KAMAL I.M. AL-MALAH

ASPEN PLUS®

CHEMICAL ENGINEERING APPLICATIONS

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ASPEN PLUS®

Chemical Engineering Applications

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To my creator who taught humans things they did not know before;
To the last prophet Mohammad and to the preceding prophets, peace be upon all of them;
To my first lovely teachers in this life: mom and dad;
To my wife (Fadia), daughters (Anwar and Lama), and sons (Abdallah and Mohammad);
To my biological brothers and sisters;
To my first class teacher (Mr Raslan Al-Malah), mercy be upon him;
To my succeeding teachers and professors between the first class and until I got my Ph.D. degree;
To my last professor (my Ph.D. supervisor, Dr Joe McGuire);
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To SPi Global, book production team.
Finally to my brothers and sisters in humanity worldwide;
To the first, I say: I owe you everything and you are the first and last.
To the rest, I say: my sincere and warm greetings to all of you.

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PREFACE

Aspen Plus® is a process flowsheet simulator. A flowsheet simulator is a computer software that is used to quantitatively model a chemical processing plant. In general, a chemical processing plant is comprised of the core reactor unit and different additional unit operations, in the form of pre- and post-treatment steps, as well.

In this regard, Aspen Plus is a very powerful tool that can be used to tackle different chemical process and unit operation calculation-based tasks, in the form of modeling, simulation, optimization, data regression, design specifications, sensitivity analysis, solids handling, dynamics and control, energy saving, safety compliance, and finally process economic analysis.

The book comprises 18 chapters. Each chapter, except the last chapter, constitutes a running tutorial that mainly covers one or more of common unit operations or chemical processes found in chemical industries. Moreover, the book has end-of-chapter contextual problems. The last chapter contains comprehensive problems (or term projects) that require an extensive knowledge of Aspen Plus features and tools that are already explained in previous chapters.

Overall, the book reflects the full-fledge nature of Aspen Plus implementation to versatile chemical process industries.

THE BOOK THEME

Let me briefly visualize my endeavor or approach in writing this book.

I am acting as the car-driving trainer and I have the student as the trainee who will be prepared to get the driving license.

The training quality (or quality training) on my behalf (as a trainer) is merely governed by two important factors: the first is the car itself, which includes all built-in electromechanical features that will help the trainer and later the driver to carry out their mission, and the second is the high-caliber skilled trainer who knows well what he/she presents to the trainee so that both can maximize their performance and that of the car.

On behalf of the trainee (student), the process of mastering car driving is to maintain the burning desire to love and not fear of driving in parallel with the internal burning/combustion of the car itself, without overburdening the learner's shoulders by the intricate details of how a car starts/stops, moves fast/slowly, forward/backward, and right/left.

The sophisticated car in our case is the Aspen Plus® full-fledge package. Humbly speaking, I am the trainer and I am presenting the training material in a very simplified way (a text in parallel with image) to let the trainee grasp and grab the training courseware real fast with a minimum yet persistent effort. At the same time, I do not really have to compromise the genuineness of both the Aspen Plus package itself and chemical engineering fundamentals.

ABOUT THE AUTHOR

Kamal I.M. Al-Malah, Professor of Chemical Engineering, graduate of Oregon State University, is currently at Higher Colleges of Technology, Abu-Dhabi, United Arab Emirates. Professor Al-Malah is Windows-based software developer (https://sites.google.com/site/almalahweb/software) and MATLAB® book author (http://mhprofessional.com/product.php?isbn=0071831282).

WHAT DO YOU GET OUT OF THIS BOOK?

The goal of writing this book is to get you started using Aspen Plus® successfully and fast. I pinpoint the parts of Aspen Plus, which you need to know without overwhelming details. I do my best to avoid presenting cumbersome Aspen Plus features. In each chapter, I demonstrate an Aspen Plus-based, running tutorial that you can refer to when you are doing your own homework, classwork, term project, or even your own project. When you are done with this recipe textbook, you will be able to efficiently use Aspen Plus. You will also be ready to explore more of Aspen Plus features on your own. You might not be an Aspen Plus expert when you finish this textbook, but you will be prepared to become one – if that is what you like and persist to be. I hope you are probably more interested in being an expert at your own specialty, as a professional chemical engineer. This textbook is designed to help you become a proficient Aspen Plus user as quickly as possible and, toward the end of our virtual journey, you will be able to examine different profitability indices of an investment project related to chemical industries.

WHO SHOULD READ THIS BOOK?

The book is primarily written for Chemical Engineering students, who plan to have a course in computer-aided design (CAD) or what is called virtual simulation (i.e., dry lab). Nevertheless, the book is expanded to reflect the broad-spectrum nature of Chemical Engineering realm in terms of courses being taught and applications being tackled. The virtual journey starts at the main station of basic principles of Chemical Engineering, while it passes through transit stations of transport phenomena, thermodynamics, chemical reaction engineering, process modeling, optimization, and simulation, the "love boat" glides down at the final stations of process dynamics and control, energy saving scenarios and safety measures, and finally process economic analysis, which declares the end of the journey.

As far as applications are concerned, in addition to classical chemical processes and unit operations, special processes are also discussed in the book, namely electrolytes, polymerization, drug characterization, and solids handling.

Professional chemical engineers can also benefit from the book as it gives them an opportunity to replenish their skills in mastering a powerful tool, such as Aspen Plus®, and stay updated at the same time. Keep in mind that Aspen Plus technology is progressively used in petroleum, petrochemical, and chemical industries, at large. Moreover, the developers of Aspen Plus keep augmenting their software with new features that will help the chemical engineer better achieve his/her mission at a pace of the speed of light compared with the manual (decrepit) mode of any calculation-based model testing or case study. Once the chemical engineer masters such a powerful tool, he/she can use it in his/her daily professional life. The book can be recommended to all chemical engineering unions, chapters, and organizations.

Aspen Plus is a full-fledge package and appears cumbersome for beginners; we need to facilitate the process of learning and later master such a powerful tool in a very short time without really making their life miserable. This textbook is recipe or cookbook type and the solution for the problem in hand is algorithmically presented via successive images (i.e., snapshots for the relevant Aspen Plus platform) in parallel with the textual explanation.

NOTES FOR INSTRUCTORS

For me, who has been spending his life digging in and pondering on chemical engineering pathways, while passing from student to instructor side, where I have been learning and teaching at different schools in the Middle East and the United States, I found that the typical classical undergraduate chemical engineering fundamental course ends up with design-oriented chapters. Toward the end of the semester (or a quarter/dime), the instructor will find it difficult to elaborate on the direct application(s) of what the student learns in the first few chapters. My recommendation is that it is time to make a gearshift and make use of CAD flowsheet simulators, such as Aspen Plus®, and have it customized to fit the instructor's needs, starting from the basic principles all the way up to the capstone design or senior project course. Many chapters of this textbook can be tuned-up to serve different fundamental chemical engineering courses, in addition to the computer-aided design course itself.

Bear in mind that the first three chapters of this textbook serve as introductory chapters for those who never used Aspen Plus technology before. I would recommend that the instructor goes first over the first three chapters before he/she moves to upcoming chapters. The instructor has to familiarize himself/herself with the new platforms of Aspen Plus, and their newly added features, which definitely look different from previous versions of Aspen Plus.

The book has contextual problems at the end of each chapter and one last dedicated chapter that encompasses term project problems. In addition, there will be additional problems for the instructor where the instructor can adjust numbers in exam/quiz problems such that each student will have his/her own version. This will minimize the process of cheating or the convective, illegal knowledge transfer among students should the instructor attempt to ask the students to solve problems in a computer lab using Aspen Plus software. For example, the first or last five numbers of a student's ID (alternatively, the national ID or social security number) can be taken as an input, in the form of ***abcde***, and plugged in the question statement such that each student ends up with his/her own version.

ACKNOWLEDGMENT

I would like to thank Aspen Technology, Inc. for their support and co-operation. It should be emphasized that screen images of Aspen Plus®, Aspen Plus Dynamics, Aspen Properties®, Aspen Energy Analyzer, and Aspen Process Economic Analyzer are reprinted with permission by Aspen Technology, Inc. AspenTech®, aspenONE®, Aspen Plus®, Aspen Properties®, and the AspenTech leaf logo are trademarks of Aspen Technology, Inc. All rights reserved.

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ABOUT THE COMPANION WEBSITE

This book is accompanied by a companion website:
www.wiley.com/go/Al-Malah/AspenPlusApplications

The website includes:

- Exam and quiz problems for instructors only
- Solution manual for instructors only

1

INTRODUCING ASPEN PLUS

1.1 WHAT DOES ASPEN STAND FOR?

ASPEN is an acronym of **A**dvanced **S**ystem for **P**rocess **EN**gineering. It is based on a flowsheet simulation. Notice that **Aspen** was replaced by **Aspen Plus**® in latest versions. A flowsheet simulation is a computer software that is used to quantitatively model a chemical processing plant, which, in addition to the core reactor unit, also includes pre- and post-treatment steps. Thus, simulation of an entire chemical process, starting from the raw material to the final finished product, is symbolically represented by different icons where each icon stands for a unit operation, chemical process, input/output material stream, input/output energy stream, or input/output electric/pneumatic signal. In terms of Aspen Plus flowsheet notation, there will be a block icon and stream icon. The iconic flowsheet simulator, such as Aspen Plus, allows us to predict the behavior of a process using basic engineering relationships. As taught in process modeling and simulation course that we describe a given physical (i.e., real) process by a set of linearly independent algebraic/differential equations such that the number of written equations will be equal to the number of variables (or unknown quantities) and the physical process as such is said to be specified or described by an equivalent mathematical portray. In general, writing such equations stems from

- balance equations of extensive thermodynamic properties, such as mass, mole, and energy;
- thermodynamic relationships for reacting and non-reacting medium, such as phase and chemical equilibrium;
- rate correlations for momentum, heat, and mass transfer;
- reaction stoichiometry and kinetic data;
- physical constraints imposed on the process.

Aspen Plus®: Chemical Engineering Applications, First Edition. Kamal I.M. Al-Malah.

Companion Website: www.wiley.com/go/Al-Malah/AspenPlusApplications

Given reliable thermodynamic data, sensible operating conditions, and rigorous equipment models, Aspen Plus can simulate actual plant behavior. Aspen Plus flowsheet simulation enables us to run many tasks, such as

- conduct “what if” tests;
- design specification (plant configuration) checks;
- carry out “de-bottlenecking of constricting parts of a process” studies;
- perform sensitivity analyses;
- run optimization investigations.

With Aspen Plus process simulator, we can design better plants and increase profitability in existing plants. Aspen Plus flowsheet simulation is useful throughout the entire lifecycle of a process, starting from a rough R&D concept/idea and zooming to a refined projected idea with a different level of details, including conceptual engineering, basic engineering, detailed engineering, and finally plant operations and revamps.

1.2 WHAT IS ASPEN PLUS PROCESS SIMULATION MODEL?

In general, a chemical process consists of chemical components, or different species, that are subject to physical or chemical treatment, or both. The goal of applying such treatment steps is basically to add a value or convert the raw, cheap material(s) into valuable, final finished products (gold). The physical treatment steps may include mixing, separation (de-mixing), such as absorption, distillation, and extraction, and heating/cooling with or without a phase change. On the other hand, the chemical treatment step involves a single or set of parallel, series, or mixed reactions, which results in a change of chemical identity of each of reacting species. Such treatment steps are visualized in the flowsheet simulator as components being transported from a unit (or block) to another through process streams.

We can translate a process into an Aspen Plus process simulation model by performing the following skeletal necessary steps:

1. Specify the chemical components in the process. We can fetch these components from Aspen Plus databanks, or we can introduce them to Aspen Plus platform.
2. Specify thermodynamic models to represent the physical properties of the components and mixtures in the process. These models are built into Aspen Plus.
3. Define the process flowsheet:
   - Define the unit operations in the process.
   - Define the process streams that flow into and out of the unit operations.
   - Select models from Aspen Plus Model Library to describe each unit operation or chemical synthesis and place them onto the process flowsheet.
   - Label each unit operation model (i.e., block) as part of the process flowsheet and connect the blocks via process streams.
4. Specify the component flow rates and the thermodynamic conditions (temperature, pressure, and composition) of all feed streams.
5. Specify the operating conditions for the unit operation models (i.e., blocks).

We can deliberately change any of the specifications listed in steps 1–5, such as flowsheet scheme, operating conditions, and feed compositions, run the show, compare the new results with the old (previous) results, and then decide whether to accept or reject new process alternatives. Keep in mind that changing the list of components means that we, in general, test for a new, alternative process type rather than simply a modified version of the same process, in terms of the type and number of physical and/or chemical treatment steps, needed to end up with the same final, finished product.

1.3 LAUNCHING ASPEN PLUS V8.8

Figure 1.1 shows where to look up Aspen Plus through Windows 8.1 Startup menu. First, click on the Windows icon keyboard button (or click on the bottom left Windows screen icon) to bring the first tile-based interface (the Metro UI) and second, on the down arrow to help the user bring the second tile-based interface to front, where it shows Aspen Plus V8.8 icon.

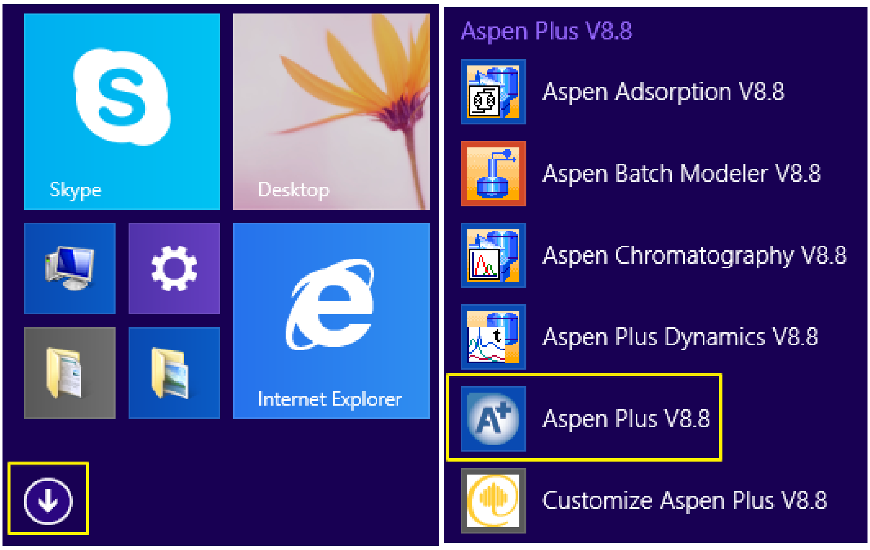


Figure 1.1 Go to Windows 8.1 Startup menu, click on the down arrow key icon (*left*), and look for "Aspen Plus V8.8" icon (*right*).

Alternatively, on the first tiled interface for tablets, key in the keyword "aspen" in Windows Search text box and Windows 8.x will furnish the menu with applications that are related to "aspen"; and finally click on "**Aspen Plus V8.8**" icon, as shown in Figure 1.2. On the other hand, for Windows 10, type the word "aspen" at the bottom-left corner of the main desktop, just right to the Windows icon, and Windows Cortana will populate the user with a list of potential aspen-based applications or files.

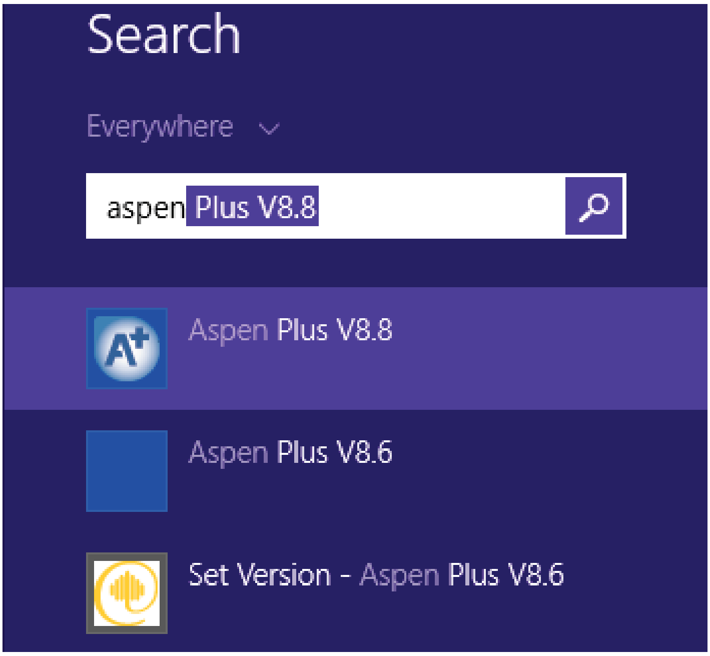


Figure 1.2 On the first tiled interface for tablets, key in the keyword “aspen” in Windows Search text box and Windows 8.x will furnish the menu with applications that are related to “aspen”. Click on “**Aspen Plus V8.8**” to open.

1.4 BEGINNING A SIMULATION

Figure 1.3 shows the first (main) window where the user may select different online (or offline) available resources, including product updates and training materials. You have to be a registered user to benefit from the online available resources. Click on “**Product Updates**” icon to see whether your software is up to date or requires installing new patches or packs. The user can select “**Open**” icon to open an existing file or select “**New**” icon to open a new file. We will discuss this issue shortly.

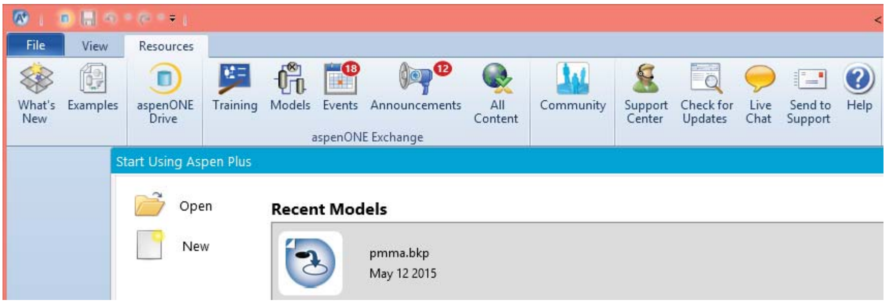
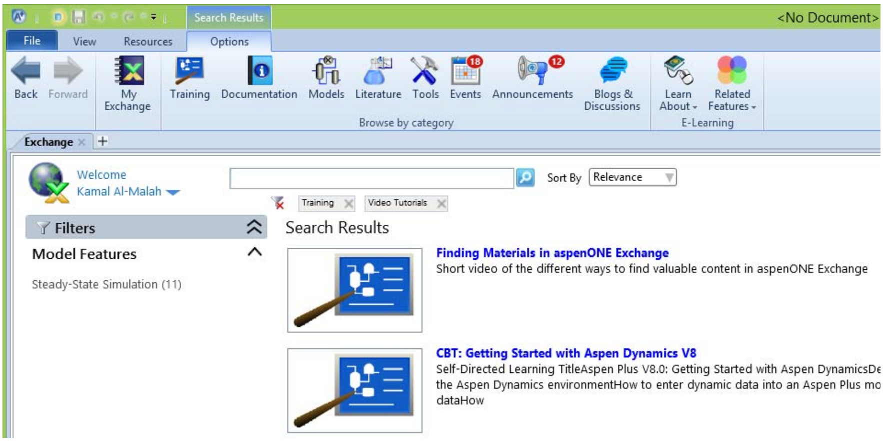


Figure 1.3 Aspen Plus first window where the user is furnished with “**Resources**” ribbon and the choice to open either an existing or new file (i.e., simulation project).

On the other hand, clicking on "**Training**" icon and selecting "**Video Tutorials**" subcategory under the main category called "**Filters**", which appears on the left pane, will populate your screen with different available online training resources, under "**Options**" tab, as shown in Figure 1.4.

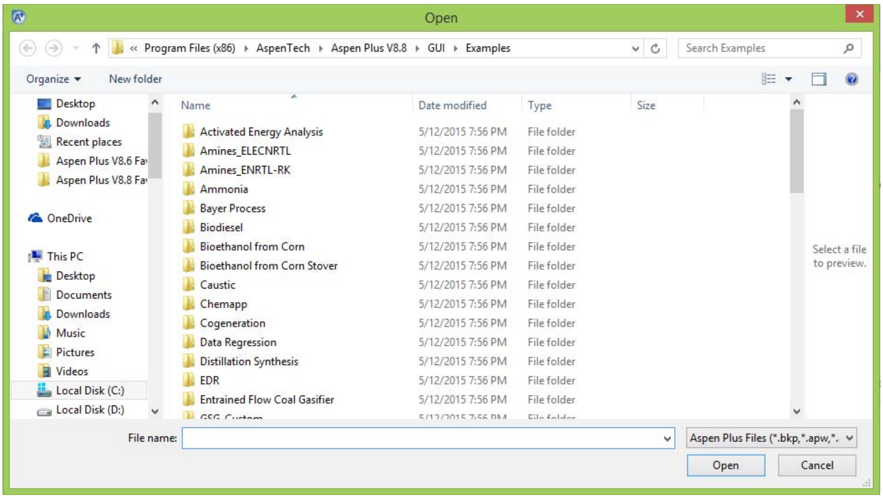


Finding Materials in aspenONE Exchange
Short video of the different ways to find valuable content in aspenONE Exchange

CBT: Getting Started with Aspen Dynamics V8
Self-Directed Learning TitleAspen Plus V8.0: Getting Started with Aspen DynamicsDe
the Aspen Dynamics environmentHow to enter dynamic data into an Aspen Plus mo
dataHow

Figure 1.4 Clicking on "**Training**" icon will populate the user's screen with different online training media that are available to the registered user.

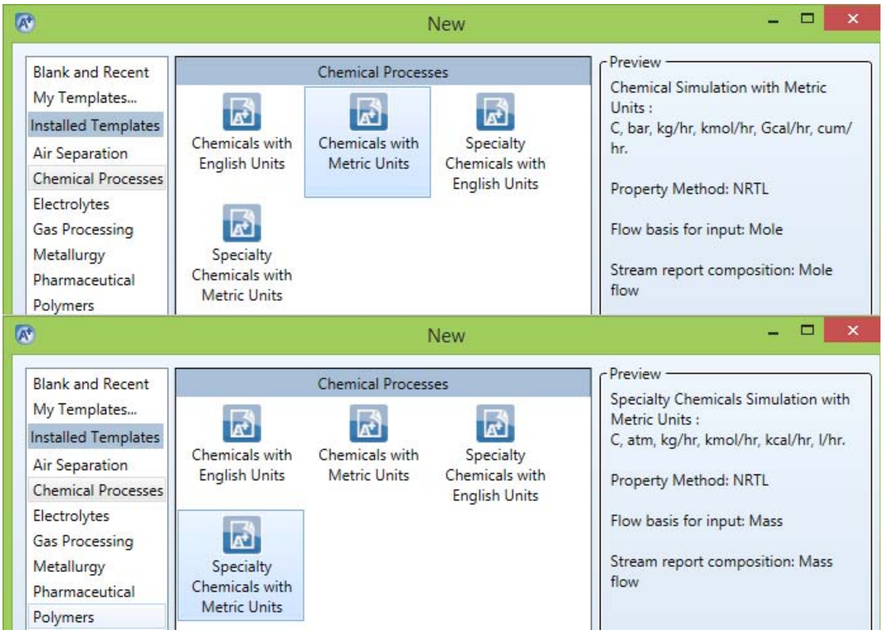
In addition, the user may benefit from offline available resources via clicking on "**Examples**" icon where she/he can select from different prepared case studies. Those can be found in the installation folder, for example: "**C:\Program Files (x86)\AspenTech\Aspen Plus V8.8\GUI\Examples**". Figure 1.5 shows a portion of such offline examples that are delivered with Aspen Plus package.



Name	Date modified	Type	Size
Activated Energy Analysis	5/12/2015 7:56 PM	File folder	
Amines_ELECNRTL	5/12/2015 7:56 PM	File folder	
Amines_ENRTL-RK	5/12/2015 7:56 PM	File folder	
Ammonia	5/12/2015 7:56 PM	File folder	
Bayer Process	5/12/2015 7:56 PM	File folder	
Biodiesel	5/12/2015 7:56 PM	File folder	
Bioethanol from Corn	5/12/2015 7:56 PM	File folder	
Bioethanol from Corn Stover	5/12/2015 7:56 PM	File folder	
Caustic	5/12/2015 7:56 PM	File folder	
Chemapp	5/12/2015 7:56 PM	File folder	
Cogeneration	5/12/2015 7:56 PM	File folder	
Data Regression	5/12/2015 7:56 PM	File folder	
Distillation Synthesis	5/12/2015 7:56 PM	File folder	
EDR	5/12/2015 7:56 PM	File folder	
Entrained Flow Coal Gasifier	5/12/2015 7:56 PM	File folder	

Figure 1.5 Aspen Plus provides offline examples where the user can benefit from.

As shown in Figure 1.3, we will choose opening a new file by clicking on "**New**" icon and the template window shows up where the user can select from different chemical industry–based templates. We will select "**Specialty Chemicals with Metric Units**" template, as shown in Figure 1.6 (*bottom*). Notice that the other counterpart template – "**Chemicals with Metric Units**" (*top*) – will differ in reporting the basis for stream composition and the units for pressure, volumetric flow rate, and rate of energy (power), as shown in "**Preview**" panel in Figure 1.6.



Chemical Simulation with Metric Units :
C, bar, kg/hr, kmol/hr, Gcal/hr, cum/hr.

Property Method: NRTL

Flow basis for input: Mole

Stream report composition: Mole flow

Specialty Chemicals Simulation with Metric Units :
C, atm, kg/hr, kmol/hr, kcal/hr, l/hr.

Property Method: NRTL

Flow basis for input: Mass

Stream report composition: Mass flow

Figure 1.6 The difference between "**Chemicals with Metric Units**" (*top*) and "**Specialty Chemicals with Metric Units**" template (*bottom*) lies in what metric units some physical properties are expressed.

Click on "**Create**" button, shown at the bottom of the template window, and the main window of Aspen Plus V8.8 shows up as in Figure 1.7.

STARTING from the top-left corner while moving row-wise to the right horizon until we finally reach the bottom-right corner, let us familiarize ourselves with what is seen, in the

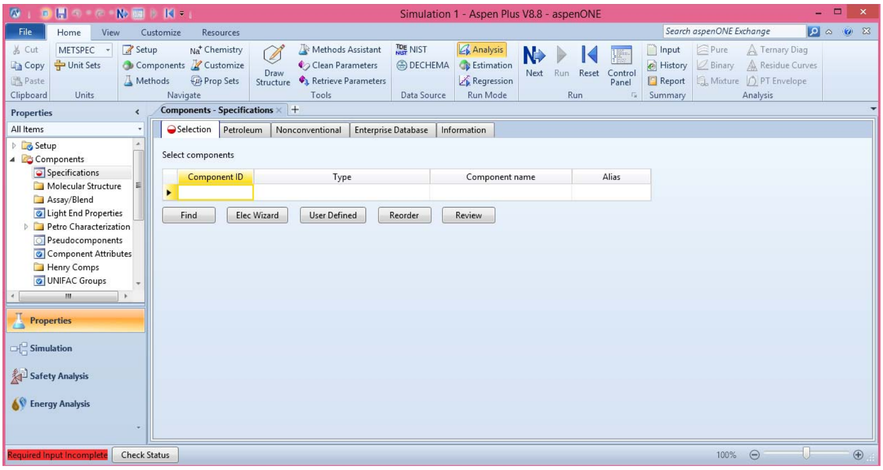


Figure 1.7 The main window of Aspen Plus flowsheet simulator.

form of a pane, ribbon, toolbar, status bar, input form, and tab, as shown in Figure 1.8. We briefly introduce each item with the understanding that, as the user keeps digging, he/she will become more comfortable because each item represents a shortcut key to one of the important features of Aspen Plus.

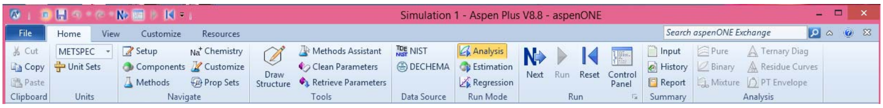


Figure 1.8 The top portion of Aspen Plus V8.8 main window contains the "**Quick Access**" toolbar (top bar), the "**Top**" toolbar, the help-related textbox and button (middle bar), and ribbon tabs associated with each "**Top**" toolbar menu (bottom bar).

The "**Quick Access**" toolbar contains the most commonly used functions in Aspen Plus, such as the "**Run**", "**Restart**", and "**Next**" buttons. Notice that other buttons can be incorporated into this toolbar simply by right-clicking on the desired function found in the "**Home**" ribbon, or in any other menu of "**Top**" toolbar, and adding it to "**Quick Access**" toolbar. The "**Top**" toolbar has "**File**", "**Home**", "**View**", "**Customize**", and "**Resources**" menus, where each menu has many submenu items that appear in the form of ribbon tabs. For example, the "**Home**" ribbon is shown in Figure 1.8 and it contains many tabs. Each "**Home**" ribbon tab will be explained shortly.

The first "**Home**" ribbon tab, called ("**Clipboard**" group), pertains to clipboard functions, such as "**Copy**", "**Cut**", and "**Paste**" buttons.

The second ("**Units**" group) tab deals with the unit sets. You can click on "**Unit Sets**" icon to open the form for entering a new set of your own (i.e., a customized set of units).

The third ("**Navigate**" group) tab represents the navigation pane where the user can open forms to choose components, select or modify property methods, and create or edit chemistry and property sets. Notice that this tab has the same functions as those of "**Navigation**" pane, shown later in Figure 1.10.

The fourth (“**Tools**” group) tab allows the user to draw chemical structures to better estimate property parameters for a user-defined component, to make use of the “**Methods Assistant**” wizard in defining the most suitable property method, and to retrieve/clean model parameters.

The fifth (“**Data Source**” group) tab deals with seeking additional components databanks, such as **N**ational **I**nstitute of **S**tandards and **T**echnology (**NIST**)/**T**hermo-**D**ata **E**ngine (**TDE**), and **DECHEMA** (experimental thermophysical properties of pure substances and mixtures available on the website; this is a paid service requiring an account setup directly with **DECHEMA**).

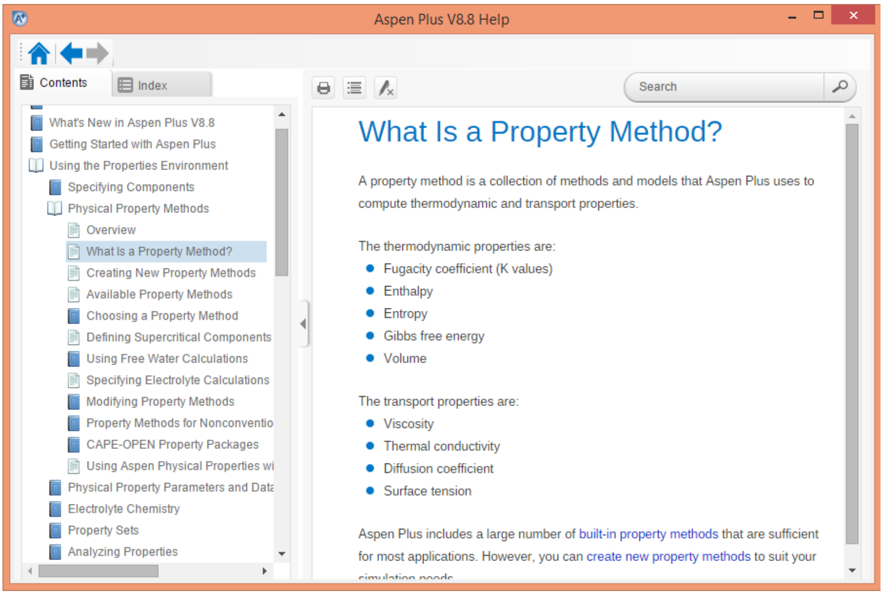
The sixth (“**Run Mode**” group) tab allows the user to select the mode of run (i.e., simulation). The run modes are analysis, estimation, and regression. In “**Analysis**” mode, the user may analyze properties of components. In “**Estimation**” mode, the user may estimate the unknown properties, such as critical properties for a known molecular structure and the model parameters for pure components and mixtures (i.e., pairwise interaction parameters). In “**Regression**” mode, the user may fit the model to data taken from Aspen Plus databanks; “**NIST/TDE**” databank; “**DECHEMA**” databank; or a user’s databank.

The seventh (“**Run**” group) tab lumps all functions related to the simulation solver, including the “**Next**”, “**Run**”, and “**Reinitialize**” (i.e., purge simulation results) buttons. The calculation status (i.e., convergence vs. divergence and presence/absence of errors and warnings) can be viewed via clicking on “**Control Panel**” button.

The eighth (“**Summary**” group) tab represents the summary where the user can view, print, and save the simulation input files, history, and reports.

The ninth and last (“**Analysis**” group) tab will become active once the user defines the property sets and property method(s) for the selected components. This will allow the user to carry out and present both tabulated and graphical types of data analysis for a single- (i.e., pure), binary-, or multicomponent system.

The help-related search text box can be used to enter a key word and let Aspen Plus search for the relevant online resources. Clicking on “**Show Help**” icon will bring the built-in offline help database as shown in Figure 1.9.



What Is a Property Method?

A property method is a collection of methods and models that Aspen Plus uses to compute thermodynamic and transport properties.

The thermodynamic properties are:

- Fugacity coefficient (K values)
- Enthalpy
- Entropy
- Gibbs free energy
- Volume

The transport properties are:

- Viscosity
- Thermal conductivity
- Diffusion coefficient
- Surface tension

Aspen Plus includes a large number of built-in property methods that are sufficient for most applications. However, you can create new property methods to suit your simulation needs

Figure 1.9 The offline built-in help database can be brought via clicking on the “**Show Help**” icon shown at the right top corner of the Aspen Plus v8.8 main window.

As shown in Figure 1.10, the “**Navigation**” pane is where the user can navigate to every stage of the property development process. This pane has a hierarchy (top to bottom) of input forms.

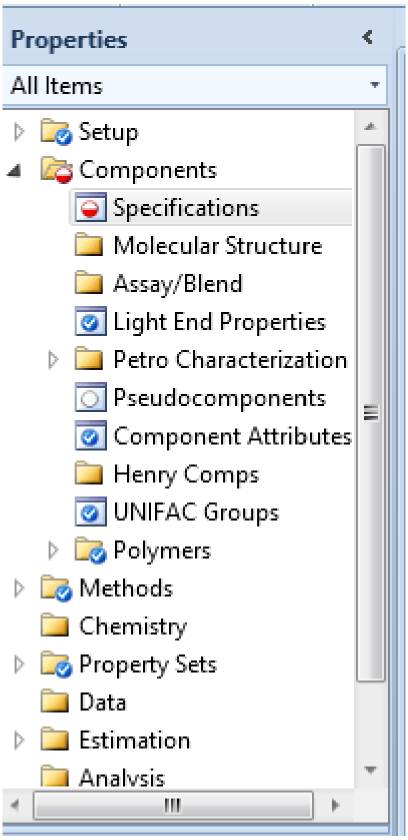


Figure 1.10 The “**Navigation**” pane that acts as folder/file explorer.

Figure 1.11 shows a sample of an input form where the user types in process components.

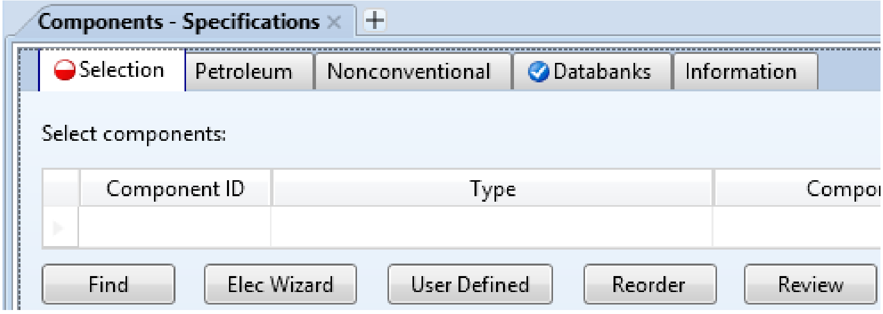


Figure 1.11 The input form for entering components involved in the process.

Figure 1.12 shows the "**Environments**" pane where the user is granted the luxury to switch from the "**Properties**" to "**Simulation**", "**Safety Analysis**", or "**Energy Analysis**" environment. Those types of environment are explained in detail in later chapters.

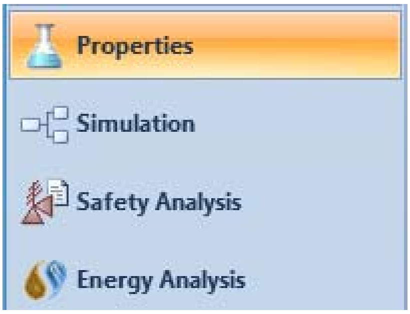


Figure 1.12 The "**Environments**" pane where the user has the flexibility to switch from one to another environment.

> <u>**NOTE #0:**</u> *Staying under "**Properties**" environment, the user does not have to specify a flowsheet; only components and the property model are needed at this stage for analysis, estimation, and regression purposes.*

Figure 1.13 shows the "**Status**" bar where the status indicator is seen, which tells the user where he/she stands in terms of the progress of process simulation, and the "**Check Status**" button, which can be used by the user to see the messages issued by Aspen Plus simulator or solver.


Required Input Incomplete

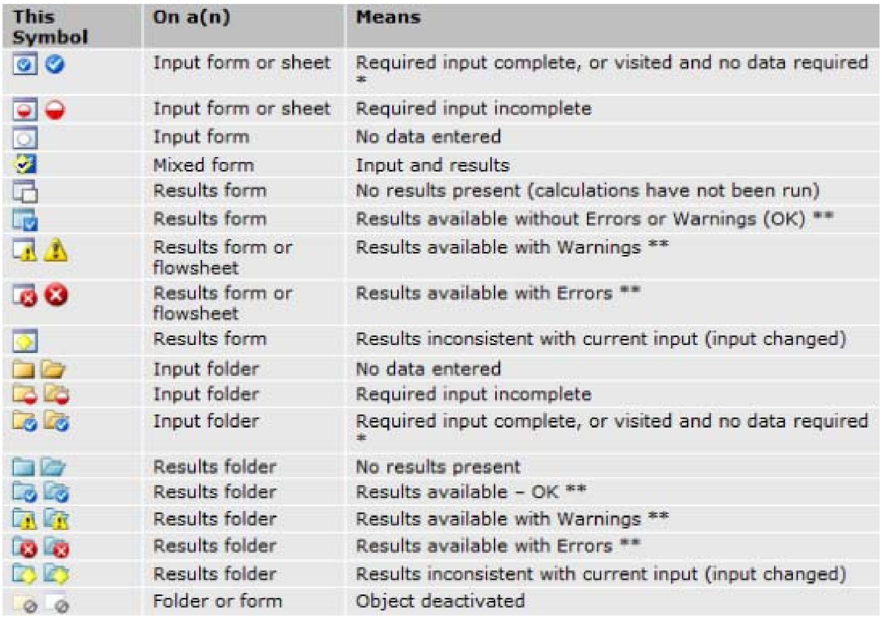
Figure 1.13 The "**Status**" bar where the user is updated about the *status quo* of Aspen Plus simulator (or solver).

Finally, Figure 1.14 shows the "**Zoom**" bar with which the user can zoom in and out the input form under concern.

Figure 1.14 The "**Zoom**" bar where the user may zoom in or out the input form under question.

After introducing the main features of Aspen Plus main window, let us pinpoint some other issues that will help the user better deal with Aspen Plus products. Notice that in "**Navigation**" pane (see Figure 1.10), there are different color codes adopted by Aspen Plus.

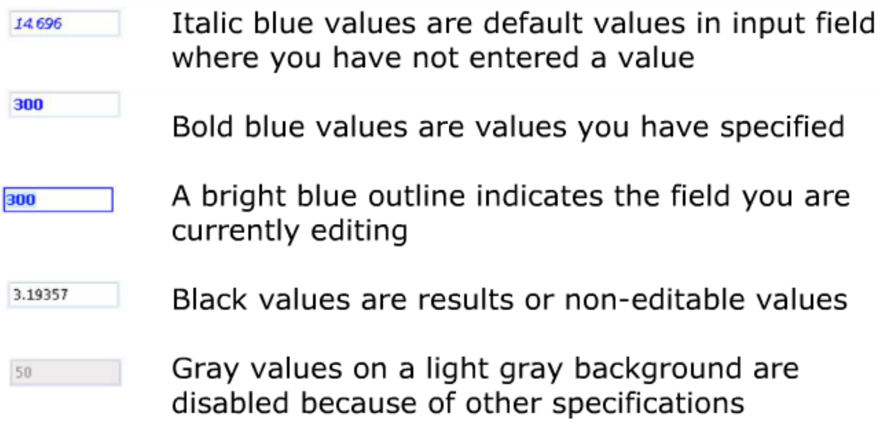
For example, a half-filled red circle indicates that input data are required for the simulator to proceed. In general, Figure 1.15 shows different color-coded symbols used by Aspen Plus.



This Symbol	On a(n)	Means
✓ ✓	Input form or sheet	Required input complete, or visited and no data required *
◒ ◒	Input form or sheet	Required input incomplete
○	Input form	No data entered
✓	Mixed form	Input and results
☐	Results form	No results present (calculations have not been run)
✓	Results form	Results available without Errors or Warnings (OK) **
⚠ ⚠	Results form or flowsheet	Results available with Warnings **
⊗ ⊗	Results form or flowsheet	Results available with Errors **
●	Results form	Results inconsistent with current input (input changed)
📁 📂	Input folder	No data entered
◒ ◒	Input folder	Required input incomplete
✓ ✓	Input folder	Required input complete, or visited and no data required *
📁 📂	Results folder	No results present
✓ ✓	Results folder	Results available – OK **
⚠ ⚠	Results folder	Results available with Warnings **
⊗ ⊗	Results folder	Results available with Errors **
● ●	Results folder	Results inconsistent with current input (input changed)
⊘ ⊘	Folder or form	Object deactivated

Figure 1.15 Different color-coded symbols used by Aspen Plus to help the user better understand the status of the solver. *See Plate section for color representation of this figure.*

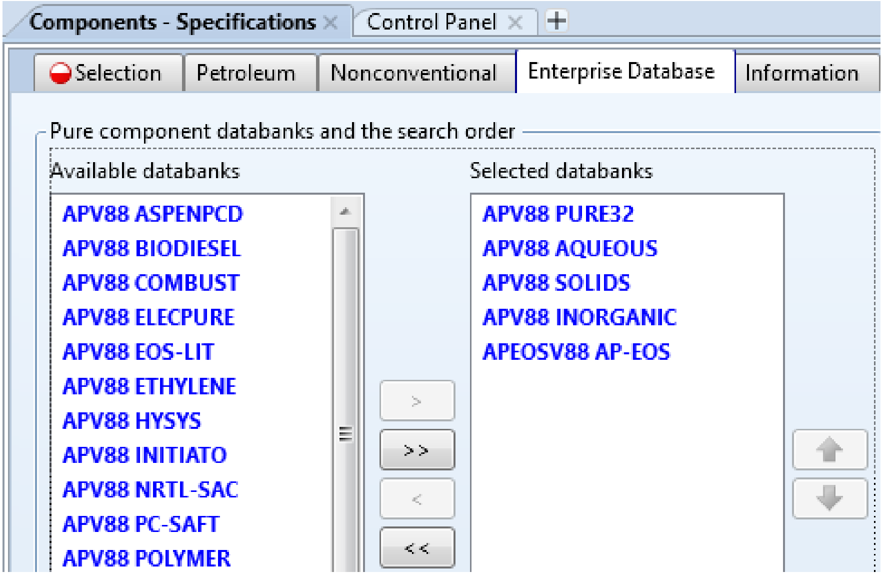
On the other hand, Figure 1.16 shows the field color coding for texts within input forms.



14.696	Italic blue values are default values in input field where you have not entered a value
300	Bold blue values are values you have specified
300	A bright blue outline indicates the field you are currently editing
3.19357	Black values are results or non-editable values
50	Gray values on a light gray background are disabled because of other specifications

Figure 1.16 The field color coding adopted by Aspen Plus for the text of an input form, which is either editable or noneditable by the user. *See Plate section for color representation of this figure.*

As shown in Figures 1.10 and 1.11, Aspen Plus requires us to enter the components involved in the process. A component can be either picked up from one of Aspen Plus built-in component databanks, or can be defined by the user and in the latter case it is considered as a non-databank member. Figure 1.17 shows the default (i.e., selected) databanks assigned by Aspen Plus, depending on, of course, the type of template initially chosen by the user. The user may select, however, one or more from the databanks available on the left side and add to the list of selected databanks on the right side, using the in-between arrow keys.



Pure component databanks and the search order

Available databanks

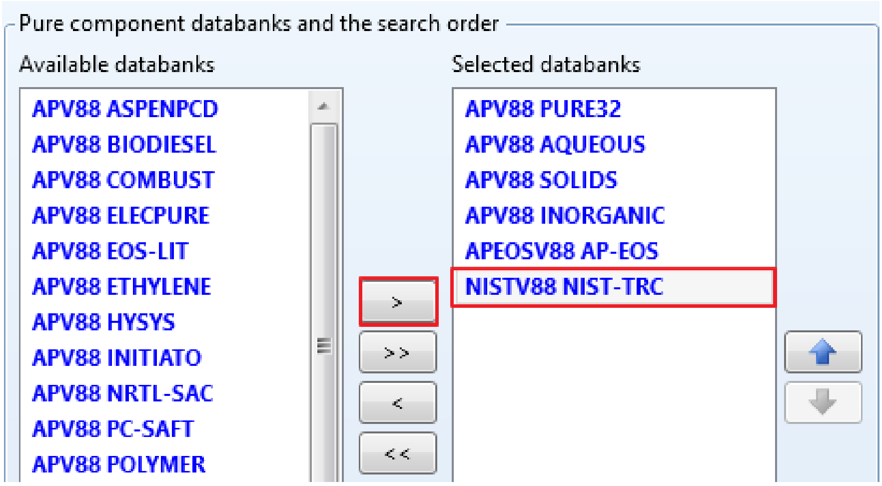
- APV88 ASPENPCD
- APV88 BIODIESEL
- APV88 COMBUST
- APV88 ELECPURE
- APV88 EOS-LIT
- APV88 ETHYLENE
- APV88 HYSYS
- APV88 INITIATO
- APV88 NRTL-SAC
- APV88 PC-SAFT
- APV88 POLYMER

Selected databanks

- APV88 PURE32
- APV88 AQUEOUS
- APV88 SOLIDS
- APV88 INORGANIC
- APEOSV88 AP-EOS

Figure 1.17 The selected databanks are shown on the right side under "**Enterprise Database**" or "**Databanks**" tab.

As shown in Figure 1.18, "**NISTV88 NIST-TRC**" databank was added to the right list. The new database is provided under an agreement with the **N**ational **I**nstitute of **S**tandards and **T**echnology's (**NIST**) Standard Reference Data Program (SRDP). The property parameters and the experimental data used were collected and evaluated by the **T**hermodynamics **R**esearch **C**enter (**TRC**) using the **NIST** Thermo**D**ata **E**ngine (**TDE**) and the **NIST-TRC** source data archival system for experimental thermophysical and thermochemical property data. The "**NIST-TRC**" source data is one of the world's most comprehensive collections of such data.



Pure component databanks and the search order

Available databanks
APV88 ASPENPCD
APV88 BIODIESEL
APV88 COMBUST
APV88 ELECPURE
APV88 EOS-LIT
APV88 ETHYLENE
APV88 HYSYS
APV88 INITIATO
APV88 NRTL-SAC
APV88 PC-SAFT
APV88 POLYMER

Selected databanks
APV88 PURE32
APV88 AQUEOUS
APV88 SOLIDS
APV88 INORGANIC
APEOSV88 AP-EOS
NISTV88 NIST-TRC

Figure 1.18 Inclusion of "**NISTV88 NIST-TRC**" databank that is comprehensive in resources.

<u>**Notice**</u> that the prefix "**APV88**" will be dropped from databank names if the user does not have the enterprise version of AspenOne and the "**Enterprise Database**" tab will be replaced by "**Databanks**" tab. Moreover, the capability to add "**NISTV88 NIST-TRC**" databank is available for the enterprise version.

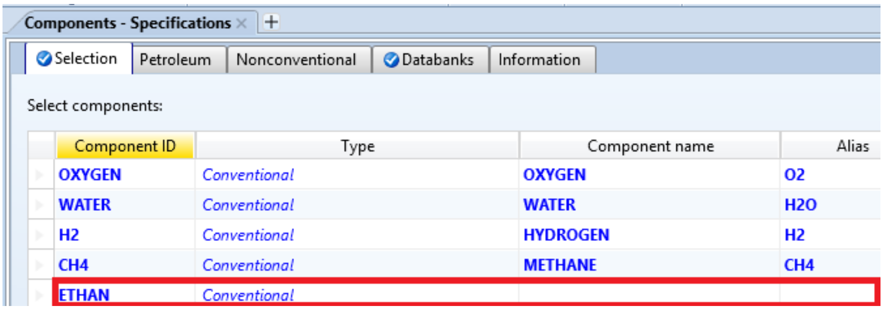
Table 1.1 gives more description on such commonly used pure component databanks. Notice that PURE## databank may change from one version of Aspen Plus to another. For example, PURE26 is the primary component databank delivered with Aspen Plus V7.3.2 and is retained in the set of databanks for upward compatibility reason. In addition, when the user attempts to search for a certain name or chemical formula, then Aspen Plus search engine will look it up in the first databank appearing on the right side of Figure 1.18, followed by the second, and so on.

TABLE 1.1 The Description and Usage of Commonly Used Pure Component Databanks.

Databank	Contents	Uses
APV88 PURE32	Data from the Design Institute for Physical Property Data (DIPPR) and AspenTech	Primary component databank in Aspen Plus
APV88 AQUEOUS	Pure component parameters for ionic and molecular species in aqueous solution	Simulations containing electrolytes
APV88 SOLIDS	Pure component parameters for strong electrolytes, salts, and other solids	Simulations containing electrolytes and solids
APV88 INORGANIC	Thermochemical properties for inorganic components in vapor, liquid, and solid states	Solids, electrolytes, and metallurgy applications
APEOSV88	Binary and pair parameters for the Cubic-Plus-Association property model	Parameters for some compound pairs. See "Cubic-Plus-Association Parameters" offline and built-in help

1.5 ENTERING COMPONENTS

The user may enter the component by typing its name, such as oxygen, water, methanol, and ethanol, or its chemical formula, such as H_2 and CH_4. As shown in Figure 1.19, once the user keys in the name of a compound or its chemical formula and clicks on either “tab” or “enter” key, Aspen Plus will complete the entries for the rest of columns titled: “**Type**”, “**Component name**”, and “**Alias**”. If the user, however, inadvertently keys in a word or formula that is not recognized by Aspen Plus, then it will not complete the missing information with the understanding that the user will introduce this new component to Aspen Plus environment (i.e., non-databank member).



Select components:

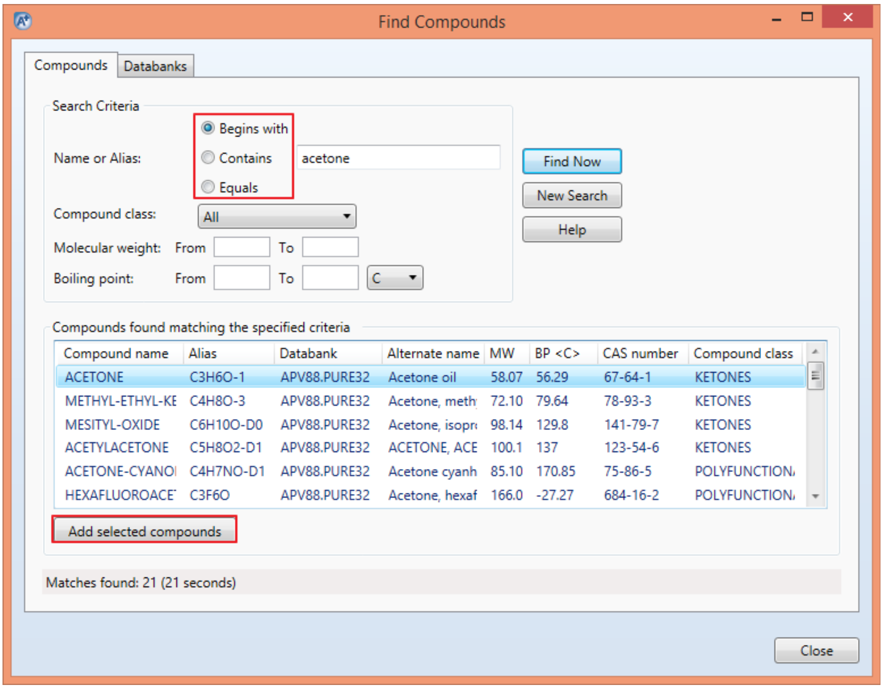
Component ID	Type	Component name	Alias
OXYGEN	Conventional	OXYGEN	O2
WATER	Conventional	WATER	H2O
H2	Conventional	HYDROGEN	H2
CH4	Conventional	METHANE	CH4
ETHAN	Conventional		

Figure 1.19 Entering “**Component ID**” by either name or chemical formula allows Aspen Plus to recognize the component. If it is not automatically recognized, then the component name and alias will be left blank.

Regarding the component type, there are six major classes that can be dealt with in Aspen Plus:

1. Conventional: Single species fluids (vapor or liquid). Typical components that may participate in vapor–liquid-phase equilibrium.
2. Solid: Single species solids. Properties are calculated by solid-based models.
3. Non-conventional: Solids that are not pure chemical species. They are not represented as molecular components, such as coal or wood pulp. They are characterized using component attributes and do not participate in chemical or phase equilibrium.
4. Pseudocomponent, Assay, and Blend: Components representing petroleum fractions, characterized by boiling point, molecular weight, specific gravity, and other properties.
5. Polymer, Oligomer, and Segment: Components used in polymer models.
6. Hypothetical liquid: A component type that is mainly used in pyrometallurgical applications when modeling a component as a liquid when its properties should be extrapolated from solid properties, for example, modeling the carbon in molten steel.

Alternatively, the user may search for a given component via clicking on “**Find**” button (see Figure 1.11) under “**Components**” | “**Specifications**” | “**Selection**” tab form. Figure 1.20 shows “**Find Compounds**” window where the user can enter the search keyword either as a name or chemical formula within the dedicated text box. Moreover, the search criterion must be specified whether the searched phrase begins with, contains,



Name or Alias: ● Begins with ○ Contains ○ Equals acetone

Compound class: All

Molecular weight: From To

Boiling point: From To C

Compound name	Alias	Databank	Alternate name	MW	BP <C>	CAS number	Compound class
ACETONE	C3H6O-1	APV88.PURE32	Acetone oil	58.07	56.29	67-64-1	KETONES
METHYL-ETHYL-KE	C4H8O-3	APV88.PURE32	Acetone, meth	72.10	79.64	78-93-3	KETONES
MESITYL-OXIDE	C6H10O-D0	APV88.PURE32	Acetone, isopr	98.14	129.8	141-79-7	KETONES
ACETYLACETONE	C5H8O2-D1	APV88.PURE32	ACETONE, ACE	100.1	137	123-54-6	KETONES
ACETONE-CYANOI	C4H7NO-D1	APV88.PURE32	Acetone cyanh	85.10	170.85	75-86-5	POLYFUNCTION/
HEXAFLUOROACE	C3F6O	APV88.PURE32	Acetone, hexaf	166.0	-27.27	684-16-2	POLYFUNCTION/

Matches found: 21 (21 seconds)

Figure 1.20 The "**Find Compounds**" window enables the user to search using either the name or chemical formula of a compound, including the flexibility to refine search results.

or exactly equals to the entered keyword. Each criterion of search will definitely give different number of matched cases. The search criterion "**Contains**" is broader than the other two criteria. In addition, you may refine the search by

1. selecting the class of compound as being aliphatic, aromatic, polymer, inorganic salt, and so on;
2. entering the range of any of the two physical properties: molecular weight and boiling point temperature.

After you decide on the right component, highlight and click on "**Add selected compounds**" button at the bottom of "**Find Compounds**" window. Finally, the set of selected databanks can be modified using the second tab "**Databanks**" present in "**Find Compounds**" window.

1.6 SPECIFYING THE PROPERTY METHOD

One of the key and most important decisions is the selection of the property method. **A property method is a set of models used to calculate thermodynamic, kinetic, and transport properties**. If the components selected by the user do not work with Aspen Plus out-of-box property (i.e., default or recommended) methods, then such methods can be modified by the user. The thermodynamic method, a subset of the property method, can be broadly classified as

1. an activity coefficient-based method;
2. an equation of state method.

The activity coefficient-based method is mainly described for subcritical and non-ideal liquid systems at pressures below 10 atm. The incorporated parameters within the model are temperature dependent. Such a method becomes problematic in the critical region. The concept of ideal versus non-ideal liquid mixture can be simplified first, before entering the intricate picture of solution thermodynamics.

In general, mixing two or more similar species, to form a solution, results in an ideal liquid mixture. For example, mixing benzene with toluene forms an ideal benzene–toluene mixture and so is the case with methanol–ethanol mixture or *n*-heptane–octane mixture. The similarity among chemical species is exemplified in terms of equal number and the same type of functional groups (i.e., —OH, —OOH, —O—, —NH_2, ═, ≡, etc.) to a large extent and of the length of the hydrocarbon chain (or tail) of the molecule, to a small extent. The deviation from an ideal liquid mixture (or formation of non-ideal liquid mixture) arises from mixing of chemical species characterized by different chemical activities (i.e., different functional groups) and by different sizes of homologous series or both. For example, mixing ethanol with water forms a non-ideal liquid mixture, as water and ethanol are of two different categories. Mixing of ethanol with hexanol also shows some sort of deviation from ideality compared with mixing of ethanol with propanol, next to ethanol in homologous series of alcohols.

From solution thermodynamics point of view, the non-ideal liquid mixture can be described by introducing the concept of fugacity, which basically accounts for the effective "thermodynamic" presence of species i in a solution. This means that its thermodynamic concentration not only reflects its count (or composition) but also extends to include its "social" interaction with its neighbors, the so-called activity coefficient. Thus, the fugacity of species i in a mixture is given by

$$\hat{f}_i = x_i \times \gamma_i \times f_i^{\mathrm{o}} \tag{1.1}$$

where

$\hat{f}_i$: the fugacity of species i in a mixture at the given pressure, temperature, and composition;
x_i : the mole fraction of species i in a mixture;
γ_i : the activity coefficient of species i in a solution at the given pressure, temperature, and composition;
f_i^{o}: the fugacity of pure liquid species i at the given pressure and temperature.

For an ideal liquid mixture, the activity coefficient is reduced to unity and the pure component fugacity is replaced by the vapor pressure of substance i at the given temperature. Thus, Equation 1.1 becomes

$$\hat{f}_i = x_i \times P_i^{\mathrm{sat}}(T) \tag{1.2}$$

In a similar manner, the gas-phase fugacity can be expressed as

$$\hat{f}_i = \hat{\varphi}_i \times y_i \times P \tag{1.3}$$

At low pressure, the fugacity coefficient of species *i* in a gas-phase mixture reduces to unity, and we have

$$\hat{f}_i = y_i \times P \tag{1.4}$$

The Raoult's case represents the simplest case, that is, ideal liquid mixture–ideal gas mixture under vapor–liquid phase equilibrium (VLE), where both fugacities are set equal.

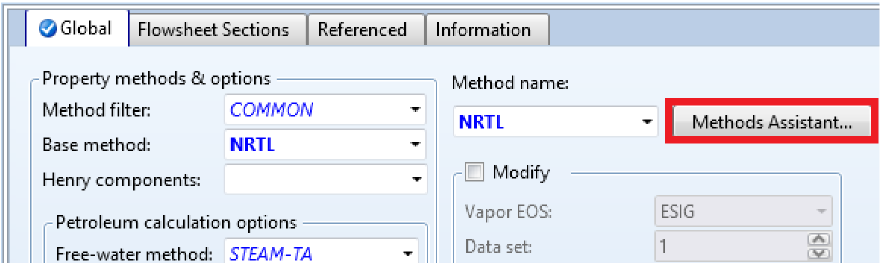
$$x_i \times P_i^{\mathrm{sat}}(T) = y_i \times P \tag{1.5}$$

Examples of activity coefficient-based model are “**NRTL**” (**N**on-**R**andom-**T**wo-**L**iquid), “**UNIFAC**” (**UNI**versal **F**unctional **A**ctivity **C**oefficient), and “**UNIQUAC**” (**UNI**versal **QU**asichemical **A**ctivity **C**oefficient). “**UNIFAC**” is based on group contributions rather than molecular contributions. With a limited number of group parameters and group–group interaction parameters, “**UNIFAC**” can predict activity coefficients. Because the “**UNIFAC**” model is a group-contribution model, it is very predictive. All published group parameters and group binary parameters are stored in the Aspen Plus physical property system. Activity coefficient models usually perform well for systems of polar compounds at low pressures and away from the critical region. They are the best way to represent highly nonideal liquid mixtures at low pressures (below 10 atm). They are used for the calculation of fugacity, enthalpy, entropy, and Gibbs free energy. Usually, an empirical correlation is used in parallel for the calculations of density when an activity coefficient model is used in phase equilibrium modeling.

On the other hand, the equation of state model operates in the critical region and when there are no polar components. It describes the holy relationship among the three variables: P, T, and $\tilde{V}$. It has few binary parameters that extrapolate well with temperature. We can use equation of state model over wide ranges of temperature and pressure, including a subcritical and supercritical region. For ideal or slightly nonideal systems, thermodynamic properties for both the vapor and liquid phases can be computed with a minimum amount of component data. An equation of state model is suitable for modeling hydrocarbon systems with light gases such as CO2, N2, and H2S. For the best representation of non-ideal systems, we must obtain binary interaction parameters from regression of experimental vapor–liquid equilibrium (VLE) data. Equation of state binary parameters for many component pairs are available in the Aspen Plus physical property system.

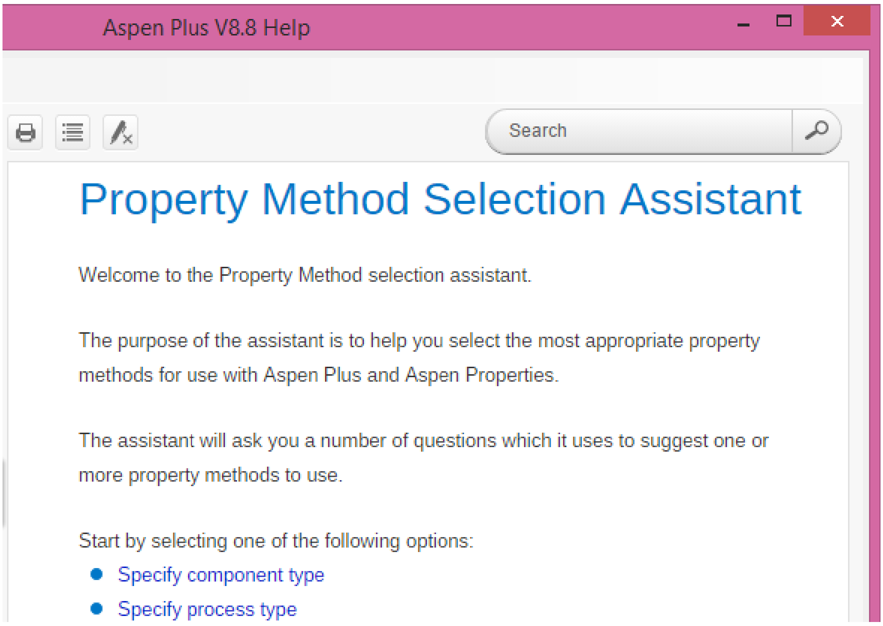
Examples of an equation of state model are “**PENG-ROB**” (**PENG-ROB**inson), “**RK-SOAVE**” (**R**edlich-**K**wong **Soave**), and “**PC-SAFT**” (**P**erturbed-**C**hain **S**tatistical **A**ssociating **F**luid **T**heory-copolymer systems).

Since the selection of a property method, for a given chemical process/component, has the first priority, Aspen Plus provides what is called the property method selection assistant (or wizard) that can be reached via clicking on the “**Methods Assistant** … ” button found in “**Methods**” **|** “**Specifications**” | “**Global**” tab window, as shown in Figure 1.21 and the “**Aspen Plus V8.8 Help**” window pops up as shown in Figure 1.22.



Property methods & options
Method filter: COMMON
Base method: NRTL
Henry components:
Petroleum calculation options
Free-water method: STEAM-TA
Method name: NRTL
☐ Modify
Vapor EOS: ESIG
Data set: 1

Figure 1.21 Aspen Plus provides a wizard for helping the user select the proper property method(s) for a given chemical process or component type.



Property Method Selection Assistant

Welcome to the Property Method selection assistant.

The purpose of the assistant is to help you select the most appropriate property methods for use with Aspen Plus and Aspen Properties.

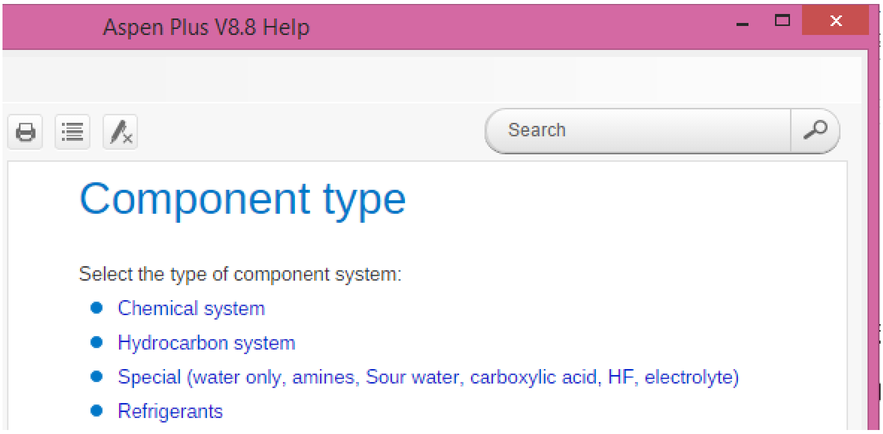
The assistant will ask you a number of questions which it uses to suggest one or more property methods to use.

Start by selecting one of the following options:

- Specify component type
- Specify process type

Figure 1.22 The property method selection wizard that helps the user refine the number of suitable property methods for a given process/component.

Here, the user is to opt between component or process type. Do not panic; both choices will guide you to the city of Rome, and upon choosing "**Specify by component type**" option, the help window updates the content as shown in Figure 1.23. It shows four different component-based categories out of which the user may select. For example, if the user selects the first category, that is, "**Chemical system**" and further selects the pressure to be less than or equal to 10 bar, then the recommended property method will be activity coefficient-based method as is the case shown later in Figure 1.27. The second category better describes hydrocarbon (non-polar) systems. The third category is dedicated for some special applications, such as amines system, carboxylic acids (such as acetic acid) in the mixture, electrolyte system, hydrogen fluoride (HF) in the mixture, refrigerants, sour water system, and water only. The last category is reserved for refrigerants.



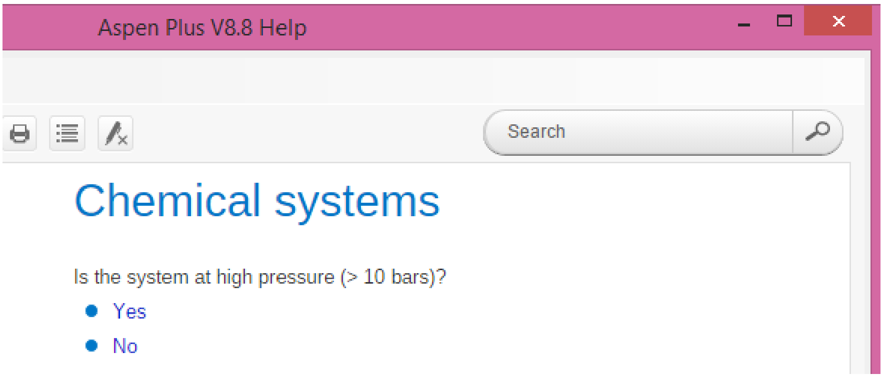
Component type

Select the type of component system:

- Chemical system
- Hydrocarbon system
- Special (water only, amines, Sour water, carboxylic acid, HF, electrolyte)
- Refrigerants

Figure 1.23 The user has to further select the type of component system in order to refine the property method selection by Aspen Plus.

Upon selecting “**Chemical system**” option, Aspen Plus opts the user to select between a low- and a high-pressure operating condition, as shown in Figure 1.24.



Chemical systems

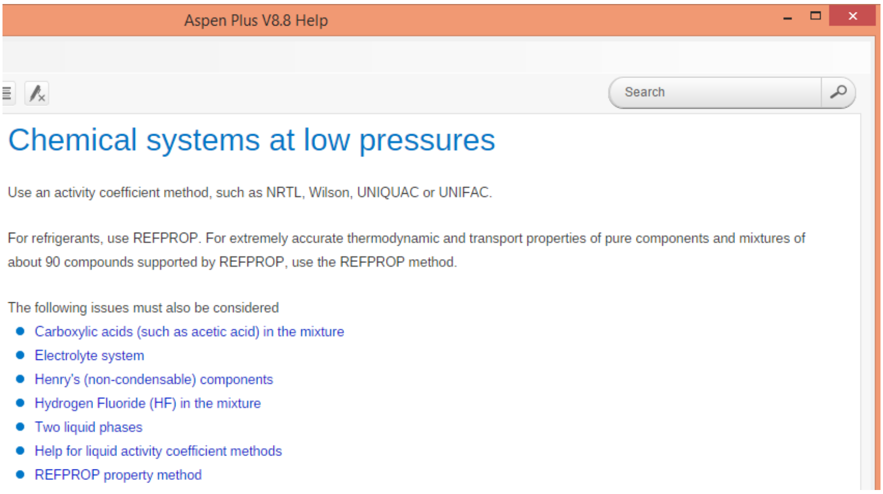
Is the system at high pressure (> 10 bars)?

- Yes
- No

Figure 1.24 Further zooming is carried out by choosing between a low- and a high-pressure operating condition.

Upon selecting a low-pressure condition, Aspen Plus help window finally shows up the recommended property method(s), as shown in Figure 1.25.

On the one hand, let us go by “**Specify process type**” choice and Figure 1.26 is the result of our choice. Notice that for “**Chemical**”, “**Environmental**”, “**Gas processing**”, “**Petrochemical**”, “**Power**”, and “**Refining process**” type of process, shown in Figure 1.26, the user will notice that there are additional subcategories from which the user can pick up his/her choice; this in turn will further refine the number of property methods recommended by the Aspen Plus property method wizard.



Chemical systems at low pressures

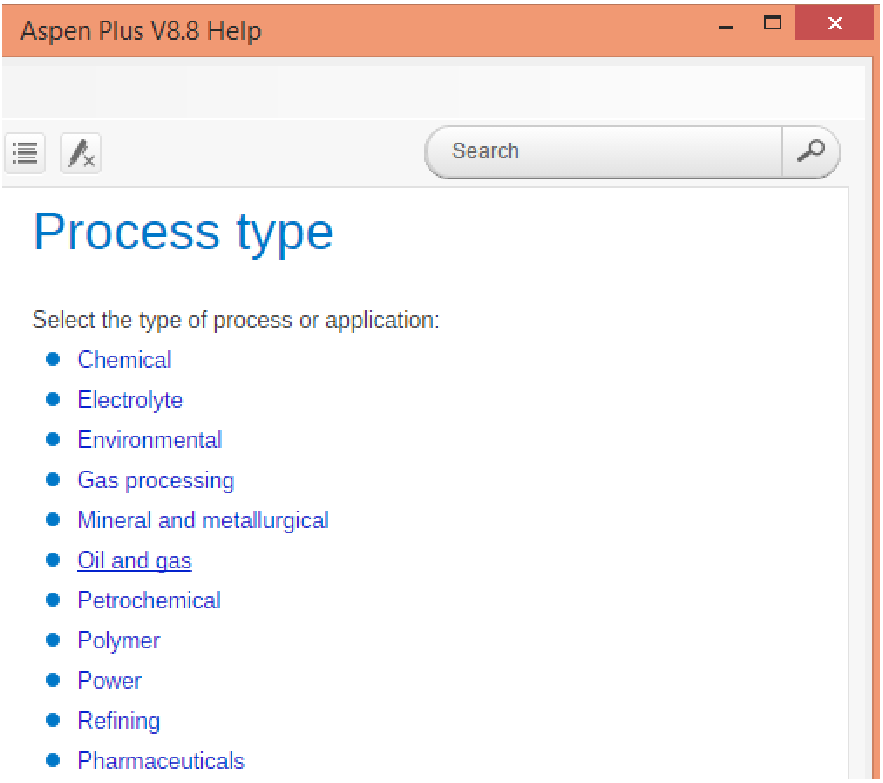
Use an activity coefficient method, such as NRTL, Wilson, UNIQUAC or UNIFAC.

For refrigerants, use REFPROP. For extremely accurate thermodynamic and transport properties of pure components and mixtures of about 90 compounds supported by REFPROP, use the REFPROP method.

The following issues must also be considered

- Carboxylic acids (such as acetic acid) in the mixture
- Electrolyte system
- Henry's (non-condensable) components
- Hydrogen Fluoride (HF) in the mixture
- Two liquid phases
- Help for liquid activity coefficient methods
- REFPROP property method

Figure 1.25 The recommendation by Aspen Plus is to use any of the activity coefficient-based method such as NRTL, Wilson, UNIQUAC, and UNIFAC.



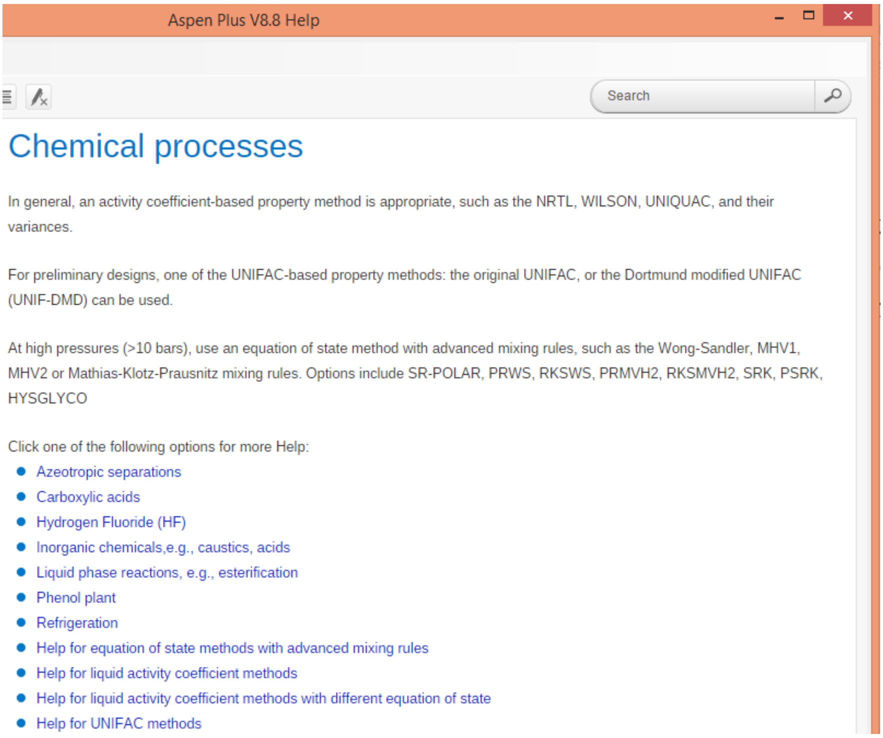
Process type

Select the type of process or application:

- Chemical
- Electrolyte
- Environmental
- Gas processing
- Mineral and metallurgical
- Oil and gas
- Petrochemical
- Polymer
- Power
- Refining
- Pharmaceuticals

Figure 1.26 The user may select one process type that best describes the process in hand.

For example, if we select the type of process to be "**Chemical**", then Figure 1.27 shows what property method(s) is (are) recommended by Aspen Plus. As one can see that Aspen Plus property method wizard recommends the activity coefficient-based method for a general chemical process for an applied pressure less than or equal to 10 bar and the equation of state method with advanced mixing rules for an applied pressure greater than 10 bar. As pointed earlier, some specialty chemical processes are also pinpointed as subcategories of chemical processes, such as azeotropic separations, and carboxylic acids.



Chemical processes

In general, an activity coefficient-based property method is appropriate, such as the NRTL, WILSON, UNIQUAC, and their variances.

For preliminary designs, one of the UNIFAC-based property methods: the original UNIFAC, or the Dortmund modified UNIFAC (UNIF-DMD) can be used.

At high pressures (>10 bars), use an equation of state method with advanced mixing rules, such as the Wong-Sandler, MHV1, MHV2 or Mathias-Klotz-Prausnitz mixing rules. Options include SR-POLAR, PRWS, RKSWS, PRMVH2, RKSMVH2, SRK, PSRK, HYSGLYCO

Click one of the following options for more Help:

- Azeotropic separations
- Carboxylic acids
- Hydrogen Fluoride (HF)
- Inorganic chemicals,e.g., caustics, acids
- Liquid phase reactions, e.g., esterification
- Phenol plant
- Refrigeration
- Help for equation of state methods with advanced mixing rules
- Help for liquid activity coefficient methods
- Help for liquid activity coefficient methods with different equation of state
- Help for UNIFAC methods

Figure 1.27 The property method wizard recommends the activity coefficient-based method for a general chemical process for pressure less than or equal to 10 bar and the equation of state method with advanced mixing rules for pressure greater than 10 bar. Some specialty chemical processes are also pinpointed.

Remember that the deeper you dive below the surface, as you move from the main into a subcategory of a chemical process/component, the higher the accuracy and predictability of the Aspen Plus-recommended property method will be. There are special common applications where Aspen Plus gives them extra attention in terms of model accuracy and predictability.

Finally, Figure 1.28 shows the tree for the property method selection, which is based on different categories, such as the nature of medium (i.e., polar vs. non-polar, electrolyte vs. non-electrolyte, or ideal vs. real), the operating conditions (i.e., high vs. low pressure), the presence/absence of interaction parameters, and the presence/absence of LLE.

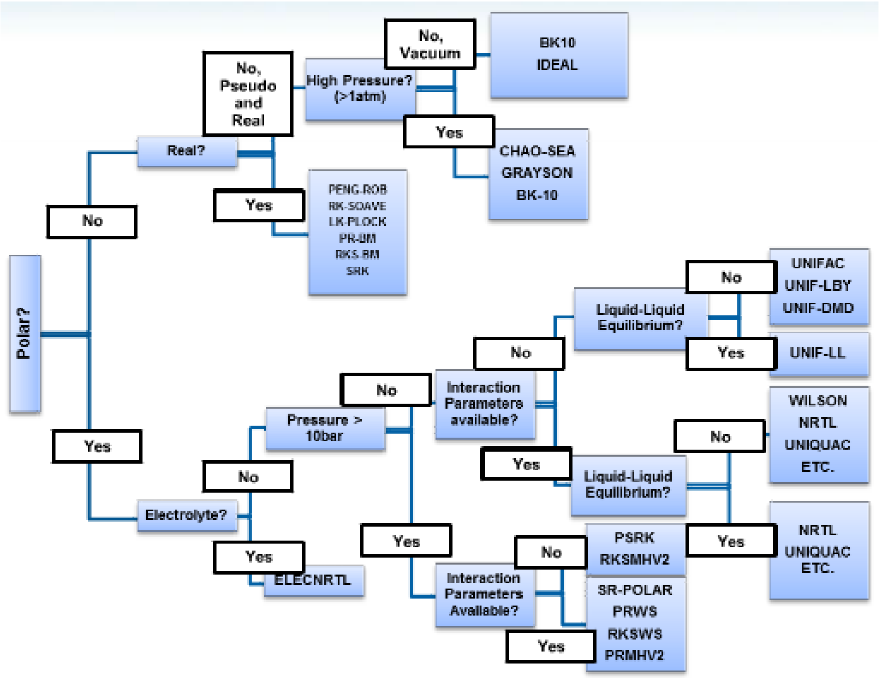


Figure 1.28 The "**Property Method**" selection tree based on different categories: The nature of medium (i.e., polar vs. nonpolar, electrolyte vs. nonelectrolyte, or ideal vs. real), the operating conditions (i.e., high vs. low pressure), the presence/absence of interaction parameters, and the presence/absence of LLE.

NOTE #1: *The property method selection is revisited in each successive chapter as it is the heart of any simulation process. Hopefully, toward the end of the book the user will grab the essence of property method selection based on the given chemical process being handled.*

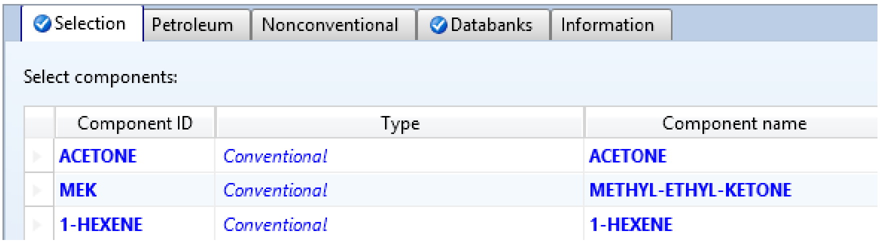
NOTE #2: *The idea behind presenting the choice of having more than one property method to try for a given process/component system is simply that one method may be superior to others in terms of getting a converging solution and realistic results. As one can see later that a given property method may fail to end up with realistic (or reasonable) results. In fact, it may not even converge to give a solution, in the first place. Thus, the built-in property method selection assistant will narrow the "search" circle for trying alternative property methods should the first suggested (or default) method fail to give reasonable results. Of course, it is intuitively assumed that the user has properly entered the flow rates, their compositions, their operating conditions (i.e., P & T), and any other physical, chemical, geometric, or thermodynamic constraint imposed on a given block or unit.*

NOTE #3: *Refer to Aspen Plus built-in help under the title: "Guidelines for Choosing a Property Method"; "Guidelines for Choosing a Property Method for Polar Non-Electrolyte Systems"; and "Guidelines for Choosing an Activity Coefficient Property Method".*

NOTE #4: *The user may assign a property method for a specified section, which is different from that assigned for the rest of the process flowsheet (i.e., global section). By default, Aspen Plus assigns a section called "GLOBAL" for the entire process flowsheet; however, the user may define a new section where it may comprise existing or newly added blocks. For further information on using more than one property method in a flowsheet, see Section 18.11.*

1.7 IMPROVEMENT OF THE PROPERTY METHOD ACCURACY

To demonstrate an example of how we can further improve the accuracy of a given model, let us look at the following set of compounds as part of a chemical process. Figure 1.29 shows three components: acetone, methyl ethyl ketone (MEK), and 1-hexene.

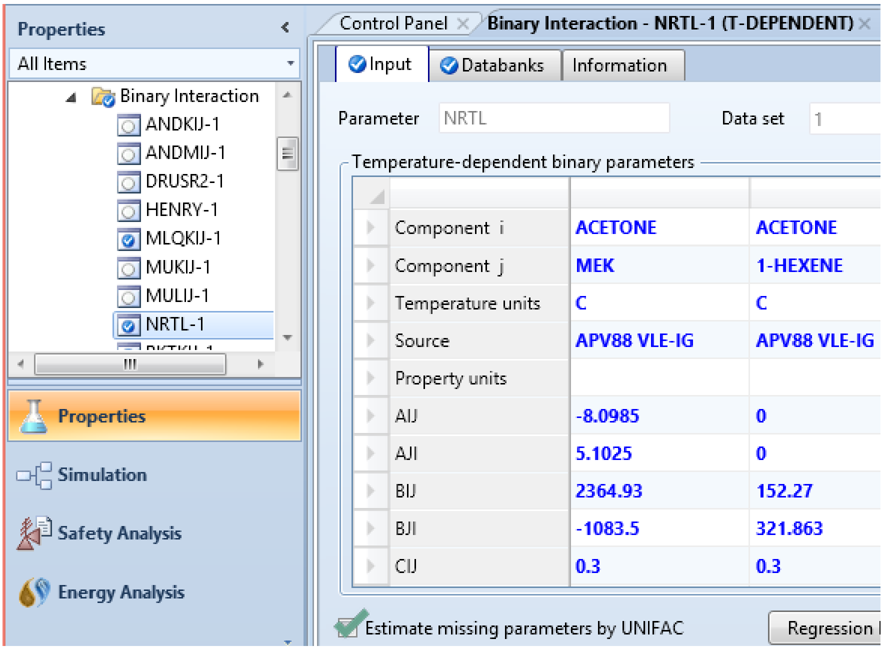


Select components:

Component ID	Type	Component name
ACETONE	Conventional	ACETONE
MEK	Conventional	METHYL-ETHYL-KETONE
1-HEXENE	Conventional	1-HEXENE

Figure 1.29 Three components are chosen to demonstrate the improvement of the accuracy of the default property method for a chemical process, that is, "**NRTL**".

Figure 1.30 shows the pairwise (i.e., binary) interaction parameters for the given three components. Notice that MEK–1-hexene interaction parameters are not given by Aspen Plus (i.e., not present in the built-in databanks. To improve the model predictability, one can select "**Estimate missing parameters by UNIFAC**", which will let Aspen Plus complete the missing information.



Parameter NRTL Data set 1

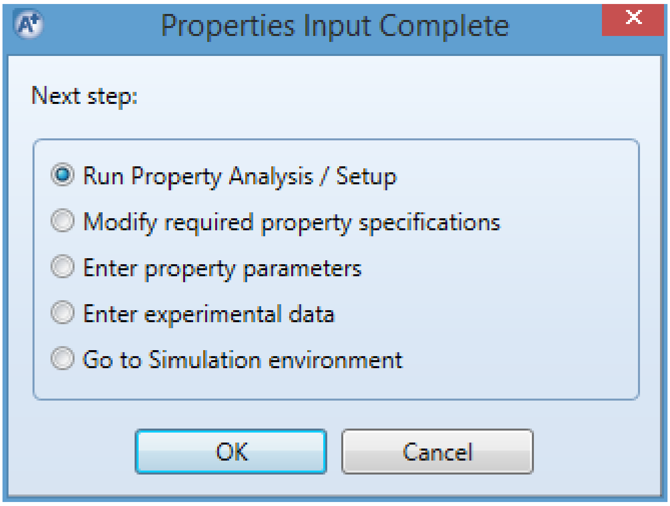
Temperature-dependent binary parameters

Component i	ACETONE	ACETONE
Component j	MEK	1-HEXENE
Temperature units	C	C
Source	APV88 VLE-IG	APV88 VLE-IG
Property units		
AIJ	-8.0985	0
AJI	5.1025	0
BIJ	2364.93	152.27
BJI	-1083.5	321.863
CIJ	0.3	0.3

☑ Estimate missing parameters by UNIFAC

Figure 1.30 Initially, the binary interaction parameters for MEK–1-hexene are missing. They can be calculated using “**UNIFAC**” method.

After selecting “**Estimate missing parameters by UNIFAC**”, while being under “**Properties**” environment | “**Analysis**” mode, click on “**Next**” button and Figure 1.31 window shows up. Select the “**Run Property Analysis/Setup**” option and click on the “**OK**” button and “**Control Panel**” tells that table generation is completed. Switch back to “**Binary Interaction - NRTL-1 (T-DEPENDENT)**” tab, you will notice that Aspen Plus has already calculated the pairwise interaction parameters for MEK–1-hexene, as shown in Figure 1.32. Notice that the source for the last column is now “**R-PCES**”, which means utilizing **P**roperty **C**onstant **ES**timation (PCES) regression. PCES provides the Bondi method for estimating the R and Q parameters for UNIFAC functional groups. The Aspen Plus physical property system uses these parameters in the UNIFAC, Dortmund UNIFAC, and Lyngby UNIFAC model. The Bondi method requires only the molecular structure as an input.

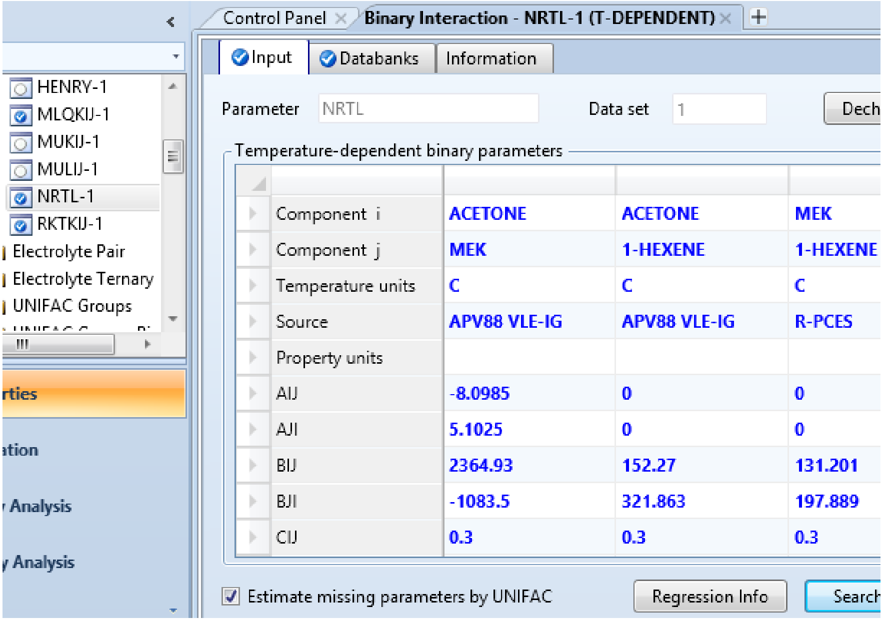


Properties Input Complete

Next step:

● Run Property Analysis / Setup
○ Modify required property specifications
○ Enter property parameters
○ Enter experimental data
○ Go to Simulation environment

Figure 1.31 Select "**Run Property Analysis/Setup**" option to calculate the missing binary interactions parameters for MEK–1-hexene.



Parameter NRTL Data set 1

Temperature-dependent binary parameters

Component i	ACETONE	ACETONE	MEK
Component j	MEK	1-HEXENE	1-HEXENE
Temperature units	C	C	C
Source	APV88 VLE-IG	APV88 VLE-IG	R-PCES
Property units			
AIJ	-8.0985	0	0
AJI	5.1025	0	0
BIJ	2364.93	152.27	131.201
BJI	-1083.5	321.863	197.889
CIJ	0.3	0.3	0.3

☑ Estimate missing parameters by UNIFAC

Figure 1.32 The binary interaction parameters are shown for MEK–1-hexene using "**UNIFAC**" method.

Under some circumstances, you may have to add additional databanks (see Figure 1.18) so that Aspen Plus can calculate the missing parameters.

The user may wish to carry out data analysis at this stage to check for the property model applicability. Click on the "**Binary Analysis**" button, at the right-top corner of "**Home**" ribbon, as shown in Figure 1.33.

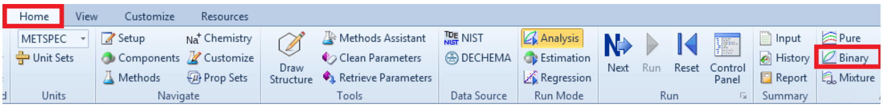
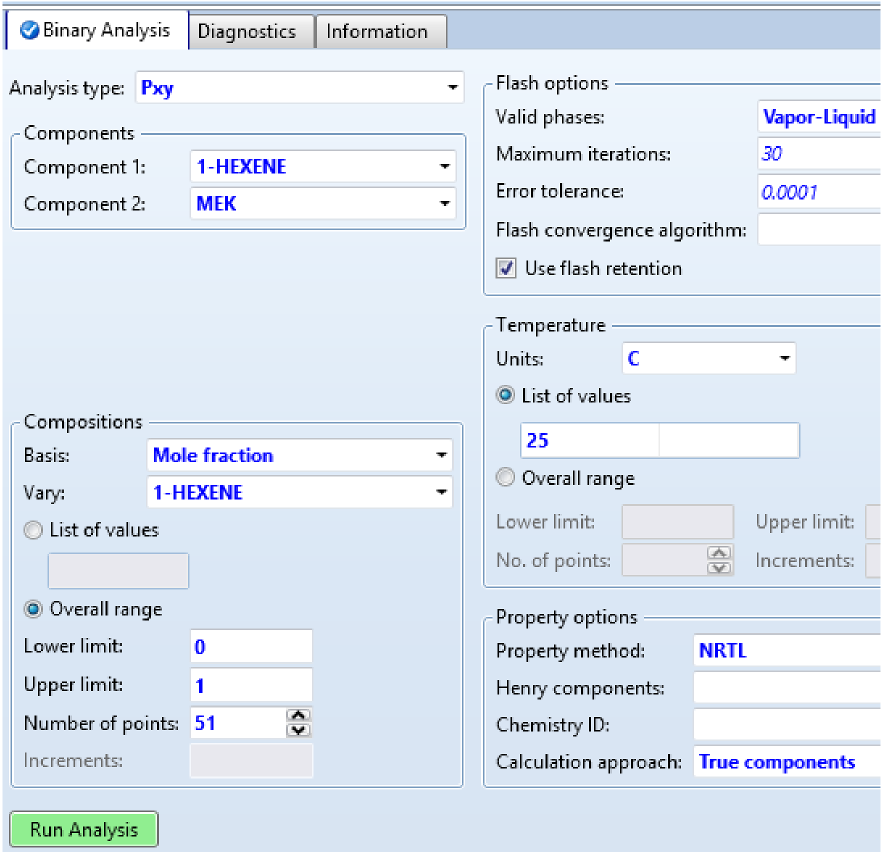


Figure 1.33 The "**Binary Analysis**" button is shown in "**Home**" ribbon.

The user may select *Gibbs energy of mixing*, *Txy*, or *Pxy* as a function of mole fraction to see whether the binary mixture of MEK–1-hexene forms an ideal mixture or deviates from ideality. For instance, Figure 1.34 shows the window for preparing the *Pxy* plot of the binary system made of 1-hexene and MEK.



Analysis type: Pxy

Components

Component 1: 1-HEXENE

Component 2: MEK

Compositions

Basis: Mole fraction

Vary: 1-HEXENE

○ List of values

● Overall range

Lower limit: 0

Upper limit: 1

Number of points: 51

Increments:

Flash options

Valid phases: Vapor-Liquid

Maximum iterations: 30

Error tolerance: 0.0001

Flash convergence algorithm:

☑ Use flash retention

Temperature

Units: C

● List of values

25

○ Overall range

Lower limit:

Upper limit:

No. of points:

Increments:

Property options

Property method: NRTL

Henry components:

Chemistry ID:

Calculation approach: True components

Figure 1.34 Carrying out analysis via plotting the isothermal dew- and bubble-point pressure as a function of mole fraction of 1-hexene to see the deviation from ideality.

Click on “**Run Analysis**” button and Aspen Plus shows the *Pxy* plot for the selected binary mixture, as shown in Figure 1.35. The figure shows a deviation from an ideal mixture in the form of an azeotrope at a mole fraction of 1-hexene higher than 0.80. An ideal liquid mixture (i.e., Raoult’s case) gives a straight line of P versus x with no formation of an azeotrope. Notice that the top blue curve, a non-straight line, represents the bubble-point pressure as $f(x_{\text{hexene}})$, which also indicates that we have a non-ideal binary mixture even below 0.8 mole fraction of 1-hexene.

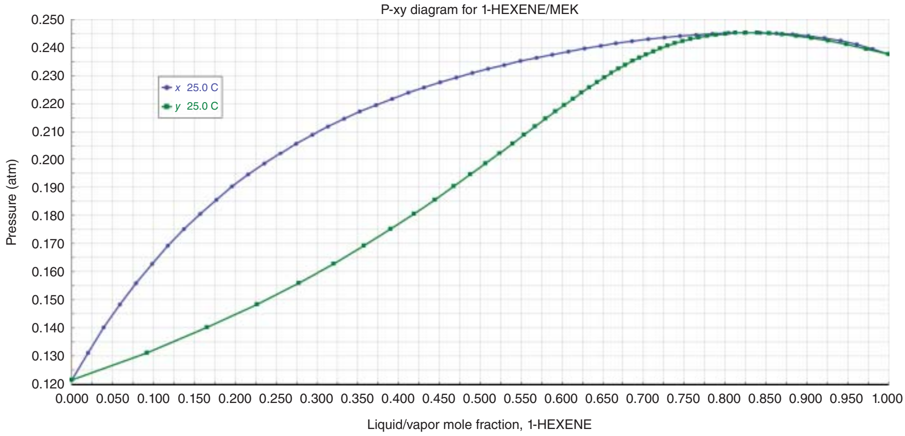


Figure 1.35 The dew- and bubble-point pressure as a function of 1-hexene mole fraction. Formation of an azeotrope can be seen at 1-hexene mole fraction greater than 0.80, in the form of an azeotrope.

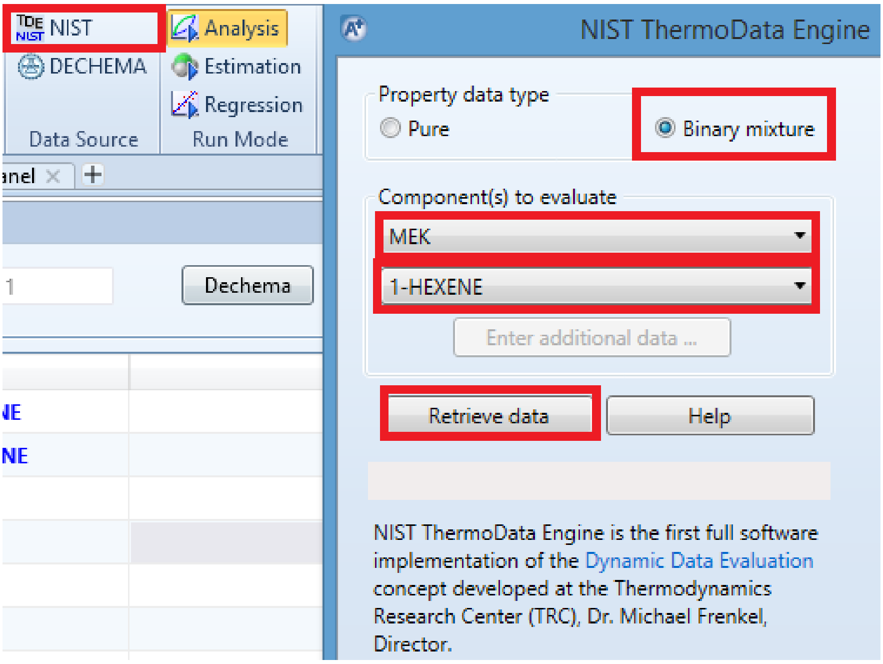
NOTE #5: *The plot format can be accessed* via “***Plot Format***” *tab window found in the* “***Top***” *toolbar. The user may carry out cosmetic changes (i.e., font type and size) on the plot format and make it look a more plausible.*

At this stage, one can say that the default property method “**NRTL**” could account for a deviation from ideality for the binary mixture of MEK–1-hexene via accounting for the azeotrope condition at higher values of 1-hexene, using UNIFAC group contribution method.

NOTE #6: *In general, it will be sufficient, within acceptable engineering accuracy limits, to calculate the missing pairwise interaction parameters using UNIFAC method. Nevertheless, if more accuracy is required, then the experimental data can be retrieved from the* ***T****hermo****D****ata* ***E****ngine (****TDE****), which is a thermodynamic data correlation, evaluation, and prediction tool provided with Aspen Plus through a long-term collaboration agreement with the* ***N****ational* ***I****nstitute of* ***S****tandards and* ***T****echnology (****NIST****). The purpose of the TDE software is to provide critically evaluated thermodynamic and transport property data based on the principles of dynamic data evaluation. Critical evaluation*

> *is based on published experimental data stored in a program database, predicted values based on molecular structure and corresponding-states methods, and user supplied data, if any. The NIST source database contains more than 24,000 pure components, more than 30,000 binary pairs, and is updated quarterly.*

Here, let us show how to improve the accuracy of pairwise interactions. Either open a new simulation with the same three components or delete the third column that belongs to MEK–1-hexene binary interaction parameters. Click on the "**NIST**" button as shown in Figure 1.36 (*left*) and the "**NIST ThermoData Engine**" window shows up as shown in Figure 1.36 (*right*). Remember to de-select "**Estimate missing parameters by UNIFAC**" option in "**Parameters**" | "**Binary Interaction**" | "**NRTL-1**" | "**Input**" tab form; otherwise, the results will be different in the following figures.



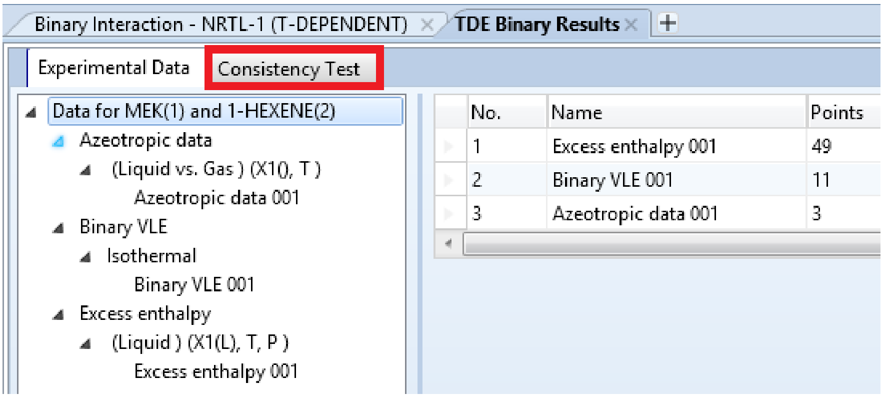
Property data type
○ Pure
● Binary mixture

Component(s) to evaluate
MEK
1-HEXENE

NIST ThermoData Engine is the first full software implementation of the Dynamic Data Evaluation concept developed at the Thermodynamics Research Center (TRC), Dr. Michael Frenkel, Director.

Figure 1.36 Retrieving experiment-based data for the binary mixture of MEK–1-hexene with the help of "**NIST/TDE**" database.

Click on the "**Retrieve data**" button and the result is shown in Figure 1.37. It shows 11 binary VLE data points for the given binary mixture. We exploit such a data set to find the parameters describing the interaction between MEK and 1-hexene.

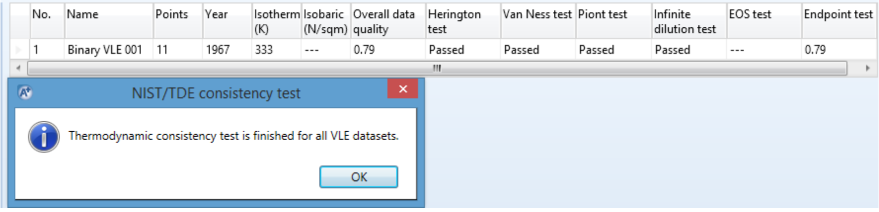


No.	Name	Points
1	Excess enthalpy 001	49
2	Binary VLE 001	11
3	Azeotropic data 001	3

Figure 1.37 A set of 11 data points are obtained from "**NIST/TDE**" databank for the given binary mixture.

> **<u>NOTE #7:</u>** *Not all experimental data are reliable or trustable; in other words, the consistency test must be carried out prior to hinging upon them for the sake of extracting further pure or binary data. See Chapter 2 as a demonstration for the possibility of having some NASTY, out of NIST, data.*

Click on the "**Consistency Test**" tab to test for the data goodness and run the consistency test via clicking on the "**Run Consistency Tests**" button shown at the bottom of the "**Consistency Test**" tab form. Figure 1.38 shows the consistency test results. The overall data quality is about 0.8, which is close to unity. The closer to one the value is, the better the data quality will be.



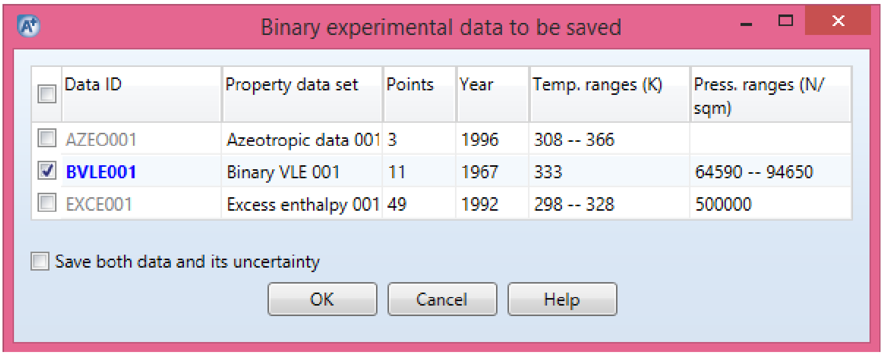
No.	Name	Points	Year	Isotherm (K)	Isobaric (N/sqm)	Overall data quality	Herington test	Van Ness test	Piont test	Infinite dilution test	EOS test	Endpoint test
1	Binary VLE 001	11	1967	333	---	0.79	Passed	Passed	Passed	Passed	---	0.79

NIST/TDE consistency test

Thermodynamic consistency test is finished for all VLE datasets.

Figure 1.38 The NIST/TDE consistency test with an overall data quality of 0.79.

Let us go back to the "**Experimental Data**" tab window (see Figure 1.37). Click on the "**Binary VLE**" | "**Isothermal**" | "**Binary VLE 001**" form and save the data set via clicking on the "**Save Data**" button at the bottom of the active form so that we can carry out some regression/estimation steps to improve the model goodness. The "**Binary experimental data to be saved**" window pops up as in Figure 1.39.

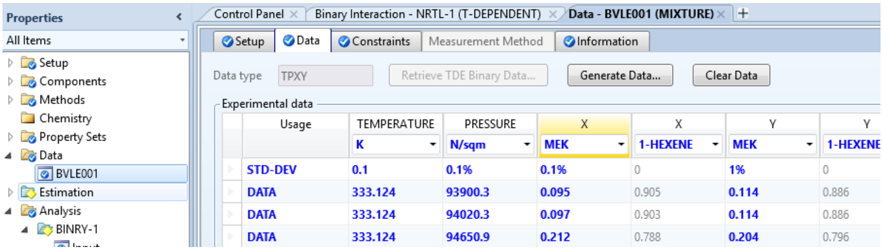


☐	Data ID	Property data set	Points	Year	Temp. ranges (K)	Press. ranges (N/sqm)
☐	AZEO001	Azeotropic data 001	3	1996	308 -- 366	
☑	BVLE001	Binary VLE 001	11	1967	333	64590 -- 94650
☐	EXCE001	Excess enthalpy 001	49	1992	298 -- 328	500000

☐ Save both data and its uncertainty

Figure 1.39 The “**Binary experimental data to be saved**” window for saving NIST/TDE data set.

A confirmation pop-up window will tell the user that the data are saved under “**Data**” folder in “**Navigation**” pane, as shown in Figure 1.40. Of course, you may rename the data set to a name of your choice by right-clicking on the data set shown under “**Data**” folder and selecting “**Rename**” submenu from the short pop-up context menu.



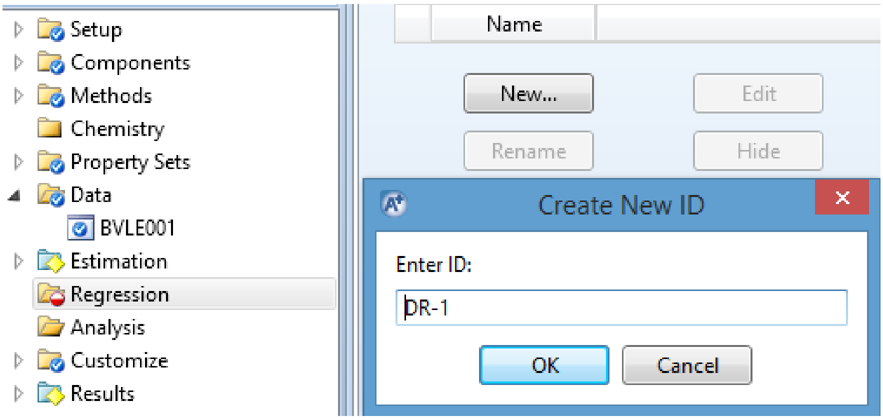
Data type TPXY

Experimental data

Usage	TEMPERATURE	PRESSURE	X	X	Y	Y
	K	N/sqm	MEK	1-HEXENE	MEK	1-HEXENE
STD-DEV	0.1	0.1%	0.1%	0	1%	0
DATA	333.124	93900.3	0.095	0.905	0.114	0.886
DATA	333.124	94020.3	0.097	0.903	0.114	0.886
DATA	333.124	94650.9	0.212	0.788	0.204	0.796

Figure 1.40 The experimental data are saved within Aspen Plus environment under “**Data**” folder.

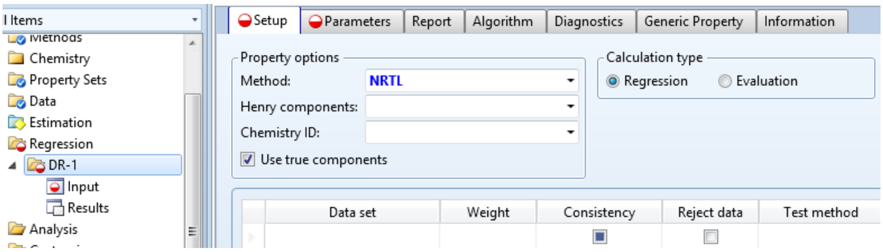
Let us switch to “**Regression**” mode (we are still under “**Properties**” environment) so that we can carry out regression or parameter evaluation step. Once the user switches to “**Regression**” mode, the “**Regression**” folder icon becomes half-filled red circle, indicating that it requires further input data to be dealt with in “**Regression**” mode. Under “**Regression**” tab form, click on “**New …** ” button where “**Create New ID**” form pops up as shown in Figure 1.41.



Enter ID: DR-1

Figure 1.41 Creation of regression data set called "**DR-1**", which will be used under "**Regression**" mode.

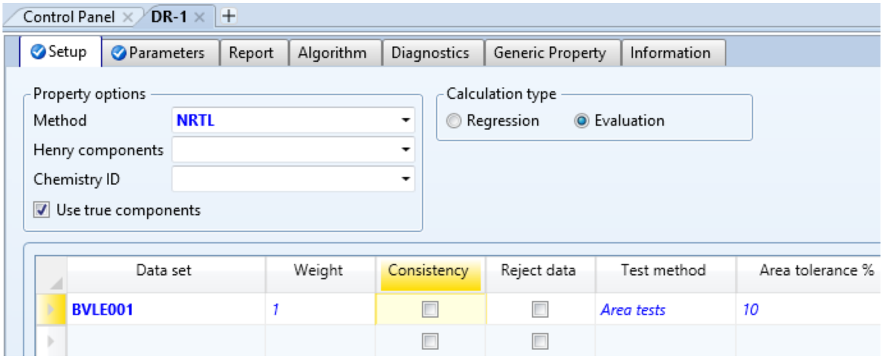
Click on "**OK**" button, and the result is as shown in Figures 1.42 and 1.43. Here, we have the choice to either carry out regression or parameter evaluation using the given model. We will try both to see how they affect the performance of the property model being examined.



Property options
Method: NRTL
Henry components:
Chemistry ID:
☑ Use true components

Calculation type
● Regression ○ Evaluation

Figure 1.42 The regression data set "**DR-1**" is ready to be examined using either regression or evaluation step.



Property options
Method NRTL
Henry components
Chemistry ID
☑ Use true components

Calculation type
○ Regression ● Evaluation

Data set	Weight	Consistency	Reject data	Test method	Area tolerance %
BVLE001	1	☐	☐	Area tests	10
		☐	☐		

Figure 1.43 The data set "**BVLE001**" contains the 11 data points for VLE of MEK–1-hexene binary mixture.

Let us try the evaluation step and retain the same property method, that is, "**NRTL**". Figure 1.43 shows the "**Setup**" window after defining the data set to be examined. Pick it up using the drop-down list.

Click on "**Next**" button, found in "**RUN**" tab, within "**Home**" ribbon, to carry out the "*Evaluation*" step. The "**Data Regression Input Complete**" window pops up; select the first option "**Run data regression cases**", and Figure 1.44 shows the "**Data Regression Run Selection**" window, which allows the user to select the right data set to be examined.

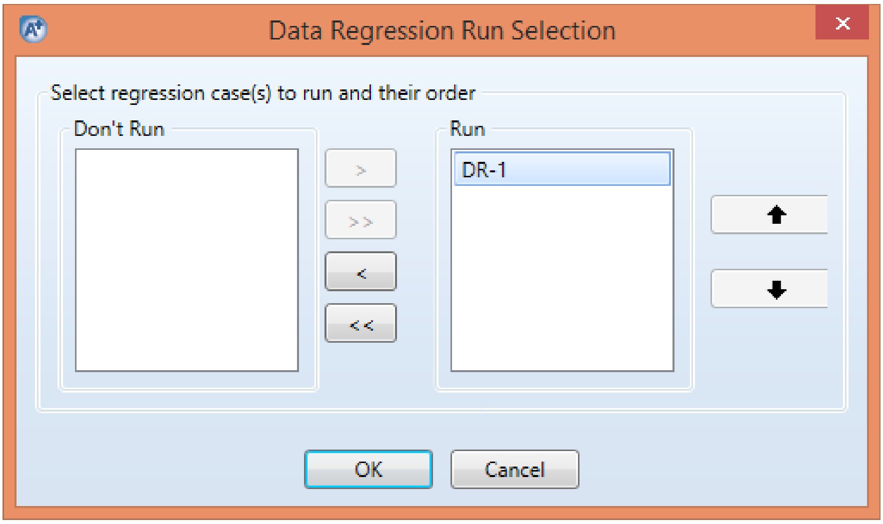
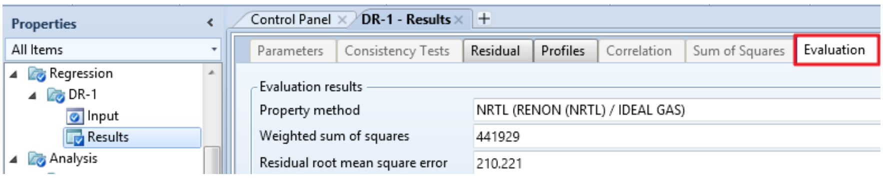


Figure 1.44 The "**Data Regression Run Selection**" window where the user selects the right data set to be examined.

Figure 1.45 shows the evaluation step results. The residual root mean square error (RRMSE) is much larger than the demarcation limit (10.0) between good and bad fit for VLE data.



Evaluation results

Property method	NRTL (RENON (NRTL) / IDEAL GAS)
Weighted sum of squares	441929
Residual root mean square error	210.221

Figure 1.45 The evaluation step results in terms of the statistical parameters that tell us about the model goodness.

NOTE #8: *Normally, RRMSE value should be less than 10 for VLE data and less than 100 for LLE data. It is calculated as* $\text{RRMSE} = \sqrt{\frac{\text{Weighted sum of squares}}{N-P}}$, *where N is the number of data points and P is number of model parameters.*

Figure 1.46 shows the plot of estimated versus experimental mole fraction of 1-hexene vapor. If the data points were to lie on the diagonal line (i.e., $y = x$), then the match would be perfect; an indication that the discrepancy between estimated and experimental data would be absent.

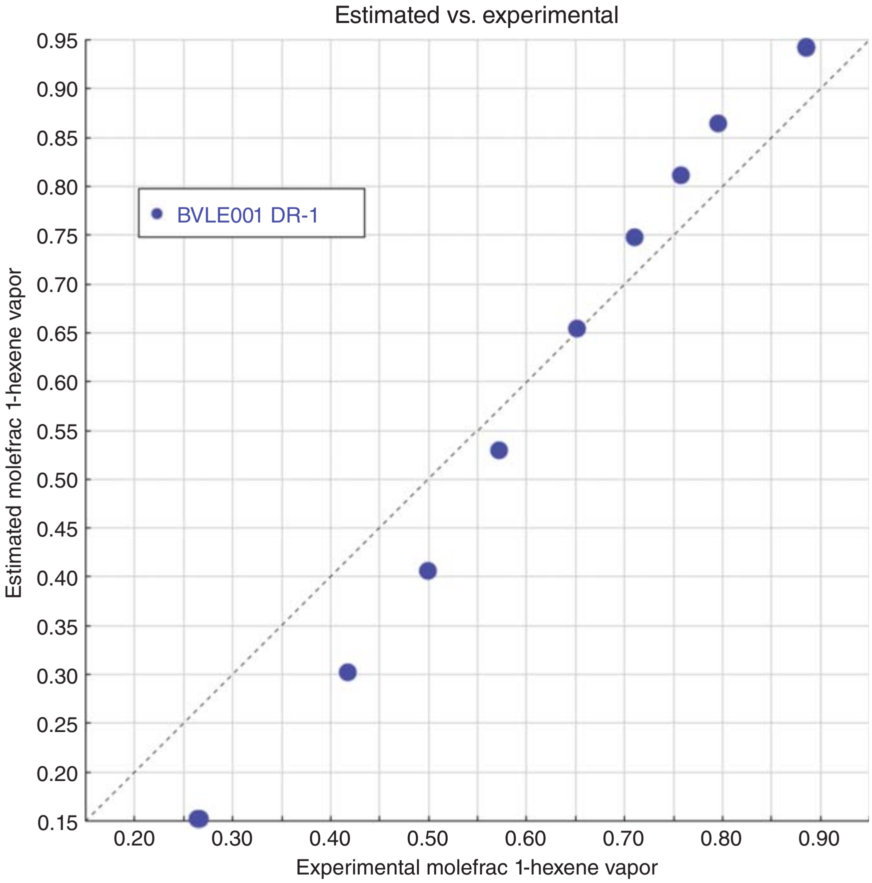
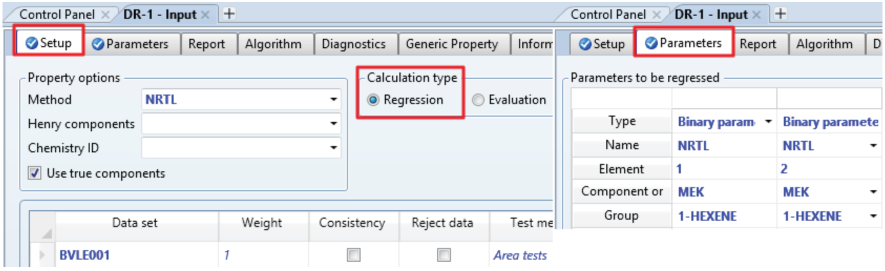


Figure 1.46 The plot of estimated versus experimental data for 1-hexene vapor mole fraction.

To improve the fit, let us switch to "*Regression*" step for "**Calculation type**" mode (Figure 1.47 *left*) and define the property model parameters and components in "**Parameters**" tab window, as shown in Figure 1.47 (*right*).



Method: NRTL

Henry components:

Chemistry ID:

☑ Use true components

● Regression ○ Evaluation

	Data set	Weight	Consistency	Reject data	Test me
	BVLE001	1	☐	☐	Area tests

Parameters to be regressed

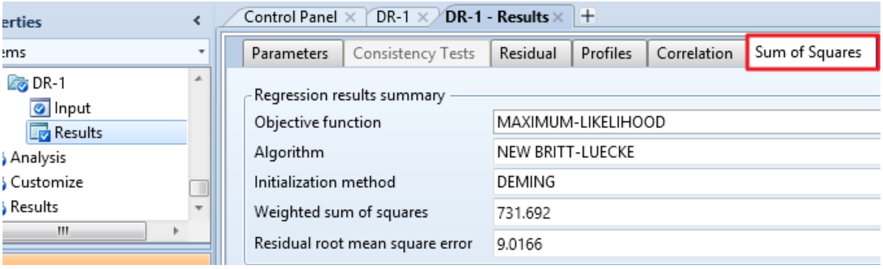
Type	Binary param	Binary paramete
Name	NRTL	NRTL
Element	1	2
Component or	MEK	MEK
Group	1-HEXENE	1-HEXENE

Figure 1.47 Defining the property model parameters and components for binary parameters calculation under "**Setup**" tab (*left*) and "**Parameters**" tab (*right*).

Notice that element 1 and 2 account for a_{ij} and b_{ij}, respectively. The activity coefficient of species i in a binary medium made of i and j is expressed as a function of the binary parameters a_{ij}, b_{ij}, c_{ij}, d_{ij}, e_{ij}, and f_{ij}. Such parameters can be determined from VLE and/or LLE data regression. Notice that a_{ij}, b_{ij}, e_{ij}, and f_{ij} are unsymmetrical, in general. In other words, a_{ij} may not be equal to a_{ji}, and so on.

The Aspen Plus physical property system has a large number of built-in binary parameters for the "**NRTL**" model. See the built-in Aspen Plus help under the topic "**NRTL (Non-Random Two-Liquid)**". In addition, the polymer NRTL ("**POLYNRTL**") model requires such binary interaction parameters to account for solvent–solvent interactions, solvent–segment interactions, and segment–segment interactions. See the built-in Aspen Plus help under the topic "**Polymer NRTL Model Parameters**".

Click on the "**Next**" button to carry out the regression step. Two pop-up windows will appear and thus follow the previous steps pertinent to Figure 1.44. Figure 1.48 shows the statistical parameters associated with the new fit. Notice that the residual root mean square error is about 9, which is smaller than that of the previous case and is also less than the demarcation limit (i.e., 10).



Regression results summary

Objective function	MAXIMUM-LIKELIHOOD
Algorithm	NEW BRITT-LUECKE
Initialization method	DEMING
Weighted sum of squares	731.692
Residual root mean square error	9.0166

Figure 1.48 RRMSE is reduced to 9 which is less than 10 for VLE data.

Figure 1.49 shows the plot of estimated versus experimental mole fraction of 1-hexene vapor. Notice how close the data points are to the diagonal line (i.e., $y = x$), an indication of a good fit and minimal discrepancy between estimated and experimental data.

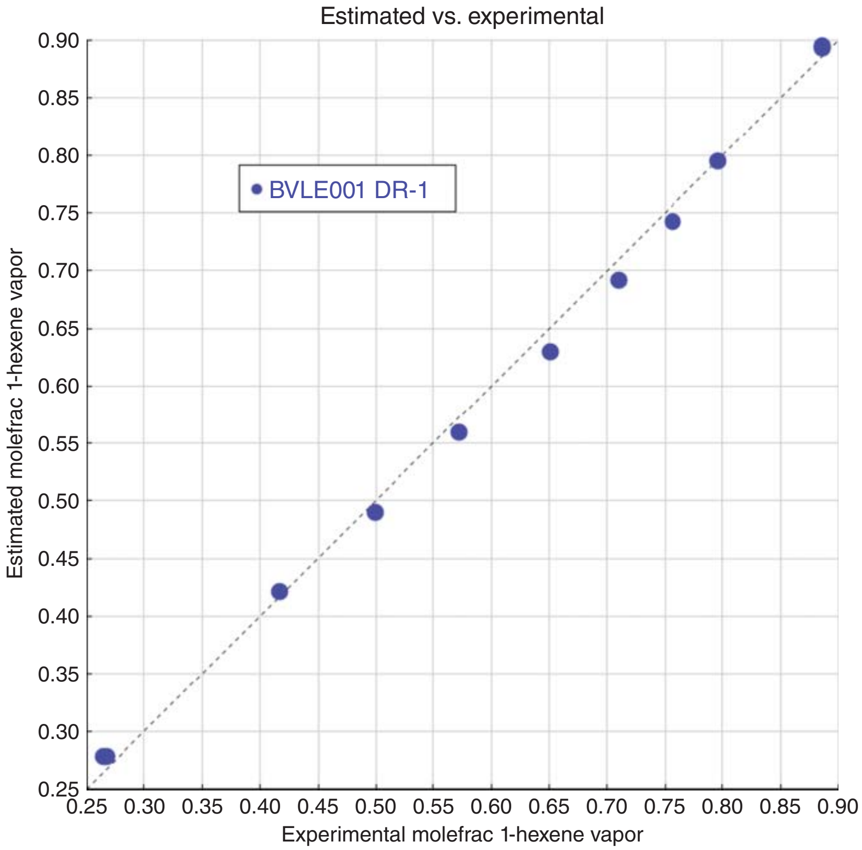
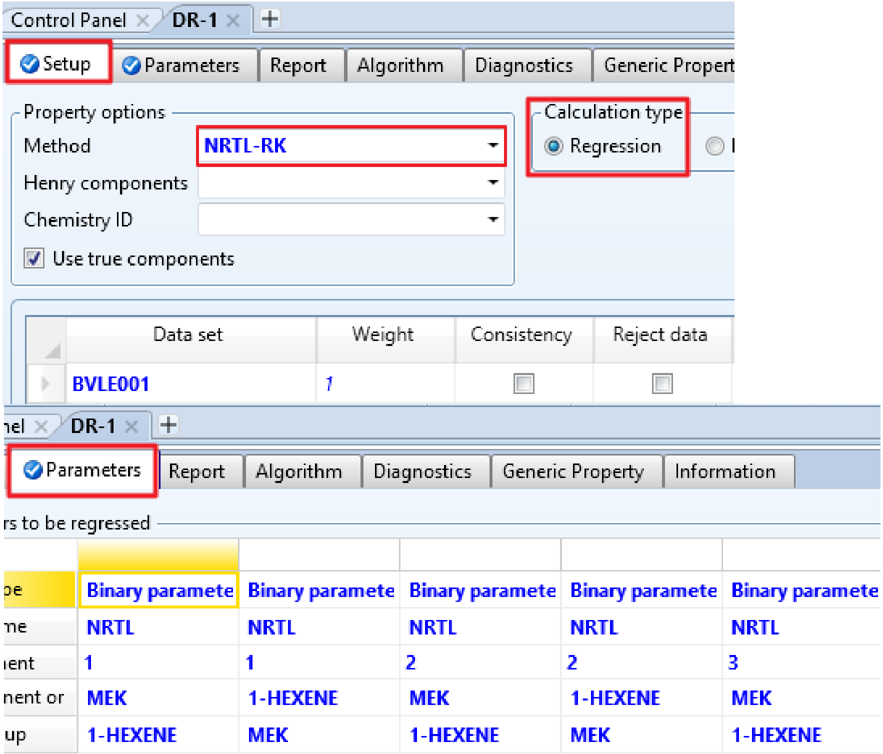


Figure 1.49 The plot of estimated versus experimental data for 1-hexene vapor mole fraction.

The model goodness can be further improved if we attempt to change the property model from "**NRTL**" to another property model, such as "**NRTL-RK**", which accounts for deviation from ideality in the gas phase in addition to accounting for deviation in the liquid phase by "**NRTL**" itself, as shown in Figure 1.50.



Property options

Method: NRTL-RK

Henry components:

Chemistry ID:

☑ Use true components

Calculation type: ● Regression

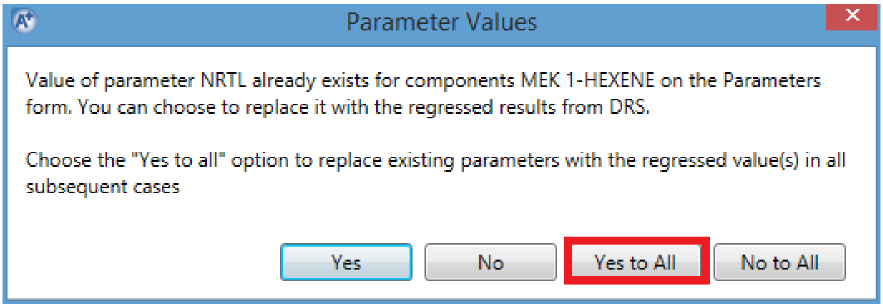
Data set	Weight	Consistency	Reject data
BVLE001	1	☐	☐

rs to be regressed

pe	Binary paramete	Binary paramete	Binary paramete	Binary paramete	Binary paramete
ne	NRTL	NRTL	NRTL	NRTL	NRTL
ent	1	1	2	2	3
nent or	MEK	1-HEXENE	MEK	1-HEXENE	MEK
up	1-HEXENE	MEK	1-HEXENE	MEK	1-HEXENE

Figure 1.50 Further improvement of model goodness using "**NRTL-RK**" model.

Click on the "**Next**" button and the simulator will find the best parameter estimates for the newly proposed property model for binary parameters. Figure 1.51 shows a pop-up window requesting to replace the old by new estimated binary parameters for the given binary system. Click on the "**Yes to All**" button to replace the old by new values.

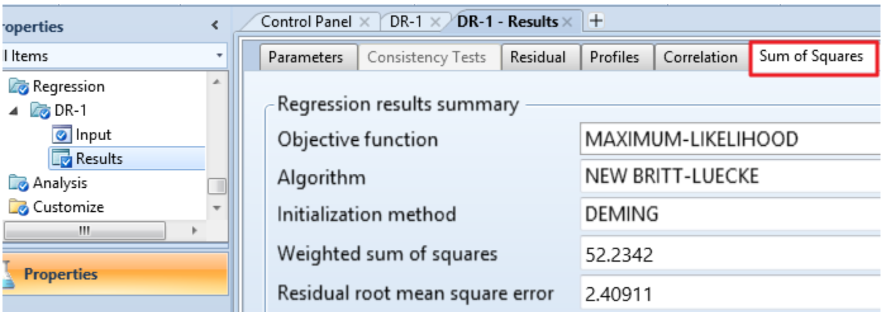


Value of parameter NRTL already exists for components MEK 1-HEXENE on the Parameters form. You can choose to replace it with the regressed results from DRS.

Choose the "Yes to all" option to replace existing parameters with the regressed value(s) in all subsequent cases

Figure 1.51 The regressed binary interaction parameters will replace the existing binary parameters for MEK–1-hexene.

Figure 1.52 shows that the new RRMSE is further reduced to 2.4.



Regression results summary

Objective function: MAXIMUM-LIKELIHOOD
Algorithm: NEW BRITT-LUECKE
Initialization method: DEMING
Weighted sum of squares: 52.2342
Residual root mean square error: 2.40911

Figure 1.52 Reduction of discrepancy between estimated and experimental data points for VLE of MEK–1-hexene mixture.

Figure 1.53 shows the plot of estimated versus experimental mole fraction of 1-hexene vapor. Notice how very close the data points are to the diagonal line (i.e., $y = x$), an indication of an excellent fit and minimal discrepancy between estimated and experimental data.

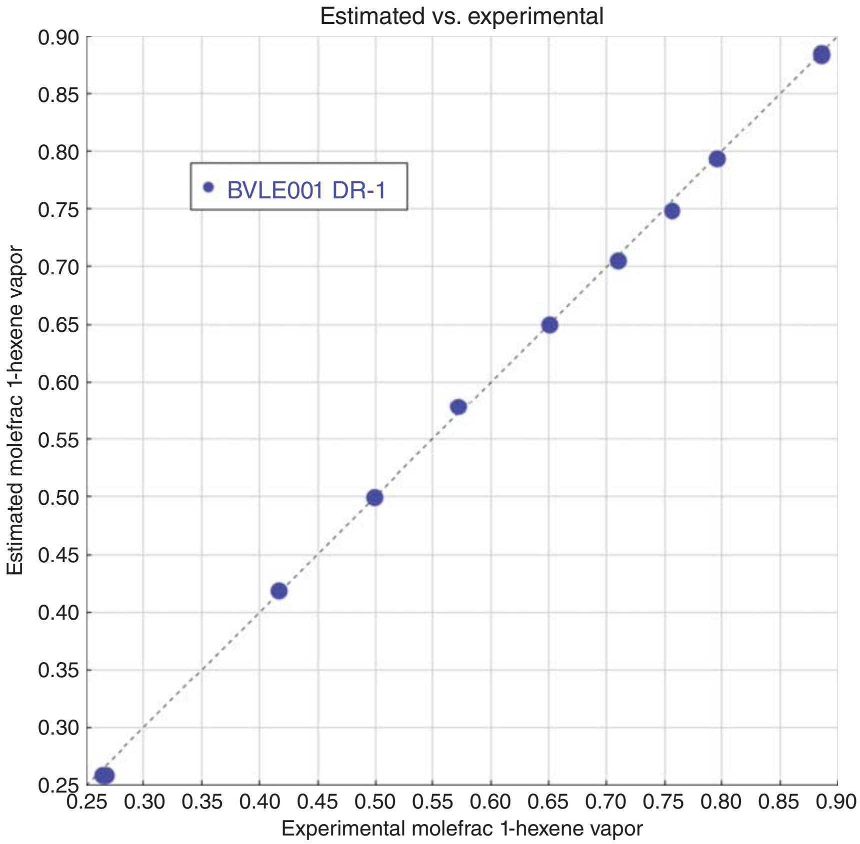
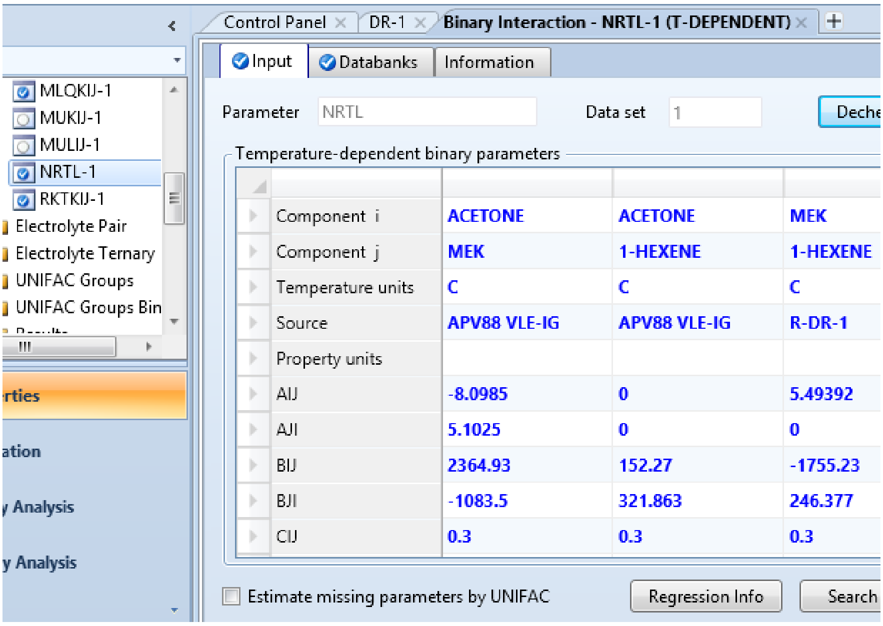


Figure 1.53 The plot of estimated versus experimental data for 1-hexene vapor mole fraction.

Finally, Figure 1.54 shows the pairwise (i.e., binary) interaction parameters for the three components present in the process flowsheet. Notice that the last column pertains to MEK–1-hexene where R-DR-1 is the source of data. "**R-DR-1**" says "**DR-1**" data set taken from "**Regression**" folder found in "**Navigation**" pane.



Parameter NRTL Data set 1

Temperature-dependent binary parameters

Component i	ACETONE	ACETONE	MEK
Component j	MEK	1-HEXENE	1-HEXENE
Temperature units	C	C	C
Source	APV88 VLE-IG	APV88 VLE-IG	R-DR-1
Property units			
AIJ	-8.0985	0	5.49392
AJI	5.1025	0	0
BIJ	2364.93	152.27	-1755.23
BJI	-1083.5	321.863	246.377
CIJ	0.3	0.3	0.3

☐ Estimate missing parameters by UNIFAC

Figure 1.54 The pairwise (binary) interaction parameters for the three components while the last column indicates that the source is taken from "**DR-1**" data set under "**Regression**" folder.

> **<u>NOTE #9:</u>** *The user should not panic about the regression aspects of experimental data. In the first place, we will be satisfied with the simplest way, that is, calculation of the missing parameters using UNIFAC group contribution method. However, the regression/evaluation step will be left as an advanced alternative approach if the accuracy of data for a given chemical process is of an immense importance.*

1.8 FILE SAVING

At this stage, we do not construct any process flowsheet, as this task is dealt with, starting from Chapter 2 onward. Yet, it is always highly recommended to save one's work, from time to time, so that it does not get lost. To save your work, you can either go to "**File**" menu found in "**Top**" toolbar (see Figure 1.8) followed by "**Save**" or "**Save As**" submenu, or click on the diskette icon found in "**Quick Access**" toolbar. The "**Save As**" dialog window pops up and you have four types of file format by which you can save your work:

1. **Aspen Plus Compound File (*.apwz):** Aspen Plus combines different file types into a single file. Such types include Backup file (*.bkp); embedded backup file (*.apmbd); Fortran files (*.dll, *.obj, *.dlopt, *.F); equipment design and rating files (e.g., *.bjt, *.edr); and custom or user model library file (*.apm).
2. **Aspen Plus Documents File (*.apw):** Aspen Plus saves the file as an Aspen Plus Document file.
3. **Aspen Plus Backup File (*.bkp):** Aspen Plus saves the file as an Aspen Plus Backup file.
4. **Aspen Plus Template File (*.apt):** Aspen Plus saves the file as a template that can be used as a basis for future simulations.

Aspen Plus compound files contain all input specifications, simulation results, and intermediate convergence information, in addition to other (normally) external files that the simulation needs. This can include user subroutines, DLOPT files, EDR input files for rigorous HeatX models, embedded Excel spreadsheets, and other files. When you save a compound file, Aspen Plus attempts to locate all related files based on the specifications in the simulation and automatically adds them to the compound file. You can add other files in your working folder to the compound file if necessary. If you save the file with a new name, Aspen Plus will save files within the compound file, which normally have the same name as the simulation file with the same new name (i.e., if you save Simu1.apwz as Mysim.apwz, Aspen Plus will save the backup file Simu1.bkp inside the compound file as Mysim.bkp). Table 1.2 gives a summary of the common Aspen Plus editable files.

TABLE 1.2 A Summary of the Common Aspen Plus Savable File Types.

File Type	Extension	Format	Description
Document	*.**apw**	Binary	Quick restart file containing simulation input and results and immediate convergence information
Compound file	*.**apwz**	Binary	Consolidated file containing all files used by a simulation
Backup	*.**bkp**	ASCII	Archive file containing simulation input and results
Template	*.**apt**	ASCII	Template containing default inputs

NOTE #10: *Files may be embedded or linked in the compound file. Files in the same folder as the Aspen Plus file or in its subfolders are embedded if referenced by relative paths. Otherwise, they are linked (not stored in the compound file). To add, remove, or extract files from a compound file, first open the file in Aspen Plus. Then, click "**File**" | "**Edit Compound File**". A dialog box appears allowing you to manipulate the current compound file. Compound files are ideal when moving simulations from one computer to another or making backups, especially for those types of simulations that need additional files. When you open a compound file in Aspen Plus, it makes a subfolder under the current folder as a working folder.*

EXERCISE 1.1

Try saving your current simulation project or any simulation project you create in the four possible file formats shown in Table 1.2 and have a look at the default location of Aspen Plus files (normally, “**C:\ProgramData\AspenTech\Aspen Plus V8.8**”) just to familiarize yourself with the file icon, size, and type of files/folder created with each choice.

1.9 A GOOD FLOWSHEETING PRACTICE

Start small and simple and then slowly grow up like a typical human being grows up.

- To build large flowsheets, you should start with a few blocks at a time. In this way, you will have a better chance to troubleshoot errors if they occur.
- Ensure that flowsheet inputs are reasonable.
- After carrying out the simulation, using Aspen Plus, check that results are consistent and realistic.

In addition, if the flowsheet is already given and has many blocks, and for some reason the solution did not converge upon modifying any input parameter as part of block specifications or setup, then the user has the flexibility to deactivate all blocks except the block(s) that has(have) convergence problems. Once the convergence problems are resolved, the user may activate other deactivated blocks one at a time and repeat the procedure until all blocks are operational (i.e., activated). To activate/deactivate a block within a flowsheet, highlight a block, right-click the mouse, and select activate/deactivate command from the pop-up shortcut context menu.

1.10 ASPEN PLUS BUILT-IN HELP

Help topics are under three categories:

- **Contents**
  - Used to browse through the documentation. The “**User Guides**” and “**Reference Manuals**” are all included in the help.
- **Index**
  - Used to search for help on a topic using the index entries
- **Search**
  - Used to search for a help on a topic that includes any word or phrase

1.11 FOR MORE INFORMATION

- ***Online Help:*** Aspen Plus has a complete system of online help and context-sensitive prompts. The help system contains both context-sensitive help and reference information. For more information about using Aspen Plus help, see the *Aspen Plus User Guide*.

- ***Aspen Plus Application Examples:*** A suite of sample online Aspen Plus simulations illustrating specific processes is delivered with Aspen Plus.
- ***Aspen Plus Installation Guide for Windows:*** This guide provides instructions on installation of Aspen Plus.
- ***Aspen Plus Getting Started Building and Running a Process Model:*** This tutorial includes several hands-on sessions to familiarize you with Aspen Plus. The guide takes you step-by-step to learn the full power and scope of Aspen Plus.
- ***Aspen Plus Getting Started Modeling Processes with Electrolytes:*** This tutorial includes several hands-on sessions to familiarize you with simulating electrolyte systems with Aspen Plus.
- ***Aspen Plus Getting Started Modeling Petroleum Processes:*** This tutorial includes several hands-on sessions to familiarize you with simulating petroleum processes with Aspen Plus.
- ***Aspen Plus Getting Started Customizing Unit Operation Models:*** This tutorial includes several hands-on sessions to familiarize you with the customization of unit operation models with Aspen Plus.
- ***Aspen Plus Getting Started Modeling Processes with Solids:*** This tutorial includes several hands-on sessions to familiarize you with simulating systems containing solids with Aspen Plus.
- ***Aspen Plus User Guide*** The three-volume *Aspen Plus User Guide* provides step-by-step procedures for developing and using an Aspen Plus process simulation model. The guide is task-oriented to help you accomplish the engineering work you need to do, using the powerful capabilities of Aspen Plus.
- ***Aspen Plus Reference Manual Series:*** Aspen Plus reference manuals provide detailed technical reference information. These manuals include background information about the unit operation models and the physical properties methods and models available in Aspen Plus, tables of Aspen Plus databank parameters, group contribution method functional groups, and a wide range of other reference information. The set comprises
  - *Unit Operation Models*
  - *Physical Property Methods and Models*
  - *Physical Property Data*
  - *User Models*
  - *System Management*
  - *System Administration*
  - *Summary File Toolkit*
  - *Input Language Guide.*

The Aspen Plus manuals are delivered in Adobe portable document format (PDF), as part of the Aspen Plus Documentation CD.

HOMEWORK/CLASSWORK 1.1 (*PXY*)

Draw *Pxy* for acetone–MIBK mixture at $T = 90°\text{C}$. At a mole fraction of 0.5, calculate the bubble-point pressure and dew-point pressure, expressed in bar.

HOMEWORK/CLASSWORK 1.2 (ΔG_{MIX})

Draw ΔG_{mix} (kcal/mol) for acetone–MIBK mixture at $T = 90°\mathrm{C}$ and $P = 2$ atm. At what mole fraction of acetone does the maximum deviation from an ideal mixture occur?

HOMEWORK/CLASSWORK 1.3 (LIKES DISSOLVE LIKES) AS ENVISAGED BY NRTL PROPERTY METHOD

Using "**Chemicals with Metric Units**" template, create an Aspen Plus file with the following components: methanol, ethanol, *n*-butanol, 1-octanol, and water. The default property method is "**NRTL**". There will be no flowsheet at this stage. We will stay under "**Properties**" environment using analysis and estimation mode. Regrettably, the NIST/TDE experimental data failed the VLE consistency tests for the following binary systems: methanol–octanol and water–octanol. So, we will not carry out any regression step. Hence, the missing binary parameters will be estimated using UNIFAC (Select "**Estimate parameters using UNIFAC**" option under "**NRTL-1**" sheet for "**Binary Interaction**" folder and run the simulator). Notice that the following sequence represents the polarity of the given molecules in descending order:

$$H_2O > \text{Methanol} > \text{Ethanol} > n\text{–Butanol} > n\text{–Octanol}$$

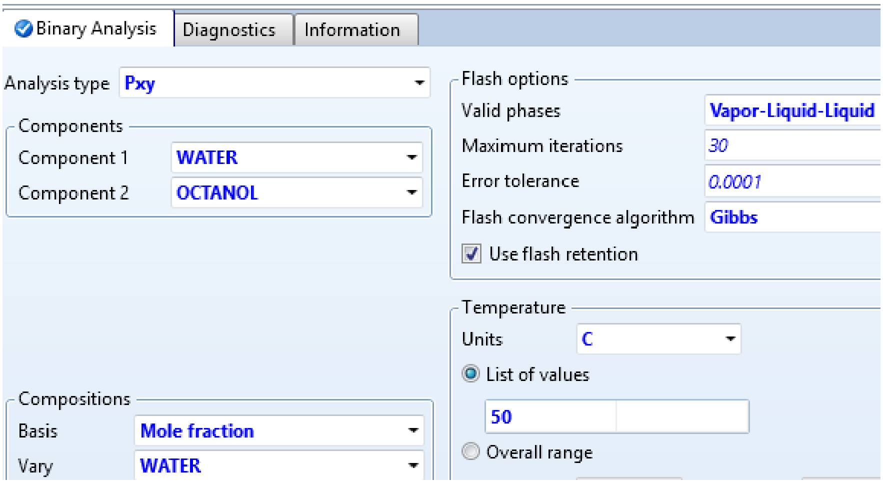
Thus, water is the most polar medium and octanol is the least. For example, methanol will be most soluble in either ethanol or water; on the contrary, *n*-octanol will be least soluble in water.

In fact, the octanol–water partition coefficient is a physical property used extensively to describe a chemical's lipophilic or hydrophobic properties. It is the ratio of a chemical's concentration in the octanol phase to its concentration in the aqueous phase of a two-phase system at equilibrium. Since measured values range from less than 10^{-4} to greater than 10^{+8} (at least 12 orders of magnitude), the logarithm (log P) is commonly used to characterize its value. Log P (or Log K_{ow}) is a valuable parameter in numerous quantitative structure–activity relationships (QSAR) that have been developed for the pharmaceutical, environmental, biochemical, and toxicological sciences.

Consequently, we explore the idea: "Likes Dissolve Likes" in this problem via utilizing the powerful feature of Aspen Plus in analyzing binary interactions and also in presenting the results.

Your job is to carry out the following analysis steps:

1. Under "**Properties**" environment and "**Analysis**" mode, click on "**Binary Analysis**"  button found in "**Home**" ribbon.
2. Create a binary isothermal ($T = 50°\mathrm{C}$) *Pxy* analysis sheet for water–octanol mixture as shown in Figure 1.55 and rename it to "**H_2O–C_8OH**". Notice that you may rename the binary analysis sheet from the default name "**BINRY-1**" to the desired new name simply by right clicking on the created binary sheet and selecting "**Rename**" submenu from the short-list pop-up context menu.



Analysis type Pxy

Components
Component 1 WATER
Component 2 OCTANOL

Compositions
Basis Mole fraction
Vary WATER

Flash options
Valid phases Vapor-Liquid-Liquid
Maximum iterations 30
Error tolerance 0.0001
Flash convergence algorithm Gibbs
☑ Use flash retention

Temperature
Units C
● List of values
50
○ Overall range

Figure 1.55 Creation of a binary isothermal *Pxy* analysis sheet for water–octanol mixture.

3. Repeat the same procedure in step #2 for the following binary mixtures:
   methanol–ethanol (MOH–C_2OH)
   methanol–butanol (MOH–C_4OH)
   methanol–octanol (MOH–C_8OH)
   methanol–water (MOH–H_2O).
4. After defining the previous list of binary sheets, click Next button shown in "**Home**" ribbon.
5. The "**Control Panel**" window will tell the user that tables are generated. Go to "**Results**" sheet under each created binary analysis sheet to explore the results in the form of different columns representing either VLE or VLLE data for the given binary mixture.
6. Using the "**Plot**" tab found in "**Home**" ribbon, click on the "**Custom**" button to plot the activity coefficient for both components making the binary mixture, except for water–octanol mixture that will have VLLE not simple VLE. Figure 1.56 (*top*) shows a liquid mixture labeled as number one (LIQUID1) activity coefficient for both water and octanol. One can see that the activity coefficient of water decreases from 5.75 down to 3; on the other hand, the activity coefficient of octanol assumes a value very close to unity. This indicates that the first liquid-phase mixture is made of water droplets being dispersed in a continuous phase (octanol). Figure 1.56 (*bottom*) shows that the activity coefficient profile of a liquid mixture labeled as number two (LIQUID2), where octanol assumes a plateau value of 1640 and that of water is unity above 0.39 mole fraction of water. This indicates that the second liquid-phase mixture is made of octanol droplets being dispersed in a continuous phase (water).

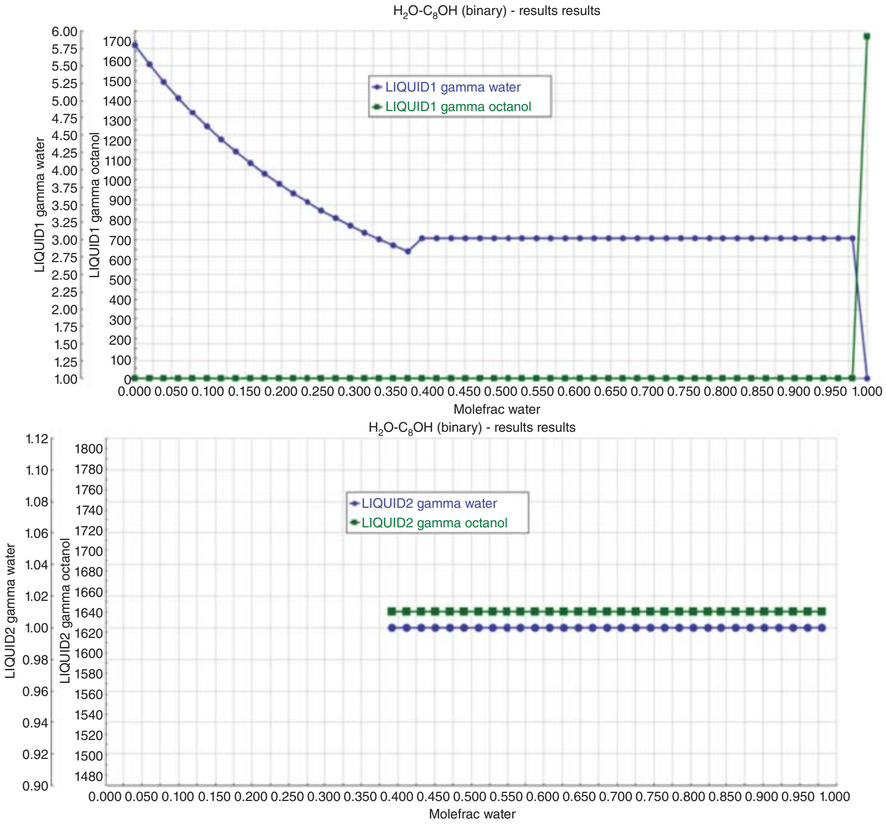


Figure 1.56 VLLE for water–octanol mixtures where two liquid mixtures exist in equilibrium with the vapor mixture. Water droplets are dispersed in liquid octanol (*top*) and octanol droplets are dispersed in water phase for a mole fraction of water greater than 0.39 (*bottom*).

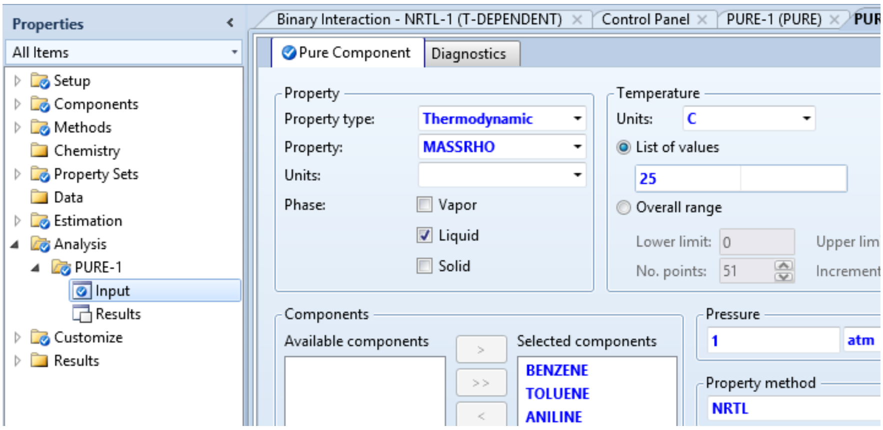
7. The activity coefficient plot for other binary mixture will be easier to track than water–octanol mixture. Go through each plot and see how the activity coefficients for both constituents change from methanol–ethanol to methanol–octanol mixture. Do not forget to compare the values in both plots: methanol–ethanol on one side and methanol–water on the other side. In particular, look at the extreme values of activity coefficients (i.e., they are called activity coefficients at infinite dilution).

HOMEWORK/CLASSWORK 1.4 (THE MIXING RULE)

We have been learning from the basic principle course found in all chemical engineering curricula that the density of a mixture, which is a mixture property, can be calculated via the additive or mixing rule that expresses the mixture property as a function of the partial molar (or partial specific) property leveraged by the mole (or mass) fraction of its constituents. A partial molar (or partial specific) property is a function of pressure, temperature, and composition of the mixture. In the absence of partial molar (or partial specific) properties data, an approximation can be drawn as a function of the pure component data of the constituents leveraged by their mole/mass fraction in solution. This applies for any thermodynamic extensive property, such as volume, internal energy, enthalpy, entropy, Gibbs free energy, and Helmholtz energy.

Let us demonstrate the concept of mixing rule via considering the density of a mixture made of benzene, toluene, and aniline, evaluated at room temperature ($T = 25°\text{C}$) and 1 atm. Using "**Specialty Chemicals with Metric Units**" template, create an Aspen Plus file with the following components: benzene, toluene, and aniline. The default property method is "**NRTL**". There will be no flowsheet at this stage. We will stay under "**Properties**" environment using analysis and estimation mode. There will be no need to use NIST/TDE experimental data; hence, the missing binary parameters (if any) will be estimated using UNIFAC (Select "**Estimate parameters using UNIFAC**" option under "**NRTL-1**" sheet for "**Binary Interaction**" folder and run the simulator). We will create two analysis tests: one for pure substances and another for a mixture. Carry out the following steps:

1. Under "**Properties**" environment and "**Analysis**" mode, click on "**Pure Analysis**" Pure button found in "**Home**" ribbon.
2. Under "**Pure Component**" tab, select "*Thermodynamic*" as the "**Property type**" and "*MASSRHO*" as the subproperty. Select the "**Phase**" to be "*Liquid*". Moreover, select "**Temperature**" to be 25°C and select all the three components as shown in Figure 1.57 for the pure property analysis.



Property
Property type: Thermodynamic
Property: MASSRHO
Units:
Phase: ☐ Vapor ☑ Liquid ☐ Solid

Temperature
Units: C
● List of values: 25
○ Overall range
Lower limit: 0
Upper lim
No. points: 51
Increment

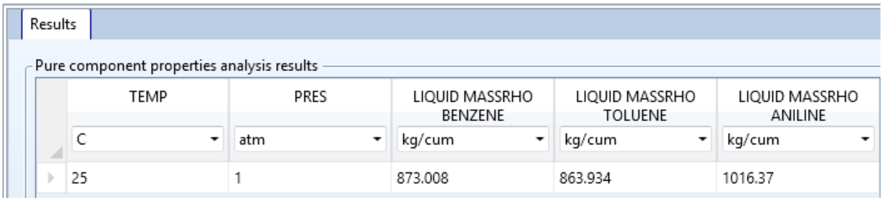
Components
Available components
Selected components: BENZENE, TOLUENE, ANILINE

Pressure: 1 atm

Property method: NRTL

Figure 1.57 Creation of a pure property analysis to evaluate the mass density of the three pure substances.

3. Click on "**Next**" Next button to run the test. Go to "**Results**" sheet below "**PURE-1**" folder. You will be able to see the estimated mass density for each pure component as shown in Figure 1.58.

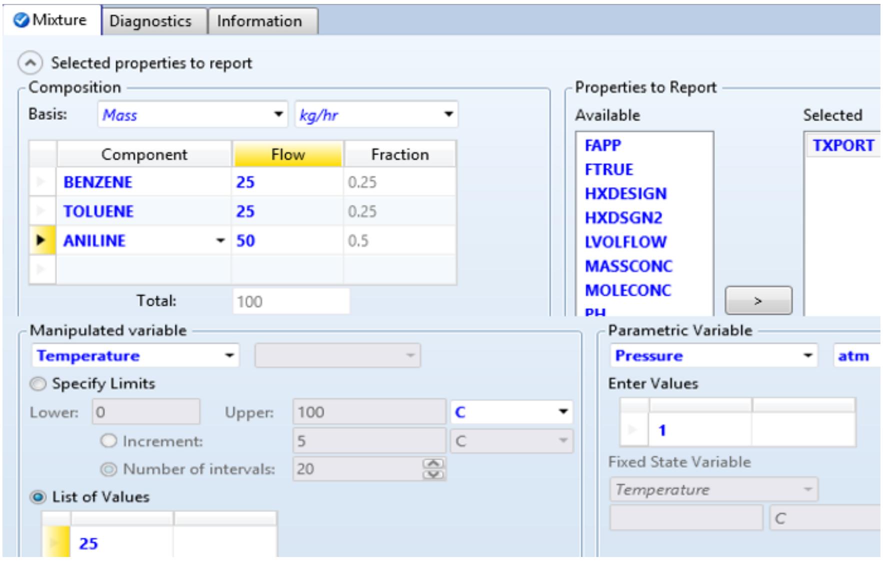


Pure component properties analysis results

TEMP	PRES	LIQUID MASSRHO BENZENE	LIQUID MASSRHO TOLUENE	LIQUID MASSRHO ANILINE
C	atm	kg/cum	kg/cum	kg/cum
25	1	873.008	863.934	1016.37

Figure 1.58 Estimation of mass density for each pure component.

4. Under “**Properties**” environment and “**Analysis**” mode, click on “**Mixture Analysis**” Mixture button found in “**Home**” ribbon.
5. Under “**Mixture**” tab, enter the required input data as shown in Figure 1.59 for the mixture property analysis. Notice that the mass fraction is automatically calculated by Aspen Plus as you enter the mass flow rate for each component. Moreover, “**TXPORT**” property is selected, as it contains the density of a mixture.



Composition

Basis: Mass kg/hr

Component	Flow	Fraction
BENZENE	25	0.25
TOLUENE	25	0.25
ANILINE	50	0.5

Total: 100

Properties to Report

Available: FAPP, FTRUE, HXDESIGN, HXDSGN2, LVOLFLOW, MASSCONC, MOLECONC, PH

Selected: TXPORT

Manipulated variable: Temperature

○ Specify Limits

Lower: 0 Upper: 100 C

○ Increment: 5 C

○ Number of intervals: 20

● List of Values: 25

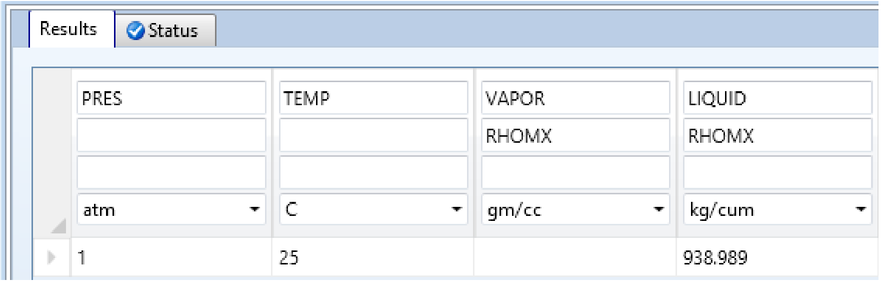
Parametric Variable: Pressure atm

Enter Values: 1

Fixed State Variable: Temperature C

Figure 1.59 Entering the input data for the mixture property analysis form. “**TXPORT**” property is selected.

6. Click on “**Next**” Next button to run the test. Go to “**Results**” sheet below “**MIX-1**” folder. You will be able to see the estimated mass density for the mixture with defined temperature, pressure, and composition, as shown in Figure 1.60.



PRES	TEMP	VAPOR	LIQUID
		RHOMX	RHOMX
atm	C	gm/cc	kg/cum
1	25		938.989

Figure 1.60 Estimation of the mass density of a liquid mixture with known temperature, pressure, and composition.

7. Check which of the following two formulae will give the closest answer to the mixture property:

   Additive rule or linear approximation: $\rho_{\text{Mix}} \cong \sum_{i=1}^{3} \rho_i^o x_i$

   Thermodynamic approximation: $V_{\text{Mix}} \cong \sum_{i=1}^{3} V_i^o x_i$

   Given that $V_{\text{Mix}} = \frac{1}{\rho_{\text{Mix}}}$ and $V_i^o = \frac{1}{\rho_i^o}$ then $\frac{1}{\rho_{\text{Mix}}} \cong \sum_{i=1}^{3} \frac{x_i}{\rho_i^o}$

8. The true value will be 938.989 kg/m^3, as given by Aspen Plus. The value given by either the linear or thermodynamic approach will be approximate. Calculate the percent relative error (PRE) associated with each approximate value as

$$\text{PRE}\,(\%) = \frac{|\text{True value-Approximate value}|}{\text{True value}} \times 100\%.$$

2

MORE ON ASPEN PLUS FLOWSHEET FEATURES (1)

2.1 PROBLEM DESCRIPTION

A mixture containing 50.0 wt% acetone and 50.0 wt% water is to be separated into two streams: one enriched in acetone and the other in water. The separation process consists of extraction of acetone from water into methyl isobutyl ketone (MIBK), which preferentially dissolves acetone but is nearly immiscible with water. The overall goal of this problem is to separate the feed stream into two streams that have greater than 95% purity of water and acetone, respectively.

In this chapter, we begin to learn the basics of running Aspen Plus® and building a process flowsheet. This episode introduces you to a number of features that must be understood to complete even a simple simulation. Our goal at the end of this episode is to understand some of the features of Aspen Plus while creating a simulation of the mixture of a feed stream of 100 kg/h of the 50/50 acetone–water mix with a solvent stream of 100 kg/h of MIBK.

2.2 ENTERING AND NAMING COMPOUNDS

Refer to Chapter 1 regarding the selection of template type and entering compounds. From installed templates, we select the "**Chemical Processes**" main template followed by "**Specialty Chemicals with Metric Units**" subtemplate. We add three compounds: acetone, water, and MIBK. To add acetone, just type in its exact name followed by hitting the Tab/Enter key, and Aspen Plus will recognize it. Repeat the same steps for adding water. For MIBK, select the first portion of its string, that is, "methyl-iso" and refine the "**Compound class**" to "*Ketones*", select either "*Begins with*" or "*Contains*" option for the "**Search Criteria**", click on "**Find Now**" search button, and finally after locating the right

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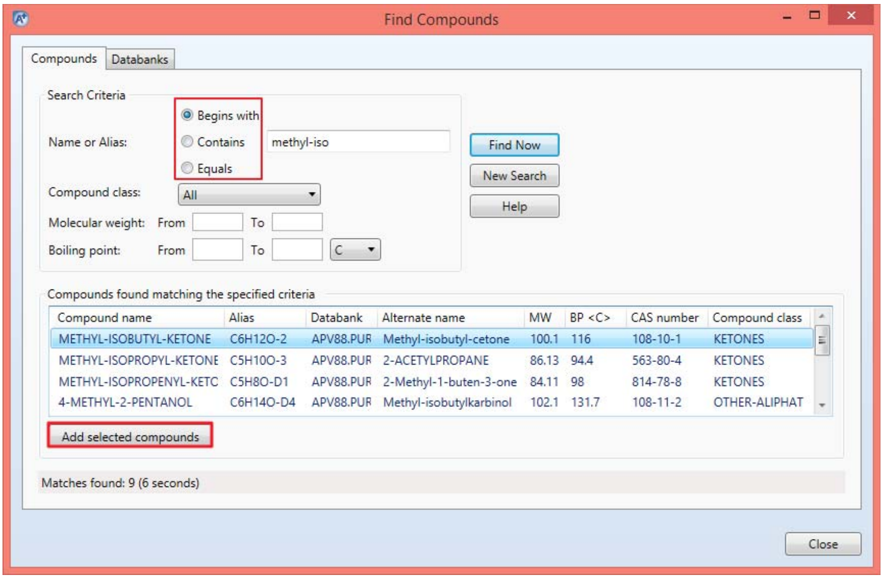
Aspen Plus®: Chemical Engineering Applications, First Edition. Kamal I.M. Al-Malah.

Companion Website: www.wiley.com/go/Al-Malah/AspenPlusApplications

compound, click on “**Add selected compounds**” button to add the desired compound, as shown in Figure 2.1.



Search Criteria

Name or Alias: ● Begins with ○ Contains ○ Equals methyl-iso

Compound class: All

Molecular weight: From To

Boiling point: From To C

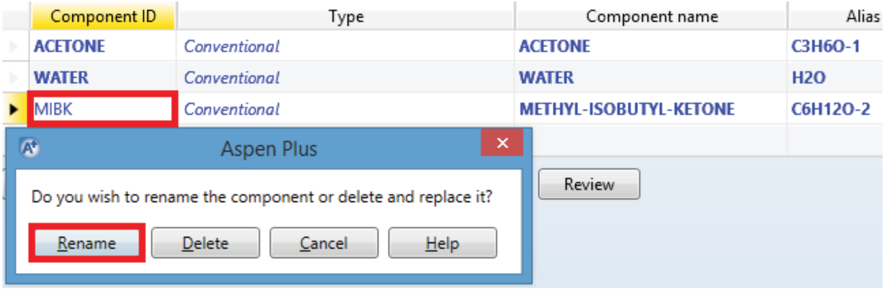
Compounds found matching the specified criteria

Compound name	Alias	Databank	Alternate name	MW	BP <C>	CAS number	Compound class
METHYL-ISOBUTYL-KETONE	C6H12O-2	APV88.PUR	Methyl-isobutyl-cetone	100.1	116	108-10-1	KETONES
METHYL-ISOPROPYL-KETONE	C5H10O-3	APV88.PUR	2-ACETYLPROPANE	86.13	94.4	563-80-4	KETONES
METHYL-ISOPROPENYL-KETC	C5H8O-D1	APV88.PUR	2-Methyl-1-buten-3-one	84.11	98	814-78-8	KETONES
4-METHYL-2-PENTANOL	C6H14O-D4	APV88.PUR	Methyl-isobutylkarbinol	102.1	131.7	108-11-2	OTHER-ALIPHAT

Matches found: 9 (6 seconds)

Figure 2.1 The “**Find Compounds**” window for locating MIBK from Aspen Plus databanks and adding it to the list of compounds.

Of course, the default assigned name “**METHY-01**” can be renamed “**MIBK**” simply via editing (or clicking on) the row pertaining to its name and entering the new name. Diligently, hit “**Tab**” or “**Enter**” key and Aspen Plus requests an answer from you as what to do with the name modification step. Click on “**Rename**” button, as shown in Figure 2.2.



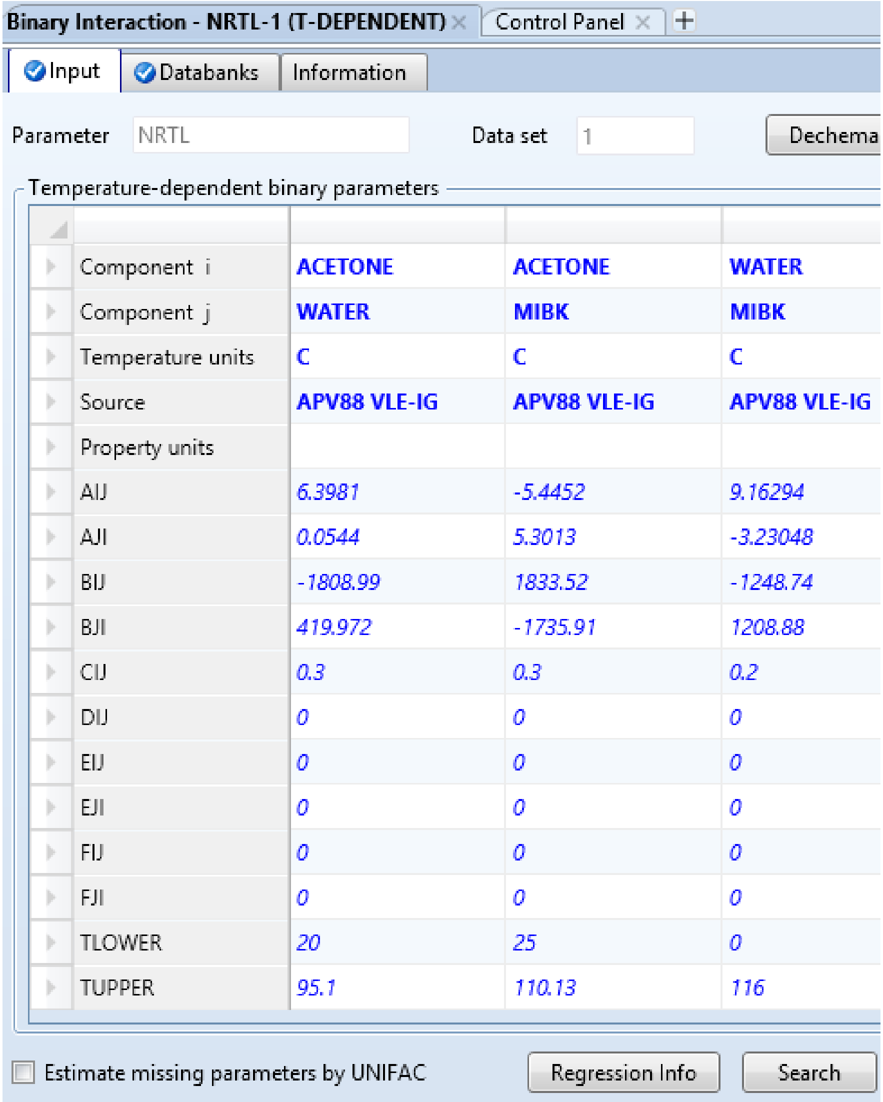
Component ID	Type	Component name	Alias
ACETONE	Conventional	ACETONE	C3H6O-1
WATER	Conventional	WATER	H2O
MIBK	Conventional	METHYL-ISOBUTYL-KETONE	C6H12O-2

Do you wish to rename the component or delete and replace it?

Figure 2.2 Renaming the default assigned name “**METHY-01**” to “**MIBK**”.

2.3 BINARY INTERACTIONS

Notice that there is a half-filled red circle under “**Methods**” folder. Click on “**Next**” button found in “**Run**” tab within “**Home**” ribbon. This brings you to “**Binary Interaction - NRTL-1 (T-Dependent)**” | “**Input**” tab window. Notice all permutations of pairwise interactions are already given and, in fact, there is no need to select “**Estimate missing parameters by UNIFAC**” option, as shown in Figure 2.3. Notice that the source of data is “**APV88 VLE-IG**”, which means that the liquid phase is handled by “**NRTL**” (i.e., activity coefficient-based model) and the gas phase is assumed to be an ideal gas mixture. Again, the prefix “**APV88**” will be dropped from either the source or databank name, if Aspen Plus is not the enterprise version.



Parameter NRTL

Data set 1

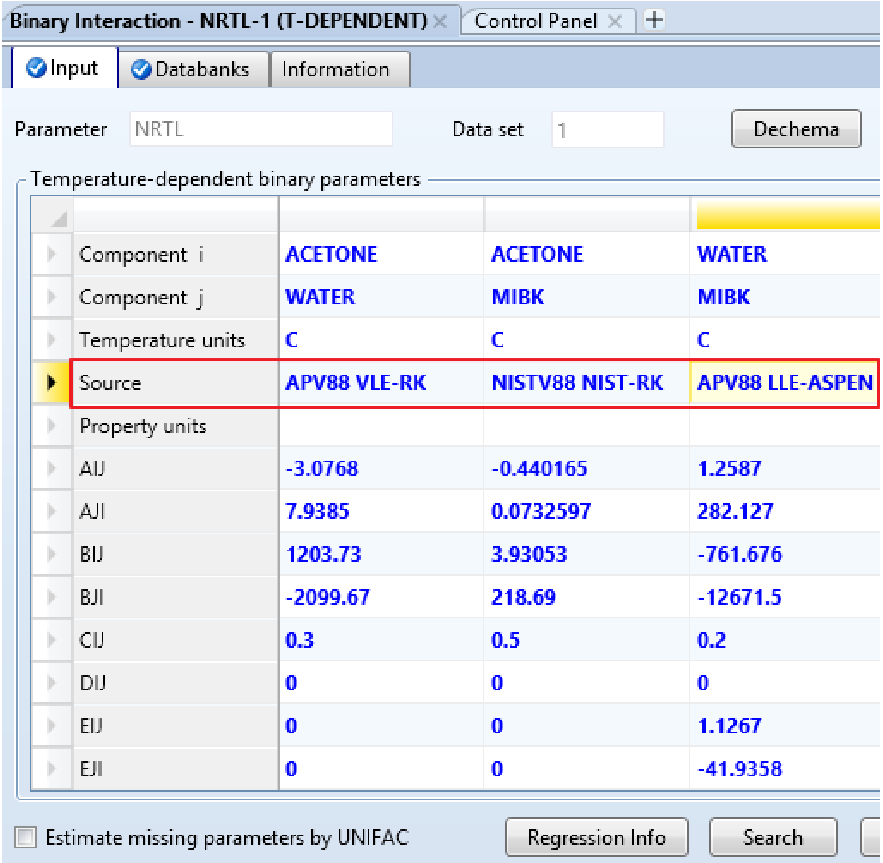
Temperature-dependent binary parameters

Component i	ACETONE	ACETONE	WATER
Component j	WATER	MIBK	MIBK
Temperature units	C	C	C
Source	APV88 VLE-IG	APV88 VLE-IG	APV88 VLE-IG
Property units			
AIJ	6.3981	-5.4452	9.16294
AJI	0.0544	5.3013	-3.23048
BIJ	-1808.99	1833.52	-1248.74
BJI	419.972	-1735.91	1208.88
CIJ	0.3	0.3	0.2
DIJ	0	0	0
EIJ	0	0	0
EJI	0	0	0
FIJ	0	0	0
FJI	0	0	0
TLOWER	20	25	0
TUPPER	95.1	110.13	116

☐ Estimate missing parameters by UNIFAC

Figure 2.3 All pairwise (binary) interaction parameters are already given by Aspen Plus.

However, if the applied pressure is relatively high (e.g., above 10 bar), then the source of data can be changed from "**APV88 VLE-IG**" to a non-ideal gas mixture, such as "**APV88 VLE-RK**" (i.e., Redlich–Kwong equation of state). Figure 2.4 shows the new binary interaction parameters after changing the source of data from "**APV86 VLE-IG**" to "**APV88 VLE-RK**", "**NISTV88 NIST-RK**", or any other available source.



Parameter: NRTL
Data set: 1

Temperature-dependent binary parameters

Component i	ACETONE	ACETONE	WATER
Component j	WATER	MIBK	MIBK
Temperature units	C	C	C
Source	APV88 VLE-RK	NISTV88 NIST-RK	APV88 LLE-ASPEN
Property units			
AIJ	-3.0768	-0.440165	1.2587
AJI	7.9385	0.0732597	282.127
BIJ	1203.73	3.93053	-761.676
BJI	-2099.67	218.69	-12671.5
CIJ	0.3	0.5	0.2
DIJ	0	0	0
EIJ	0	0	1.1267
EJI	0	0	-41.9358

☐ Estimate missing parameters by UNIFAC

Figure 2.4 Changing the source of data from "**APV88 VLE-IG**" to any other source will give a new estimate of binary interaction parameters.

In this running example, we do have an applied (operating) pressure below 10 bar; hence, there is no need to go to the non-ideal gas mixture.

> **<u>NOTE #1:</u>** *If xy plot is generated for acetone/water mixture under both cases "**APV88 VLE-IG**" and "**APV88 VLE-RK**", you will notice that both plots do exhibit the same pattern, except that they slightly differ in predicting the onset of azeotropic condition at higher values of acetone mole fraction.*

2.4 THE “SIMULATION” ENVIRONMENT: ACTIVATION DASHBOARD

After successfully completing the properties analysis and setup, switch to “**Simulation**” environment so that we can add the required blocks and input and output streams. You will notice that there exists a dashboard, which lies exactly above the flowsheet window. This dashboard initially contains three disabled large buttons that can be activated upon completing a successful task under “**Simulation**” environment. The three buttons account for economics (or cost), energy, and EDR exchanger feasibility analysis, respectively. We will come to such three dashboard items later in more details. At this stage, you may select to collapse the dashboard to make the flowsheet window a more spacious. Alternatively, you may enable/disable activation dashboard via going to “**File**” | “**Options**” | “**Advanced**” tab and then deselecting/selecting “**Disable activation dashboard**” check button. Click on “**OK**” button to close the “**Advanced Options**” window.

2.5 PLACING A BLOCK AND MATERIAL STREAM FROM MODEL PALETTE

To place a unit operation (or piece of equipment) into the flowsheet window, select it from the “**Model Palette**” ribbon, shown at the bottom of the process flowsheet, and then click on the flowsheet window where you would like the piece of equipment to appear. Do this for each piece of equipment that you would like to add to your simulation. For this simulation, we will add one “**TRIANGLE**” stream mixer (found in the “**Mixers/Splitters**” tab). You may want to go through the rest of the “**Model Palette**” tabs to see what other types of equipment are available in Aspen Plus package. Figure 2.5 shows the addition of a stream mixer, which was automatically given the name “**B1**” (stands for Block 1) by Aspen Plus. To change the default prefix assigned by Aspen Plus for an added block or stream, go to “**File**” | “**Options**” | “**Flowsheet**” tab and type in the new prefix for labeling the newly added block or stream.

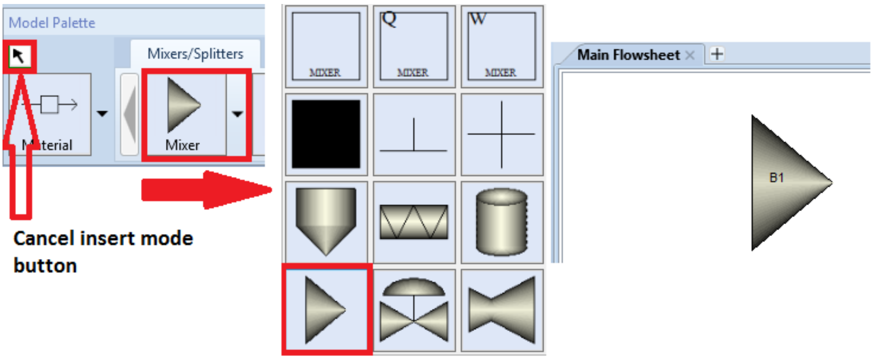


Figure 2.5 The addition of a stream mixer to the process flowsheet. The name “**B1**”, which is given by Aspen Plus, can be changed later by the user.

It should be pointed out that after adding your desired unit operations, you must click on the “**Cancel insert mode**” button to stop the insertion of additional blocks. If you do not select this button, you will continue to add equipment to the process flowsheet. To delete extraneous equipment, simply highlight that object and hit the Delete key on the keyboard. Alternatively, after adding the desired model equipment, right-click the mouse and the insert mode will turn off.

To add a material stream to your simulation, click on the "**Material stream**" icon (other options include heat and work, but we will not be using those at this time), which is the first icon appearing in the "**Model Palette**" ribbon (see Figure 2.5). In this regard, Aspen Plus has a feature that will indicate to you where streams are required. When you select the material stream option, a number of arrows will appear on each of the unit operations. **Red** arrows indicate required streams and **blue** arrows indicate optional streams (see Figure 2.6).

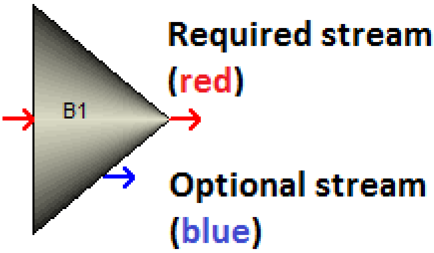


Figure 2.6 Upon selecting the stream type and moving the mouse to the workspace of the process flowsheet, the required and optional stream will show up in the red and blue color, respectively. *See Plate section for color representation of this figure.*

Streams can be added by clicking on the process flowsheet where you would like the stream to begin and clicking again where you would like the stream to end. To connect to a piece of equipment, you must have the desired stream type selected and then begin from or terminate at one of the arrows shown on the piece of equipment (depending on whether your stream is a product from or feed to the equipment). In a similar manner to the model equipment, each click will add a new stream to the process flowsheet until you click on the "**Cancel insert mode**" button.

NOTE #2: *Do not forget to save your work from time to time.*

For this running example, we will add two feed streams into the mixer, and one product stream out of the mixer. Some pertinent features of Aspen Plus are worth mentioning here.

2.6 BLOCK AND STREAM MANIPULATION

a) To rotate or rename a stream or block, simply select the object that you would like to manipulate and right click on it. This will present you with a number of options for changing each object. I suggest renaming both the material streams and the mixer to names that will better reflect their function or content (rather than the default numbers and letters).

b) To resize the block, here are the steps:
   - Left-click on the block and a rectangle, made of square-dotted (■) boxes, highlights or embraces the selected block.
   - Move the cursor to any corner of the rectangle until you notice a change in the cursor from a single to double arrow.
   - In drag (left mouse being clicked) mode, move the mouse either in or out of the rectangle.

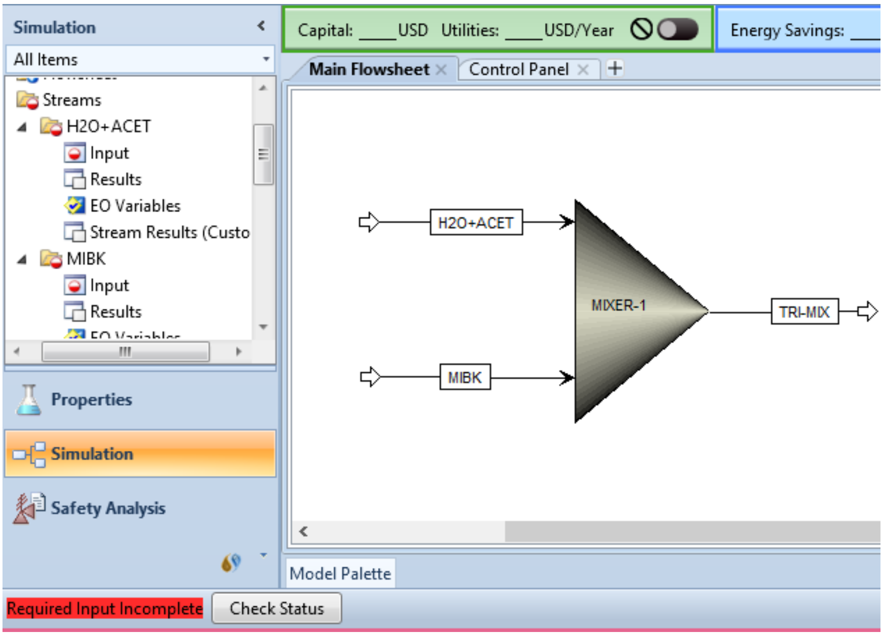
c) To relocate the entire process flowsheet as one piece or a portion of it, you need to entirely highlight it or a portion of it. To highlight an iconic object, you need to left click the mouse at some point slightly faraway from one edge and diagonally move your mouse to the opposite edge and then relax the mouse. Highlighting will impose squared dots (■) around the block itself. Use right/left and up/down arrow keys to move the highlighted object(s). After moving to a new location, left-click away from the highlighted object(s) and Aspen Plus will unhighlight the object(s) and stick to the new location.

d) To highlight a single stream, left-click anywhere on the stream where it becomes square-dotted (■) along the stream. You can also use the right/left and up/down arrow keys to lengthen/shorten or displace the stream.

e) To displace the point of contact with the block for either an input or output stream, highlight the requested stream and you will notice a small tiny portion of the selected stream becomes blue. This small tiny blue portion represents either the endpoint for the input stream or start point for the output stream. Hover the mouse over that tiny portion that is in contact with the block itself. Left-click on this tiny blue portion and you will notice that either an inlet or an outlet arrow shows up, similar to those shown in Figure 2.6. After that, you will be able to move the arrow around the block to decide on the new port for the selected stream.

f) To exchange an already existing block icon with another within the same group (such as mixers/splitters group) of blocks, right-click on the existing block and select "**Exchange Icon**" submenu from the context shortcut menu. Repeat this step more than once to probe group icons until you finally decide on or reach at the proper icon that better represents the unit operation or chemical process in hand.

At this point, your process flowsheet should be complete, and it should resemble the one shown in Figure 2.7. Notice the "**Simulation Status**" at the left-bottom corner has been changed from "*Flowsheet not Complete*" to "*Required Input Incomplete*". This switch in the simulation status means that the block and its associated input and output streams are already defined. What remains is to enter the properties of the two feed streams and this explains why the simulation status says that the required input is incomplete and we can see two half-filled red circles hooked to both input forms of the feed streams, as can be seen in Figure 2.7.



Required Input Incomplete

Figure 2.7 Connecting two input streams and one output stream to the mixer. Moreover, the name of the mixer was changed as well as the name of each input and output stream. Notice that the "**Simulation Status**" changed from "*Flowsheet not Complete*" to "*Required Input Incomplete*".

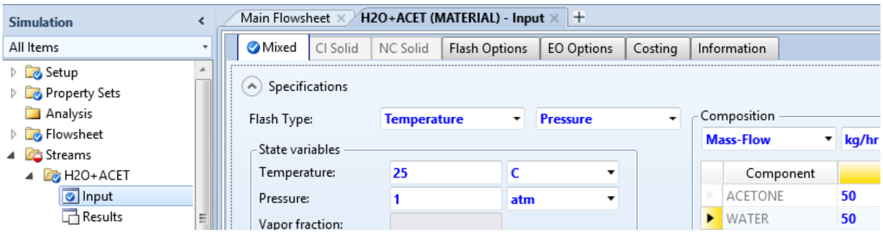
Table 2.1 gives a brief information about the three categories of mixer/splitter types.

TABLE 2.1 Description of Mixer/Splitter Types.

Model	Description	Purpose	Use
Mixer	Stream mixer	To combine multiples streams into one stream	Mixing tees, stream mixing operations, adding heat streams, and adding work
FSplit	Stream splitter	To split stream flows	Stream splitters and bleed valves
SSplit	Substream splitter	To split substream flows	Solid stream splitters and bleed valves

2.7 DATA INPUT, PROJECT TITLE, AND REPORT OPTIONS

Up to this point, all data input is complete except for the feed streams. Under the "**Simulation**" environment, and from the "**Home**" ribbon, click on the "**Next**" (Next) button (shortcut key F4 or fn/F4) and this will bring us to where we input the first feed stream properties in terms of pressure, temperature, and compositional flow rate, as shown in Figure 2.8. Notice that Aspen Plus highlights the areas where the input has been completed and has not been completed with the use of either a blue check mark or a half-filled red circle, as seen in Figure 2.8 for "**Streams**" folder because the second stream properties are not yet entered.



Flash Type: Temperature Pressure

Temperature: 25 C

Pressure: 1 atm

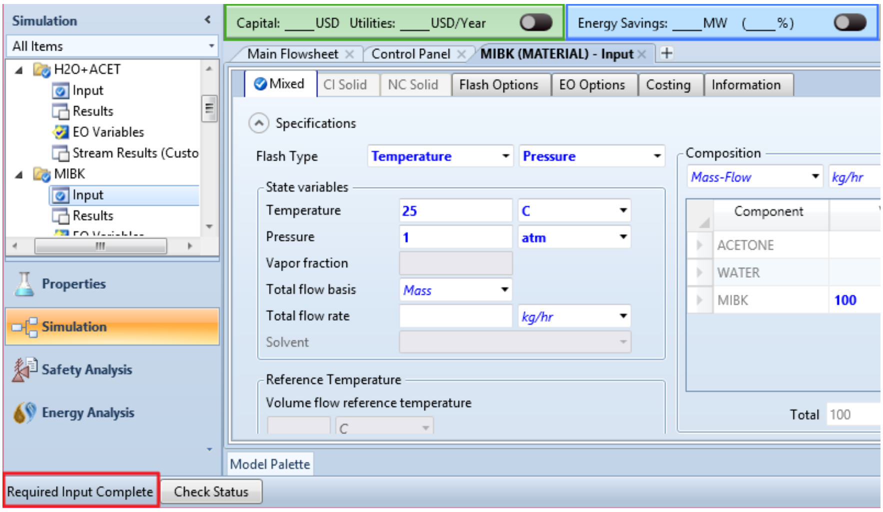
Vapor fraction:

Mass-Flow kg/hr

Component	
ACETONE	50
WATER	50

Figure 2.8 Entering the first feed stream properties in terms of P, T, and compositional flow rate.

Click (Next) button and Aspen Plus will bring us to where we enter the second feed stream properties in terms of pressure, temperature, and compositional flow rate, as shown in Figure 2.9. Notice that all input data are now complete and the "**Simulation Status**" changed from "*Required Input Incomplete*" to "*Required Input Complete*".



Flash Type Temperature Pressure

Temperature 25 C

Pressure 1 atm

Vapor fraction

Total flow basis Mass

Total flow rate kg/hr

Solvent

Volume flow reference temperature C

Mass-Flow kg/hr

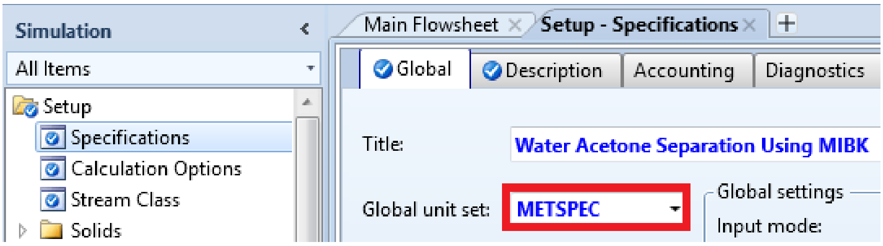
Component	
ACETONE	
WATER	
MIBK	100

Total 100

Figure 2.9 Entering the second feed stream properties in terms of P, T, and compositional flow rate.

Before showing the simulation results, let us show where to modify how the results can be presented.

Figure 2.10 shows the "**Global**" tab window where the user defines the title of the simulation project and the option to change or select the global unit set.

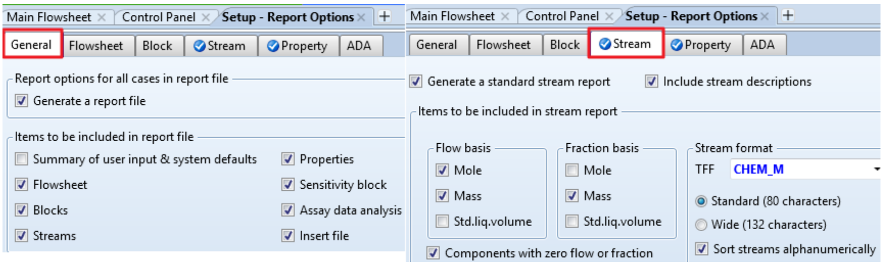


Title: Water Acetone Separation Using MIBK

Global unit set: METSPEC

Figure 2.10 The title and global unit set of the project are entered using "**Setup**" | "**Specifications**" | "**Global**" tab window.

Clicking on "**Setup**" | "**Report Options**" will bring the form shown in Figure 2.11. Here, the user instructs Aspen Plus what items are to be included in the report via the "**General**" tab form (*left*) and how Aspen Plus shall report the stream conditions whether they are reported on a molar basis, mass basis, or both via the "**Stream**" tab form (*right*).



Report options for all cases in report file

☑ Generate a report file

Items to be included in report file

☐ Summary of user input & system defaults
☑ Flowsheet
☑ Blocks
☑ Streams
☑ Properties
☑ Sensitivity block
☑ Assay data analysis
☑ Insert file

☑ Generate a standard stream report
☑ Include stream descriptions

Items to be included in stream report

Flow basis
☑ Mole
☑ Mass
☐ Std.liq.volume

Fraction basis
☐ Mole
☑ Mass
☐ Std.liq.volume

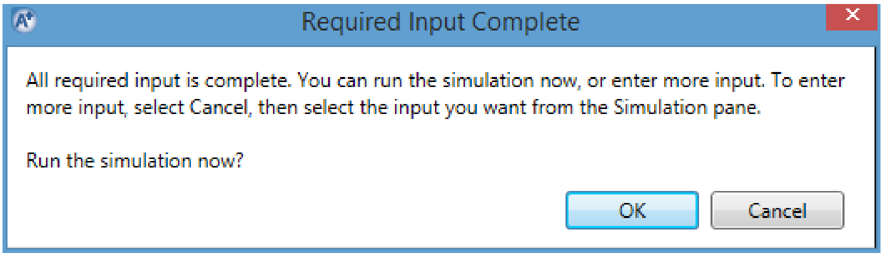
Stream format
TFF CHEM_M
● Standard (80 characters)
○ Wide (132 characters)
☑ Sort streams alphanumerically

☑ Components with zero flow or fraction

Figure 2.11 The "**General**" tab window shows what items to be included in the final generated report (*left*) and the "**Stream**" tab window how Aspen Plus shall report the process and stream conditions on a molar basis; mass basis; or both (*right*).

2.8 RUNNING THE SIMULATION

Clicking on the "Next" (Next) button will tell us that the simulator is ready as shown in Figure 2.12. Here, it indicates that the all required input data are complete, which means that Aspen Plus is happy now as it has the minimum number of input data. However, if the user has more to input, especially for a more complex process, then it is time to select "**Cancel**" button and go for the folder/subfolder property where the user can input more data. Otherwise, click on the "**OK**" button. Here, we have no more data to input; hence, we will click on the "**OK**" button. Remember that we will use the pairwise interaction parameters given in Figure 2.3 not in Figure 2.4.



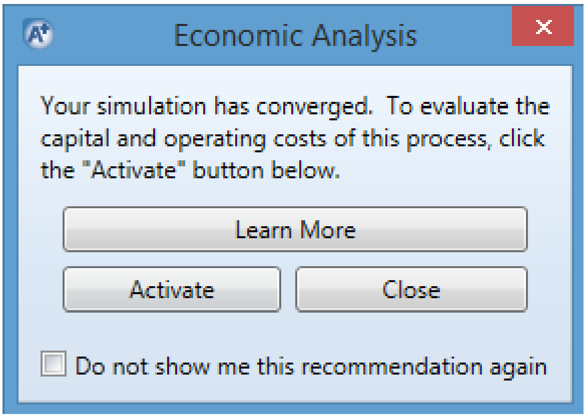
Required Input Complete

All required input is complete. You can run the simulation now, or enter more input. To enter more input, select Cancel, then select the input you want from the Simulation pane.

Run the simulation now?

Figure 2.12 The pop-up window tells the user that, after all, Aspen Plus is satisfied with input data and it will be ready for the giant step: solution of simultaneous steady-state material, component, and energy balances, augmented by other algebraic/differential equations describing stream and block properties.

Clicking on "**OK**" button in Figure 2.12 will trigger Aspen Plus simulator to carry out steady-state material, component, and energy balances simultaneously. The "**Control Panel**" will tell the user the result of attempting to solve the set of algebraic and differential equations (i.e., with time as in unsteady-state or with space as in a steady-state plug flow reactor). If there is no simulation error, a convergence is reached but not necessarily realistic. On the contrary, if there exists a simulation error, it will show up in the "**Control Panel**" and the solution diverges. In addition, there is something called warning rather than error. In this case, the user needs to pay attention to the warning statement to see whether the warning indicates a serious issue that the user need to consider or it can be ignored. We will explain this shortly. In previous versions of Aspen Plus, a window used to pop up as in Figure 2.13. Aspen Plus prompted the user to go to the next step, that is, economic analysis. Of course, to proceed, the user would click on "**Activate**" button. Else, the user would click on "**Close**" button. We handle the economic aspects in a separate chapter. The user can also activate the economic analysis feature from "**Economics**" ribbon under "**Simulation**" environment. Take into account that the default behavior for caution messages and reminder prompts issued by Aspen Plus can be reclaimed, in general, via visiting "**File**" | "**Options**" | "**Advanced**" tab and clicking on restore buttons.



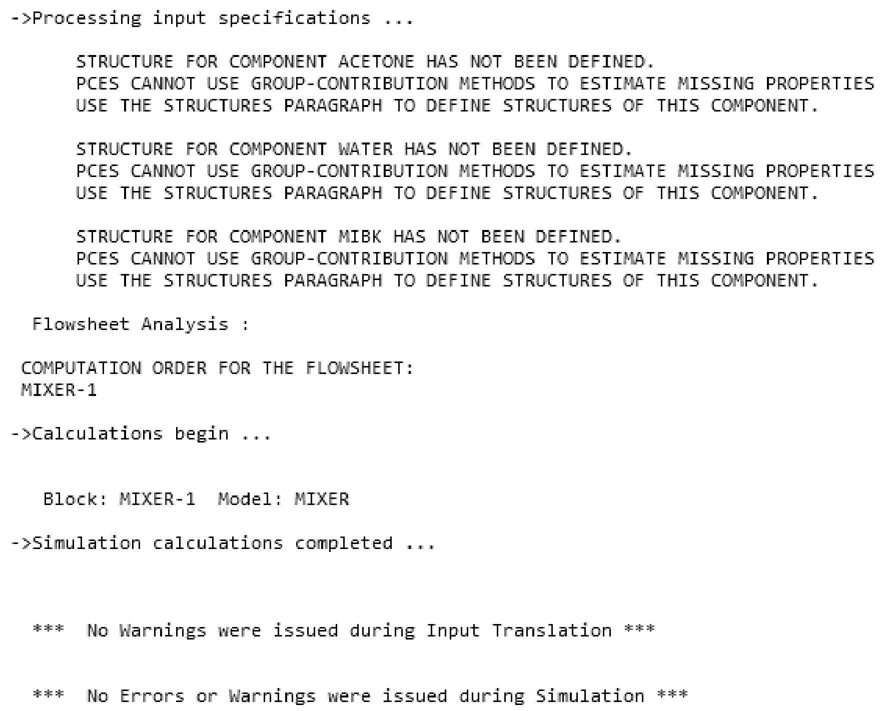
Economic Analysis

Your simulation has converged. To evaluate the capital and operating costs of this process, click the "Activate" button below.

☐ Do not show me this recommendation again

Figure 2.13 The "**Economic Analysis**" window used to pop-up, if the solution converged, ending up with results having no simulation error.

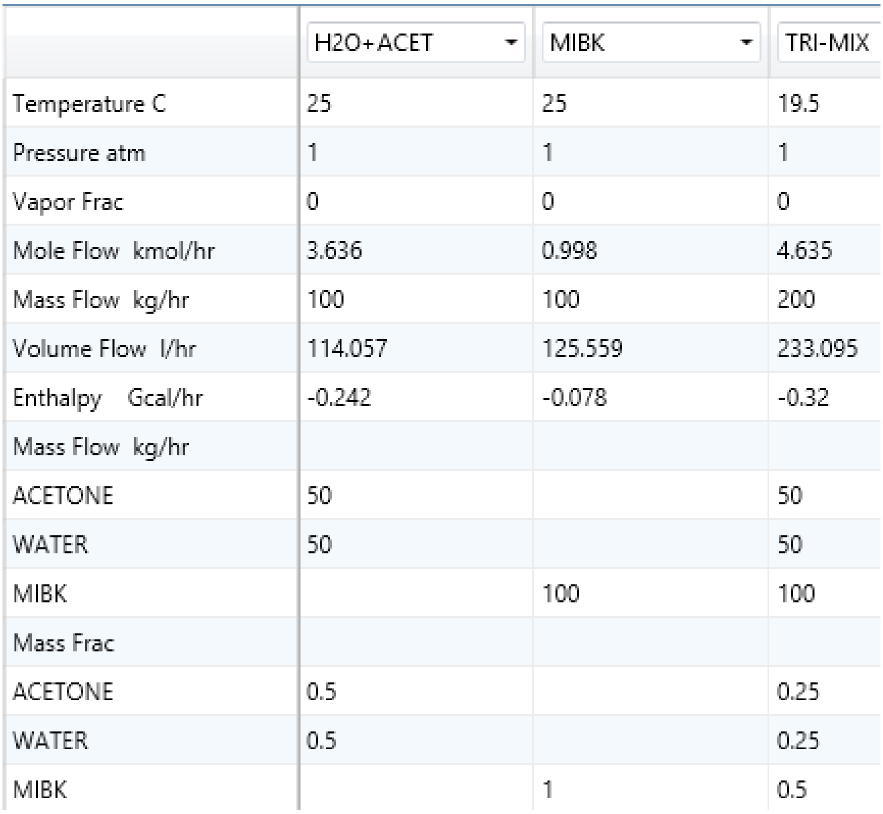
Have a look at the “**Control Panel**” where Aspen Plus shows the status of the solver after carrying out one attempt to solve for the steady-state condition of the process represented by the flowsheet. Figure 2.14 shows that there is a warning saying that “**PCES**” cannot use “Group-Contribution” methods to estimate missing properties. This warning is not serious and can be relieved if the user selects “**Estimate missing parameters using UNIFAC**” option, as shown in Figure 2.3. Moreover, the final block and stream results will not be affected whether or not the user selects to go with the previous option, as all pairwise interaction parameters are already given ahead.



```
->Processing input specifications ...

      STRUCTURE FOR COMPONENT ACETONE HAS NOT BEEN DEFINED.
      PCES CANNOT USE GROUP-CONTRIBUTION METHODS TO ESTIMATE MISSING PROPERTIES
      USE THE STRUCTURES PARAGRAPH TO DEFINE STRUCTURES OF THIS COMPONENT.

      STRUCTURE FOR COMPONENT WATER HAS NOT BEEN DEFINED.
      PCES CANNOT USE GROUP-CONTRIBUTION METHODS TO ESTIMATE MISSING PROPERTIES
      USE THE STRUCTURES PARAGRAPH TO DEFINE STRUCTURES OF THIS COMPONENT.

      STRUCTURE FOR COMPONENT MIBK HAS NOT BEEN DEFINED.
      PCES CANNOT USE GROUP-CONTRIBUTION METHODS TO ESTIMATE MISSING PROPERTIES
      USE THE STRUCTURES PARAGRAPH TO DEFINE STRUCTURES OF THIS COMPONENT.

  Flowsheet Analysis :

 COMPUTATION ORDER FOR THE FLOWSHEET:
 MIXER-1

->Calculations begin ...


   Block: MIXER-1  Model: MIXER

->Simulation calculations completed ...



  ***  No Warnings were issued during Input Translation ***


  ***  No Errors or Warnings were issued during Simulation ***
```

Figure 2.14 The Aspen Plus “**Control Panel**” flags, where it tells the user about the progress and performance of the solver (i.e., simulator).

Finally, clicking on the “**Results Summary**” | “**Streams**” sheet (shown in “**Navigation**” pane as a blue check-mark folder), or on the stream summary (Stream Summary) button, found in “**Home**” ribbon while being under “**Simulation**” environment, will enable the user to see the results, as shown in Figure 2.15



	H2O+ACET	MIBK	TRI-MIX
Temperature C	25	25	19.5
Pressure atm	1	1	1
Vapor Frac	0	0	0
Mole Flow kmol/hr	3.636	0.998	4.635
Mass Flow kg/hr	100	100	200
Volume Flow l/hr	114.057	125.559	233.095
Enthalpy Gcal/hr	-0.242	-0.078	-0.32
Mass Flow kg/hr			
ACETONE	50		50
WATER	50		50
MIBK		100	100
Mass Frac			
ACETONE	0.5		0.25
WATER	0.5		0.25
MIBK		1	0.5

Figure 2.15 The stream results can be seen if a converging solution is reached by Aspen Plus solver.

NOTE #3: *DO NOT FORGET TO SAVE YOUR FILE.*

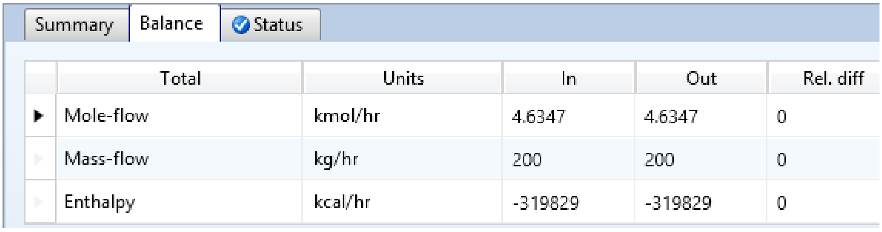
2.9 THE DIFFERENCE AMONG RECOMMENDED PROPERTY METHODS

For a chemical process, three methods are suggested by the "**Property Method Selection Assistant**" (see: Section 1.6). These are "**NRTL**", "**WILSON**", and "**UNIQUAC**". We will show how each method affects the estimation of the mixer mass and energy balance.

If we select "**WILSON**" as the property method, then we will notice that not all pairwise interactions are initially given by Aspen Plus. So, let us instruct Aspen Plus to complete the mission (i.e., estimate the missing parameters using UNIFAC). On the other hand, "**UNIQUAC**", such as "**NRTL**" method, has all three pairwise interaction parameters initially given.

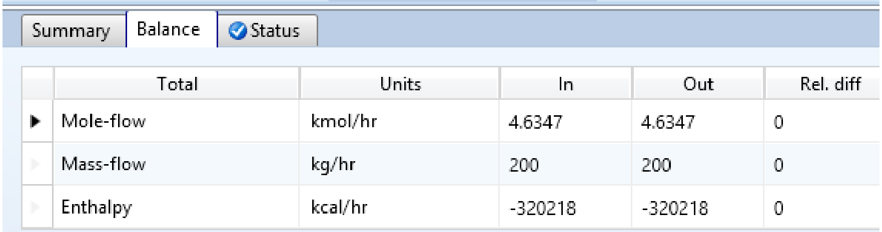
Figure 2.16 shows the mixer material and energy balance using the three recommended property methods: "**NRTL**", "**WILSON**", and "**UNIQUAC**". The difference lies in estimating the enthalpy value of input and output stream but the difference is quite insignificant between one method and another.

Mixer mass & energy balance using NRTL



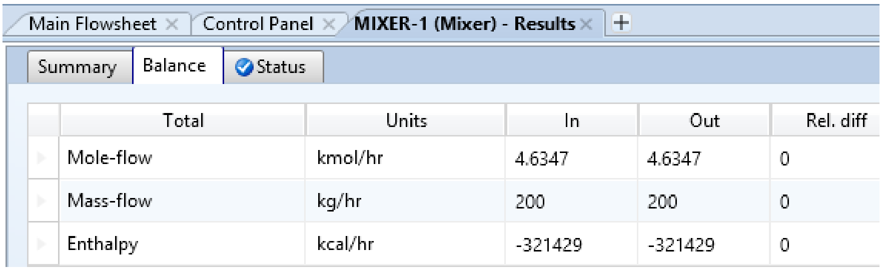
Total	Units	In	Out	Rel. diff
Mole-flow	kmol/hr	4.6347	4.6347	0
Mass-flow	kg/hr	200	200	0
Enthalpy	kcal/hr	-319829	-319829	0

Mixer mass & energy balance using WILSON



Total	Units	In	Out	Rel. diff
Mole-flow	kmol/hr	4.6347	4.6347	0
Mass-flow	kg/hr	200	200	0
Enthalpy	kcal/hr	-320218	-320218	0

Mixer mass & energy balance using UNIQUAC



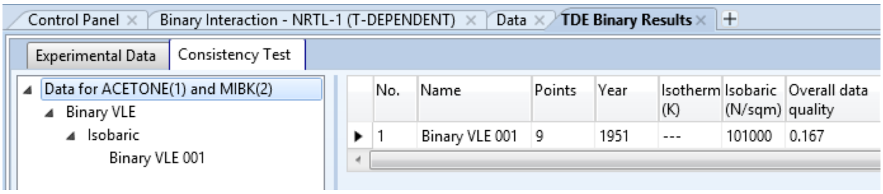
Total	Units	In	Out	Rel. diff
Mole-flow	kmol/hr	4.6347	4.6347	0
Mass-flow	kg/hr	200	200	0
Enthalpy	kcal/hr	-321429	-321429	0

Figure 2.16 The material and energy balance around the mixer as estimated by the three recommended property methods for a chemical process type.

2.10 NIST/TDE EXPERIMENTAL DATA

An attempt was made to make use of the experimental data available through NIST/TDE databank.

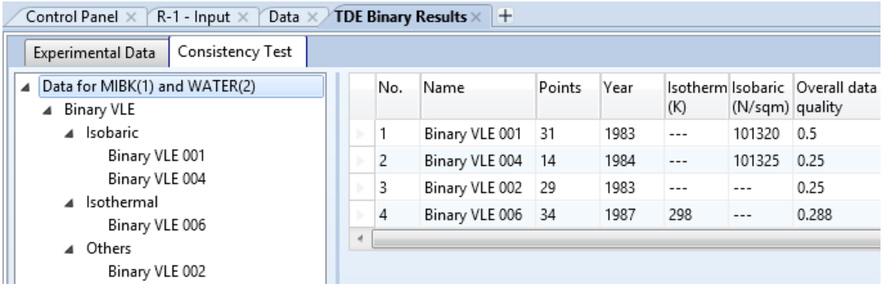
Figure 2.17 shows the overall data quality for acetone–MIBK binary interaction parameters. Obviously, the experimental data failed the consistency tests and thus are not recommended as an alternative for group-contribution method calculated binary data.



No.	Name	Points	Year	Isotherm (K)	Isobaric (N/sqm)	Overall data quality
1	Binary VLE 001	9	1951	---	101000	0.167

Figure 2.17 The overall data quality for acetone–MIBK binary interaction parameters.

Figure 2.18 shows the overall data quality for MIBK–water binary interaction parameters. Again, the experimental data failed the consistency tests and thus are not recommended as an alternative for group-contribution method calculated binary data.

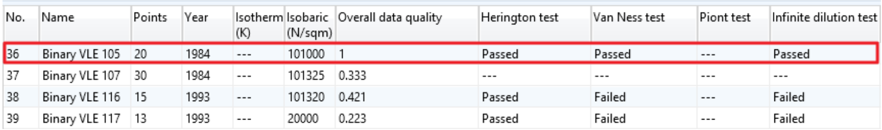


- Data for MIBK(1) and WATER(2)
  - Binary VLE
    - Isobaric
      - Binary VLE 001
      - Binary VLE 004
    - Isothermal
      - Binary VLE 006
    - Others
      - Binary VLE 002

No.	Name	Points	Year	Isotherm (K)	Isobaric (N/sqm)	Overall data quality
1	Binary VLE 001	31	1983	---	101320	0.5
2	Binary VLE 004	14	1984	---	101325	0.25
3	Binary VLE 002	29	1983	---	---	0.25
4	Binary VLE 006	34	1987	298	---	0.288

Figure 2.18 The overall data quality for MIBK–water binary interaction parameters.

Figure 2.19 shows the overall data quality for acetone–water binary interaction parameters. Here, some experimental data sets failed the consistency tests and others passed. Hence, one set of isobaric VLE data with an overall data quality equal to unity was selected for regression purposes. The data source is from [Huang, R., Gu, Y. and Hou, Y. (1984) VLE of acetone-water-isobutyraldehyde system. *Chemical Engineering (China)*, **4**, 26–29].



No.	Name	Points	Year	Isotherm (K)	Isobaric (N/sqm)	Overall data quality	Herington test	Van Ness test	Piont test	Infinite dilution test
36	Binary VLE 105	20	1984	---	101000	1	Passed	Passed	---	Passed
37	Binary VLE 107	30	1984	---	101325	0.333	---	---	---	---
38	Binary VLE 116	15	1993	---	101320	0.421	Passed	Failed	---	Failed
39	Binary VLE 117	13	1993	---	20000	0.223	Passed	Failed	---	Failed

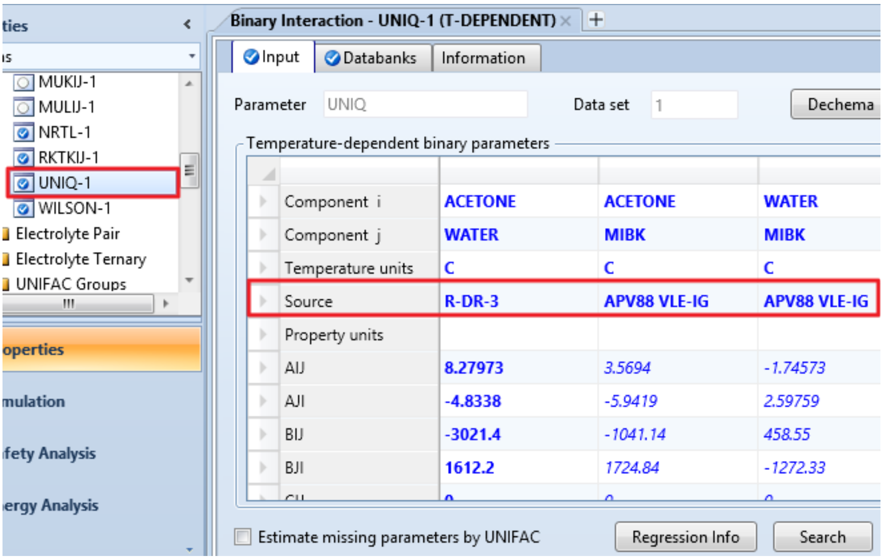
Figure 2.19 NIST/TDE binary interaction parameters for acetone–water mixture.

The regression step was carried out for such a set of isothermal VLE data for water–acetone solution, using the three recommended activity coefficient-based methods: “**NRTL**”, “**WILSON**”, and “**UNIQUAC**”. Two elements or parameters were used in the regression step. It was found that “**UNIQUAC**” method gave the minimum residual root mean square error (RRMSE), as shown in Table 2.2.

TABLE 2.2 The Regression Quality Results Using the Three Recommended Methods for a Chemical Process.

Property Method	Parameter Name/Element	Component *i*	Component *j*	RRMSE
NRTL	NRTL/1, NRTL/2	Acetone	Water	8.75792
WILSON	WILSON/1, WILSON/2	Acetone	Water	20.0062
UNIQUAC	UNIQ/1, UNIQ/2	Acetone	Water	5.01786

Figure 2.20 shows the pairwise interaction parameters for the three components using “**UNIQUAC**” as the property method. Notice that the source for the first data column is taken from regression folder with a regression data set called “**DR-3**”, which exploits “**UNIQUAC**” as the regression property method; the other two data columns are automatically calculated or given by Aspen Plus.



Parameter UNIQ Data set 1

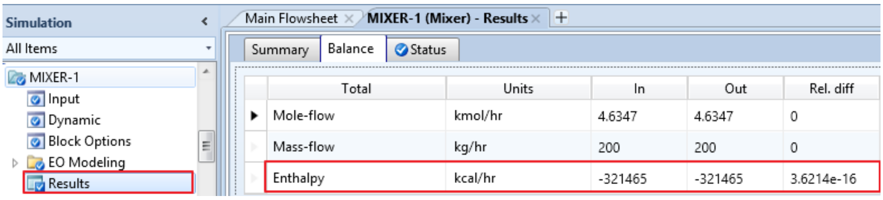
Temperature-dependent binary parameters

Component i	ACETONE	ACETONE	WATER
Component j	WATER	MIBK	MIBK
Temperature units	C	C	C
Source	R-DR-3	APV88 VLE-IG	APV88 VLE-IG
Property units			
AIJ	8.27973	3.5694	-1.74573
AJI	-4.8338	-5.9419	2.59759
BIJ	-3021.4	-1041.14	458.55
BJI	1612.2	1724.84	-1272.33

☐ Estimate missing parameters by UNIFAC

Figure 2.20 The pairwise interaction parameters for three components using “**UNIQUAC**” as the property method. The source of the first column is from regression data set “**DR-3**” with the least RRMSE.

Figure 2.21 shows the material and energy balance around the mixer using the estimated binary parameters for water–acetone, based on NIST/TDE experimental data.



Total	Units	In	Out	Rel. diff
Mole-flow	kmol/hr	4.6347	4.6347	0
Mass-flow	kg/hr	200	200	0
Enthalpy	kcal/hr	-321465	-321465	3.6214e-16

Figure 2.21 The mixer material and energy balance using “**UNIQUAC**” as the property method with NIST/TDE experimental data.

One can see that the value of enthalpy for the outlet stream is lower than any of those given earlier in Figure 2.16. Claiming that the experiment-based, “**UNIQUAC**”-regressed value has more credit than that estimated by the group contribution (**PCES**) method, the maximum percent relative error (PRE) among the three tested methods will be

$$\mathrm{PRE} = \frac{|-321\,465 - (-319\,829)|}{|-321\,465|} \times 100\% = 0.509\% \ll 10.0\%$$

NOTE #4: *This PRE value of 0.51% lies way below the generally accepted PRE borderline of 10% for measured or estimated quantities in engineering applications. Moreover, what really matters will be the enthalpy difference between in and out, which will reflect the amount of heat added into or extracted out of the control volume under study. This will make the PRE value associated with the heat duty even smaller and smaller as a result of using different property methods. In brief, we are quite confident to use the auto calculated binary parameters by Aspen Plus using the group contribution method (i.e., UNIFAC). Be happy!*

NOTE #5: *For the sake of having a linear learning curve with time (i.e., while proceeding from here onward), we will walk in parallel with the pace and content of each presented chapter. Consequently, for a given problem statement, we will start with a simple process and as we move onward, the process will continuously grow up as far as the corresponding flowsheet that describes the real process is concerned. Once we are done with covering the essential features of Aspen Plus we will have a complete stand-alone task.*

HOMEWORK/CLASSWORK 2.1 (WATER–ALCOHOL SYSTEM)

We have a 50/50 wt% mixture of water and n-hexanol. We plan to separate this mixture into its constituents and ultimately end up with almost pure streams of water and alcohol. Figure 2.22 shows the starting (i.e., simple) process flowsheet where we mix water–hexanol stream with 1-octanol to end-up with a ternary mixture ("**TRI-MIX**").

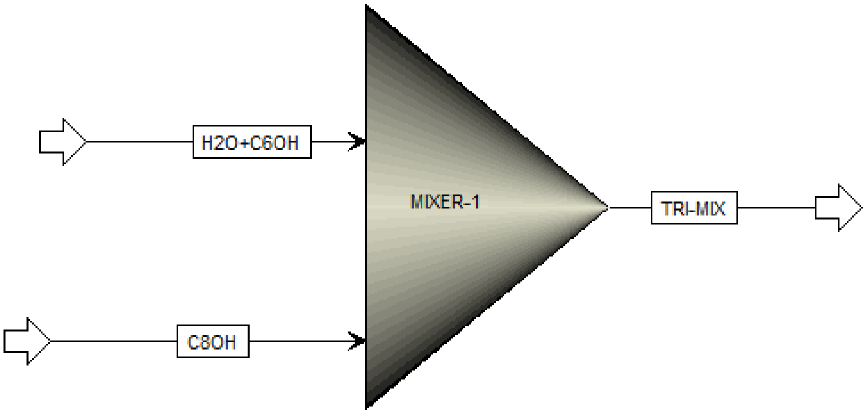


Figure 2.22 A simple process flowsheet for mixing water–hexanol mixture with 1-octanol.

Create an Aspen Plus flowsheet via selecting “**Specialty Chemicals with Metric Units**”. The default property method assigned by Aspen Plus is “**NRTL**”. We use the mass as the flow-basis throughout the flowsheet, unless otherwise specified. Initially, add the following three components: water, 1-hexanol, and 1-octanol.

The total flow rate of “**H2O+C6OH**” stream is 100 kg/h at 25°C and 2 atm. The flow rate of “**C8OH**” stream is also 100 kg/h of pure octanol at 25°C and 2 atm. The mixer exists under the same conditions of pressure and temperature. Perform the following tasks:

1. Add the three components from the assigned component databanks.
2. Under “**Properties**” environment while in “**Analysis**” mode and using NIST/TDE experimental data, carry out the consistency tests on the binary VLE data of water–hexanol, water–octanol, and hexanol–octanol systems to see whether it is possible to use the experimental VLE data instead of UNIFAC-estimated parameters for such binary interactions.
3. If in step #2, it is found that the experimental data fail the consistency tests and to avoid the little bit annoying warning appearing later in “**Control Panel**”, select “**Estimate missing parameters by UNIFAC**” option under “**Methods**” | “**Parameters**” | “**Binary Interaction**” | “**NRTL-1**” sheet. Click on “**Next**” button, select “**Run Property Analysis/Setup**” option from “**Properties Input Complete**” window, and click on “**OK**” button to estimate any missing property that is needed for further calculations.
4. Switching to “**Simulation**” environment and using the “**Model Palette**”, add one mixer from “**Mixers/Splitters**” tab and three required material streams. Name the block and streams as shown in Figure 2.22.
5. Add the feed stream conditions in terms of pressure, temperature, and compositional flow rate for both feed streams.
6. For the first mixer, you do not have to enter any input data; Aspen Plus will do the job for you.
7. Click on “**Next**” button and then on “**OK**” button found in “**Required Input Complete**” pop-up window, where the latter confirmation lets Aspen Plus run the simulation immediately.
8. Watch out any simulation error or serious warning in “**Control Panel**” of Aspen Plus. If there is any warning or error then you need to fix the problem. Aspen Plus will not give you error-free results unless you do everything correctly.
9. Check for the results via inspecting “**TRI-MIX**” stream properties.
10. It is reported in literature that azeotropic conditions exist for some of those binary systems. Using the “**Azeotrope Search**”  button found in “**Home**” ribbon, carry out an inspection for the possibility of azeotropic condition and, if any, report the azeotropic composition and temperature for such binary systems.

HOMEWORK/CLASSWORK 2.2 (WATER–ACETONE–EIPK SYSTEM WITH NIST/DTE DATA)

We have a <u>50/50 wt% mixture of water and acetone</u>. We plan to separate this mixture into its constituents and ultimately end up with almost pure streams of water and acetone. Figure 2.23 shows the starting (i.e., simple) process flowsheet where we mix water–acetone stream with ethyl-isopropyl-ketone (“**EIPK**”) stream to end-up with a ternary mixture (“**TRI-MIX**”) product stream.

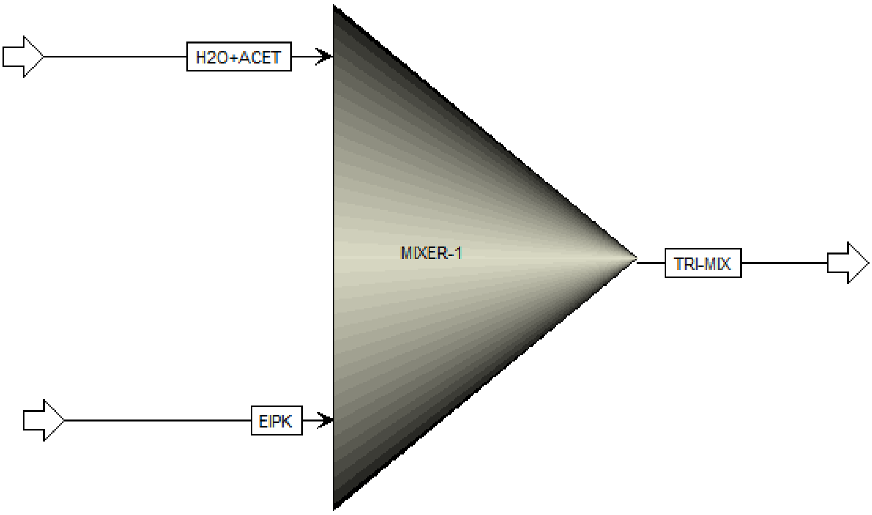
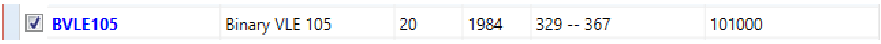


Figure 2.23 A simple process flowsheet for mixing water–acetone mixture with EIPK.

Create Aspen Plus flowsheet via selecting “**Specialty Chemicals with Metric Units**”. The default property method assigned by Aspen Plus is “**NRTL**”. We use the mass as the flow-basis throughout the flowsheet, unless otherwise specified. Initially, add the following three components: water, acetone, and ethyl-isopropyl-ketone (EIPK).

The total flow rate of “**H2O+ACET**” stream is 100 kg/h at 25°C and 1 atm. The flow rate of “**EIPK**” stream is also 100 kg/h of pure EIPK at 25°C and 1 atm. The mixer exists under the same conditions of pressure and temperature. Perform the following tasks:

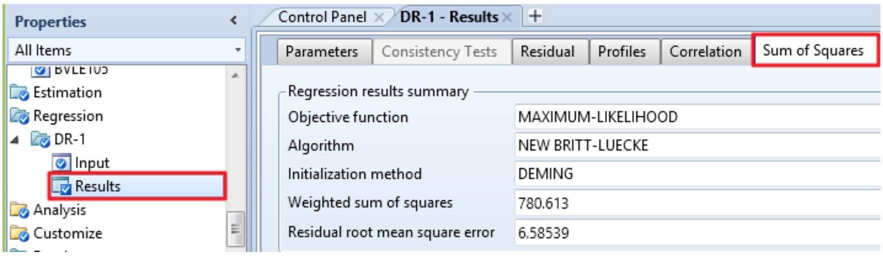
1. Add the three components from the assigned component databanks.
2. Under “**Properties**” environment while in “**Analysis**” mode and using NIST/TDE experimental data, carry out the consistency tests on the binary VLE data of water–acetone, water–EIPK, and acetone–EIPK systems to see whether it is possible to use the experimental VLE data instead of UNIFAC-estimated parameters for such binary interactions.
3. For water–acetone system, you will find that the following VLE data set is the most reliable in terms of the overall data quality index and consistency tests passed.
   Binary VLE 105: “Huang, R., Gu, Y. and Hou, Y. (1984) VLE of acetone-water-isobutyraldehyde system. *Chemical Engineering (China)*, **4**, 26–29”.
4. Save the data set in step #3 as shown in Figure 2.24.



☑ BVLE105	Binary VLE 105	20	1984	329 -- 367	101000

Figure 2.24 Saving the binary VLE data set as BVLE105.

5. Using “**NRTL**” method, carry out the regression step under “**Properties**” environment while in “**Regression**” mode. Use the first entry in Table 2.2 and define parameters, under “**Parameters**” tab, as in Figure 1.47. You should be able to obtain the regressed NRTL parameters with RMMSE less than 10 for such a VLE data set as shown in Figure 2.25.

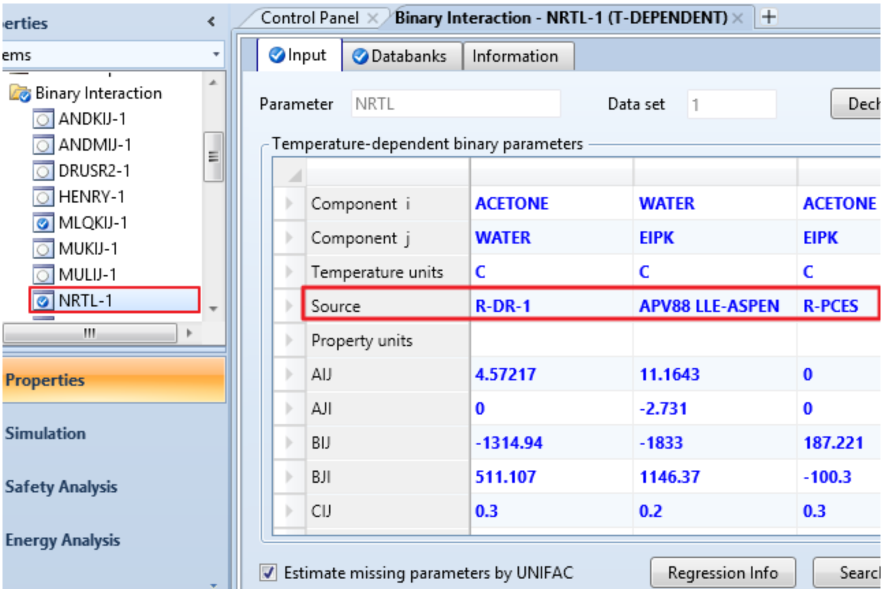


Regression results summary

Objective function	MAXIMUM-LIKELIHOOD
Algorithm	NEW BRITT-LUECKE
Initialization method	DEMING
Weighted sum of squares	780.613
Residual root mean square error	6.58539

Figure 2.25 Regressing water–acetone VLE data using a two-parameter “**NRTL**” model.

6. After successfully completing the regression step, click on “**Yes to all**” button appearing in the pop-up window to replace the existing binary interaction parameters with the newly regressed ones, for water–acetone system as shown in Figure 2.26.



Parameter: NRTL
Data set: 1

Temperature-dependent binary parameters

Component i	ACETONE	WATER	ACETONE
Component j	WATER	EIPK	EIPK
Temperature units	C	C	C
Source	R-DR-1	APV88 LLE-ASPEN	R-PCES
Property units			
AIJ	4.57217	11.1643	0
AJI	0	-2.731	0
BIJ	-1314.94	-1833	187.221
BJI	511.107	1146.37	-100.3
CIJ	0.3	0.2	0.3

☑ Estimate missing parameters by UNIFAC

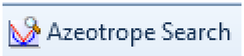
Figure 2.26 The binary interaction parameters for acetone–water system based on the regression step (R-DR-1).

7. To avoid the little bit annoying warning appearing later in “**Control Panel**”, select “**Estimate missing parameters by UNIFAC**” option under “**Methods**” | “**Parameters**” | “**Binary Interaction**” | “**NRTL-1**” sheet. Click on “**Next**” button, select “**Run Property Analysis/Setup**” option from “**Properties Input Complete**” window, and click on “**OK**” button to estimate any missing property that is needed for further calculations.
8. Switching to “**Simulation**” environment and using the “**Model Palette**”, add one mixer from “**Mixers/Splitters**” tab and three required material streams. Name the block and streams as shown in Figure 2.23.
9. Add the feed stream conditions in terms of pressure, temperature, and compositional flow rate for both feed streams.
10. For the first mixer, you do not have to enter any input data; Aspen Plus will do the job for you.
11. Click on “**Next**” button and then on “**OK**” button found in “**Required Input Complete**” pop-up window, where the latter confirmation lets Aspen Plus run the simulation immediately.
12. Watch out any simulation error or serious warning in “**Control Panel**” of Aspen Plus. If there is any serious warning or error then you need to fix the problem. Aspen Plus will not give you error-free results unless you do everything correctly.
13. Check for the results via inspecting “**TRI-MIX**” stream properties.
14. Using the “**Azeotrope Search**”  button found in “**Home**” ribbon, carry out inspection for the possibility of an azeotropic condition and, if any, report the azeotropic composition and temperature for such binary systems.

HOMEWORK/CLASSWORK 2.3 (WATER–ACETONE–EIPK SYSTEM WITHOUT NIST/DTE DATA)

Consider the same problem of Homework/Classwork 2.2 and trace all steps except for those pertaining to using NIST/DTE experimental data.

1. Add the three components from the assigned component databanks.
2. To avoid the little bit annoying warning appearing later in “**Control Panel**”, select “**Estimate missing parameters by UNIFAC**” option under “**Methods**” | “**Parameters**” | “**Binary Interaction**” | “**NRTL-1**” sheet. Click on “**Next**” button, select “**Run Property Analysis/Setup**” option from “**Properties Input Complete**” window, and click on “**OK**” button to estimate any missing property that is needed for further calculations.
3. Switching to “**Simulation**” environment and using the “**Model Palette**”, add one mixer from “**Mixers/Splitters**” tab and three required material streams. Name the block and streams as shown in Figure 2.23.
4. Add the feed stream conditions in terms of pressure, temperature, and compositional flow rate for both feed streams.
5. For the first mixer, you do not have to enter any input data; Aspen Plus will do the job for you.
6. Click on “**Next**” button and then “**OK**” button found in “**Required Input Complete**” pop-up window, where the latter confirmation lets Aspen Plus run the simulation immediately.

7. Watch out any simulation error or serious warning in “**Control Panel**” of Aspen Plus. If there is any serious warning or error then you need to fix the problem. Aspen Plus will not give you error-free results unless you do everything correctly.
8. Check for the results via inspecting “**TRI-MIX**” stream properties. See whether the results here are different from those in Homework/Classwork 2.2.
9. Using the “**Azeotrope Search**”  button found in “**Home**” ribbon, carry out inspection for the possibility of an azeotropic condition and, if any, report the azeotropic composition and temperature for such binary systems. See whether the azeotropic condition reported here is different from that in Homework/Classwork 2.2.

3

MORE ON ASPEN PLUS FLOWSHEET FEATURES (2)

3.1 PROBLEM DESCRIPTION: CONTINUATION TO THE PROBLEM IN CHAPTER 2

A mixture containing 50.0 wt% acetone and 50.0 wt% water is to be separated into two streams—one enriched in acetone and another in water. The separation process consists of extraction of acetone from water into methyl isobutyl ketone (MIBK), which dissolves acetone but is nearly immiscible with water. The overall goal of this problem is to separate the feed stream into two streams, which have greater than 95% purity of water and acetone, respectively.

In this episode, we emphasize the importance of checking for simulation results convergence and assure that the solution determined by Aspen Plus® is reasonable. In addition, we explore some features of Aspen Plus for presenting simulation results. We use our simulations from Chapter 2 to cover these topics.

3.2 THE CLEAN PARAMETERS STEP

As pointed out in Chapter 2, it was found that while accounting for the reliable NIST/TDE VLE data, the difference in estimating energy flow around the mixer between one recommended property method and another lies within the universally accepted engineering limit; that is, an associated PRE value being smaller than 10% for a typical measured or estimated quantity in engineering applications. In addition to its dependence on experimental data in terms of their validity or reliability, the regression goodness of any experimental data will also depend on the thermodynamic model being tackled and the number of parameters to plug in that model. This will make the entire process of regression non-calibrated and thus will vary from one user to another. To avoid confusion and inconsistency, we set the

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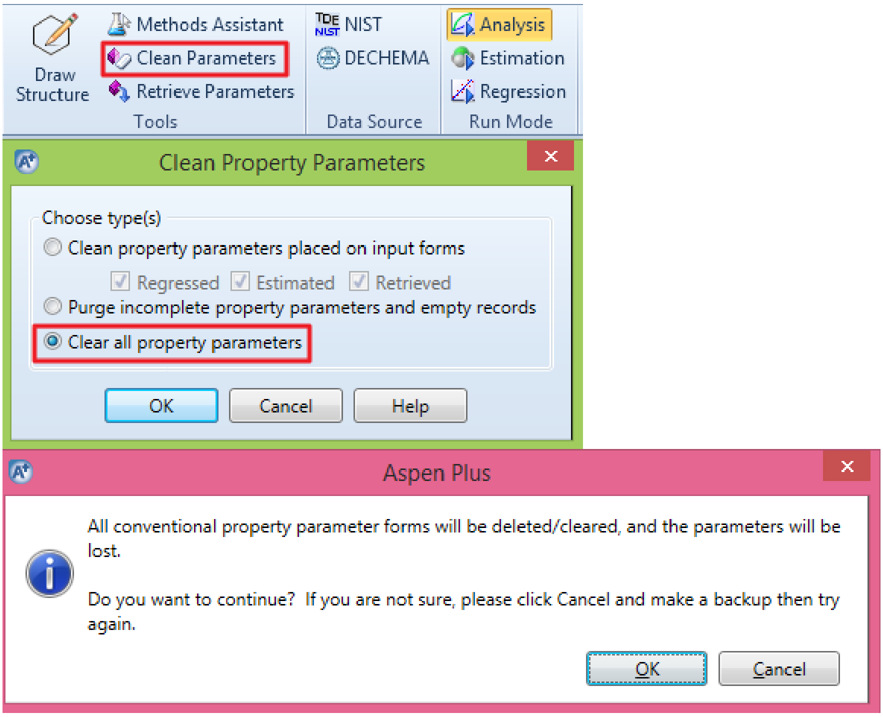
property method to "**NRTL**" and clear all estimated binary parameters of NIST/TDE VLE data regression, which was carried out in Chapter 2, for the sake of comparison between the results shown here and any results generated by the user should he/she attempt to rerun the same problem at hand.

Reopen your simulation by using "**Open**" folder and under "**Recent Models**" select the file that pertains to Chapter 2. We will rerun the existing simulation of Chapter 2. The selection of the property method is explained in detail in Chapters 1 and 2. Regarding clearing any estimated parameters, click on the "**Clean Parameters**" button found in "**Home**" ribbon while running the simulator under "**Properties**" environment. Figure 3.1 (*top*) shows the "**Clean Property Parameters**" window where the user may select more than a choice.



Choose type(s)

○ Clean property parameters placed on input forms

☑ Regressed ☑ Estimated ☑ Retrieved

○ Purge incomplete property parameters and empty records

● Clear all property parameters

All conventional property parameter forms will be deleted/cleared, and the parameters will be lost.

Do you want to continue? If you are not sure, please click Cancel and make a backup then try again.

Figure 3.1 The "**Clean Property Parameters**" window for cleaning any previously estimated or regressed property parameter.

The first choice removes property parameters that have been added to input forms as a result of running regressions, estimations, and/or retrieving property parameters from the databanks for review.

The second choice removes property parameters that are incomplete because of missing value, component ID, or parameter name. Such parameters can exist because the forms were incompletely filled out, or because a component with a property parameter data was removed, or because a property method was removed and there were parameters specified that only exist for that particular property method.

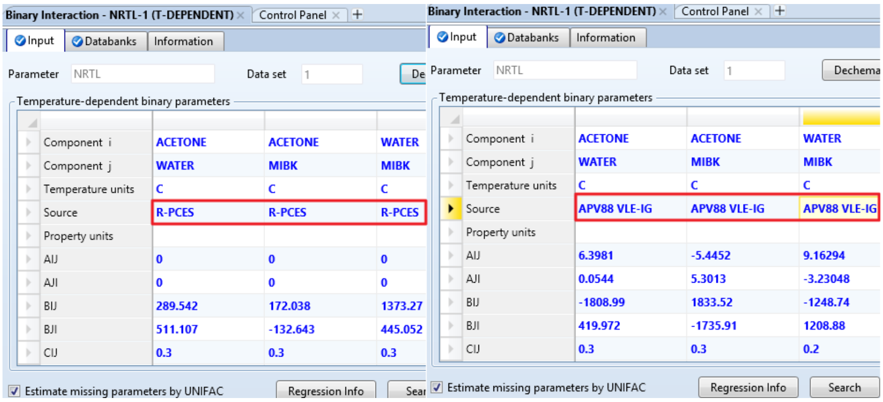
The third and last choice removes all specified data for conventional parameters and UNIFAC binary parameters. This restores these forms under “**Methods**” **|** “**Parameters**” to their initial state in a new simulation.

So, we will select “*Clear all property parameters*” option to clear out any residue and be back to the new born baby condition.

Clicking on the “**OK**” button will pop up another window (Figure 3.1 *bottom*) that will tell the user what such a cleaning step will do. Click on the “**OK**” button of the bottom window to complete the execution of the cleaning step.

After carrying out the cleaning step, you will notice that all binary interaction parameters were cleared out. Next, be sure that under “**Methods**” | “**Parameters**” | “**Binary Interaction**” | “**NRTL-1**” sheet the “*Estimate missing parameters by UNIFAC*” option is selected. Click on the “**Next**” button and select “*Run Property Analysis/Setup*” option from the pop-up window titled “**Properties Input Complete**”. Click on the “**OK**” button to complete estimating missing parameters.

Figure 3.2 (*left*) shows “**NRTL-1**” sheet where the binary interactions parameters are now estimated utilizing **R**egression by **P**roperty **C**onstant **ES**timation (“*R-PCES*”) method (see Chapter 1). For each of the three columns, select “*APV88 VLE-IG*” as the source for binary data to replace “*R-PCES*”, as shown in Figure 3.2 (*right*). Click on the “**Next**” button and select “*Run Property Analysis/Setup*” option from the pop-up window titled: “**Properties Input Complete**”. Click on the “**OK**” button to assure that the new values take into effect.



Parameter NRTL
Data set 1

Temperature-dependent binary parameters

Component i	ACETONE	ACETONE	WATER
Component j	WATER	MIBK	MIBK
Temperature units	C	C	C
Source	R-PCES	R-PCES	R-PCES
Property units			
AIJ	0	0	0
AJI	0	0	0
BIJ	289.542	172.038	1373.27
BJI	511.107	-132.643	445.052
CIJ	0.3	0.3	0.3

☑ Estimate missing parameters by UNIFAC

Parameter NRTL
Data set 1

Temperature-dependent binary parameters

Component i	ACETONE	ACETONE	WATER
Component j	WATER	MIBK	MIBK
Temperature units	C	C	C
Source	APV88 VLE-IG	APV88 VLE-IG	APV88 VLE-IG
Property units			
AIJ	6.3981	-5.4452	9.16294
AJI	0.0544	5.3013	-3.23048
BIJ	-1808.99	1833.52	-1248.74
BJI	419.972	-1735.91	1208.88
CIJ	0.3	0.3	0.2

☑ Estimate missing parameters by UNIFAC

Figure 3.2 The binary interaction parameters after cleaning followed by “**UNIFAC**” estimation step (*left*). Changing the source of binary data from “*R-PCES*” to “*APV88 VLE-IG*” (*right*).

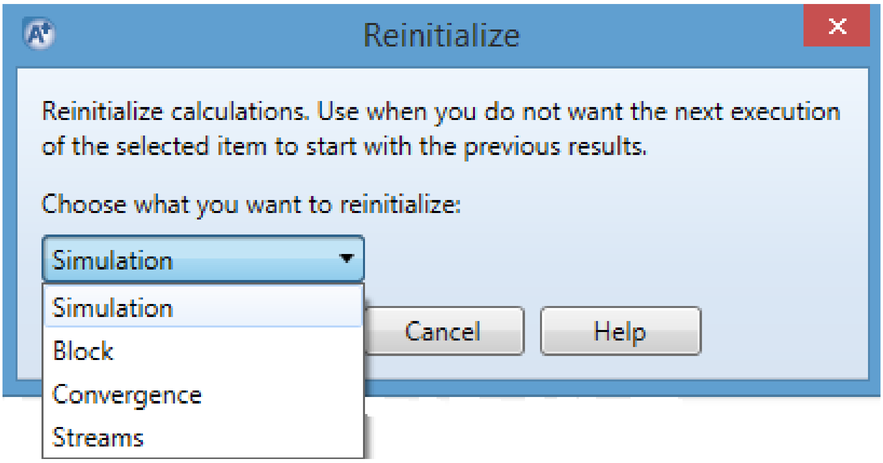
Doing so will bring us back to the simulation state (or status) as if we were to create a new Aspen Plus file from “**Chemicals**” template, add the three components, and run the simulation under “**Properties**” environment. *The theme here is to learn how to deal with parameters clearing/cleaning step without requiring us to create a new file from scratch.*

Switch from “**Properties**” to “**Simulation**” environment.

3.3 SIMULATION RESULTS CONVERGENCE

One should recall that when using a computer simulation package, the incorrect input data or programming can lead to solutions that are superficially "correct" based on the user's entered specifications, but unrealistic with respect to real-life applications. For this reason, it is very important that the user scrutinizes at least the basic balances to make sure that the simulation results are reasonable, based on his/her experience and the expected results.

At the end of Chapter 2, we had completed a simulation of the first mixer in our acetone separation process. Let us reset the simulator back to the initial state (or point) via using the "**Reset**" button, found in "**Home**" ribbon under "**Simulation**" environment this time. Figure 3.3 shows the "**Reinitialize**" window where it tells the user that upon executing this step, the solver will not proceed from where it stopped last run; instead it will make a step back to the initial state, of course, depending on the level of reinitialization to be carried out. If the user selects "*Simulation*", then Aspen Plus will reinitialize the entire process of calculations. Any other choice such as "*Block*", "*Convergence*", or "*Streams*" will result in a partial reinitialization to a block, streams, or convergence (i.e., the solver for design specifications, sensitivity analysis, optimization procedure, and data fit testing).



Reinitialize

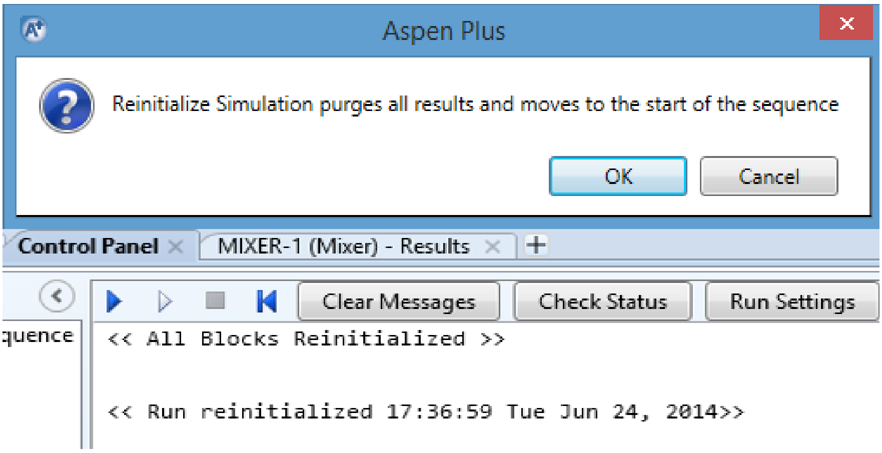
Reinitialize calculations. Use when you do not want the next execution of the selected item to start with the previous results.

Choose what you want to reinitialize:

Simulation

Figure 3.3 The reinitialization step is carried out to purge out any calculated block, convergence, stream properties, or all of the above.

Figure 3.4 shows the pop-up warning window (*top*) about the reset step and what it does upon execution and "**Control Panel**" (*bottom*) shows the solver message upon clicking on the "**OK**" button.



Reinitialize Simulation purges all results and moves to the start of the sequence

```
<< All Blocks Reinitialized >>


<< Run reinitialized 17:36:59 Tue Jun 24, 2014>>
```

Figure 3.4 The pop-up warning window for the reset step (*top*) and the confirmation of reinitialization step via the "**Control Panel**" message (*bottom*).

NOTE #1: *The reset feature is useful when modifying an existing simulation in terms of input data, operating condition(s), and/or any constraint imposed on a given block. The solver, for example, may converge for all blocks except for a few (i.e., one or two) blocks, then the user's duty is to keep changing specifications for that particular non-converging block until a converging and reasonable solution is reached. So does the case for any "**Flowsheeting Options**" or "**Model Analysis Tools**" case study. In this regard, the reset feature for that particular non-converging "**Block**" or "**Convergence**" will be very useful and time saving. Moreover, I occasionally found that the "**Reset**" button did nothing upon clicking; alternatively, one may click on the "* Reset *" button at the top of "**Control Panel**", as shown in Figure* 3.4.

Now that the simulation has been reset, run it again, using the "**Next**" button. On clicking the "**Next**" button to run the simulation, the program will show information about its convergence in "**Control Panel**". This means that Aspen Plus will make "**Control Panel**" as the active window, which can be seen by the user.

On the other hand, if you click the "**Run**" button instead of the "**Next**" button, after executing the "**Reset**" process, the status of the run can be seen via clicking the "**Control Panel**" button found in "**Home**" ribbon, given that "**Control Panel**" is not active.

Since our simulation is very basic, we should not have any convergence problems. However, as our simulation becomes more intricate in the coming chapters; that is, we will be adding more complicated unit operations (blocks), which may require multiple iterations to solve. In this case, we examine both the "**Control Panel**" messages and convergence algorithm results to make sure that the simulation did converge with reasonable tolerance (or accuracy).

NOTE #2: *Some factors that usually lead to convergence difficulties are a poor choice for the property method (i.e., thermodynamics) and the creation of recycle streams.*

The “**Control Panel**” will also list any warnings or errors that may arise based on your input choices.

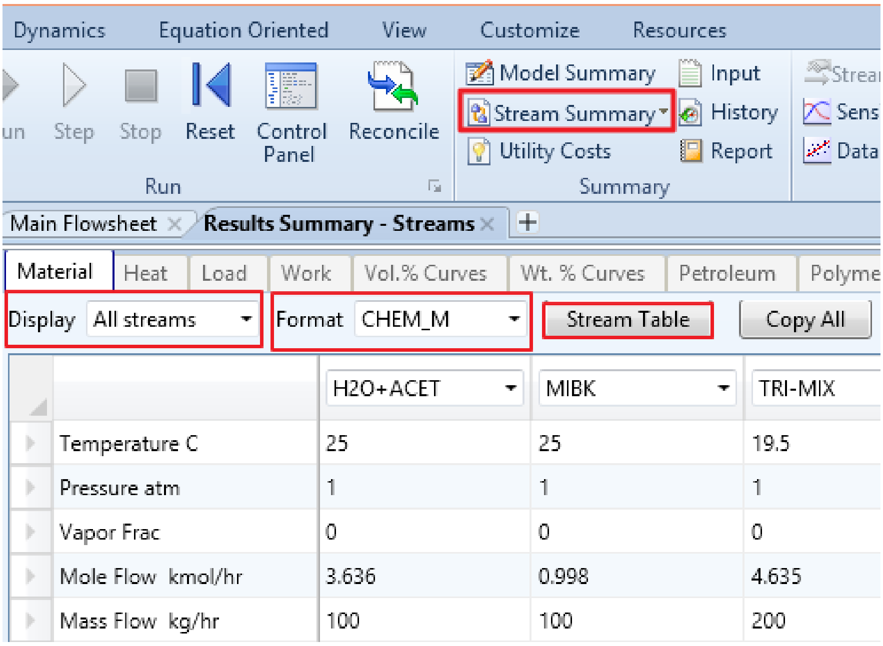
If our simulation normally converges, it does not necessarily mean that the solution will be reasonable. We now move on to another basic check that should be done when completing simulations. Click on the “**Stream Summary**” button found in “**Home**” ribbon. When you do this you will be presented with a stream material summary table as shown earlier in Figure 2.15. While we expect Aspen Plus to be correct, it is advisable to run a few simple checks on the data presented in this table.

As mentioned earlier, Aspen Plus can give “correct” but unreasonable results due to convergence or the selected thermodynamic properties, so it is highly recommended that you verify the results presented in this table. Some checks to perform include a quick material balance, a quick heat balance, and a comparison to available experimental or operating data. Later in your professional life, you will be able to use your experience to quickly tell whether the results do not appear to make sense. However, even then you should look at every number that is presented in the results. If your results appear to be acceptable, you can move on and add the simulation results to the process flowsheet for ease of demonstration. On the other hand, clicking on “**Home**” ribbon | “**Summary**” tab | “**Model Summary**” button will provide the user with the used property method and a summary view of important variables of all unit operations (i.e., blocks) models and, if applicable, design specs, utilities, and stream prices.

3.4 ADDING STREAM TABLE

Click on the “**Stream Summary**” button found in “**Home**” ribbon. Go over some options for formatting and modifying your stream tables. As shown in Figure 3.5, you will see two of the options for varying the stream table: “**Display**” and “**Format**”. Under “**Display**” drop-down menu, there are three options, “*All streams*”, “*Hierarchy streams*”, or “*Streams*”. “*All streams*” will show all streams found within the flowsheet. The “*Hierarchy streams*” has to deal with hierarchy blocks to provide hierarchical structure to complex simulations. Hierarchy blocks may be added automatically when importing templates into a simulation. Hierarchy blocks may contain streams and other blocks (even other hierarchy blocks) as well other features such as design specifications and sensitivity problems. Hierarchy blocks contain Setup and Methods form with some of the same information as the top-level Setup form and the Methods form from the Properties environment. The settings on these forms override the settings on the corresponding forms in higher-level hierarchy blocks or at the top level of the simulation for blocks within the hierarchy block. The scope of this textbook is not meant to deal with complex simulations; hence, we do not have hierarchical streams.

The “*Streams*” option allows the user to choose the streams he/she would like to see or show, one by one. Under the “**Format**” drop-down menu there are several types of stream tables. Each of the options presents the data in a slightly different manner, depending on the intended application. Finally, click on the “**Stream Table**” button to display the stream table on the main flowsheet window.



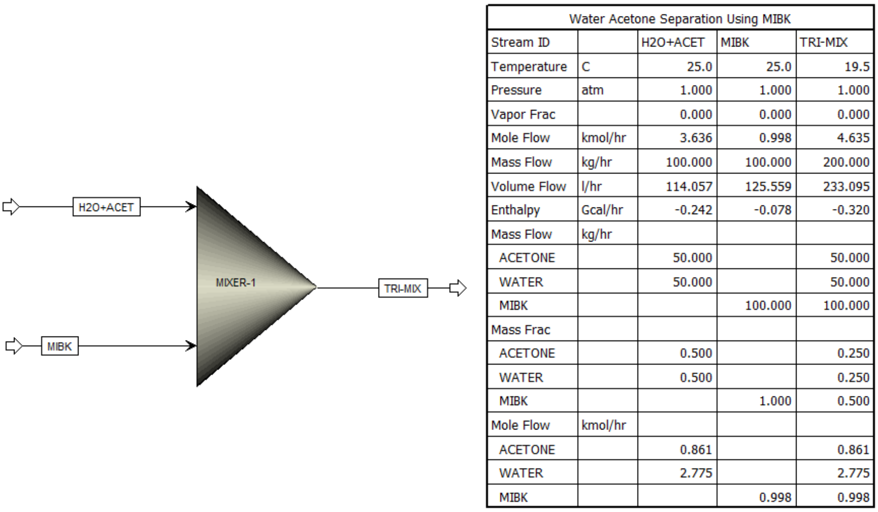
Display: All streams

Format: CHEM_M

	H2O+ACET	MIBK	TRI-MIX
Temperature C	25	25	19.5
Pressure atm	1	1	1
Vapor Frac	0	0	0
Mole Flow kmol/hr	3.636	0.998	4.635
Mass Flow kg/hr	100	100	200

Figure 3.5 "**Display**" and "**Format**" options for adding the stream table to the main flowsheet window.

If we use "*CHEM_M*" option from the "**Format**" drop-down menu, and click the "**Stream Table**" button, then the stream table will be added to the main flowsheet window, as shown in Figure 3.6.



Water Acetone Separation Using MIBK

Stream ID		H2O+ACET	MIBK	TRI-MIX
Temperature	C	25.0	25.0	19.5
Pressure	atm	1.000	1.000	1.000
Vapor Frac		0.000	0.000	0.000
Mole Flow	kmol/hr	3.636	0.998	4.635
Mass Flow	kg/hr	100.000	100.000	200.000
Volume Flow	l/hr	114.057	125.559	233.095
Enthalpy	Gcal/hr	-0.242	-0.078	-0.320
Mass Flow	kg/hr			
ACETONE		50.000		50.000
WATER		50.000		50.000
MIBK			100.000	100.000
Mass Frac				
ACETONE		0.500		0.250
WATER		0.500		0.250
MIBK			1.000	0.500
Mole Flow	kmol/hr			
ACETONE		0.861		0.861
WATER		2.775		2.775
MIBK			0.998	0.998

Figure 3.6 The main process flowsheet with added stream table. The property method is "**NRTL**".

3.5 PROPERTY SETS

A property set is a collection of thermodynamic, transport, and other properties that you can use in physical property tables and analysis. The list of built-in property sets is determined by the template you choose when creating a new run. You can use a built-in property set and modify it to fit your needs, or you can create your own property sets. To see the built-in sets available or select one, use the drop-down list on any property set list box. Figure 3.7 shows the built-in property sets associated with "*Specialty Chemicals with Metric Units*" template. Keep in mind that the active environment is "**Simulation**".

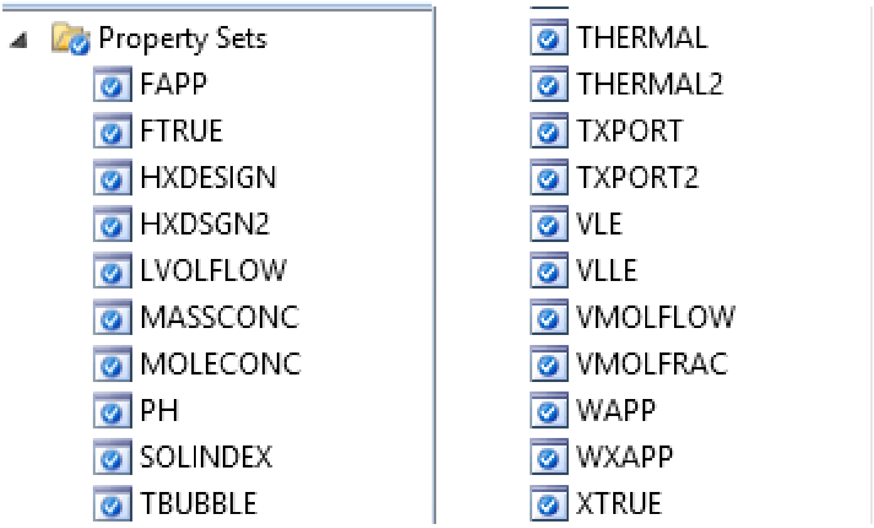
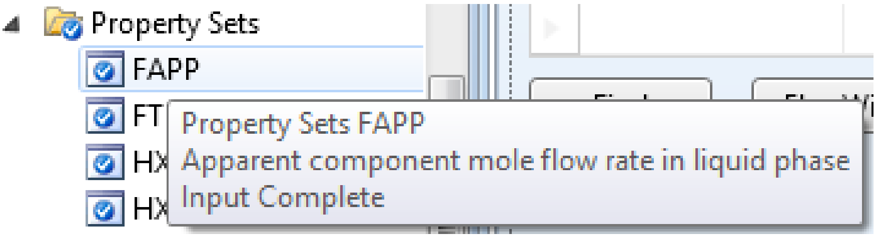

Property Sets
FAPP
FTRUE
HXDESIGN
HXDSGN2
LVOLFLOW
MASSCONC
MOLECONC
PH
SOLINDEX
TBUBBLE
THERMAL
THERMAL2
TXPORT
TXPORT2
VLE
VLLE
VMOLFLOW
VMOLFRAC
WAPP
WXAPP
XTRUE

Figure 3.7 The built-in property sets for "*Specialty Chemicals with Metric Units*" template.

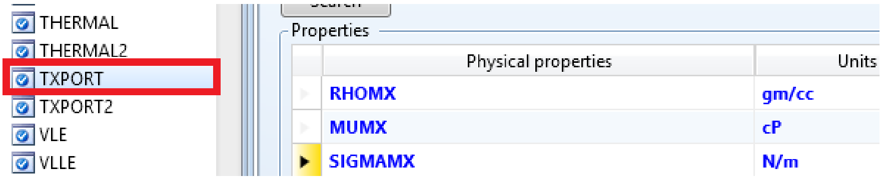
For more details on any property set, just hover the mouse over a particular set and Aspen Plus will prompt the user with a few descriptions, as shown in Figure 3.8.



Property Sets FAPP
Apparent component mole flow rate in liquid phase
Input Complete

Figure 3.8 An information summary can be obtained via hovering the mouse over a particular set, such as "**FAPP**".

For each property set, there may exist more than one thermodynamic, transport, or thermal property being defined so that they can be evaluated by Aspen Plus for a given stream. Figure 3.9 shows an example of a property set that contains more than one property to be



Physical properties	Units
RHOMX	gm/cc
MUMX	cP
SIGMAMX	N/m

Figure 3.9 The property set “**TXPORT**” includes three properties of a mixture to be evaluated by Aspen Plus.

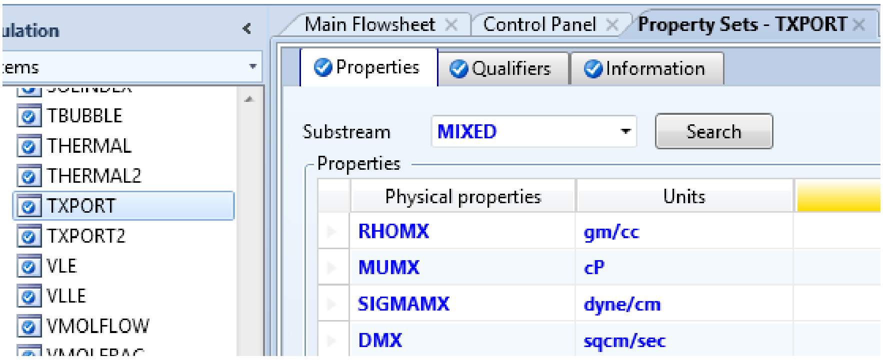
evaluated. “**RHOMX**” stands for density of a mixture; “**MUMX**” for a mixture viscosity; and “**SIGMAMX**” for surface tension of a mixture.

Mass diffusivity is not one of the default variables that are reported by Aspen Plus, and it is only reported if the user defines a specific property set. The easiest way to do this is to modify an existing property set that reports other parameters of interest and then have Aspen Plus report this property set.

We will modify the “**TXPORT**” property set so that it includes diffusivity values for our system. In the “**Prop-Sets**” window, select “**TXPORT**” and hit the “**Edit**” button at the bottom of the screen. Alternatively, you may directly go to the property set itself and Aspen Plus will open up its associated form.

Select the last row (or record) in the first column that is currently blank. In doing so, you will be presented with a scrolling window of physical properties that Aspen Plus can calculate for the user. Scroll down until you find “**DMX**” (Diffusivity of a mixture), which is the variable for diffusivity in Aspen Plus. You will notice that a description of each physical property appears as you hover the mouse over the variable name.

Figure 3.10 shows “**TXPORT**” of “**Prop-Sets**” in “**Navigation**” pane where “**DMX**” is added.

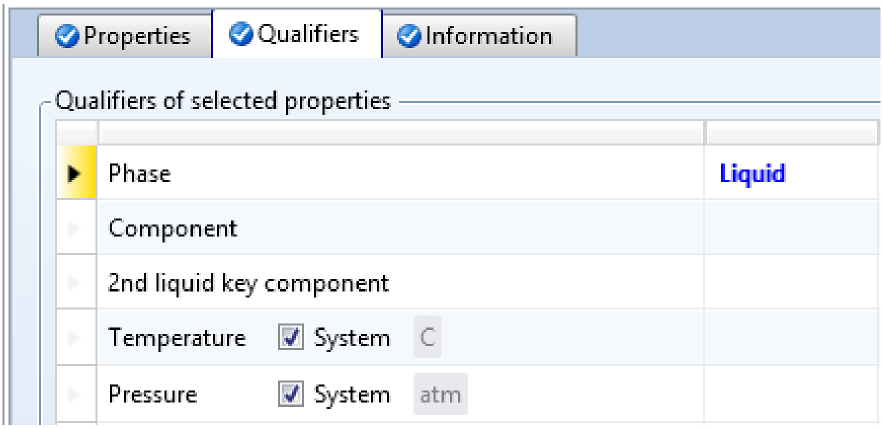


Substream MIXED

Physical properties	Units
RHOMX	gm/cc
MUMX	cP
SIGMAMX	dyne/cm
DMX	sqcm/sec

Figure 3.10 The “**DMX**” property will be added to streams. “**DMX**” is the diffusivity with units of cm^2/s.

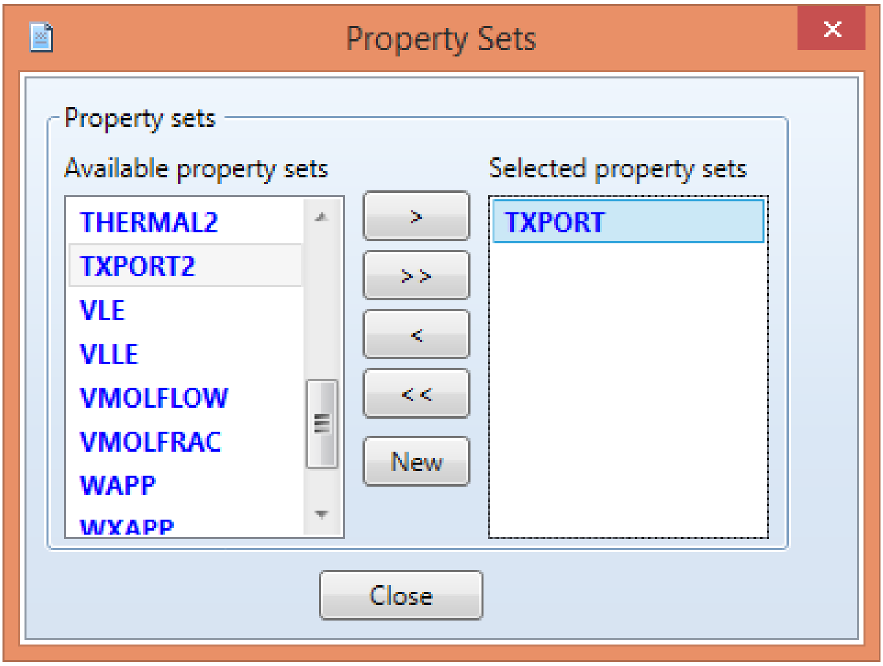
Figure 3.11 shows the “**Qualifiers**” tab. This window allows the user to input the phases they would like the property set to be reported for. Because we are not concerned about the vapor phase at this point, we keep only the liquid phase. The “**Qualifiers**” tab should now look like that seen in Figure 3.11.



Phase	Liquid
Component	
2nd liquid key component	
Temperature ☑ System C	
Pressure ☑ System atm	

Figure 3.11 The “**Qualifiers**” tab window, where it allows the user to input the phase he/she would like the property set to be reported for.

We must now add the “**TXPORT**” property set to the stream table that is shown in the process flowsheet. While “**Simulation**” environment is the active mode and using “**Navigation**” pane, go to “**Setup**” | “**Report Options**” | “**Stream**” tab form and click on the “**Property Sets**” button. Doing so will open up the window shown in Figure 3.12.



Available property sets:
- THERMAL2
- TXPORT2
- VLE
- VLLE
- VMOLFLOW
- VMOLFRAC
- WAPP
- WXAPP

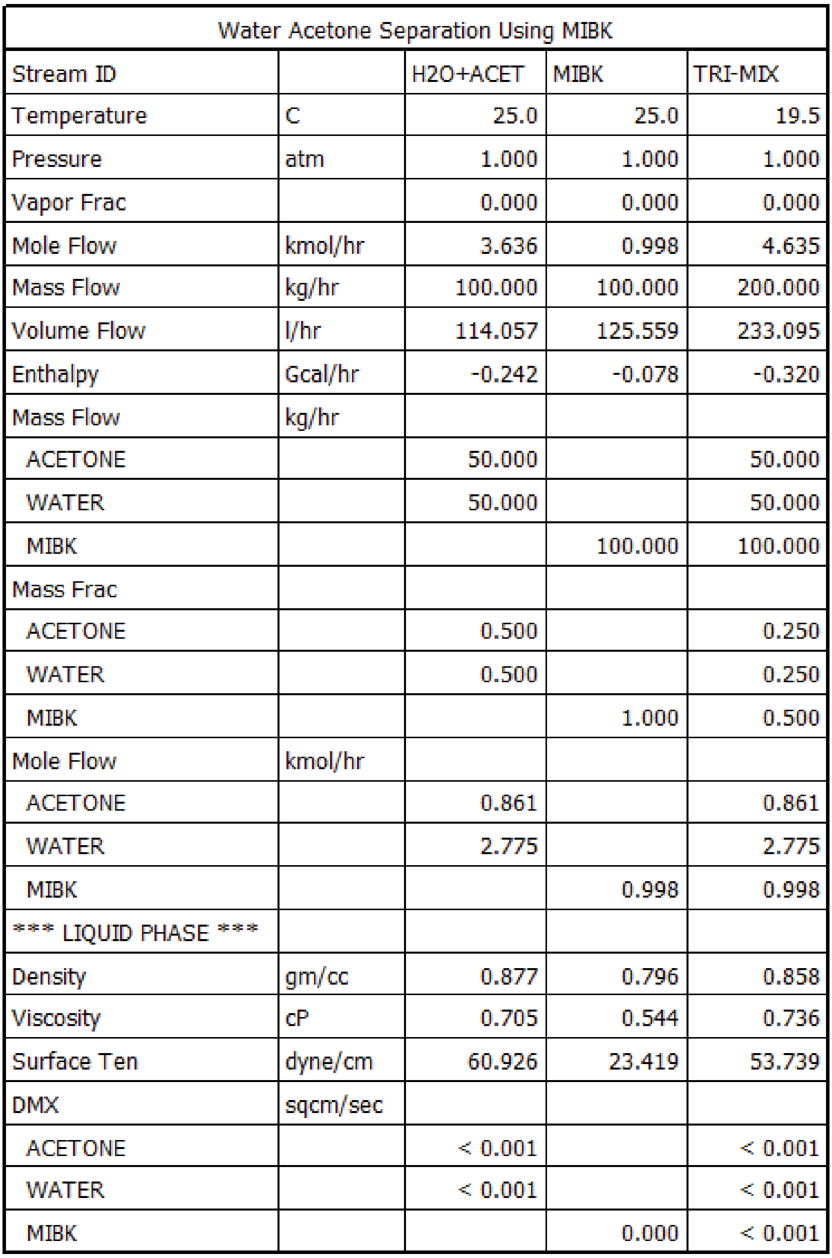
Selected property sets:
- TXPORT

Figure 3.12 The “**Property Sets**” window that is invoked by hitting the “**Property Sets**” button under the “**Stream**” tab in the “**Report Options**” sheet of “**Setup**” folder in “**Navigation**” pane.

Select “**TXPORT**” and hit the single arrow button pointing to the right. This will move “**TXPORT**” to the side labeled “*Selected property sets*”, and it will now be displayed in the stream table. After doing this, close the “**Property Sets**” window.

When you have done this, reset and rerun your simulation. In order to update the stream table, you will most likely need to click on the stream table and then click away from it. Another option is to delete the existing stream table and add a new one to the process flowsheet.

Figure 3.13 shows the stream table where its transport properties ("**TXPORT**") are listed.



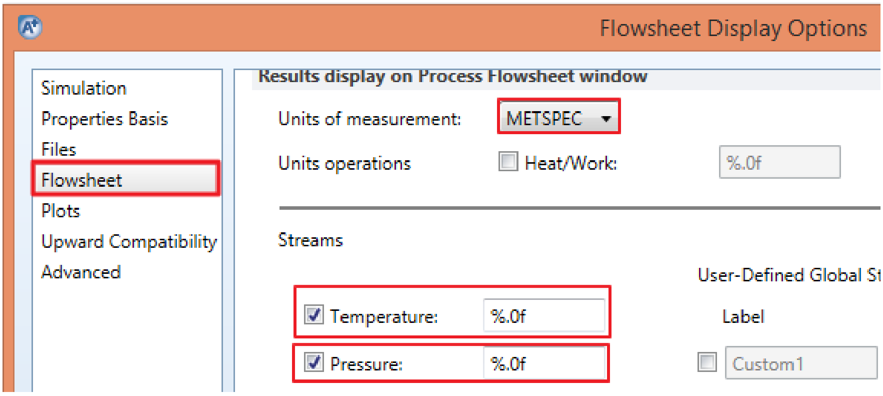
Water Acetone Separation Using MIBK

Stream ID		H2O+ACET	MIBK	TRI-MIX
Temperature	C	25.0	25.0	19.5
Pressure	atm	1.000	1.000	1.000
Vapor Frac		0.000	0.000	0.000
Mole Flow	kmol/hr	3.636	0.998	4.635
Mass Flow	kg/hr	100.000	100.000	200.000
Volume Flow	l/hr	114.057	125.559	233.095
Enthalpy	Gcal/hr	-0.242	-0.078	-0.320
Mass Flow	kg/hr			
ACETONE		50.000		50.000
WATER		50.000		50.000
MIBK			100.000	100.000
Mass Frac				
ACETONE		0.500		0.250
WATER		0.500		0.250
MIBK			1.000	0.500
Mole Flow	kmol/hr			
ACETONE		0.861		0.861
WATER		2.775		2.775
MIBK			0.998	0.998
*** LIQUID PHASE ***				
Density	gm/cc	0.877	0.796	0.858
Viscosity	cP	0.705	0.544	0.736
Surface Ten	dyne/cm	60.926	23.419	53.739
DMX	sqcm/sec			
ACETONE		< 0.001		< 0.001
WATER		< 0.001		< 0.001
MIBK			0.000	< 0.001

Figure 3.13 The stream table where the stream transport properties ("**TXPORT**") are listed.

3.6 ADDING STREAM CONDITIONS

In a large simulation, it is common to add stream conditions directly to the streams themselves so the user does not have to search through a large stream table for values. Although this is not the case in our simulation, however, we will tag each stream by its temperature and pressure value, for the sake of learning. This can be done via clicking on "**Options**" submenu under "**File**" menu found in the "**Top**" toolbar, as shown in Figure 3.14. The number format (i.e., how many significant numbers) of these variables can be changed by changing the number in the format edit-box. For example, the default value is "*%.0f*", which means that the data will be presented as integer with no fraction. If you change the default format to "*%.1f*" then the value of temperature (°C) will be shown as *25.0* instead of *25*. On the other hand, the associated units of measurement can be changed from the drop-down menu of "**Units of measurement**" option. For example, Figure 3.14 shows that "*METSPEC*" is selected as the "**Units of measurement**".


Flowsheet Display Options

Results display on Process Flowsheet window

Units of measurement: METSPEC

Units operations ☐ Heat/Work: %.0f

Streams

☑ Temperature: %.0f

☑ Pressure: %.0f

User-Defined Global St

Label

☐ Custom1

Figure 3.14 The "**Flowsheet Display Options**" window under "**File**" | "**Options**" submenu. Select "**Temperature**" and "**Pressure**" options and hit "**Apply**" and/or "**OK**" button.

Go to the main flowsheet window and you will notice those two properties will now be shown in the process flowsheet, as shown in Figure 3.15.

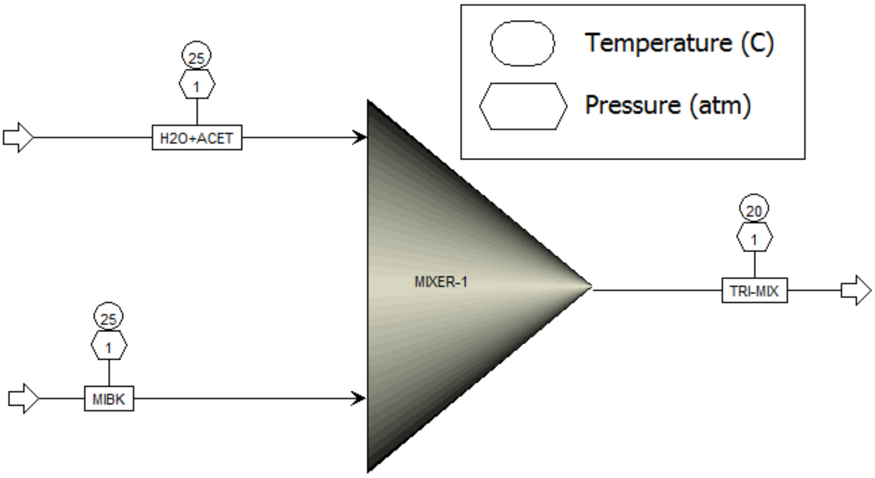
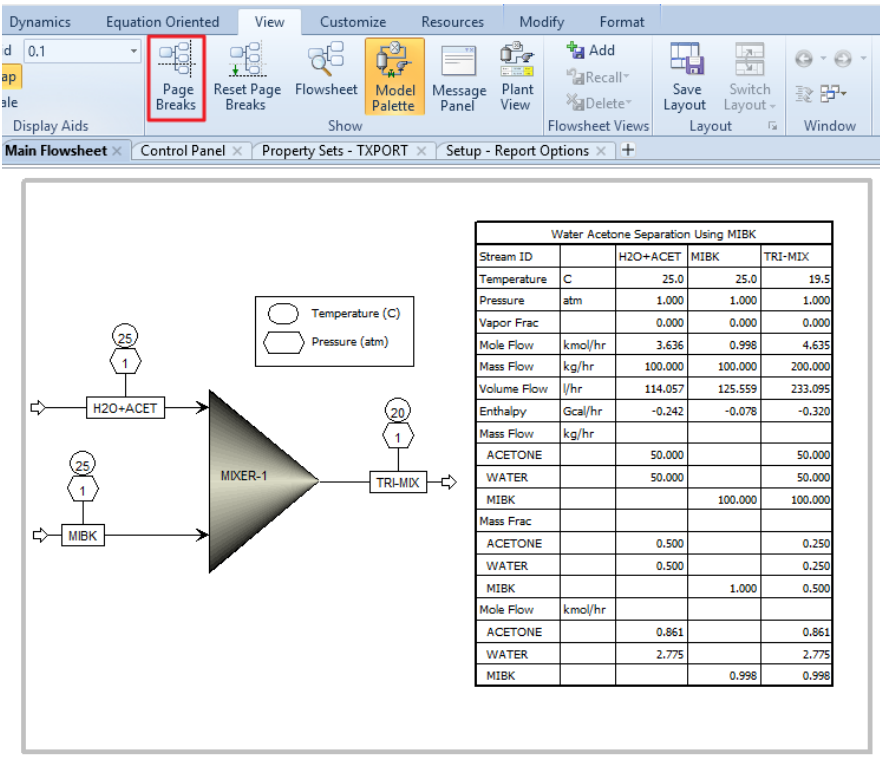


Figure 3.15 Showing *P* and *T* in each stream of the process flowsheet.

3.7 PRINTING FROM ASPEN PLUS

Printing a process flowsheet can be easily completed from "**File**" | "**Print**" submenu found in "**Top**" toolbar. However, the user may want to select only a portion of a process flowsheet to print. To do this, either right-click on the flowsheet window and select "**Page Break Preview**" submenu, or go to "**Top**" toolbar | "**View**" | "**Page Breaks**" found in "**Show**" group. Doing so will place a gray box around your entire process diagram in the flowsheet window as shown in Figure 3.16. This box represents the area that will be printed, similar to the print preview option in other programs. This box can be moved around on the screen and/or reduced/enlarged to fit the user's need. When the box is positioned to the users need, the flowsheet can be printed as mentioned here.

To change the printer type or page setup (i.e., page size and orientation), go to "**File**" | "**Print Preview**" and "**Print Preview**" window shows up. Select the first top-left icon that represents the printer type and the second top-left icon that represents the page setup.

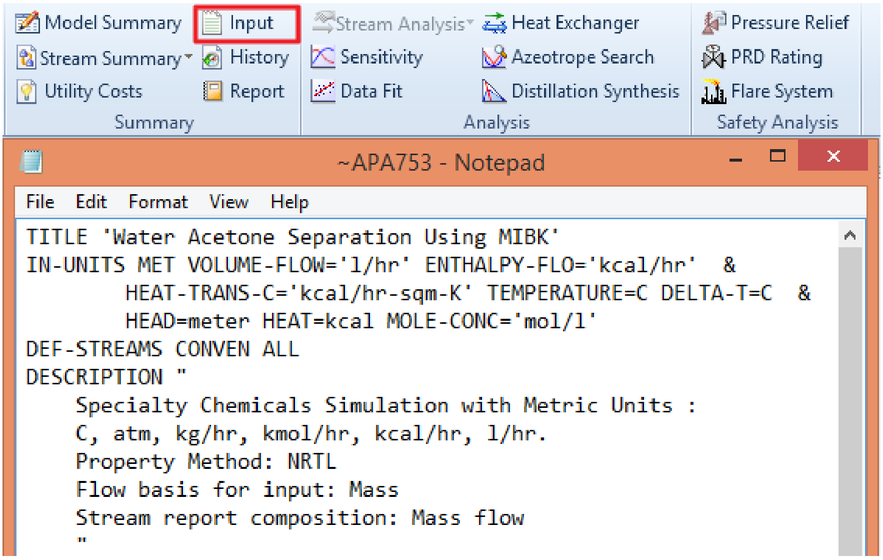


Water Acetone Separation Using MIBK				
Stream ID		H2O+ACET	MIBK	TRI-MIX
Temperature	C	25.0	25.0	19.5
Pressure	atm	1.000	1.000	1.000
Vapor Frac		0.000	0.000	0.000
Mole Flow	kmol/hr	3.636	0.998	4.635
Mass Flow	kg/hr	100.000	100.000	200.000
Volume Flow	l/hr	114.057	125.559	233.095
Enthalpy	Gcal/hr	-0.242	-0.078	-0.320
Mass Flow	kg/hr			
ACETONE		50.000		50.000
WATER		50.000		50.000
MIBK			100.000	100.000
Mass Frac				
ACETONE		0.500		0.250
WATER		0.500		0.250
MIBK			1.000	0.500
Mole Flow	kmol/hr			
ACETONE		0.861		0.861
WATER		2.775		2.775
MIBK			0.998	0.998

Figure 3.16 A gray box is drawn around the entire process diagram in the flowsheet window via right-clicking the mouse and selecting "**Page Break Preview**" submenu from the shortcut context menu. Go to "**Top**" toolbar | "**File**" | "**Print**" submenu to print the selected page break preview, if you want to print to a file (i.e., ***.PDF**) or to a printer.

3.8 VIEWING THE INPUT SUMMARY

Another way for Aspen Plus users to present their results is through the input file of Aspen Plus. This is a useful way to check your input data for errors (or for a supervisor to check a junior engineer's work quickly to look for bad assumptions etc.). The input summary is easily generated by clicking on "**Home**" ribbon **|** "**Summary**" tab **|** "**Input File**" button. The summary will be opened up in Notepad and it can be saved or printed directly from there. Figure 3.17 shows a portion of the Notepad file that is created upon invoking the "**Input File**" button.



```
TITLE 'Water Acetone Separation Using MIBK'
IN-UNITS MET VOLUME-FLOW='l/hr' ENTHALPY-FLO='kcal/hr'  &
        HEAT-TRANS-C='kcal/hr-sqm-K' TEMPERATURE=C DELTA-T=C  &
        HEAD=meter HEAT=kcal MOLE-CONC='mol/l'
DEF-STREAMS CONVEN ALL
DESCRIPTION "
    Specialty Chemicals Simulation with Metric Units :
    C, atm, kg/hr, kmol/hr, kcal/hr, l/hr.
    Property Method: NRTL
    Flow basis for input: Mass
    Stream report composition: Mass flow
    "
```

Figure 3.17 A portion of Notepad file that is created upon invoking the “**Input File**” button.

3.9 REPORT GENERATION

Clicking on “**Home**” ribbon | “**Summary**” tab | “**Report File**” button will open up the dialog box titled “**Report**”, where the user has the choice to select the item in the form of block, streams, convergence, sensitivity, and so on that will be included in the report as shown in Figure 3.18. For each drop-down menu item, shown in Figure 3.18, there may exist a corresponding flowsheet object, depending on the complexity of your flowsheet and the analysis you have already included.

After clicking on the “**Apply**” button for each selected item, in Figure 3.18, a Notepad file is created as a generated report, as shown in Figure 3.19. On the other hand, clicking on the “**OK**” button will do the same job but will also close the dialog box.

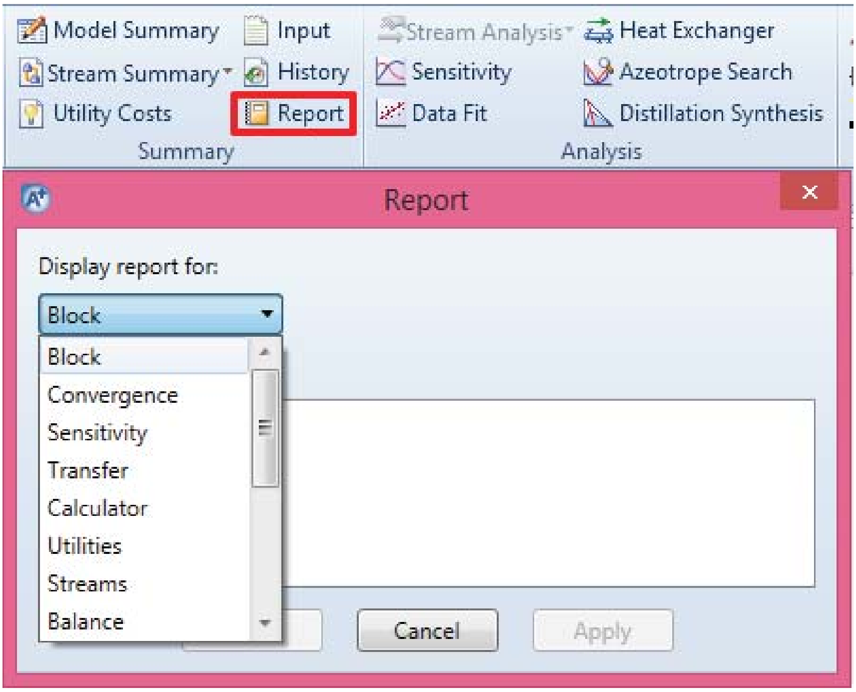
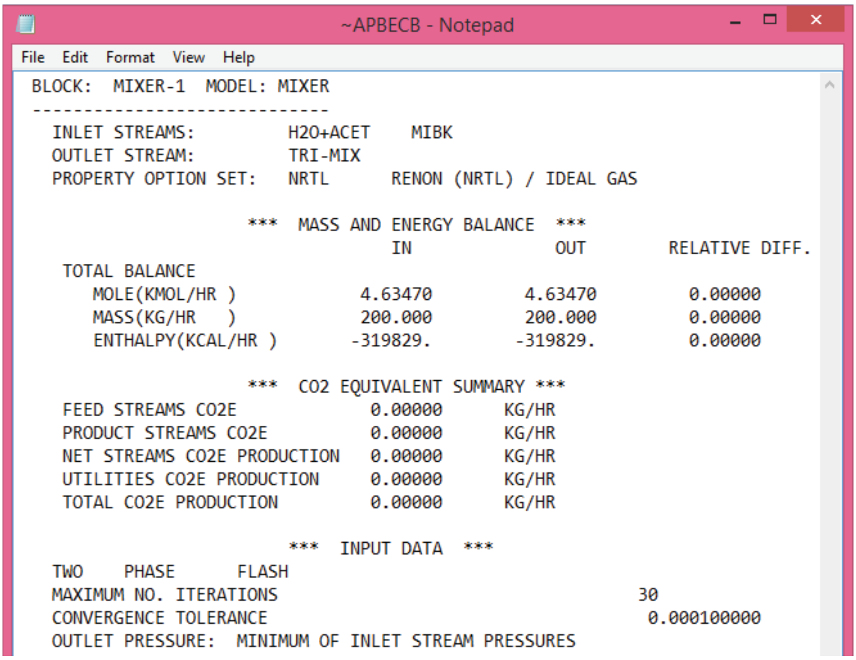


Figure 3.18 Aspen Plus will give the user the choice for the items to include in the generated report.



```
BLOCK:  MIXER-1  MODEL: MIXER
-----------------------------
  INLET STREAMS:         H2O+ACET    MIBK
  OUTLET STREAM:         TRI-MIX
  PROPERTY OPTION SET:   NRTL       RENON (NRTL) / IDEAL GAS

                   ***  MASS AND ENERGY BALANCE  ***
                                IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(KMOL/HR )         4.63470         4.63470         0.00000
      MASS(KG/HR    )        200.000         200.000         0.00000
      ENTHALPY(KCAL/HR )    -319829.        -319829.         0.00000

                   ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E              0.00000       KG/HR
   PRODUCT STREAMS CO2E           0.00000       KG/HR
   NET STREAMS CO2E PRODUCTION    0.00000       KG/HR
   UTILITIES CO2E PRODUCTION      0.00000       KG/HR
   TOTAL CO2E PRODUCTION          0.00000       KG/HR

                       ***  INPUT DATA  ***
  TWO    PHASE      FLASH
  MAXIMUM NO. ITERATIONS                                   30
  CONVERGENCE TOLERANCE                                     0.000100000
  OUTLET PRESSURE:  MINIMUM OF INLET STREAM PRESSURES
```

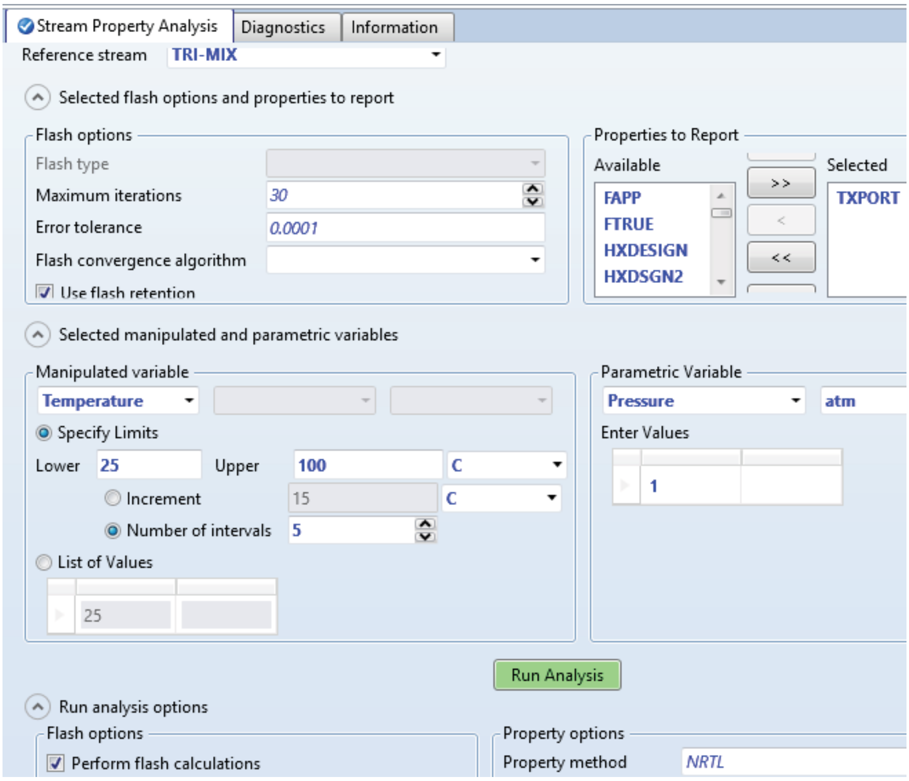
Figure 3.19 Report generation by Aspen Plus for a selected block (“**MIXER-1**”). Mass, mole, and energy balances around the mixer are shown.

NOTE #3: *What to include in the report (i.e., level of details) is done via "**Report Options**" in "**Setup**" folder of "**Navigation**" pane.*

3.10 STREAM PROPERTIES

To show stream thermodynamic, transport, or both properties at specified temperature and pressure, make the flowsheet window active and select a given stream by right-clicking the mouse on that stream then go to "**Analysis** … " menu | "**Stream Properties**" submenu. Alternatively, you may click on "**Home**" ribbon | "**Analysis**" group | "**Stream Analysis**" button and then select "**Stream Properties**" item from the drop-down list.

A stream property analysis ("**SPROP-1**") form is created under "**Analysis**" folder in "**Navigation**" pane, as shown in Figure 3.20 for "**TRI-MIX**" stream. The "**TXTPORT**" property set was selected, the manipulated variable is temperature, and the parametric variable is pressure. Clicking on the "**Run Analysis**" button, Aspen Plus will refresh the user by the analysis results in the form of a parametric plot for transport mixture properties as a function of temperature at a fixed value of pressure in this case.



Reference stream TRI-MIX

Flash type

Maximum iterations 30

Error tolerance 0.0001

Flash convergence algorithm

☑ Use flash retention

Available: FAPP, FTRUE, HXDESIGN, HXDSGN2

Selected: TXPORT

Temperature

● Specify Limits

Lower 25 Upper 100 C

○ Increment 15 C

● Number of intervals 5

○ List of Values

25

Pressure atm

Enter Values

1

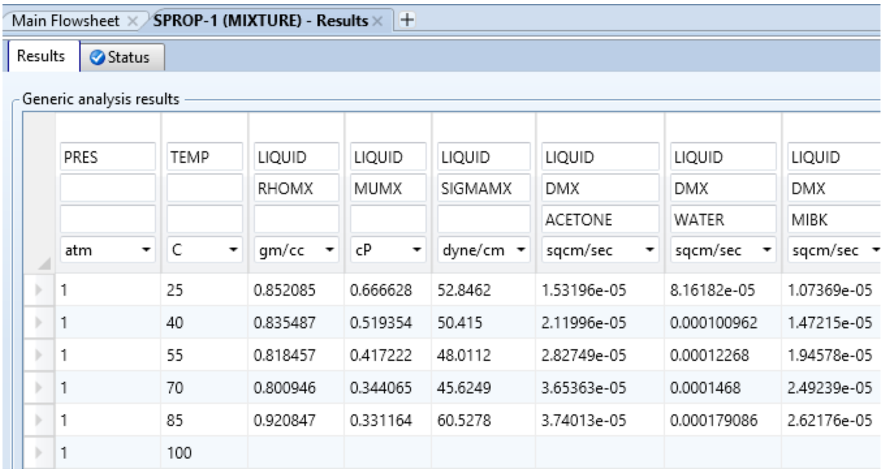
☑ Perform flash calculations

Property method NRTL

Figure 3.20 Stream "**TRI-MIX**" was selected first and its transport properties will be shown using the stream property analysis tool provided by Aspen Plus.

Notice that if the “**Run Analysis**” button is not active, then this means that the simulation status is such that no successful results are available. Consequently, Click on “**Reset**” followed by the “**Next**” button to run the simulator, which will then calculate the transport properties of “**TRI-MIX**” stream. Moreover, the property method to be used in analysis can be changed, as well.

Clicking on “**Analysis**” **|** “**SPROP-1**” **|** “**Results**” sheet will reveal the transport properties of “**TRI-MIX**” stream in tabulated form, as shown in Figure 3.21. Again, if no results are shown, then you have to run the simulator and arrive at successful results (i.e., a converging solution).



Generic analysis results

PRES	TEMP	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID
		RHOMX	MUMX	SIGMAMX	DMX	DMX	DMX
					ACETONE	WATER	MIBK
atm	C	gm/cc	cP	dyne/cm	sqcm/sec	sqcm/sec	sqcm/sec
1	25	0.852085	0.666628	52.8462	1.53196e-05	8.16182e-05	1.07369e-05
1	40	0.835487	0.519354	50.415	2.11996e-05	0.000100962	1.47215e-05
1	55	0.818457	0.417222	48.0112	2.82749e-05	0.00012268	1.94578e-05
1	70	0.800946	0.344065	45.6249	3.65363e-05	0.0001468	2.49239e-05
1	85	0.920847	0.331164	60.5278	3.74013e-05	0.000179086	2.62176e-05
1	100						

Figure 3.21 The calculated transport (“**TXPORT**”) properties of “**TRI-MIX**” stream, using “**NRTL**” as the property method.

3.11 ADDING A FLASH SEPARATION UNIT

From “**Model Palette**”, select the “**Separators**” tab. We will be using “**Flash3**” type separator using a rigorous vapor–liquid–liquid equilibrium (VLLE) to separate our stream for further purification. Remember that MIBK is immiscible with water; hence, this explains why we have to use VLLE. On the other hand, “**Flash2**” type is used to describe vapor–liquid equilibrium (VLE). Table 3.1 shows a brief description of different types of separators used in Aspen Plus.

TABLE 3.1 Types of Separators Used in Aspen Plus.

Model	Description	Purpose	Use
Flash2	Two-outlet flash	Determine thermal and phase conditions	Flashes, evaporators, knockout drums, single stage separator, and free water
Flash3	Three-outlet flash	Determine thermal and phase conditions	Stream splitters and bleed valves
Decanter	Liquid–liquid decanter	Determine thermal and phase conditions	Solid stream splitters and bleed valves
Sep	Multi-outlet component separator	Separate inlet stream components into any number of outlet streams	Solid stream splitters and bleed valves
Sep2	Two-outlet component separator	Separate inlet stream components into two outlet streams	Solid stream splitters and bleed valves

Select the "**Flash3**" type separator and add one to your process flowsheet. Select the "**Material**" stream from the "**Model Palette**" and add three product streams leaving the flash separator from the top side, the middle, and the bottom side (where the red arrows indicate a product is required). Rename the three added streams as shown in Figure 3.22.

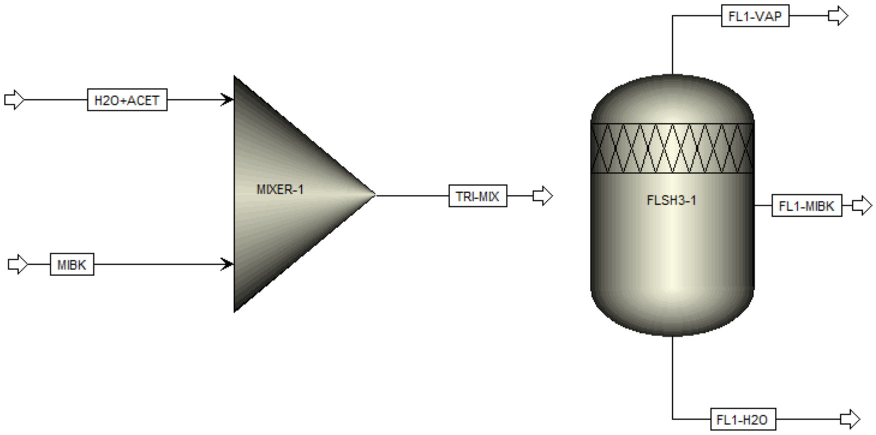


Figure 3.22 Addition of "**Flash3**"-type separator and three product streams to the flowsheet.

To hook "**TRI-MIX**" stream to the flash separator right-click on "**TRI-MIX**" stream, out of "**MIXER-1**". Select "**Reconnect**" menu → "**Reconnect Destination**" submenu and attach this stream to the inlet arrow (a short red arrow appear at the inlet) of the flash separator. The modified process flowsheet is shown in Figure 3.23.

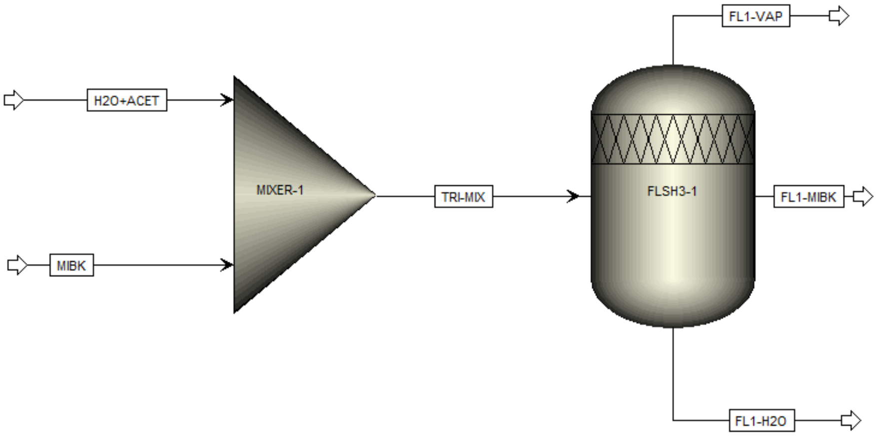
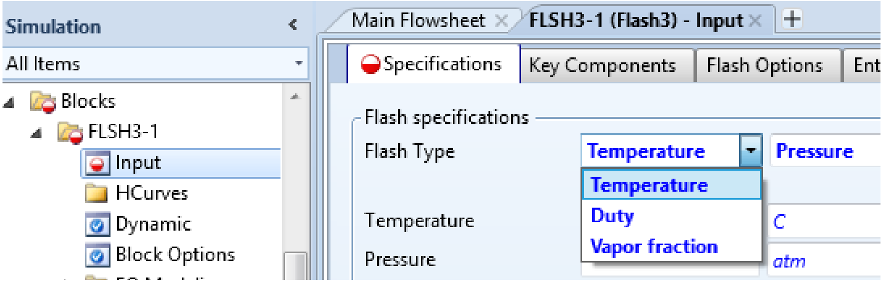


Figure 3.23 Connecting the “**MIXER-1**” to “**FLSH3-1**” via “**TRI-MIX**” stream.

3.12 THE REQUIRED INPUT FOR “FLASH3”-TYPE SEPARATOR

You will notice that the simulation status has changed to “Required Input Incomplete” because of the new unit operation that we have added to our process flowsheet. All of the user input is complete except for that in the “**Blocks**” folder. One of the interesting and facilitating features of Aspen Plus is that you only need to add input data to new feed streams and new equipment and it will complete calculations to determine the missing properties, such as composition, *P*, and *T*, of all of the new intermediate and product streams. However, there is a drawback to this feature: if the selected thermodynamic method is not appropriate for the newly added unit or block, Aspen Plus will not force the users to go back to the thermodynamic selection to confirm that the user has properly selected the thermodynamic base for his/her problem and this can lead to convergence problems and unrealistic results if the selection is not appropriately considered.

Click on the “**Next**” button and Aspen Plus will bring you to “**Blocks**” folder | “**FLSH3-1**” subfolder | “**Input**” file | “**Specifications**” form. You will notice that the user can specify two out of four variables for the flash separator, depending on a particular application. These options are shown in Figure 3.24. In our simulation, we specify the temperature and pressure of our first flash separator to be 50°C and 1.0 atm, respectively. After inputting these two values you will notice that the “**Simulation Status**”, at the bottom-left corner, changes from “Required Input Incomplete” to “Required Input Complete”.

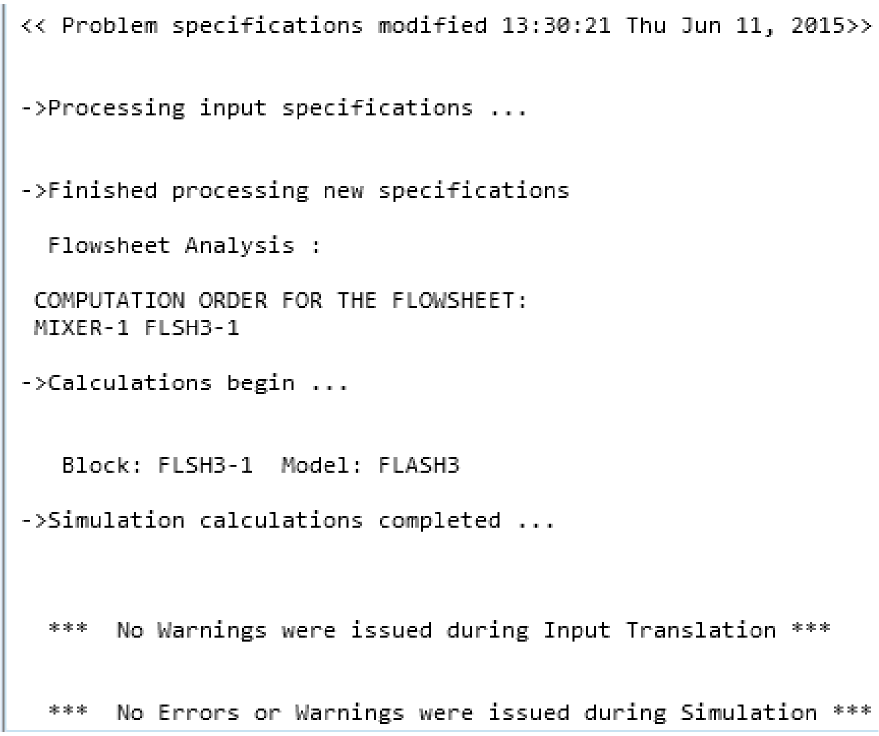


Flash specifications
Flash Type: Temperature, Pressure
Temperature: C
Pressure: atm

Figure 3.24 Two out of four variables can be specified for a flash separator: *T*, *P*, vapor fraction, and heat duty.

3.13 RUNNING THE SIMULATION AND CHECKING THE RESULTS

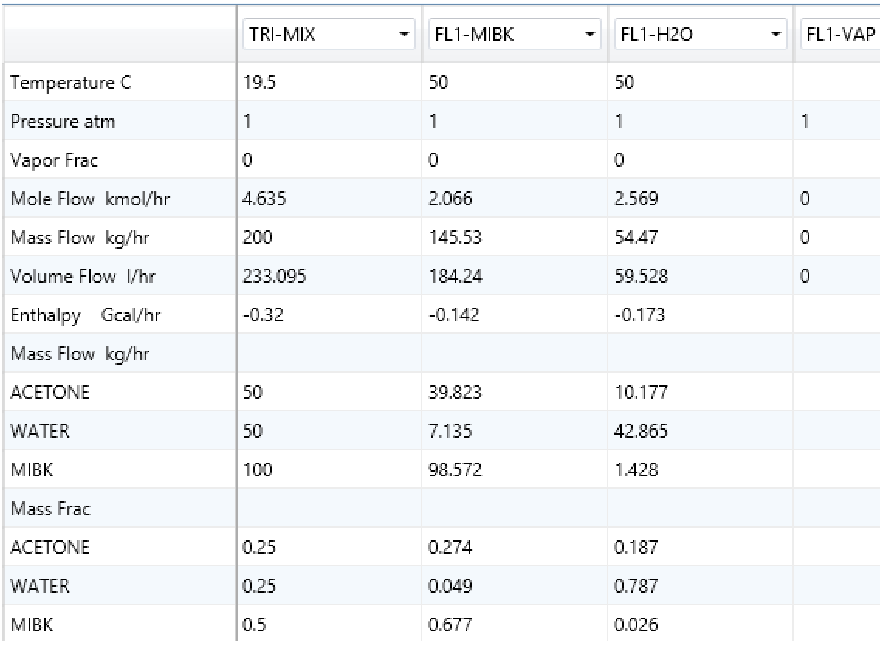
Run your simulation at this time. As pointed earlier, be sure to check your results for both convergence and run status. Figure 3.25 shows the “**Control Panel**” window that shows messages related to convergence and warnings.



```
<< Problem specifications modified 13:30:21 Thu Jun 11, 2015>>


->Processing input specifications ...


->Finished processing new specifications

  Flowsheet Analysis :

 COMPUTATION ORDER FOR THE FLOWSHEET:
 MIXER-1 FLSH3-1

->Calculations begin ...


   Block: FLSH3-1  Model: FLASH3

->Simulation calculations completed ...



  ***  No Warnings were issued during Input Translation ***


  ***  No Errors or Warnings were issued during Simulation ***
```

Figure 3.25 The “**Control Panel**” shows messages related to convergence and warnings.

Figure 3.26 shows the composition of the “**Flash3**”-type separator outlet streams. Notice that “**FL1-H2O**” stream is higher in water but it did not hit the target value; that is, the mass fraction should be at least 0.95 for H_2O. In Chapter 4, we discuss about how to tackle this deficiency.



	TRI-MIX	FL1-MIBK	FL1-H2O	FL1-VAP
Temperature C	19.5	50	50	
Pressure atm	1	1	1	1
Vapor Frac	0	0	0	
Mole Flow kmol/hr	4.635	2.066	2.569	0
Mass Flow kg/hr	200	145.53	54.47	0
Volume Flow l/hr	233.095	184.24	59.528	0
Enthalpy Gcal/hr	-0.32	-0.142	-0.173	
Mass Flow kg/hr				
ACETONE	50	39.823	10.177	
WATER	50	7.135	42.865	
MIBK	100	98.572	1.428	
Mass Frac				
ACETONE	0.25	0.274	0.187	
WATER	0.25	0.049	0.787	
MIBK	0.5	0.677	0.026	

Figure 3.26 The composition of the first flash separator outlet steams. Notice that “**FL1-H2O**” stream did not hit the target value of 0.95 mass fraction of water.

HOMEWORK/CLASSWORK 3.1 (OUTPUT OF INPUT DATA AND RESULTS)

Continue working on Homework/Classwork 2.1 and complete the following tasks:

1. Add a stream table showing flow and operating conditions for all streams.
2. Add stream conditions (*P* and *T tags*) for all streams. You may need to reinitialize and rerun the simulation to have the tags appear on each stream. Show a snapshot for the process flowsheet.
3. As shown in Figure 3.16, define the “**Page Break Preview**” area and print the framed image to a PDF file.
4. Create an input file for the given process, using the “**Input File**” button.
5. Generate a report file that includes the mixer block and the input and output streams, using the “**Report File**” button.

HOMEWORK/CLASSWORK 3.2 (OUTPUT OF INPUT DATA AND RESULTS)

Continue working on Homework/Classwork 2.2 and complete the following tasks:

1. Add a stream table showing flow and operating conditions for all streams.
2. Add stream conditions (*P* and *T tags*) for all streams. You may need to reinitialize and rerun the simulation to have the tags appear on each stream. Show a snapshot for the process flowsheet.
3. As shown in Figure 3.16, define the "**Page Break Preview**" area and print the framed image to a PDF file.
4. Create an input file for the given process, using the "**Input File**" button.
5. Generate a report file that includes the mixer block and the input and output streams, using the "**Report File**" button.

HOMEWORK/CLASSWORK 3.3 (OUTPUT OF INPUT DATA AND RESULTS)

Continue working on Homework/Classwork 2.3 and complete the following tasks:

1. Add a stream table showing flow and operating conditions for all streams.
2. Add stream conditions (*P* and *T tags*) for all streams. You may need to reinitialize and rerun the simulation to have the tags appear on each stream. Show a snapshot for the process flowsheet.
3. As shown in Figure 3.16, define the "**Page Break Preview**" area and print the framed image to a PDF file.
4. Create an input file for the given process, using the "**Input File**" button.
5. Generate a report file that includes the mixer block and the input and output streams, using the "**Report File**" button.

HOMEWORK/CLASSWORK 3.4 (THE PARTITION COEFFICIENT OF A SOLUTE)

One of the useful features of Aspen Plus "**Flash3**"-type separator model is to use it in predicting the partition coefficient of a solute between 1-octanol and water phase. The octanol–water partition coefficient is a physical property that is extensively used to describe a chemical's lipophilic or hydrophobic properties. It is the ratio of a chemical's concentration in the octanol phase to its concentration in the aqueous phase of a two-phase system at equilibrium. Since measured values range from less than 10^{-4} to greater than 10^{+8} (at least 12 orders of magnitude), the logarithm (Log *P*) is commonly used to characterize its value. Log *P* (or, Log K_{ow}) is a valuable parameter in numerous quantitative structure–activity relationships (QSARs) that have been developed for the pharmaceutical, environmental, biochemical, and toxicological sciences. Let us demonstrate the application of this concept via the following process flowsheet. We have three streams: "H_2O" with a flow rate of 45 kmol/h of pure water at 25°C and 1 atm; "**SOLUTE**" with a flow rate of 10 kmol/h of pure <u>solute</u> at 25°C and 1 atm; and "**OCTANOL**" with a flow rate of 45 kmol/h of pure 1-octanol at 25°C and 1 atm. The <u>solute</u> will be varied from one to another case study. The three streams enter the mixer to form “**TRI-MIX**” product stream, which will be sent, as a feed, to the “**Flash3**” type separator. The “**Flash3**” type separator will basically split the feed into two immiscible liquid phases: the organic solvent (**C8OHFAZE**) and aqueous (**H2OPHASE**). Figure 3.27 shows this process flowsheet. The solute will assume one of the following alcohol compounds: methanol, ethanol, 1-propanol, 1-butanol, 1-pentanol, and 1-hexanol.

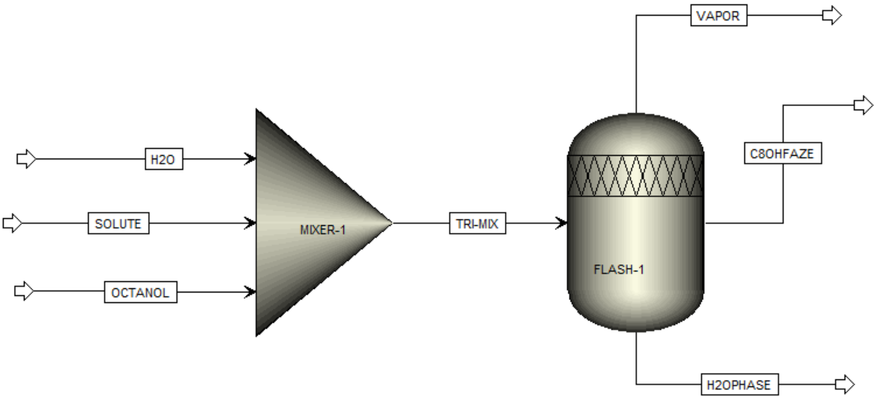
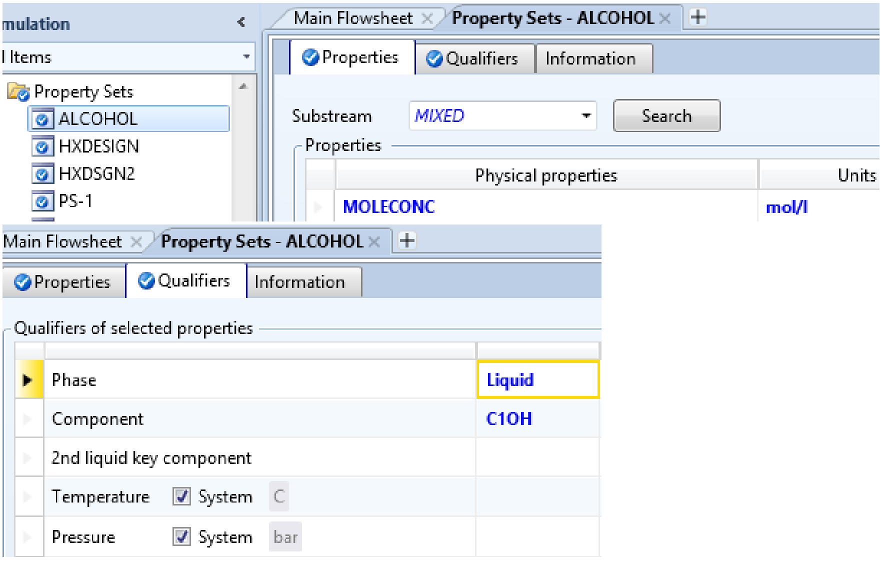


Figure 3.27 A simple process flowsheet for predicting the partition coefficient of a solute between octanol and water phase.

Using “*Chemicals with Metric Units*” template, create an Aspen Plus project. Under “**Properties**” environment, add the following components: methanol, ethanol, 1-propanol, 1-butanol, 1-pentanol, 1-hexanol, 1-octanol, and water. The default property method is “**NRTL**”. Assure that the option: “Estimate missing parameters by UNIFAC” is selected under “**Methods**” | “**Parameters**” | “**Binary Interaction**” | “**NRTL-1**” sheet. Click on “**Reset**” followed by the “**Next**” button to run the simulation under the “**Properties**” environment and watch out messages of “**Control Panel**” for any error or serious warning.

Switch to “**Simulation**” environment and under “**Property Sets**” folder, click on “**New …** ” button to create a new property set named “**ALCOHOL**” and its attributes are defined as in Figure 3.28.



Substream: MIXED

Properties

Physical properties	Units
MOLECONC	mol/l

Qualifiers of selected properties

Phase	Liquid
Component	C1OH
2nd liquid key component	
Temperature ☑ System C	
Pressure ☑ System bar	

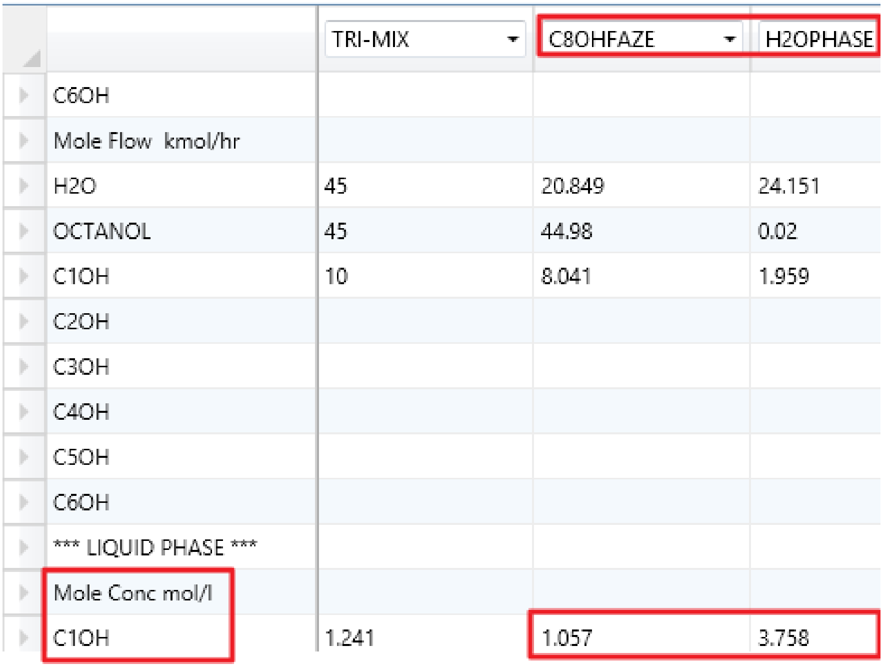
Figure 3.28 The property set: "**ALCOHOL**" is defined as "**MOLECONC**" (molar concentration) of "**C1OH**" (methanol) component in liquid phase.

After defining "**ALCOHOL**" property set, go to "**Setup**" | "**Reports Option**" | "**Stream**" tab and click on "**Property Sets**" button to select "**ALCOHOL**".

Then, complete the following tasks.

1. Add one "**TRIANGLE**" type mixer from "**Model Palette**" under "**Mixers/Splitters**" tab and rename it "**MIXER-1**".
2. Add three feed streams: "**H2O**", "**SOLUTE**", and "**OCTANOL**".
3. Add one product stream: "**TRI-MIX**".
4. For "**H2O**" stream, enter $T = 25°\text{C}$, $P = 1$ atm, and flow rate = 45 kmol/h pure water.
5. For "**OCTANOL**" stream, enter $T = 25°\text{C}$, $P = 1$ atm, and flow rate = 45 kmol/h pure octanol.
6. For "**SOLUTE**" stream, enter $T = 25°\text{C}$, $P = 1$ atm, and flow rate = 10 kmol/h pure methanol.
7. Enter "**MIXER-1**" temperature as 25°C.
8. Click on "**Reset**" followed by "**Next**" button to run the simulation.
9. In the "**Control Panel**", see whether there is any serious warning or error that requires an action by the user.
10. Save your work.
11. Once you manage to get successful and reasonable results, add the "**Flash3**"-type separator from "**Model Palette**" under "**Separators**" tab and name it as "**FLASH1**". Reconnect "**TRI-MIX**" stream destination as the feed to "**FLASH1**" block.
12. Add the three required output streams: "**VAPOR**", "**C8OHFAZE**", and "**H2OPHASE**".
13. Enter "**FLSH3-1**" temperature and pressure as 25°C and 1.0 atm.

14. Click on “**Reset**” followed by “**Next**” button to run the simulation.
15. In the “**Control Panel**”, see whether there is any serious warning or error that requires an action by the user.
16. Save your work.
17. Once you manage to get successful and reasonable results, go to “**Results Summary**” | “**Streams**” sheet and look at the alcohol solute (in this case **C1OH**) molar concentration in the two output liquid streams: “**C8OHFAZE**” and “**H2OPHASE**”, as shown in Figure 3.29.



	TRI-MIX	C8OHFAZE	H2OPHASE
C6OH			
Mole Flow kmol/hr			
H2O	45	20.849	24.151
OCTANOL	45	44.98	0.02
C1OH	10	8.041	1.959
C2OH			
C3OH			
C4OH			
C5OH			
C6OH			
*** LIQUID PHASE ***			
Mole Conc mol/l			
C1OH	1.241	1.057	3.758

Figure 3.29 The molar concentration of methanol in the two immiscible liquid phases: octanol and water.

18. Calculate $\text{Log}_{10}\,K_{ow} = \text{Log}_{10}\,([\text{C1OH}_{\text{octanol}}]/[\text{C1OH}_{\text{water}}]) = \text{Log}_{10}\,[(1.057/3.758)]$.
19. Change where necessary from methanol to the second member of alcohol solute family, that is, ethanol. In particular, the definition of the property set: “**ALCOHOL**” and the type of flow rate of “**SOLUTE**”.
20. Click on “**Reset**” followed by “**Next**” button to run the simulation.
21. In the “**Control Panel**”, see whether there is any serious warning or error that requires an action by the user.
22. Once you manage to get successful and reasonable results, go to “**Results Summary**” | “**Streams**” sheet and look at the alcohol solute (in this case **C2OH**) molar concentration in the two output liquid streams: “**C8OHFAZE**” and “**H2OPHASE**”.
23. Calculate $\text{Log}_{10}\,K_{ow} = \text{Log}_{10}\,([\text{C2OH}_{\text{octanol}}]/[\text{C2OH}_{\text{water}}])$

24. Repeat steps: 19 through 23 for the rest of solute alcohol family members.
25. What does a negative value of $\mathrm{Log}_{10}\ K_{\mathrm{ow}}$ mean? What does a positive value mean? What does a zero value mean?
26. You may add as many as you wish from the list of components found in Aspen Plus databanks, in the form of groups of homologous series. For example, alkanes, alkenes, aldehydes, ketones, ethers, peroxides, carboxylic acids, and aromatics can be sorted in ascending or descending manner in terms of aqueous solubility. Doing so will give you a better insight into the chemical's lipophilic (or hydrophobic) nature in terms of preferential solubilization in organic, aqueous, or both phases.

4

FLASH SEPARATION AND DISTILLATION COLUMNS

4.1 PROBLEM DESCRIPTION

A mixture containing 50.0 wt% acetone and 50.0 wt% water is to be separated into two streams: one enriched in acetone and another in water. The separation process consists of extraction of the acetone from water into methyl isobutyl ketone (MIBK), which dissolves acetone but is nearly immiscible with water. The overall goal of this problem is to separate the feed stream into two streams that have greater than 95 wt% purity of water and acetone.

In this episode, we resume from where we stopped in Chapter 3 by adding both a mixer and flash separation unit to our existing product line. The flash separation unit can be used to represent a number of real-life pieces of equipment including feed surge drums in refining processes and settlers as is the case here. A flash separation is a one-stage separation process and for our problem we plan to split our mixture into two streams: one is mainly aqueous and another mainly organic phase. Acetone is partitioned in between based on its relative solubility in both phases. Finally, a distillation tower is installed to end up with almost a pure stream both from top and bottom. Different built-in distillation column models are explained.

4.2 ADDING A SECOND MIXER AND FLASH

Open the previous chapter's simulation project. Add a second mixer and a second flash separation unit to the process flowsheet and properly rename them. Connect the stream that is primarily water and acetone (the stream off the bottom of the first flash separator) to the new mixer and add in a new feed stream of MIBK that also feeds into this new mixer. Next, connect the product from the second mixer to the new "**Flash3**" type separation unit and add the required product streams. Your process flowsheet should be similar to that shown in Figure 4.1.

Aspen Plus®: Chemical Engineering Applications, First Edition. Kamal I.M. Al-Malah.

Companion Website: www.wiley.com/go/Al-Malah/AspenPlusApplications

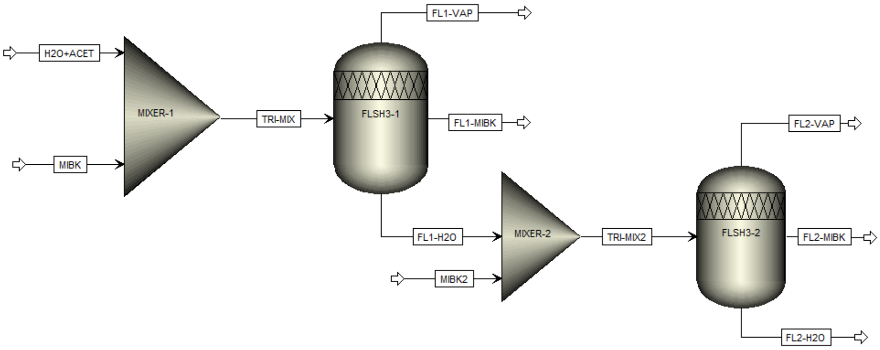
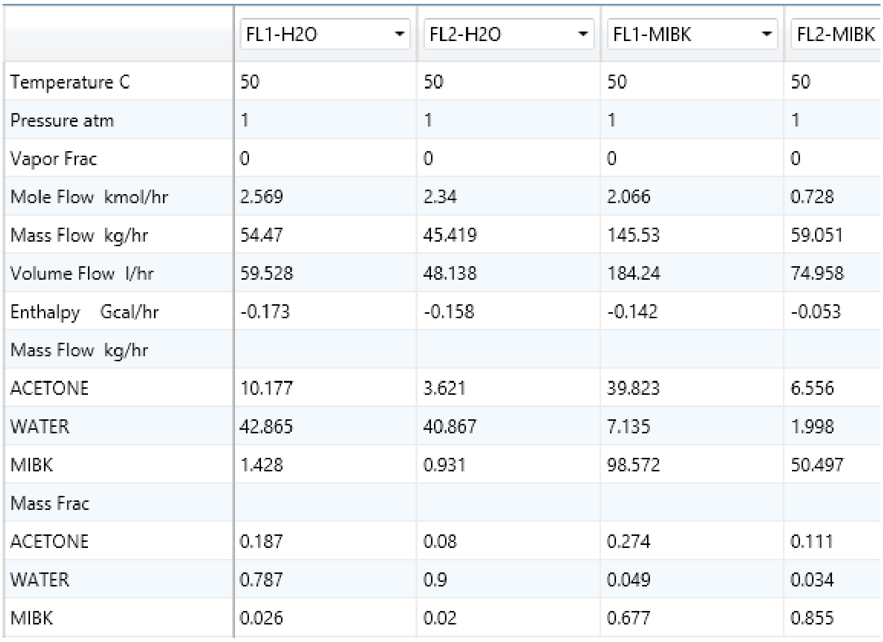


Figure 4.1 The addition of a second mixer and "**Flash3**" type separator.

Click "**Reset**" followed by "**Next**" button to update the inputs for the new additions to the process flowsheet. The new feed stream **MIBK2** should have a flow rate of 50 kg/h of pure MIBK at a temperature of 25°C and a pressure of 1.0 atm. The second mixer requires to specify that pressure drop is zero (i.e., assign a value of zero for the pressure in the input form) and the second flash separation unit should be operated at 50°C and 1.0 atm. Notice that "**Simulation Status**", at the bottom-left corner, changes from "Required Input Incomplete" to "Required Input Complete".

Run the simulation at this point and check "**Control Panel**" for any warning or error. You should get results similar to those seen in the stream results shown in Figure 4.2. You



	FL1-H2O	FL2-H2O	FL1-MIBK	FL2-MIBK
Temperature C	50	50	50	50
Pressure atm	1	1	1	1
Vapor Frac	0	0	0	0
Mole Flow kmol/hr	2.569	2.34	2.066	0.728
Mass Flow kg/hr	54.47	45.419	145.53	59.051
Volume Flow l/hr	59.528	48.138	184.24	74.958
Enthalpy Gcal/hr	-0.173	-0.158	-0.142	-0.053
Mass Flow kg/hr				
ACETONE	10.177	3.621	39.823	6.556
WATER	42.865	40.867	7.135	1.998
MIBK	1.428	0.931	98.572	50.497
Mass Frac				
ACETONE	0.187	0.08	0.274	0.111
WATER	0.787	0.9	0.049	0.034
MIBK	0.026	0.02	0.677	0.855

Figure 4.2 The addition of mixer and flash separator results in a more purification for water and MIBK streams. The water mass fraction increased from 0.787 for "**FL1-H2O**" to 0.90 for "**FL2-H2O**".

will notice that we did not get yet the desired 95% purity of the water stream, which is specified in the problem statement. While we can simply rerun the simulation more than once such that a feed rate of "**MIBK2**" will give us this desired purity, we will instead instruct Aspen Plus® to complete the iterations for us before reporting the results. You may notice that the stream table shown in Figure 4.2 does not include all the streams. Remember that this is discussed in Section 3.4.

NOTE #0: *The simulation and design specification results in this chapter will be subject to how we let Aspen Plus calculate binary interaction parameters among the three components. So, be sure that, under "**Methods**" | "**Parameters**" | "**Binary Interaction**" | "**NRTL-1**" sheet, the source for each of the three columns is selected as "APV88 VLE-IG" not "R-PCES". See Chapter 3 on how to set the source as "APV88 VLE-IG". Keep in mindthat this does not advocate using "APV88 VLE-IG" as the source for binary data. This only serves the calibration of process of learning by the user. The validity of simulation results are always governed by experimental data for a given chemical process/components. We have elaborated on this critical issue in the first two chapters.*

4.3 DESIGN SPECIFICATIONS STUDY

One of the powerful features of Aspen Plus is the ability to examine how a given independent variable will affect another dependent variable. Select the "**Flowsheeting Options**" folder in the "**Navigation**" pane and open up the "**Design Specs**" subfolder. At the bottom of the screen, select the "**New**" button and choose a name for this design specification. When you have done this, the "**Define**" tab form should look like that seen in Figure 4.3.

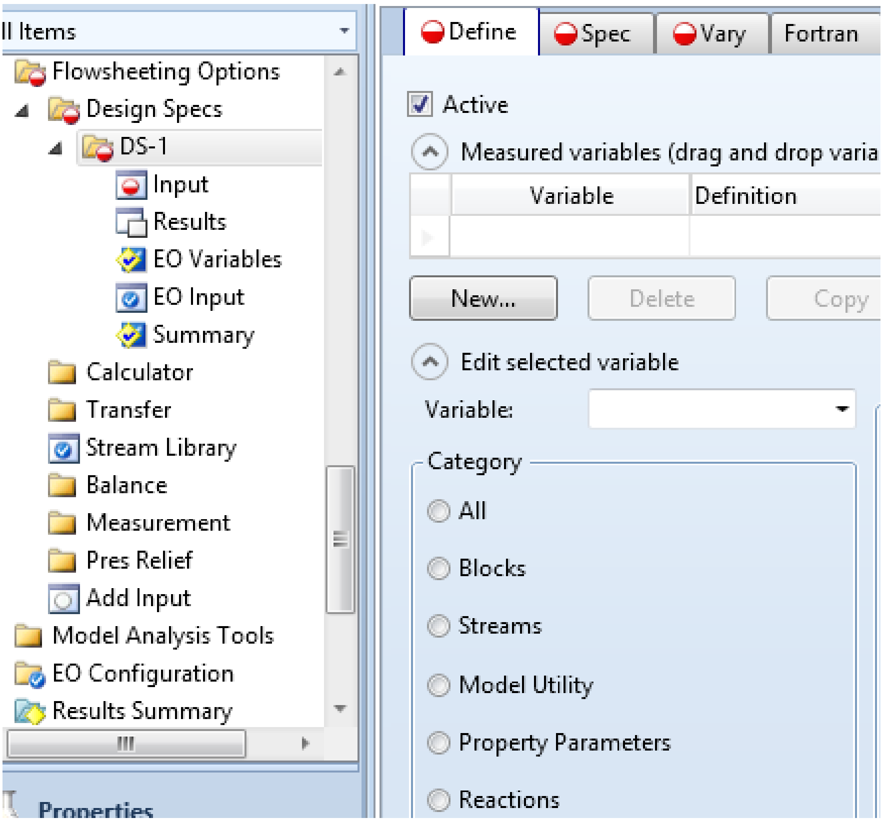
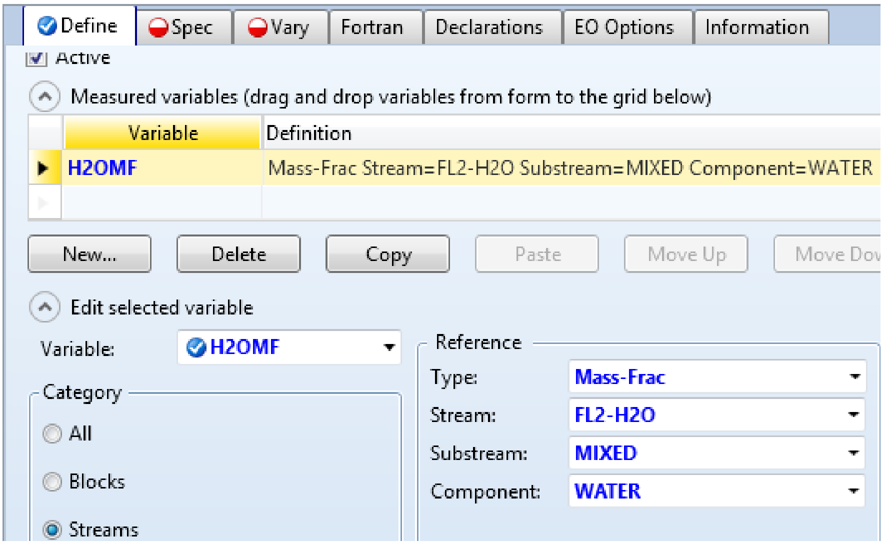


Figure 4.3 The first "**Define**" tab form of the "**Design Specs**" subfolder, under "**Flowsheeting Options**" folder, where one can define the dependent and independent variable.

You will notice that there are three areas where we must input data in order for the required input to be complete. These are "**Define**", "**Spec**", and "**Vary**" tab.

In the "**Define**" tab window, the user must set the dependent variable that he/she is interested in. For our case, this is the purity of the water product stream (or mass fraction of water). Either you click on "**New** … " button and name the new variable as "**H2OMF**" (i.e., water mass fraction) or directly key in the variable name under "**Variable**" column, as shown in Figure 4.4. Moreover, we need to specify that our variable is the mass fraction of water in the water-rich product stream "**FL2-H2O**". Under "**Category**", select "*Streams*". From the "**Type**" drop-down menu, select "*Mass-Frac*". In the "**Stream**" box, select your water product stream (*FL2-H2O*) and under the "**Component**" box, select "*WATER*". Figure 4.4 shows the filled-in "**Define**" tab window.

We are now done with the required input of the "**Define**" tab window and can move on to the "**Spec**" tab window. You will notice that we have three values that we must input into this form. The first, "**Spec**", is the dependent variable that we want to set a target value for.



☑ Active

Measured variables (drag and drop variables from form to the grid below)

Variable	Definition
H2OMF	Mass-Frac Stream=FL2-H2O Substream=MIXED Component=WATER

Edit selected variable

Variable: H2OMF

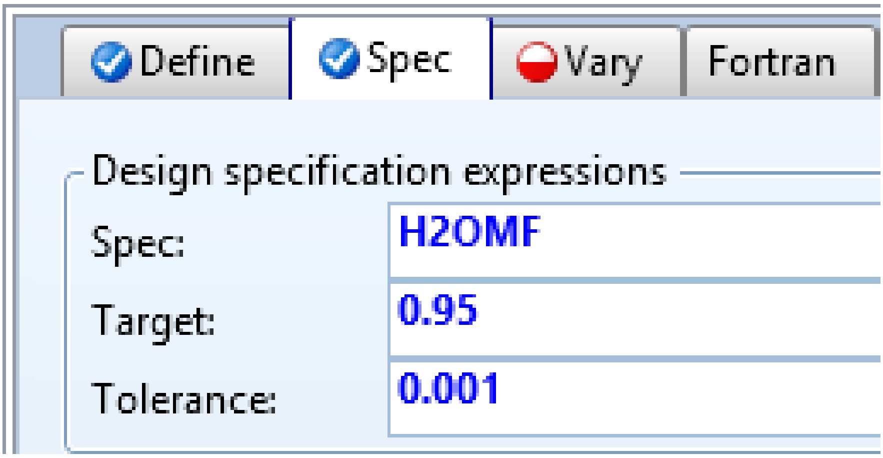
Category
○ All
○ Blocks
● Streams

Reference
Type: Mass-Frac
Stream: FL2-H2O
Substream: MIXED
Component: WATER

Figure 4.4 Defining the "**Design Spec**" variable name as "**H2OMF**", which accounts for mass fraction of water in "**FL2-H2O**" stream.

This is the variable that we just defined in the "**Define**" tab window as "**H2OMF**". Type this into this box. "**Target**" is the numeric value that we would like our dependent variable to be equal to at the completion of the calculation iterations. Our target value is 95% or 0.95.

Finally, "**Tolerance**" entry accounts for the margin of acceptance. For our purpose, a tolerance of 0.1% is acceptable (this means 0.95 ± 0.001 or [0.949–0.951] target value). After inputting those three parameters, the "**Spec**" tab window should be as shown in Figure 4.5.

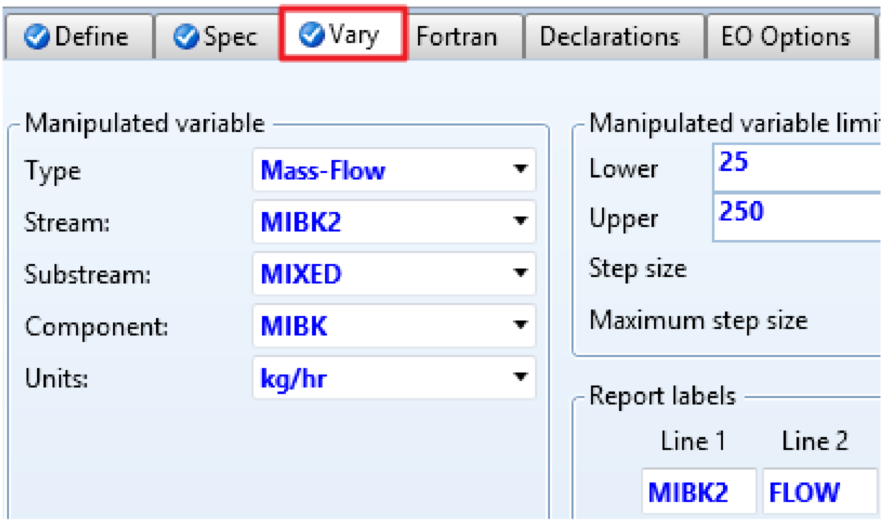


Design specification expressions
Spec: H2OMF
Target: 0.95
Tolerance: 0.001

Figure 4.5 Entering parameter values appearing in "**Spec**" tab window of the design spec: **DS-1** for **H2OMF** variable. The "**Spec**" value is allowed to fluctuate around 0.95 by a magnitude of 0.001.

To complete the input for our sensitivity analysis, we must input the variable that is to be varied or manipulated. This is done under the "**Vary**" tab. In this simulation, we are varying the flow rate of MIBK2 feed stream. Under the "**Vary**" tab, select "*Mass-Flow*" under the "**Type**" list. Under "**Stream**", select the stream that corresponds to your second feed stream of MIBK (i.e., *MIBK2*). Next, select "*MIBK*" from the "**Component**" list. The values placed into the "**Manipulated variable limits**" boxes indicate the range that Aspen Plus can use during its iteration calculations. One thing to note is that the original input value under the stream inputs must fall within the range that is input here. Remember our original input is 50 kg/h. For this case, input a variable range from 25 to 250 kg/h.

The other blocks that can be filled on this screen relate to the step size that Aspen Plus takes during its iteration calculations. It is not necessary for the user to input values into these blocks, and we will use the default Aspen Plus values. At this point, the "**Vary**" tab window should look like that seen in Figure 4.6.



Type: Mass-Flow
Stream: MIBK2
Substream: MIXED
Component: MIBK
Units: kg/hr

Lower: 25
Upper: 250
Step size
Maximum step size

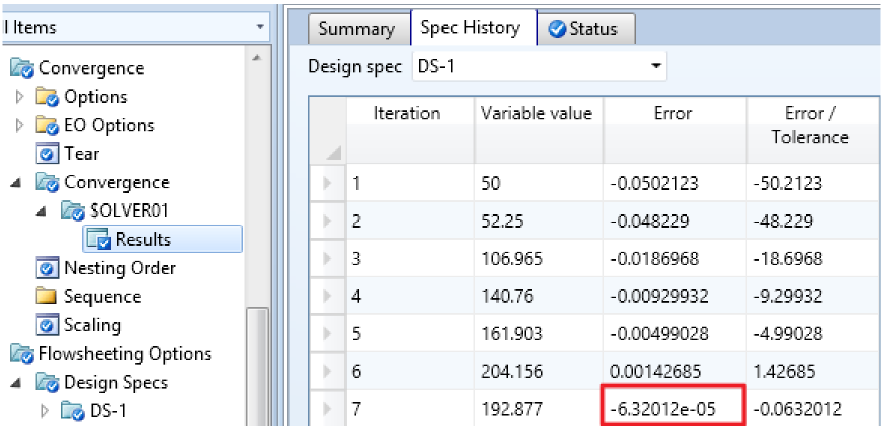
MIBK2 FLOW

Figure 4.6 Defining parameters of the manipulated variable appearing in "**Vary**" tab window of the design spec: "**DS-1**".

We are now ready to run the simulation again and check its convergence based on our input design specifications. Click on the "**Run**" button at this time and when the computer has finished its calculations, open up "**Control Panel**".

"**Control Panel**" indicates how many iterations Aspen Plus made during its determination of the flow rate that met our design specification (i.e., "**DS-1**"). If completed correctly, your simulation should contain neither warnings nor errors in this window.

Let us get information regarding the convergence of a simulation. In "**Navigation**" pane, go to "**Convergence**" | "**Convergence**" | "**Solver01**" | "**Results**" | "**Spec History**" tab sheet, as shown in Figure 4.7. In this sheet, one can see each of the values attempted by Aspen Plus during its iteration cycle.



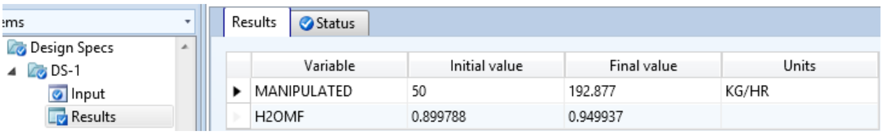
Design spec DS-1

Iteration	Variable value	Error	Error / Tolerance
1	50	-0.0502123	-50.2123
2	52.25	-0.048229	-48.229
3	106.965	-0.0186968	-18.6968
4	140.76	-0.00929932	-9.29932
5	161.903	-0.00499028	-4.99028
6	204.156	0.00142685	1.42685
7	192.877	-6.32012e-05	-0.0632012

Figure 4.7 The convergence "**Spec History**" tab sheet where it shows the number of iterations needed to converge to the final solution within the prescribed accuracy given by the "**Tolerance**" and "**Target**" value. The "**Error / Tolerance**" column indicates the division of "**Error**" by "**Tolerance**" value.

You will also notice that Aspen Plus simulator executed seven iterations to determine **MIBK2** flow rate such that the absolute value of error is less than the tolerance value (i.e., $0.0000632 < 0.001$) that is specified in "**Spec**" tab sheet. Moreover, the final value of the manipulated variable **MIBK2** flow rate is 192.877 kg/h of pure MIBK. The "**Error**" column indicates how far the final dependent variable (**H2OMF**) is from the specified value (i.e., "**Target**" in Figure 4.5) and the "**Error / Tolerance**" column indicates the division of "**Error**" value by "**Tolerance**" (0.001) value. An absolute large value in this column means that the simulation does not converge while an absolute value near 0 indicates an excellent convergence.

Figure 4.8 shows "**Design Specs**" | "**DS-1**" | "**Results**" sheet, which shows the value of the final manipulated variable ("**MIBK2**" mass flow rate) and the mass fraction of water in the outlet stream as obtained by Aspen Plus simulator after seven iterations.



Variable	Initial value	Final value	Units
MANIPULATED	50	192.877	KG/HR
H2OMF	0.899788	0.949937	

Figure 4.8 At the initial value of "**MIBK2**" flow rate, "**H2OMF**" is 0.899788 and it jumped to 0.949937 at the final value of "**MIBK2**" flow rate, fulfilling the design specifications (i.e., the target and tolerance value) imposed by the user.

EXERCISE 4.1 (DESIGN SPEC)

What flow rate of "**MIBK2**" is necessary to achieve 97% purity of the water stream? Show your results with the stream table from your simulation.

Hint: Modify your existing design specifications by changing both the target spec and the range for the independent variable.

NOTE #1: *For more details on how to utilize the "**Calculator**" option under "**Flowsheeting Options**", see Section 18.10.*

4.4 ASPEN PLUS DISTILLATION COLUMN OPTIONS

Aspen Plus has multiple unit operation options for completing distillation problems, based on the complexity of the user's application. Click on the "**Separators**" tab in the "**Model Palette**". In this tab, you will see one of the options that users can choose for completing a distillation process, "**Sep2**". This unit operation can be used to model separation processes with only two possible outlet streams. This process can be used to simulate distillations, but it does not provide the level of detail that is available when using some of the other distillation options. "**Sep2**" model does not include, for example, the number of trays and the reflux ratio. For this reason, such an option is not recommended except as an oversimplified approach for testing/starting purposes.

Now select the "**Columns**" tab in the "**Model Palette**". You will notice a number of distillation column models, as shown in Figure 4.9. Here, we will use the first three general distillation choices: "**DSTWU**", "**Distl**", and "**RadFrac**". The fourth column (i.e., extraction unit operation) is covered in detail in Chapter 5. The last five unit operation columns complete much more rigorous calculations than we require for applications presented in this textbook and they are intended for use in more difficult separations and specific applications. Briefly, "**MultiFrac**" option is a rigorous approach used for complex columns such as crude units, "**SCFrac**" option is a shortcut approach for complex columns such as crude units and vacuum towers, "**PetroFrac**" option is a rigorous approach for petroleum refining applications such as preflash towers, "**ConSep**" option performs feasibility and design calculations for distillation columns, and finally "**BatchSep**" option is used for a batch separation.

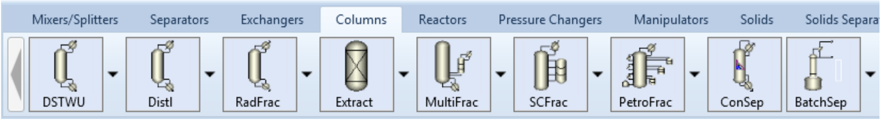


Figure 4.9 Different distillation column models can be found under "**Columns**" tab in "**Model Palette**".

The "**DSTWU**" unit operation is designed for a single feed, two product distillation process. This column performs calculations using *Gilliland's, Winn's, and Underwood's method* for calculation of stages and reflux ratios. Such a method assumes a *constant molar overflow and constant relative volatilities*.

For a specified product recovery (both light and heavy), the "**DSTWU**" column first estimates the minimum number of stages and the minimum reflux ratio, and then it calculates either the required reflux ratio or the required number of theoretical stages based on the user's input. During these calculations, Aspen Plus will also estimate the optimum feed stage location and the condenser and reboiler duties. Finally, when the calculations are complete, Aspen Plus can produce tables and plots for the reflux ratio and stage profile.

> **NOTE #2:** *If you plan to work with more complicated simulations later, you can use this column to get a quick idea about a process, and use its results as inputs to a more detailed simulation. Aspen Plus makes it easy for the user to start simple in approach and become more complicated as the user moves from "**DSTWU**" to "**RadFrac**" column. So, you may start with "**DSTWU**" column, get more intermediate results, utilize such results in the second or third option and get more and more results. For advanced users in distillation columns, they may attempt to directly use "**RadFrac**" option without having to try the first two options.*

On the other hand, the "**Distl**" unit operation is also designed for a single-feed, two-product distillation process. However, this column calculates product compositions based on the Edmister approach. It is a shortcut multicomponent distillation rating model used to separate an inlet stream into two product streams. The user must specify

- number of theoretical stages
- reflux ratio
- overhead product rate.

"**Distl**" model estimates the condenser and reboiler duties. The user can specify a partial or a total condenser. Again, the calculations are based on the assumptions of constant molar overflow and constant relative volatilities. Thus, "**Dist1**" column option requires more input parameters than "**DSTWU**" case to be plugged in by the user.

The final general distillation unit operation is the "**RadFrac**" column. This distillation unit involves much more rigorous calculations than the first two methods and can be used to simulate absorption, stripping, extractive distillation, and azeotropic distillation for solids, liquids, and gases. This column can also be used for highly nonideal liquid solutions or processes with an ongoing chemical reaction. Finally, the "**RadFrac**" column can have multiple feed and product streams (including pump-around streams) and it can simulate columns with trays, random packing, or structured packing. As one can see, this "**RadFrac**" column option is much more complicated than the previous two methods, and is covered in depth throughout this chapter.

4.5 "DSTWU" DISTILLATION COLUMN

The first update we will make to our simulation is the addition of a third mixer. Add the third mixer such that it combines the two streams of acetone and MIBK mixture from the two flash separators "**FLSH3-1**" and "**FLSH3-2**". This can be seen in the process flowsheet window shown in Figure 4.10.

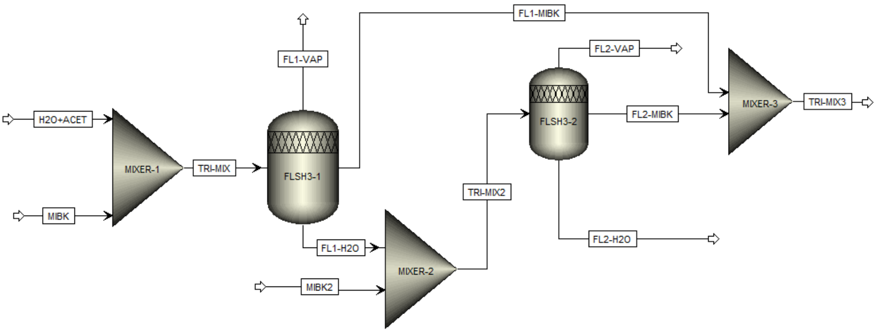


Figure 4.10 The addition of a third mixer where it combines the two MIBK-based product streams from the two flash separators "**FLSH3-1**" and '**FLSH3-2**".

At this point, save your current Aspen Plus simulation project under three names. We will use the first version to complete a distillation with the "**DSTWU**" distillation column, the second with "**Distl**" column, and the third with "**RadFrac**" column. It is recommended that you save them with names that reflect the distillation method that is being used.

Now select the "**Columns**" tab in the "**Model Palette**" and place a "**DSTWU**" column into the process flowsheet window. Connect the product stream from the third mixer to the "**DSTWU**" column and add in two product streams where Aspen Plus indicates that they are required. We will also be adding in a third product stream off the condenser, to account for any free water product that can be separated from within the condenser. Rename the streams and column as you see fit. At this point, your flowsheet should look similar to that in Figure 4.11.

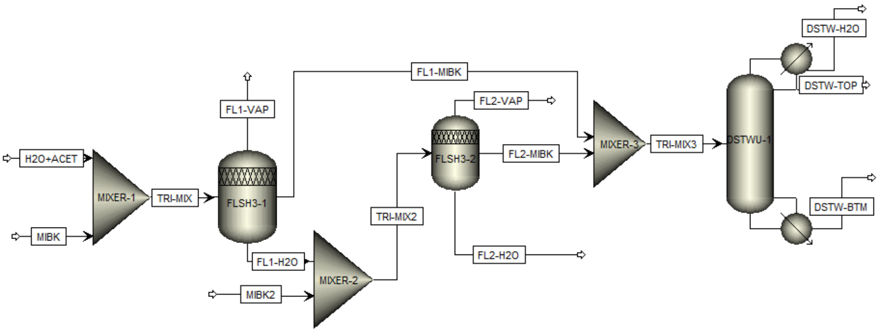
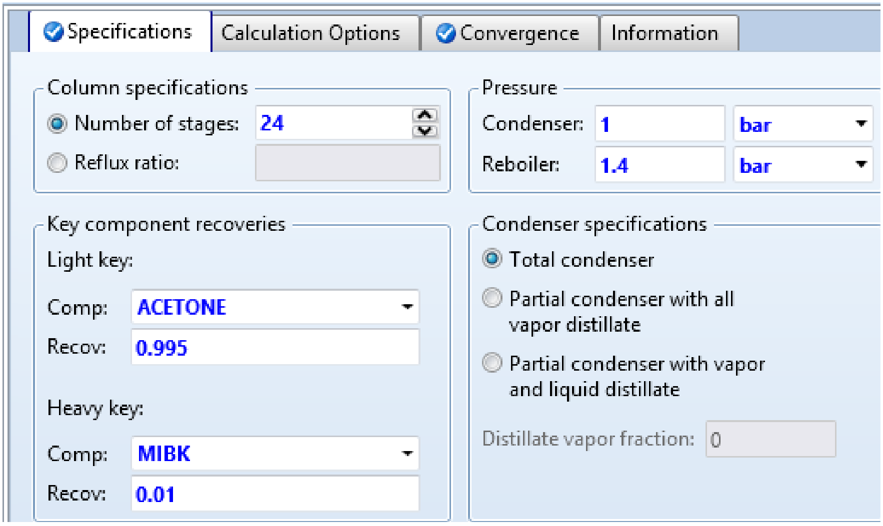


Figure 4.11 The addition of "**DSTWU**" distillation column.

Click on "**Reset**" followed by "**Next**" button. You will notice that we are only required to update our data input in the "**Blocks**" tab. Under the appropriate option for the third mixer, input 0 for pressure to indicate that the pressure drop is zero across the mixing unit. Then, open up the appropriate option for the distillation column.

For this simulation, we will be inputting the number of stages, the key component recoveries, and the tower pressures. The condenser and reboiler pressures are 1.0 and 1.4 bar, respectively. We will start with the number of stages equal to 24 and vary the number until the required degree of purity is achieved for acetone product stream. The component recovery values that are input are equal to the amount of each component in the distillate divided by the amount of each component in the feed. For this reason, a recovery of 99.5% for acetone and 1% for the MIBK are applicable if our distillation tower is operating well. The completed input screen is shown in Figure 4.12.



Column specifications

● Number of stages: 24

○ Reflux ratio:

Pressure

Condenser: 1 bar

Reboiler: 1.4 bar

Key component recoveries

Light key:

Comp: ACETONE

Recov: 0.995

Heavy key:

Comp: MIBK

Recov: 0.01

Condenser specifications

● Total condenser

○ Partial condenser with all vapor distillate

○ Partial condenser with vapor and liquid distillate

Distillate vapor fraction: 0

Figure 4.12 Inputting the number of stages, the key component recoveries, and the tower pressures.

For our benefit, we would also like Aspen Plus to produce a table of reflux ratio versus the total number of calculated theoretical trays. This can be easily done by selecting the "**Calculation Options**" tab (second from left) at the top of the "**DSTWU**" input window. Check the box corresponding to this calculation.

At this point, our simulation is complete. *Reset* and *run* your simulation.

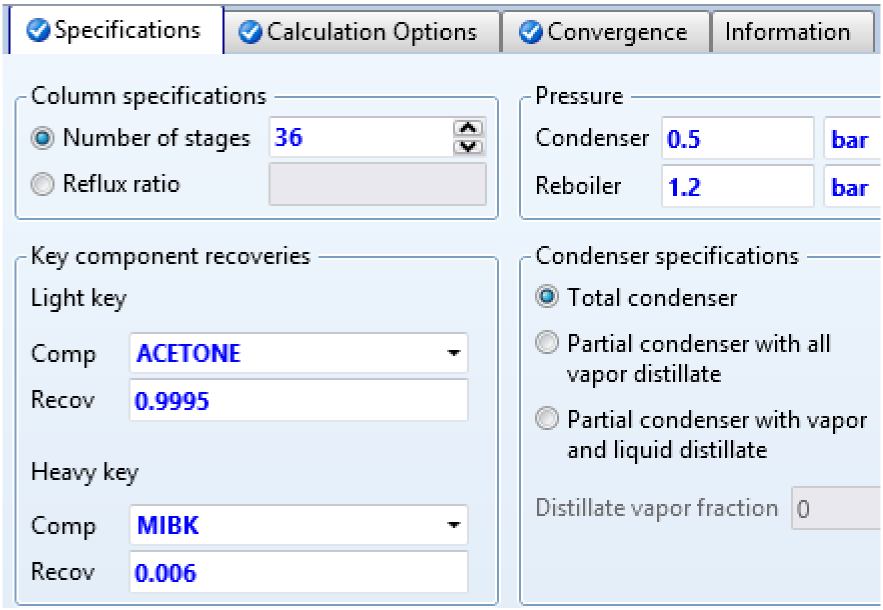
NOTE #3: *You may get a warning like this:* *WARNING WHILE CHECKING INPUT SPECIFICATIONS*

```
INCONSISTENT FREE WATER SETTING DETECTED FOR 1 STREAMS
SOURCE BLOCK        FREE WATER STREAM   DESTINATION BLOCK   FREE WATER
=================== ========== ======== =================== ==========
MIXER-3             NO         TRI-MIX3 DSTWU-1             YES.
```

*This can be removed if you set the "**Free water**" to Yes, under "**Setup**" | "**Specifications**" | "**Global**" sheet while being under "**Simulation**" environment.*

The results shown here are calculated with the fact that the flowsheet design specifications (DS-1) in the previous section are still active or operational. In addition, the binary interaction parameters are as indicated in NOTE #0.

If you closely look at the results, you will notice that with the given input parameters, we could not achieve the desired 95% purity of acetone in this simulation. Hence, we have to manipulate the input parameters by trial-and-error procedure to achieve the required target of acetone mass fraction higher than 0.95. Figure 4.13 shows the newly modified input parameters such that acetone mass fraction in the top stream is 0.96 and MIBK mass fraction is 0.998 in the bottom stream. Moreover, the feed stage number (i.e., location) is 17 from top, the actual reflux ratio is 1.387, and distillate to feed fraction is 0.3486. This can be seen under "**Blocks**" | "**DSTWU-1**" | "**Results**" | "**Summary**" tab window.



Column specifications
● Number of stages 36
○ Reflux ratio

Pressure
Condenser 0.5 bar
Reboiler 1.2 bar

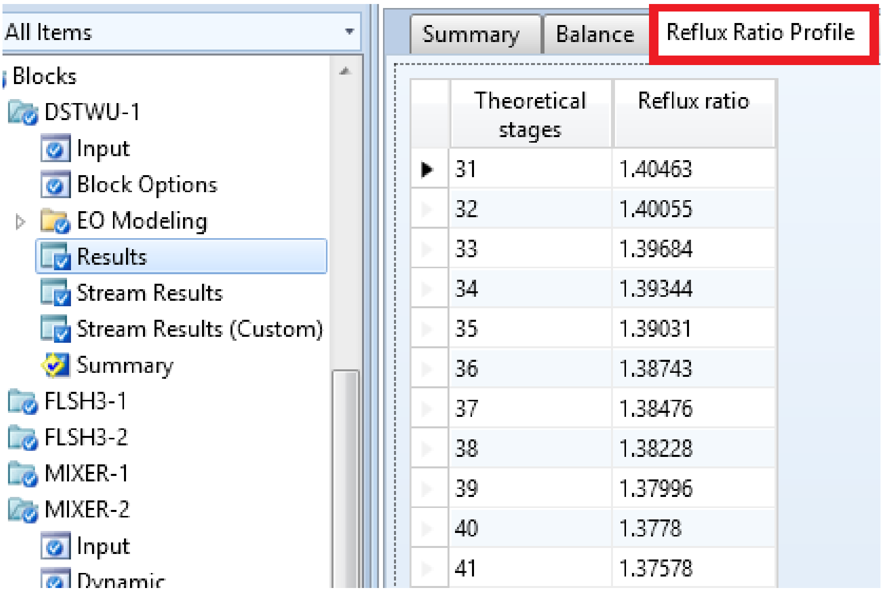
Key component recoveries
Light key
Comp ACETONE
Recov 0.9995
Heavy key
Comp MIBK
Recov 0.006

Condenser specifications
● Total condenser
○ Partial condenser with all vapor distillate
○ Partial condenser with vapor and liquid distillate
Distillate vapor fraction 0

Figure 4.13 The newly modified input parameters for "**DSTWU**" unit such that we end up with a mass fraction of acetone in top stream equals 0.96 and that of MIBK in bottom stream is 0.998.

Figure 4.14 shows "**Reflux Ratio Profile**" for "**DSTWU**" column. Keep in mind that there is a trade-off between the number of stages and the reflux ratio. Each additional tray will add up to the equipment cost, while the increase in reflux will add up to the operating costs of the column. We will use some of this information in our input for the "**Distl**" column.

NOTE #4: *It is worth mentioning here that because of the simplifications that are used in the model of "**DSTWU**"-type column, the design specifications "**Design Specs**" will not be appropriate; for example, the purity level of acetone in the acetone product stream (here, "**DSTW-TOP**" stream) will not be affected by the block variable, that is, the reflux ratio (RR) of the distillation tower; the truth of matter it is. In conclusion, although the shortcut methods, in general, appear to provide a quick way to obtain results, they do not always guarantee the accuracy that is desired. For this reason, any case study in the form of design specifications, sensitivity analysis, or optimization should be carried out using rigorous models such as the "**RadFrac**" column.*



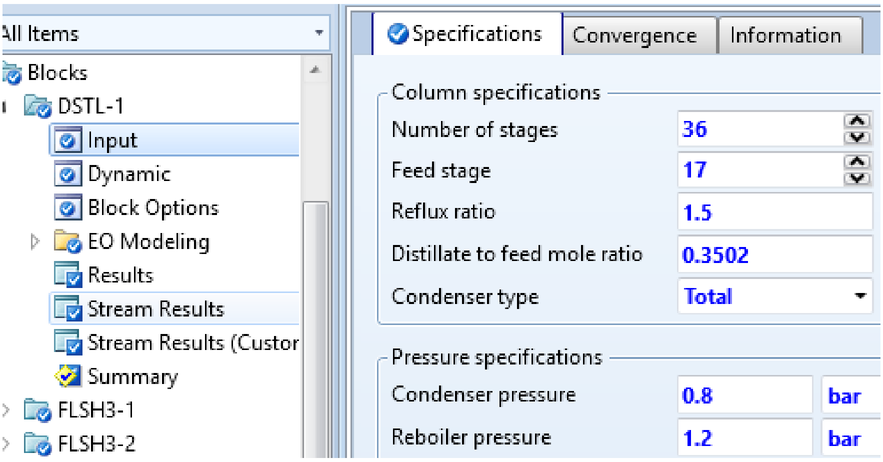
Theoretical stages	Reflux ratio
31	1.40463
32	1.40055
33	1.39684
34	1.39344
35	1.39031
36	1.38743
37	1.38476
38	1.38228
39	1.37996
40	1.3778
41	1.37578

Figure 4.14 The “**Reflux Ratio Profile**” for “**DSTWU**” column.

4.6 “DISTL” DISTILLATION COLUMN

Let us consider the second type, that is, the “**Distl**” column. Open the second file that you saved earlier for the current Aspen Plus simulation project. Now select the “**Columns**” tab in “**Model Palette**” and place a “**Distl**” column into the process flowsheet window. Connect the product stream from the third mixer to the “**Distl**” column and add the two product streams where Aspen Plus indicates they are required. Add a third product stream off the condenser, to account for any free water product that can be separated from within the condenser. Rename the streams and column as you see fit. At this point, your flowsheet should look similar to that in Figure 4.11 with one exception, that is, we replaced the “**DSTWU**” by “**Distl**” column.

Click on “**Reset**” followed by “**Next**” button. The newly added “**Distl**” column to the process flowsheet requires some input parameters, as shown in Figure 4.15. Here, the input parameters were entered in light of the results of “**DSTWU**” column (see the previous section), but not exactly the same.



Column specifications

Number of stages 36

Feed stage 17

Reflux ratio 1.5

Distillate to feed mole ratio 0.3502

Condenser type Total

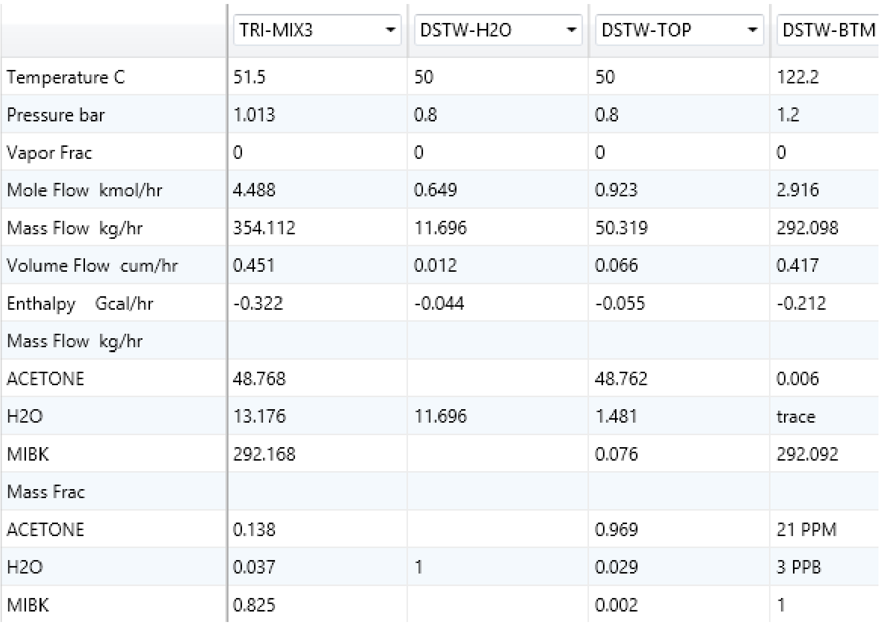
Pressure specifications

Condenser pressure 0.8 bar

Reboiler pressure 1.2 bar

Figure 4.15 Entering input parameters for "**Distl**" column, which were entered in light of "**DSTWU**" column results.

Figure 4.16 shows the "**Distl**" results for product streams. The product stream chemical composition is different from that of "**DSTWU**" column for the same stream. Remember that both "**DSTWU**" and "**Distl**" column models are not rigorous in approach; hence, an approximate solution is expected. Keep also in mind that the entered parameters, shown in Figure 4.15, will affect the composition and flow rate of final product streams. It will be left



	TRI-MIX3	DSTW-H2O	DSTW-TOP	DSTW-BTM
Temperature C	51.5	50	50	122.2
Pressure bar	1.013	0.8	0.8	1.2
Vapor Frac	0	0	0	0
Mole Flow kmol/hr	4.488	0.649	0.923	2.916
Mass Flow kg/hr	354.112	11.696	50.319	292.098
Volume Flow cum/hr	0.451	0.012	0.066	0.417
Enthalpy Gcal/hr	-0.322	-0.044	-0.055	-0.212
Mass Flow kg/hr				
ACETONE	48.768		48.762	0.006
H2O	13.176	11.696	1.481	trace
MIBK	292.168		0.076	292.092
Mass Frac				
ACETONE	0.138		0.969	21 PPM
H2O	0.037	1	0.029	3 PPB
MIBK	0.825		0.002	1

Figure 4.16 The product stream results for "**Distl**" column.

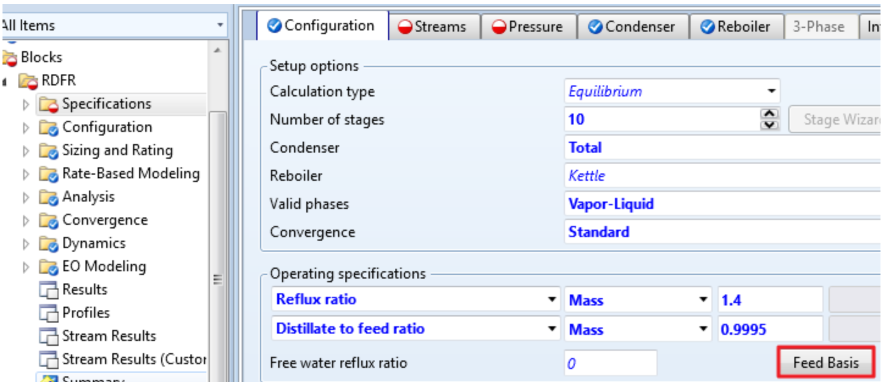
as a mini-exercise for the user to see how each of the entered parameters affects the final product stream amount and quality.

We will not work hard here to make the acetone composition to be higher than 0.95 in the top stream; instead, we will move to the third type of column models, that is, “**RadFrac**”, which is more rigorous than any of its two predecessors.

4.7 “RADFRAC” DISTILLATION COLUMN

Let us consider the third type, that is, “**RadFrac**” column. Open the third file that you saved earlier for the current Aspen Plus simulation project. Now select the “**Columns**” tab in “**Model Palette**” and place a “**RadFrac**” column into the process flowsheet window. Connect the product stream from the third mixer to the “**RadFrac**” column and add in two product streams where Aspen Plus indicates they are required. Add a third product stream off the condenser, to account for any free water product that can be separated from within the condenser. Rename the streams and column as you see fit. At this point, your flowsheet should look similar to that in Figure 4.11 with one exception, that is, we replaced the “**DSTWU**” by “**RadFrac**” column.

Click on “**Reset**” followed by “**Next**” button. The newly added “**RadFrac**” column to the process flowsheet requires some input parameters. The input window is shown in Figure 4.17. As one can see, “**RadFrac**” column requires more input than either the “**DSTWU**” or “**Distl**” column does. For example, this column model requires us to enter the number of theoretical stages as well as the reflux ratio RR. Notice that in Figure 4.17, we used a total condenser with “*Vapor-Liquid*” option as “**Valid phases**”.

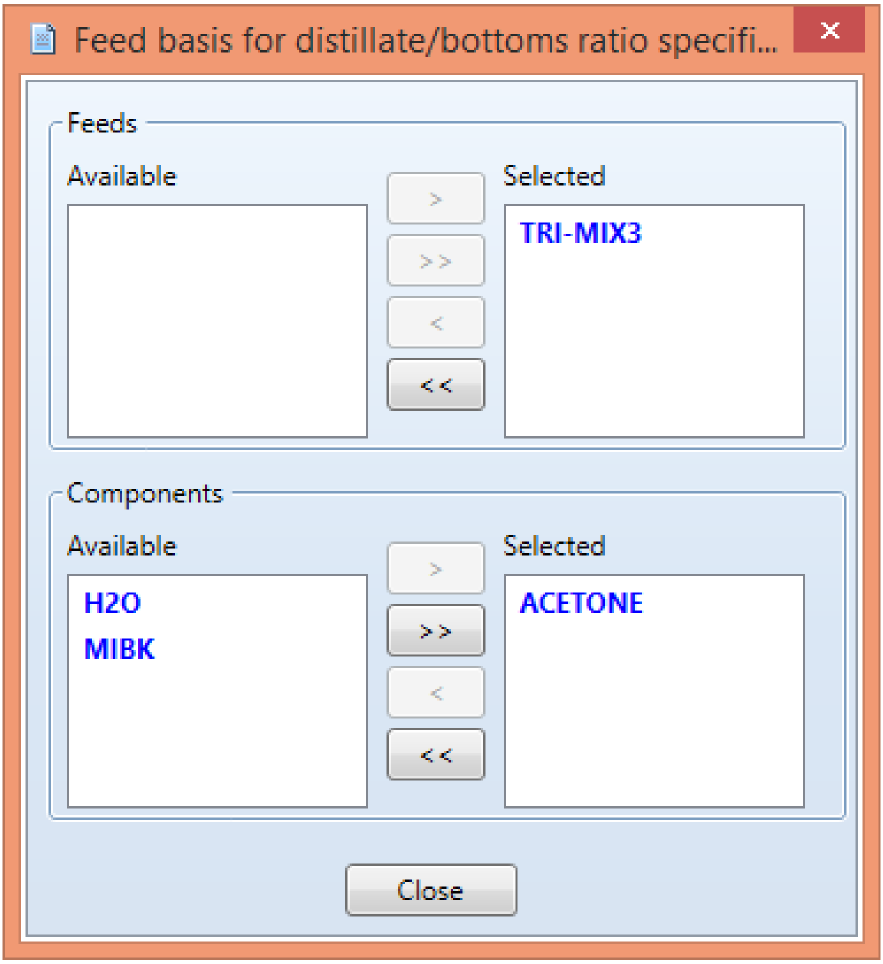


Setup options
Calculation type: Equilibrium
Number of stages: 10
Condenser: Total
Reboiler: Kettle
Valid phases: Vapor-Liquid
Convergence: Standard

Operating specifications
Reflux ratio: Mass: 1.4
Distillate to feed ratio: Mass: 0.9995
Free water reflux ratio: 0

Figure 4.17 The required input “**Configuration**” parameters for “**RadFrac**” type of distillation columns.

Click on the “**Feed basis**” button, shown at the bottom of Figure 4.17, where you need to tell Aspen Plus what the feed basis is and what component is to be used for distillate to feed ratio, as shown in Figure 4.18.



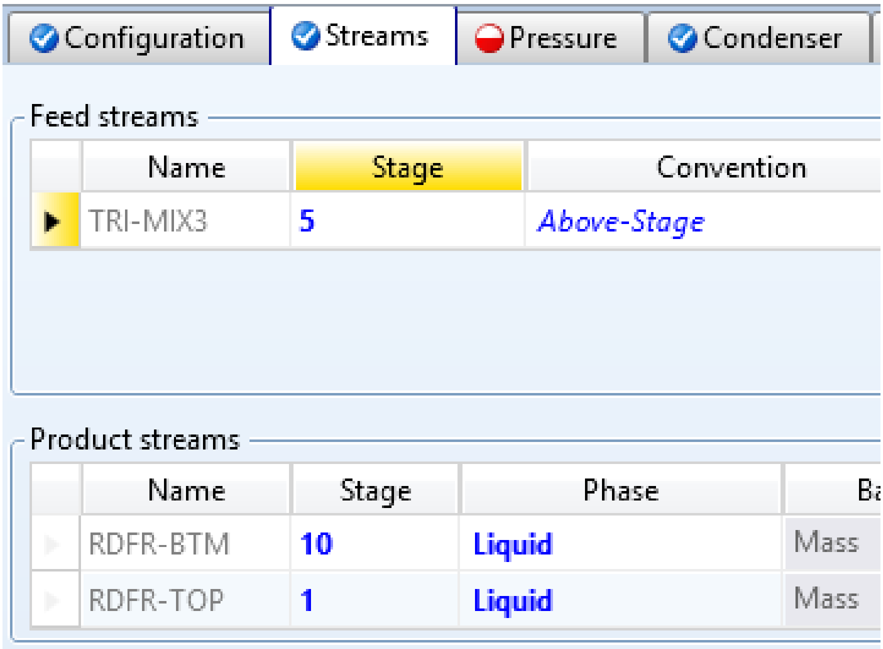
Feeds — Selected: TRI-MIX3

Components — Available: H2O, MIBK

Components — Selected: ACETONE

Figure 4.18 Selection of the feed basis and component to be used for distillate to feed ratio.

Under the “**Streams**” tab, we need to input the location of the feed stream. As discussed in the mass transfer/separation process class, we will locate the feed at the middle stage of the column, tray #5. This completes the “**Streams**” tab input (Figure 4.19).



Feed streams

	Name	Stage	Convention
▶	TRI-MIX3	5	Above-Stage

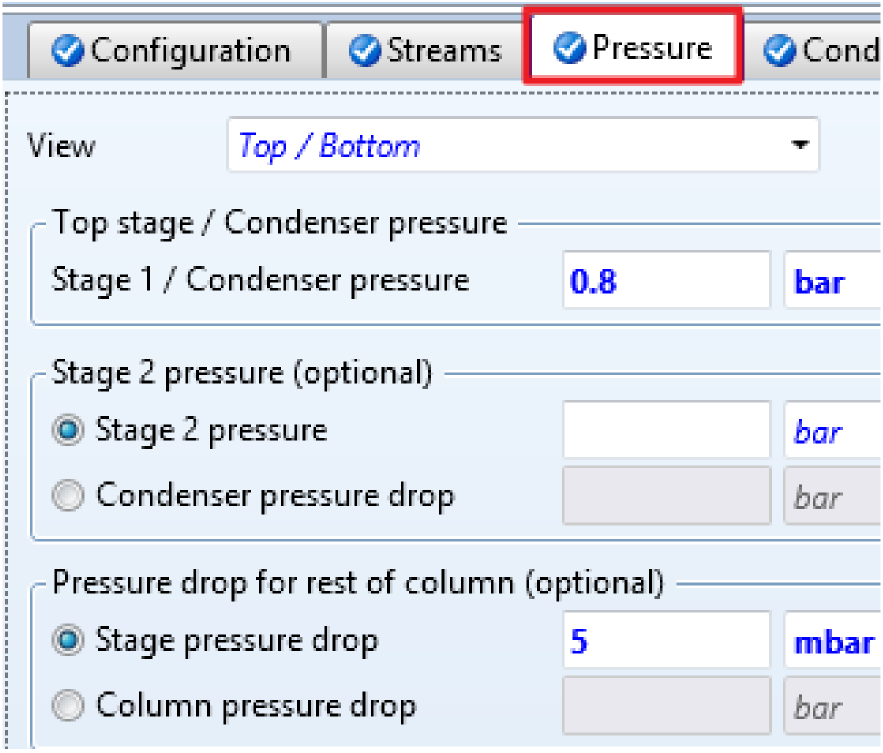
Product streams

	Name	Stage	Phase	Ba
	RDFR-BTM	10	Liquid	Mass
	RDFR-TOP	1	Liquid	Mass

Figure 4.19 Entering the location of feed tray under "**Streams**" tab and phase type of each product stream.

Notice that the tray corresponding to each product stream is shown in this window. If we have any side stream from our tower or an additional feed, we will need to input the tray that it issues from or merges to and it should appear here in this tab window.

Under the "**Pressure**" tab, we will simulate a distillation column that is operating at 0.8 bar with 5 mbar drop. Input this as the operating pressure at Stage 1 (Figure 4.20). At this point, our required input is again complete and we are ready to run our simulation. Notice that in real operations, there exists a pressure drop along the column from the bottom (highest pressure) to the top (lowest pressure), which is accounted for via specifying either a stage pressure or column pressure drop.



View: Top / Bottom

Top stage / Condenser pressure

Stage 1 / Condenser pressure: 0.8 bar

Stage 2 pressure (optional)

● Stage 2 pressure: bar

○ Condenser pressure drop: bar

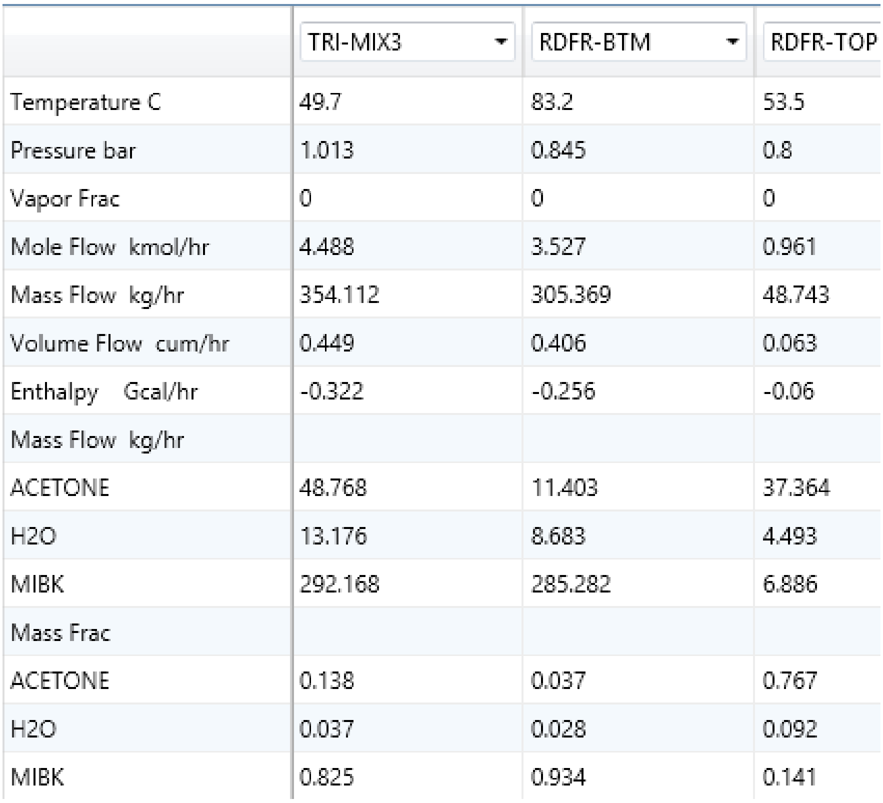
Pressure drop for rest of column (optional)

● Stage pressure drop: 5 mbar

○ Column pressure drop: bar

Figure 4.20 Inputting the pressure value at Stage 1 (i.e., condenser pressure) and pressure drop per stage.

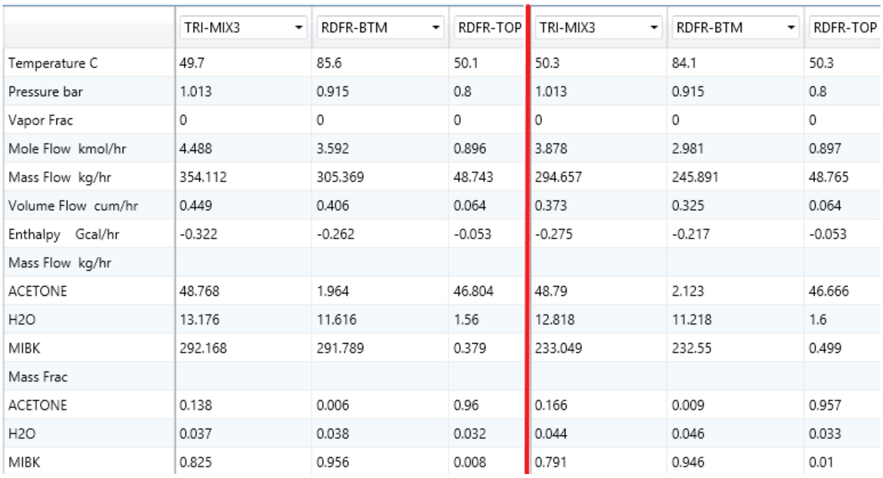
Click on "**Reset**" followed by "**Next**" button and run the simulation at this point. Figure 4.21 shows results of product streams of "**RadFrac**" distillation column where "**RDFR-TOP**" did not fulfill the minimum required degree of purity (i.e., 95 wt% acetone).



	TRI-MIX3	RDFR-BTM	RDFR-TOP
Temperature C	49.7	83.2	53.5
Pressure bar	1.013	0.845	0.8
Vapor Frac	0	0	0
Mole Flow kmol/hr	4.488	3.527	0.961
Mass Flow kg/hr	354.112	305.369	48.743
Volume Flow cum/hr	0.449	0.406	0.063
Enthalpy Gcal/hr	-0.322	-0.256	-0.06
Mass Flow kg/hr			
ACETONE	48.768	11.403	37.364
H2O	13.176	8.683	4.493
MIBK	292.168	285.282	6.886
Mass Frac			
ACETONE	0.138	0.037	0.767
H2O	0.037	0.028	0.092
MIBK	0.825	0.934	0.141

Figure 4.21 The composition of inlet and outlet stream for "**RadFrac**" distillation column. The desired degree of product stream purity is not yet fulfilled.

The ability to split a feed stream into almost one or two pure streams depends on many input parameters as can be seen in Figures 4.17–4.20. For example, increasing both the number of trays and reflux ratio will grant us more luxury to have a higher degree of separation. Let us increase the number of trays to 24 and the molar reflux ratio to 3.5. We will be able to end up with almost pure product streams as shown in Figure 4.22 (*left*). Remember to relocate the feed tray to 12, although it is not necessary that the feed tray location be exactly in the middle between the top and bottom trays. On the other hand, Figure 4.22 (*right*) shows the final product stream properties for rerunning the same flowsheet while regressing the binary interaction parameters for acetone–water quoted from "**NIST/TDE**" databank. In other words, "**UNIQUAC**" was used as the property method, and the source for binary interaction parameters are exactly those shown in Figure 2.20. The qualitative and quantitative behavior in terms of separability is the same regardless of the property method being used. Notice that the final composition for each product stream is practically the same for both property methods. However, there is a difference in behavior in predicting the amount of MIBK needed to accomplish the same degree of water purity for "**FL2−H2O**" stream. In the design specs ("**DS−1**") case study using "**UNIQUAC**"



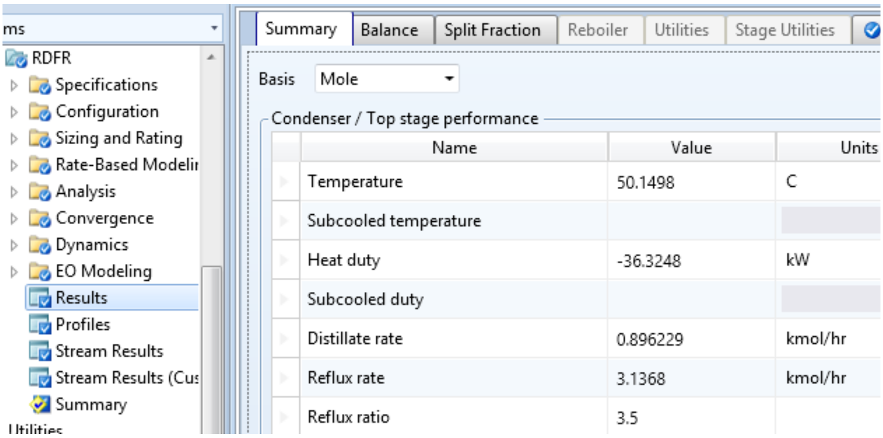
	TRI-MIX3	RDFR-BTM	RDFR-TOP	TRI-MIX3	RDFR-BTM	RDFR-TOP
Temperature C	49.7	85.6	50.1	50.3	84.1	50.3
Pressure bar	1.013	0.915	0.8	1.013	0.915	0.8
Vapor Frac	0	0	0	0	0	0
Mole Flow kmol/hr	4.488	3.592	0.896	3.878	2.981	0.897
Mass Flow kg/hr	354.112	305.369	48.743	294.657	245.891	48.765
Volume Flow cum/hr	0.449	0.406	0.064	0.373	0.325	0.064
Enthalpy Gcal/hr	-0.322	-0.262	-0.053	-0.275	-0.217	-0.053
Mass Flow kg/hr						
ACETONE	48.768	1.964	46.804	48.79	2.123	46.666
H2O	13.176	11.616	1.56	12.818	11.218	1.6
MIBK	292.168	291.789	0.379	233.049	232.55	0.499
Mass Frac						
ACETONE	0.138	0.006	0.96	0.166	0.009	0.957
H2O	0.037	0.038	0.032	0.044	0.046	0.033
MIBK	0.825	0.956	0.008	0.791	0.946	0.01

Figure 4.22 The composition of inlet and outlet streams for "**RadFrac**" distillation column, based on "**NRTL**" property method (*left*) and "**UNIQUAC**"-fitted "**NIST/TDE**" binary data for water–acetone system (*right*).

property method, it was found that the mass flow rate of "**MIBK2**" stream is 133.8 as opposed to 192.9 kg/h for that of "**NRTL**" method (see Figure 4.8) to achieve a degree of water purity equal to at least 95 wt% in "**FL2−H2O**" product stream. We should not panic (or freak out) at all, given the fact that it is only after an adequate experience the R&D engineer will be able to identify the property method that is the most adequate among all other recommended methods for a given process type or set of components.

It is worth mentioning here that since we have in hand a rigorous column model (i.e., "**RadFrac**" model), for example, a design specification case study can be conducted here where the design specs variable will be the mass fraction of acetone in the top stream with a target value of 0.95 and tolerance value of 0.001 (see Figure 4.5) and the manipulated variable will be the block variable, namely, the molar reflux ratio.

Let us look at the results for the "**RadFrac**" distillation tower. Select the appropriate unit operation under the "**Blocks**" option. Scroll down until you see the "**RDFR**" subfolder and click on the "**Results**" file. This is shown in Figure 4.23. This window shows the final operating conditions for the distillation column that were calculated by the program. You can see in this window that the molar reflux ratio is 3.5. You can also see the required condenser cooling duty, which is equal to −36.3248 kW. Of course, the negative sign indicates that heat will be taken off the condenser.



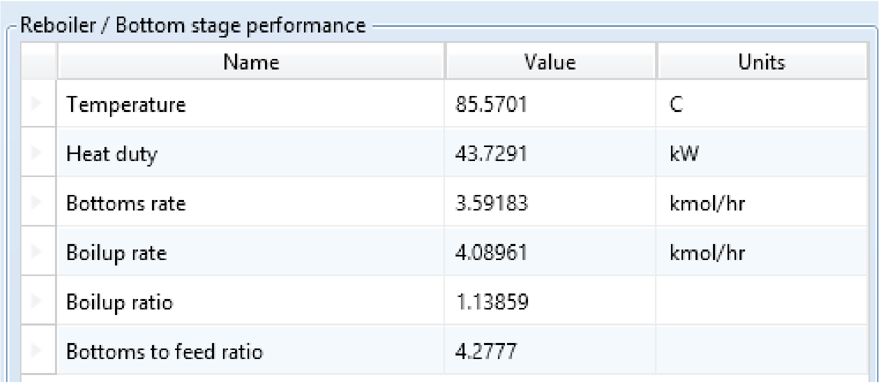
Basis Mole

Condenser / Top stage performance

Name	Value	Units
Temperature	50.1498	C
Subcooled temperature		
Heat duty	-36.3248	kW
Subcooled duty		
Distillate rate	0.896229	kmol/hr
Reflux rate	3.1368	kmol/hr
Reflux ratio	3.5	

Figure 4.23 The results summary for the "*Condenser / Top stage performance*" table of the "**RadFrac**" distillation tower under "**Results**" | "**Summary**" tab.

On the other hand, the "*Reboiler / Bottom stage performance*" table, shown immediately below the condenser table, gives the required heat added to the reboiler (Figure 4.24). The reboiler heat duty is 43.7291 kW. If you select the "**Balance**" tab at the top of the screen in Figure 4.23, you can see the overall heat and material balances for the column. You can also see the relative difference in the values, indicating that no simulation is 100% perfect.

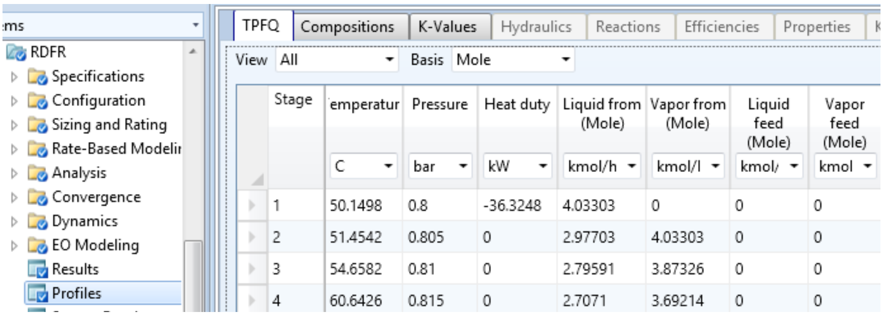


Reboiler / Bottom stage performance

Name	Value	Units
Temperature	85.5701	C
Heat duty	43.7291	kW
Bottoms rate	3.59183	kmol/hr
Boilup rate	4.08961	kmol/hr
Boilup ratio	1.13859	
Bottoms to feed ratio	4.2777	

Figure 4.24 The results summary for the "*Reboiler / Bottom stage performance*" table of the "**RadFrac**" distillation tower.

Finally, under the "**Profiles**" sheet of "**RadFrac**" block, Aspen Plus presents a summary of the operating conditions for this simulation. Under the "**TPFQ**" tab you can see a breakdown of the liquid and vapor flow rates from each tray. From the "**View**" drop-down menu, under the "**TPFQ**" tab, you may select all or a subset of profile results, such as summary, feeds and products, stage flows, and heat duty and enthalpy profile. Under the "**Compositions**" tab on the top of the screen, you can see a profile of each of the components throughout the column (Figure 4.25).



View All Basis Mole

Stage	emperatur	Pressure	Heat duty	Liquid from (Mole)	Vapor from (Mole)	Liquid feed (Mole)	Vapor feed (Mole)
	C	bar	kW	kmol/h	kmol/l	kmol/	kmol
1	50.1498	0.8	-36.3248	4.03303	0	0	0
2	51.4542	0.805	0	2.97703	4.03303	0	0
3	54.6582	0.81	0	2.79591	3.87326	0	0
4	60.6426	0.815	0	2.7071	3.69214	0	0

Figure 4.25 Temperature, Pressure, Flow, and Heat duty, Q, (TPFQ) is shown at each stage in "**Profiles**" | "**TPFQ**" tab sheet of the distillation tower.

HOMEWORK/CLASSWORK 4.1 (WATER–ALCOHOL SYSTEM)

Continue working on Homework/Classwork 2.1 and complete the process flowsheet as shown in Figure 4.26. The property method is set to "**NRTL**" while allowing Aspen Plus to estimate any missing binary parameters by "**UNIFAC**". The goal of the entire process is to separate 1-hexanol from water using 1-octanol while at the same time end up with pure streams and recycle water–hexanol stream from the top of the **Flash2**-type separator back to the inlet of the first mixer. Since this is the first problem that contains several unit operations (i.e., blocks), we will give more details on how to consecutively add a block and its associated input and output stream(s). The following step-by-step standard procedure should be used as a general guideline in creating and simulating any typical process flowsheet. Under "**Simulation**" environment, execute (without mercy) the following tasks:

1. Add one "**Flash3**"-type ("**FLSH3-1**") separator from "**Model Palette**" under "**Separators**" tab and reconnect "**TRI-MIX**" stream destination as the required feed to "**FLSH3-1**" block.
2. Add the three required output streams: "**VAP**", "**TOPLIQ**", and "**BTMLIQ**".
3. Enter "**FLSH3-1**" temperature and pressure as 25°C and 1.9 atm.

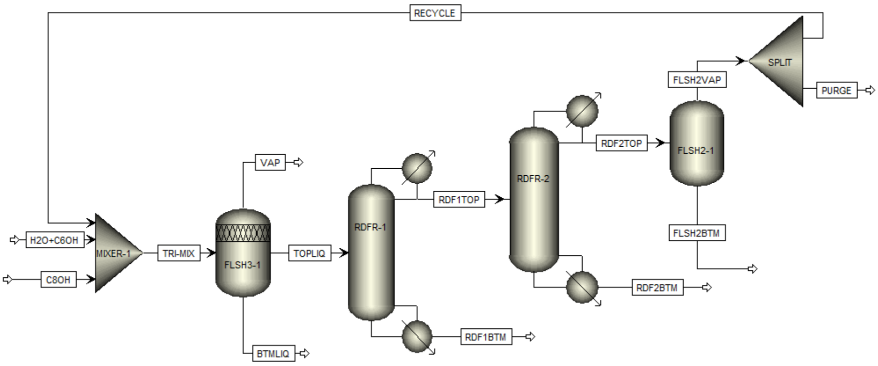
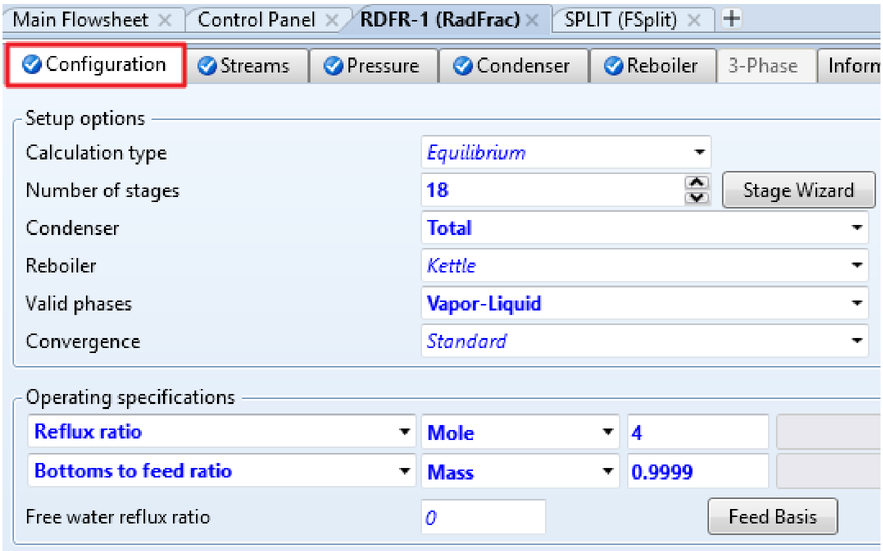


Figure 4.26 The process flowsheet for separating hexanol from water using octanol.

4. Click on “**Reset**” followed by “**Next**” button to run the simulation.
5. In “**Control Panel**”, see if there is any serious warning or error that requires an action by the user.
6. Save your work.
7. Once you manage to get successful and reasonable results, add the “**RadFrac**” distillation column from “**Model Palette**” under “**Columns**” tab and give it a name “**RDFR-1**”. Reconnect “**TOPLIQ**” stream destination as the feed to “**RDFR-1**” block.
8. Add the two required output streams: “**RDF1TOP**” and “**RDF1BTM**”.
9. Enter the following specifications for “**RDFR-1**”, as shown in Figure 4.27.
10. Within “**Operating specifications**” box, click on “**Feed Basis**” button, shown in Figure 4.27, to select “**TOPLIQ**” stream as the feed basis and octanol compound as the basis for *Bottoms to feed ratio*.



Setup options

Calculation type Equilibrium
Number of stages 18
Condenser Total
Reboiler Kettle
Valid phases Vapor-Liquid
Convergence Standard

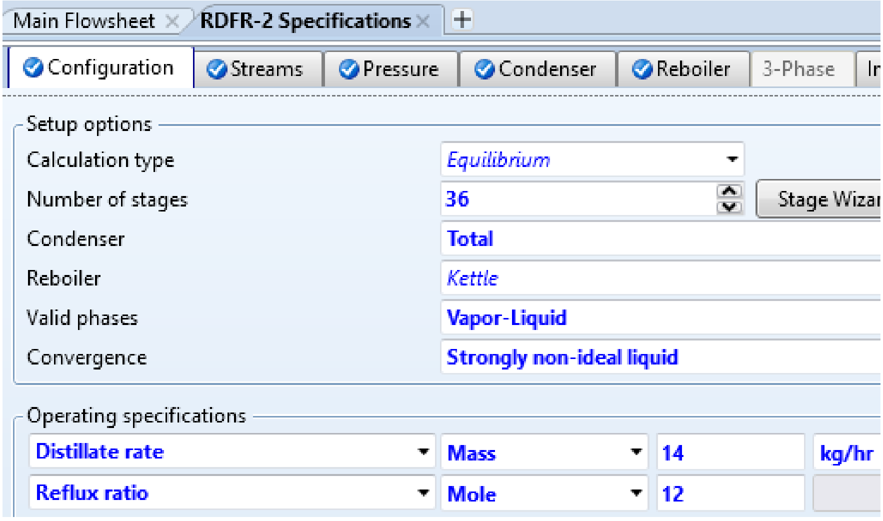
Operating specifications

Reflux ratio Mole 4
Bottoms to feed ratio Mass 0.9999
Free water reflux ratio 0

Figure 4.27 “**RDFR-1**” specifications, under “**Configuration**” tab.

11. Under “**Streams**” tab, mount the feed stream at tray location #9.
12. Under “**Pressure**” tab, set the condenser pressure to 1.8 atm.
13. Click on “**Reset**” followed by “**Next**” button to run the simulation.
14. In “**Control Panel**”, see if there is any serious warning or error that requires an action by the user.
15. Save your work.
16. Once you manage to get successful and reasonable results, add the “**RadFrac**” distillation column from “**Model Palette**” under “**Columns**” tab and give it a name “**RDFR-2**”. Reconnect “**RDF1TOP**” stream destination as the feed to “**RDFR-2**” block.

17. Add the two required output streams: “**RDF2TOP**” and “**RDF2BTM**”.
18. Enter the following specifications for “**RDFR-2**”, as shown in Figure 4.28:



Setup options

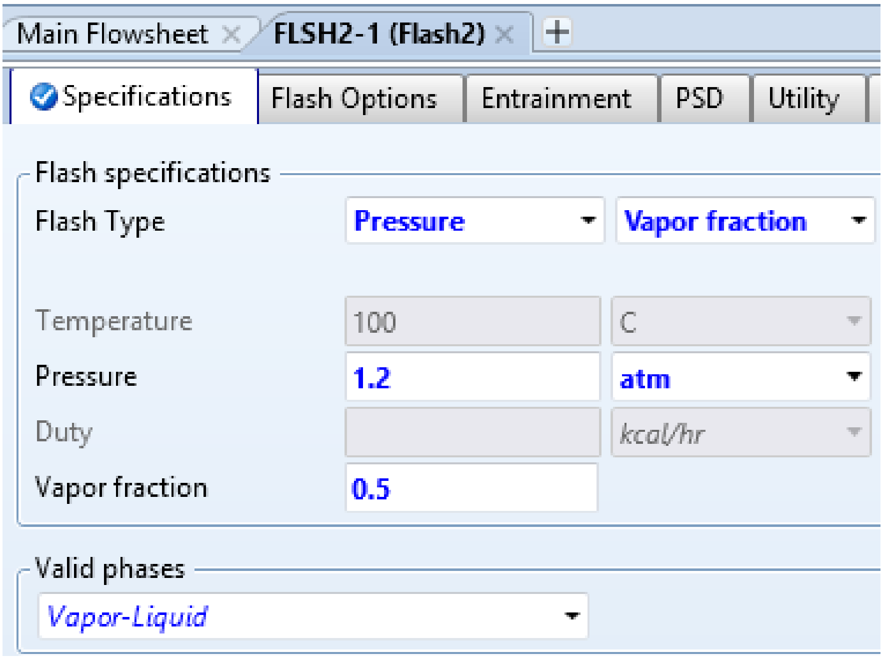
Calculation type: Equilibrium
Number of stages: 36
Condenser: Total
Reboiler: Kettle
Valid phases: Vapor-Liquid
Convergence: Strongly non-ideal liquid

Operating specifications

Distillate rate	Mass	14	kg/hr
Reflux ratio	Mole	12	

Figure 4.28 “**RDFR-2**” specifications, under “**Configuration**” tab.

19. Under “**Streams**” tab, mount the feed stream at tray location #20.
20. Under “**Pressure**” tab, set the condenser pressure to 1.4 atm.
21. Click on “**Reset**” followed by “**Next**” button to run the simulation.
22. In “**Control Panel**”, see if there is any serious warning or error that requires an action by the user.
23. Save your work.
24. Once you manage to get successful and reasonable results, add the “**Flash2**” separator from “**Model Palette**” under “**Separators**” tab and give it a name “**FLSH2-1**”. Reconnect “**RDF2-TOP**” stream destination as the feed to “**FLSH2-1**” block.
25. Add the two required output streams: “**FLSH2VAP**” and “**FLSH2BTM**”.
26. Enter the following specifications for “**FLSH2-1**”, as shown in Figure 4.29.



Flash specifications

Flash Type: Pressure, Vapor fraction

Temperature: 100 C

Pressure: 1.2 atm

Duty: kcal/hr

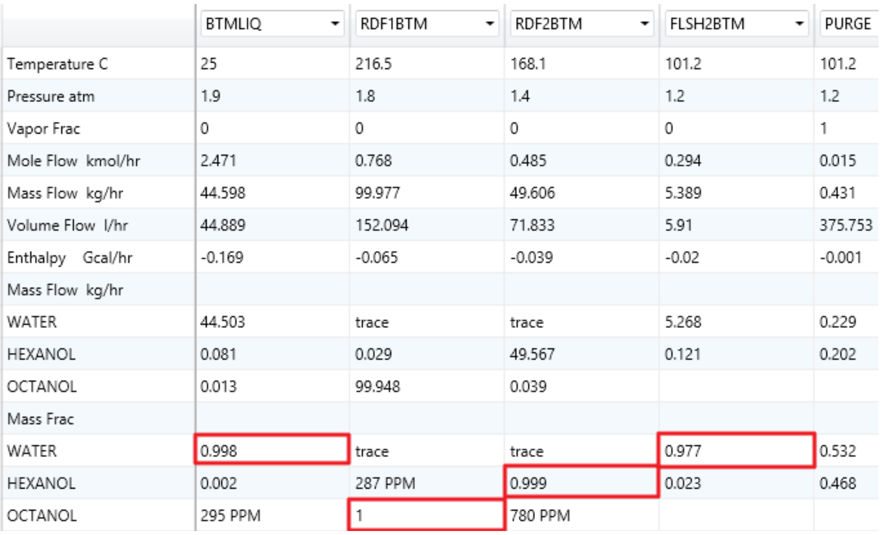
Vapor fraction: 0.5

Valid phases: Vapor-Liquid

Figure 4.29 “**FLSH2-1**” specifications, under “**Specifications**” tab.

27. Click on “**Reset**” followed by “**Next**” button to run the simulation.
28. In “**Control Panel**”, see if there is any serious warning or error that requires an action by the user.
29. Save your work.
30. Show a streams table for the following output streams: “**BTMLIQ**”, “**RDF1BTM**”, “**RDF2BTM**”, “**FLSH2BTM**”, and “**FLSH2VAP**”. Of course, “**VAP**” is essentially zero.
31. Up to this point there is no recycling and “**FLSH2VAP**” is purged out to a storage facility; nevertheless, we would like to recycle this stream to the inlet of the first mixer.
32. Add the “**FSplit**” splitting unit from “**Model Palette**” under “**Mixers/Splitters**” tab and give it a name “**SPLIT**”. Reconnect “**FLSH2VAP**” stream destination as the feed to “**SPLIT**” block.
33. Add the two required output streams: “**PURGE**” and “**RECYCLE**”.
34. In “**Blocks**” | “**SPLIT**” | “**Input**” | “**Specifications**” tab window, enter a value of *0.05* as a split fraction for “**PURGE**” stream.
35. Click on “**Reset**” followed by “**Next**” button to run the simulation.
36. In the “**Control Panel**”, see if there is any serious warning or error that requires an action by the user.
37. Save your work.
38. Reconnect “**RECYCLE**” stream destination to the inlet of “**MIXER-1**” block.
39. Click on “**Reset**” followed by “**Next**” button to run the simulation.

40. In “**Control Panel**”, see if there is any serious warning or error that requires an action by the user.
41. Save your work.
42. Make a stream table for the following output streams: “**BTMLIQ**”, “**RDF1BTM**”, “**RDF2BTM**”, “**FLSH2BTM**”, and “**PURGE**”. Of course, “**FLSH2VAP**” stream should not appear now because it is no longer an outlet but an intermediate stream with recycling.
43. Figure 4.30 shows typical results for the outlet streams. Notice the high level of purity for each output stream, except for the sacrificial “**PURGE**” stream, which serves as a mixture of water–hexanol yet with a low mass flow rate.



	BTMLIQ	RDF1BTM	RDF2BTM	FLSH2BTM	PURGE
Temperature C	25	216.5	168.1	101.2	101.2
Pressure atm	1.9	1.8	1.4	1.2	1.2
Vapor Frac	0	0	0	0	1
Mole Flow kmol/hr	2.471	0.768	0.485	0.294	0.015
Mass Flow kg/hr	44.598	99.977	49.606	5.389	0.431
Volume Flow l/hr	44.889	152.094	71.833	5.91	375.753
Enthalpy Gcal/hr	-0.169	-0.065	-0.039	-0.02	-0.001
Mass Flow kg/hr					
WATER	44.503	trace	trace	5.268	0.229
HEXANOL	0.081	0.029	49.567	0.121	0.202
OCTANOL	0.013	99.948	0.039		
Mass Frac					
WATER	0.998	trace	trace	0.977	0.532
HEXANOL	0.002	287 PPM	0.999	0.023	0.468
OCTANOL	295 PPM	1	780 PPM		

Figure 4.30 Operating conditions and compositions for each of the outlet streams.

The Perpetual Cycle!!!

The theme here is simply that we managed to separate the original water–hexanol mixture into its constituents as pure water and pure hexanol while at the same time we recovered the solvent octanol, which was used as a chemical agent to liberate hexanol from water. Of course, the recovered solvent can be reused on and on. In other words, “**RDF1BTM**” stream is pure octanol that can be reused as “**C8OH**” feed stream to the inlet of the first mixer.

Ideally, the purge stream can be collected from time to time and be mixed with the incoming “**H2O+C6OH**” stream in a certain proportion (or fraction) to minimize the load disturbance effect on the entire process flowsheet. In general, the control unit is operated with the mode that the feed mixture enters at some nominal (or steady-state) values in terms of pressure, temperature, and mole fraction of hexanol.

In real life, however, the situation might be slightly different from this ideally depicted picture. Given the fact other constituents may be encountered as a result of impurities present in the feed streams as well as the by-products resulting from inevitable processes, such as erosion, corrosion, oxidation, decomposition, and exchange (or cross contamination) with the surrounding environment. This being the case, it will be practically impossible to end up with the concept of having a permanent or perpetual process with 100% efficiency (i.e., 100% recovery of solvent while attaining zero "PURGE" flow rate or 100% separation of the mixture into pure water and hexanol). So, we have to pay the price for that in the form of either a nonrecoverable solvent or sacrifice with some amount of a purged mixture (or waste).

HOMEWORK/CLASSWORK 4.2 (WATER–ACETONE–EIPK SYSTEM WITH NIST/DTE DATA)

Continue working on Homework/Classwork 2.2 and complete the process flowsheet as shown in Figure 4.31. The property method is set to "**NRTL**" while utilizing NIST/DTE experimental VLE data for acetone–water mixture to generate the binary interaction parameters.

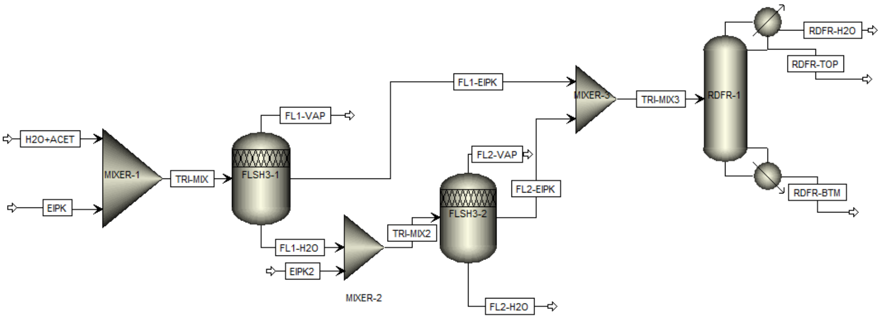


Figure 4.31 The process flowsheet for water–acetone separation utilizing EIPK.

Follow the same procedure outlined in Homework/Classwork 4.1 as far as adding one block at a time with its associated input and output streams, checking for successful simulation results, and then adding the next block in series until we add all required blocks. Figure 4.32 shows the annotated and reduced version of the "**Input File**" that was generated by Aspen Plus for the process flowsheet. The annotation starts with the pound sign (#) and ends up with the colon (:), for a given line. This is another exercise for the user to learn how to properly read the data within the input file and be able to use them in a similar simulation project. Your job is to enter the required input data for each block or stream.

```
DESCRIPTION”: Specialty Chemicals Simulation with Metric Units: C, atm, kg/h, kmol/h,
kcal/h, l/h.
   Property Method: NRTL, Flow basis for input: Mass, Stream report composition: Mass flow
STREAM EIPK
   SUBSTREAM MIXED TEMP=25°C. PRES=1 atm.
   MASS-FLOW EIPK 50 kg/h.
STREAM EIPK2
   SUBSTREAM MIXED TEMP=25°C. PRES=1 atm.
   MASS-FLOW EIPK 50 kg/h.
STREAM H2O+ACET
   SUBSTREAM MIXED TEMP=25°C. PRES=1 atm.
   MASS-FLOW ACETONE 50 kg/h. / WATER 50 kg/h.
# NOTE: No need to enter any parameter for the three mixers
BLOCK MIXER-1 MIXER
   PARAM
BLOCK MIXER-2 MIXER
   PARAM
BLOCK MIXER-3 MIXER
   PARAM MAXIT=60
BLOCK FLSH3-1 FLASH3
   PARAM TEMP=10°C. PRES=1 atm.
BLOCK FLSH3-2 FLASH3
   PARAM TEMP=15°C. PRES=1 atm.
BLOCK RDFR-1 RADFRAC
# The number of stages: PARAM NSTAGE=10 ALGORITHM=STANDARD MAXOL=25
# Valid phases: NPHASE=2 (Vapor-Liquid-FreeWaterCondenser) & DAMPING=NONE
# Condenser type: COL-CONFIG CONDENSER=TOTAL
# Feed tray location: FEEDS TRI-MIX3 5
# Top stream: PRODUCTS RDFR-TOP 1 (Tray #1) L1 (First liquid)/
# Bottom stream: RDFR-BTM 10 (Tray # 10) L (Liquid)/
# Condensed liquid: RDFR-H2O 1 (Tray #1) W (Free water).
# The condenser pressure at tray #1 (Under “Pressure” tab): P-SPEC 1 (Tray #) 0.5 atm.
# The distillate to feed ratio (Under “Configuration” tab, Figure 4.23): COL-SPECS D/F=1.
# The reflux molar ratio (Under “Configuration” tab): MOLE-RR=6.
# The “Feed Basis” (Under “Configuration” tab, see Figure 4.23): DB: F-PARAMS
STREAMS=TRI-MIX3
# The component for distillate over feed ratio: COMPS=ACETONE
BLOCK-OPTION FREE-WATER=YES
# Under “Flowsheeting Options” | “Design Spec” | “DS-1” sheet (See Figure (4.8) through
(4.11)):
# The name of design spec: DESIGN-SPEC DS-1
# The “DS-1” variable named WMF under “Define” tab: DEFINE WMF MASS-FRAC
STREAM=FL2-H2O SUBSTREAM=MIXED & COMPONENT=WATER
# The “DS-1” parameters under “Spec” tab: SPEC "WMF"
# “Target”: TO "0.90",
# “Tolerance”: TOL-SPEC "0.001"
# The “DS-1” variable under “Vary” tab: VARY MASS-FLOW STREAM=EIPK2
SUBSTREAM=MIXED COMPONENT=EIPK, & UOM="kg/h", LIMITS "50" (Lower) "250"
(Higher)
```

Figure 4.32 The annotated and reduced version of “**Input File**” pertinent to the process flowsheet shown in Figure 4.31.

In addition, carry out the design specification study shown at the bottom of Figure 4.32, where the user is required to find the minimum mass flow rate of EIPK via “**EIPK2**” stream such that the water mass fraction (**WMF**) in “**FL2-H2O**” stream is at least 0.9 within a tolerance of ±0.001.

After you carry out the design spec study, show a stream table of the process output streams.

HOMEWORK/CLASSWORK 4.3 (WATER–ACETONE–EIPK SYSTEM WITHOUT NIST/DTE DATA)

Continue working on Homework/Classwork 2.3 and complete the process flowsheet as shown in Figure 4.31. The property method is set to “**NRTL**” while allowing Aspen Plus to estimate any missing binary parameters by “**UNIFAC**”. The required input data for blocks and streams are replicates of those shown in Figure 4.32. Your job is to enter the required input data for each block or stream.

In addition, carry out the design specification study shown at the bottom of Figure 4.32, where the user is required to find the minimum mass flow rate of EIPK via “**EIPK2**” stream such that the water mass fraction (**WMF**) in “**FL2-H2O**” stream is at least 0.9 within a tolerance of ±0.001.

NOTE #5: *Here, reduce the lower limit of “**Vary**” tab variable to 10 instead of 50 kg/h of “**EIPK2**” mass flow rate (10–250). Alternatively, you may increase the target value to 0.96 for the same “**EIPK2**” mass flow rate range (50–250).*

After you carry out the design spec study, show a stream table of the process product streams.

Compare the results here with those in Homework/Classwork 4.2, in terms of the mass fraction for each output stream and in terms of the result of “**DS-1**” study.

Consider the recycling of a major portion of “**RDFR-BTM**” stream with 0.05 split fraction assigned for “**PURGE**” stream, as shown in Figure 4.33.

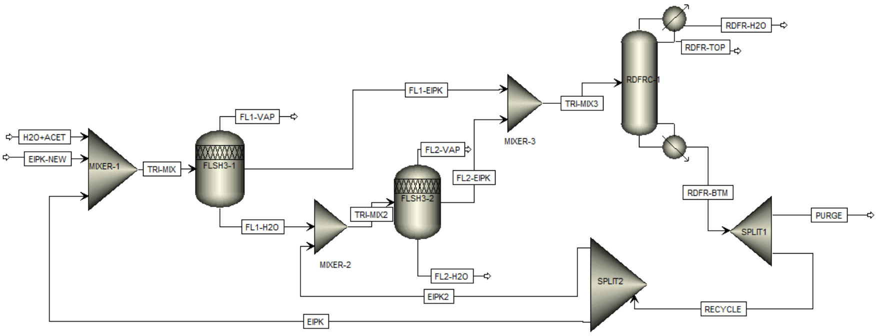


Figure 4.33 The recycling of EIPK-based product stream to the inlet of the first and second mixers.

In light of "**DS-1**" results, decide on the two output splitting fractions for the second ("**SPLIT2**") splitter, which will be returned as MIBK feed for the first and second mixers. Also, estimate the amount of make-up MIBK, which is introduced as "**EIPK-NEW**" stream. Notice that with recycling, you should expect that the make-up stream will be less than "**EIPK**" feed stream without recycling. Show the stream table for the process output streams. You should end up with practically pure output streams.

HOMEWORK/CLASSWORK 4.4 (SCRUBBER)

There are different routes through which acetic acid can be produced. One route is carried out via oxidation of ethylene (C_2H_4) into acetic acid. In addition, the parallel reaction, that is, oxidation of ethylene into water and CO_2, also takes place. The reactor product stream will contain 89.9 wt% acetic acid, 7.1 wt% CO_2, 2.9 wt% water, and trace amounts of inert N_2 (from the liquefaction process of air), unreacted ethylene, and unreacted O_2. Using a "**Flash2**" type drum (i.e., cooling tank), 99.96% of entering acetic acid and all water will be knocked out, in addition to a small fraction of CO_2. The vapor stream will contain 98.1 wt% CO_2, 1.2 wt% N_2, 0.6 wt% acetic acid, and trace amounts of C_2H_4, water, and O_2.

To simplify your task, we will assume that 100 kg/h of vapor feed stream with a composition of 98.2 wt% CO_2, 1.2 wt% N_2, and 0.6 wt% acetic acid, at 40°C and 10 bar, will be fed to a "**RadFrac**" distillation tower. From the top of the distillation tower, a second feed stream of 150 kg/h fresh water at 25°C and 10 bar will be introduced, as shown in Figure 4.34.

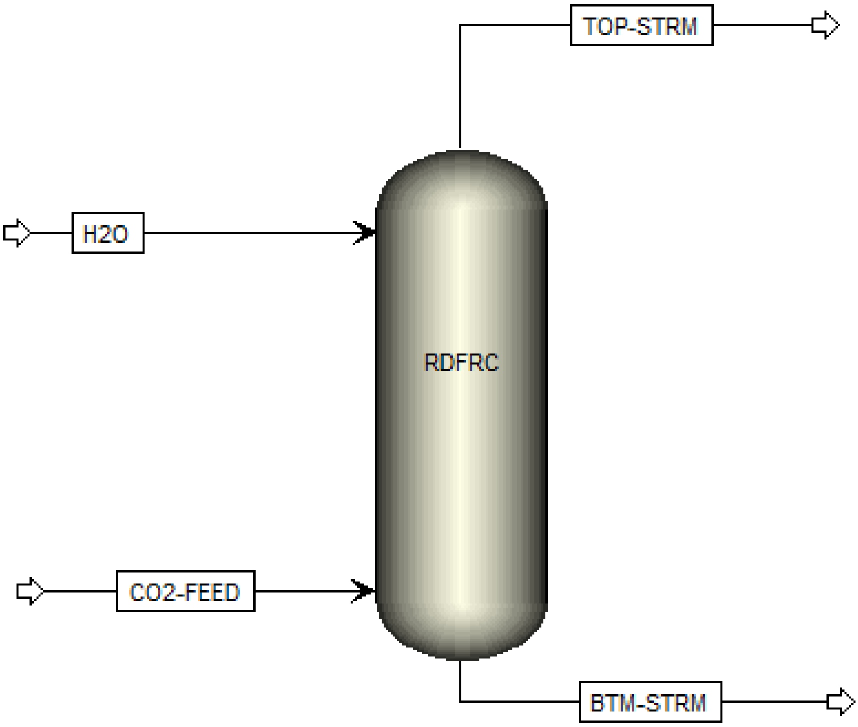
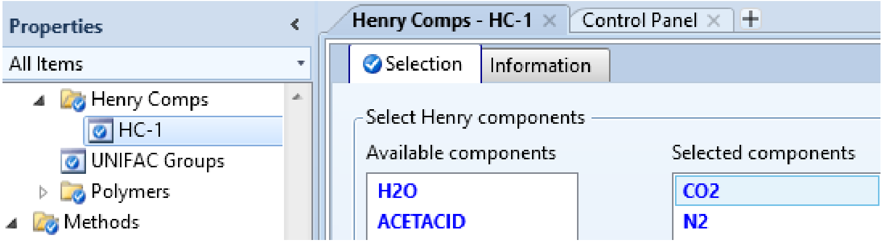


Figure 4.34 A schematic for scrubbing acetic acid off CO_2 gas using fresh water as liquid scrubber.

Your task is to design a “**RadFrac**” absorption unit that will scrub acetic acid from CO_2 (“**CO2-FEED**”) stream so that we end up with an inert outlet gas stream, mainly composed of CO_2 and trace amounts of N_2. This CO_2-based gas stream can be used as a blanket (inert) atmosphere purged onto hydrocarbon storage vessels. Report the composition, P, T, and flow rate for top and bottom streams, the reflux ratio, and number of theoretical stages.

Use “**NRTL**” method, which is automatically assigned by Aspen Plus upon selecting the template as “*Specialty Chemicals with Metric Units*”. Add the following components: water, acetic acid, carbon dioxide, and nitrogen. However, you need to define CO_2 and N_2 as Henry’s components as both are noncondensable gases at the given P and T. To do this, in “**Navigation**” pane, while under “**Properties**” environment, go to “**Components**” folder | “**Henry Comps**” subfolder. Define a new set that, by default, is given the name “**HC-1**”. Select CO_2 and N_2 from the list of available components and move them to Henry’s components side, as shown in Figure 4.35. Of course, use the forward and backward arrows to move one component from right to left or vice versa.

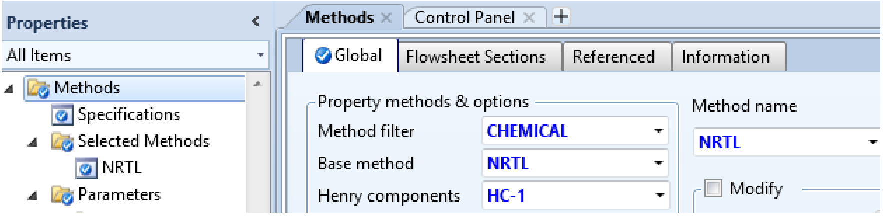


Available components: H2O, ACETACID

Selected components: CO2, N2

Figure 4.35 Selection of CO_2 and N_2 as Henry’s components.

Then, in “**Navigation**” pane, while under “**Properties**” environment, go to “**Methods**” folder | “**Specifications**” file | “**Global**” tab window, where you must define Henry’s group (“**HC-1**”) of components, which are defined in the previous step. This is shown in Figure 4.36.



Method filter: CHEMICAL

Base method: NRTL

Henry components: HC-1

Method name: NRTL

Figure 4.36 Selecting Henry’s components via “**HC-1**” group found in “**Methods**” | “**Specification**” | “**Global**” tab window.

> **NOTE #6:** *There is no need in this case for condenser and reboiler (i.e., heat duties are zero). Moreover, a gas scrubber is modeled via* “***RadFrac***”*-column model.*

5

LIQUID–LIQUID EXTRACTION PROCESS

5.1 PROBLEM DESCRIPTION

A mixture of water and methyl ethyl ketone (MEK) is to be separated using a third component *n*-octanol. For testing the goodness of property methods, the separation process initially is made of a single-stage (mixer) extraction unit and is later replaced by a multistage extraction column. MEK will migrate from water solution into *n*-octanol phase, which dissolves MEK but is nearly immiscible with water. The overall goal of this problem is to separate the feed stream into two streams that have greater than 90% purity of water and MEK. In addition, *n*-octanol will be recovered so that it can be reused.

Liquid–liquid extraction, or simply solvent extraction, is a method to separate compounds based on their relative solubilities in two different immiscible liquids, usually water and an organic solvent. It is an extraction of a substance from one liquid into another liquid phase. Liquid–liquid extraction is a basic technique in chemical industries. The term partitioning is commonly used to refer to the underlying chemical and physical processes involved in liquid–liquid extraction. The term solvent extraction can also refer to the separation of a substance from a mixture by preferentially dissolving that substance in a suitable solvent. Solvent extraction is used in roasted coffee beans, ore processing, production of fine organic compounds, processing of perfumes, and production of vegetable oils and food flavoring agents.

5.2 THE PROPER SELECTION FOR PROPERTY METHOD FOR EXTRACTION PROCESSES

As pointed in the previous chapters, selection of the thermodynamic method is one of the most critical and important steps in process simulation; nevertheless, the selection of the

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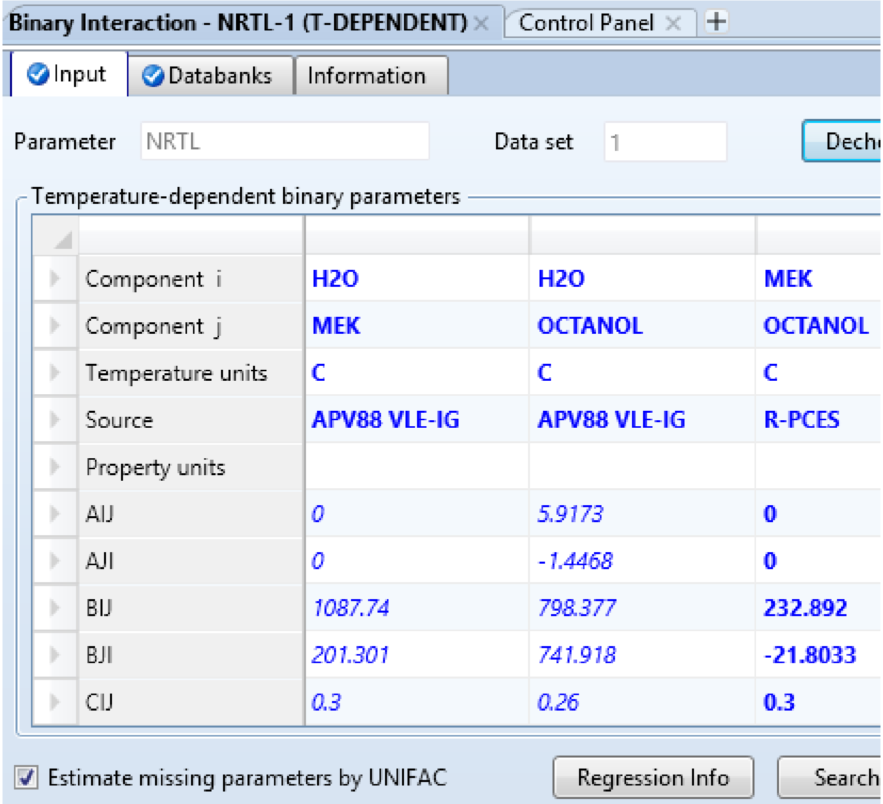
method, to a large extent, is affected by the property of the chemical species making up the liquid mixture and the applied pressure and temperature. Each of such chemicals has its own specific characteristics in terms of the types of intra- and intermolecular forces involved and its molecular volume (i.e., the size of the building block of the compound). Consequently, each method has its own application limitation, and a thermodynamic method of a particular type is only applicable to a particular group of chemical compounds. Finally, the presence of experimental data will help the engineer identify the method that will be the most adequate for his/her own process/chemicals.

With extraction processes, we need a thermodynamic model that accounts for the activity coefficient of a given species in liquid media. This can be done using activity-coefficient property methods. In general, the activity-coefficient models are versatile, accommodating a high degree of solution non-ideality into the model. On the other hand, when applied to vapor–liquid equilibrium (VLE) calculations, they can only be used for the liquid phase and another model (usually an equation of state) is needed for the vapor phase. Activity coefficient models usually perform well for systems of polar compounds at low pressures and away from the critical region. They are the best way to represent highly non-ideal liquid mixtures at low pressure systems. Examples are NRTL, Pitzer, Van Laar, UNIFAQ, UNIQUAC, and Wilson. For the sake of brevity, we examine three of them. The first is the **N**on-**R**andom **T**wo **L**iquid ("**NRTL**") model, recommended for highly non-ideal chemical systems, which can be used for VLE and LLE applications. The second is the **UNI**versal **QUA**si-**C**hemical ("**UNIQUAC**") model that can be used in the description of phase equilibria (SLE, LLE, and VLE). "**UNIQUAC**" model is also called the lattice model and has been derived from a first-order approximation of interacting molecular surfaces in statistical thermodynamics. The third and last is the **UNI**QUAC **F**unctional-group **A**ctivity **C**oefficients ("**UNIFAC**"), which is a semiempirical system for the prediction of non-electrolyte activity in non-ideal mixtures. "**UNIFAC**" uses the group contribution method (i.e., atomic functional groups that make up the given solute and solvent molecules) for a liquid mixture to calculate activity coefficients.

To demonstrate this, we show the single-stage extraction simulation results using the three selected property models: "**NRTL**", "**UNIFAC**", and "**UNIQUAC**". We use a simple (single-) stage extraction unit to differentiate the fitness of the property method from one another and then we move to a multistage extraction column. So, open Aspen Plus® and select the template as "**Specialty Chemicals with Metric Units**".

In the first property method test, the property method called "**NRTL**" will be automatically assigned. Make sure your simulation is set to this base method.

Under "**Properties**" environment, assure that the option "*Estimate missing parameters by UNIFAC*" is selected under "**Methods**" | "**Parameters**" | "**Binary Interaction**" | "**NRTL-1**" sheet. Click on "**Reset**" followed by "**Next**" button to run the simulation and watch out messages of "**Control Panel**" for any error or serious warning. You will notice that the missing MEK–octanol binary interaction parameters will be estimated by "**UNIFAC**" method, as shown in Figure 5.1.



Parameter NRTL Data set 1

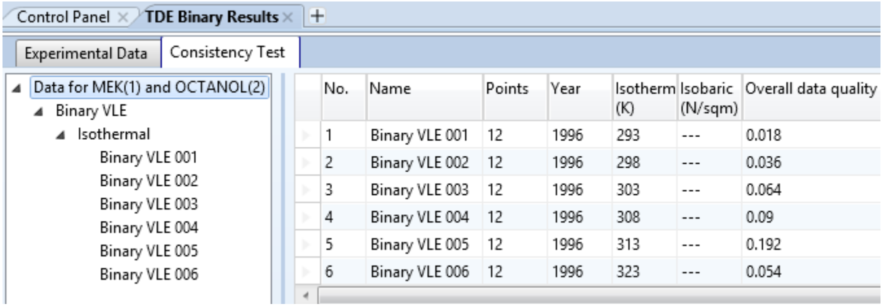
Temperature-dependent binary parameters

Component i	H2O	H2O	MEK
Component j	MEK	OCTANOL	OCTANOL
Temperature units	C	C	C
Source	APV88 VLE-IG	APV88 VLE-IG	R-PCES
Property units			
AIJ	0	5.9173	0
AJI	0	-1.4468	0
BIJ	1087.74	798.377	232.892
BJI	201.301	741.918	-21.8033
CIJ	0.3	0.26	0.3

☑ Estimate missing parameters by UNIFAC

Figure 5.1 The missing MEK–octanol binary interaction parameters are estimated by “**UNIFAC**” method.

In this regard, it is worth mentioning here that no “**NIST/TDE**” LLE experimental data for the MEK–octanol binary mixture is available. Moreover, VLE data are of a bad quality (having low overall data quality indices in consistency tests) for such a binary mixture as shown in Figure 5.2.



Data for MEK(1) and OCTANOL(2)
- Binary VLE
  - Isothermal
    - Binary VLE 001
    - Binary VLE 002
    - Binary VLE 003
    - Binary VLE 004
    - Binary VLE 005
    - Binary VLE 006

No.	Name	Points	Year	Isotherm (K)	Isobaric (N/sqm)	Overall data quality
1	Binary VLE 001	12	1996	293	---	0.018
2	Binary VLE 002	12	1996	298	---	0.036
3	Binary VLE 003	12	1996	303	---	0.064
4	Binary VLE 004	12	1996	308	---	0.09
5	Binary VLE 005	12	1996	313	---	0.192
6	Binary VLE 006	12	1996	323	---	0.054

Figure 5.2 “**NIST/TDE**” binary VLE data for MEK–octanol mixture is of a bad quality having low data quality indices in consistency test.

Switch to “**Simulation**” environment to add the required blocks and streams. Choose the mixing tank from “**Model Palette**” under “**Mixer**” tab, as shown in Figure 5.3.

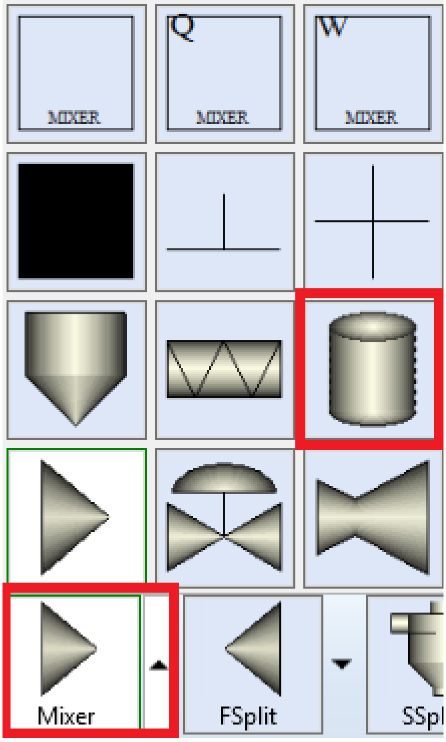


Figure 5.3 Selection of the mixing tank from “**Model Palette**” to represent a single-stage extraction unit.

Add two feed and two product streams and name them as shown in Figure 5.4. The mixer in this case mimics a single-stage extraction unit, where water–MEK mixture is mixed with *n*-octanol for the sake of separating MEK from water. “**H2O+MEK**” stream is set at 25°C and 1 atm with 75 kg/h water and 21 kg/h MEK. “**OCTANOL**” stream is 100 kg/h of pure *n*-octanol at 25°C and 1 bar. Properties of “**EXTRCT**” and “**RFFNTE**” streams will be calculated by Aspen Plus simulator based on the assigned property method. Notice here that the location of feed streams, with respect to the block’s inlet port, is immaterial as we have only a single stage. On the other hand, for the extraction column, the location of a feed stream matters because it may represent the feed mixture or the extracting solvent stream.

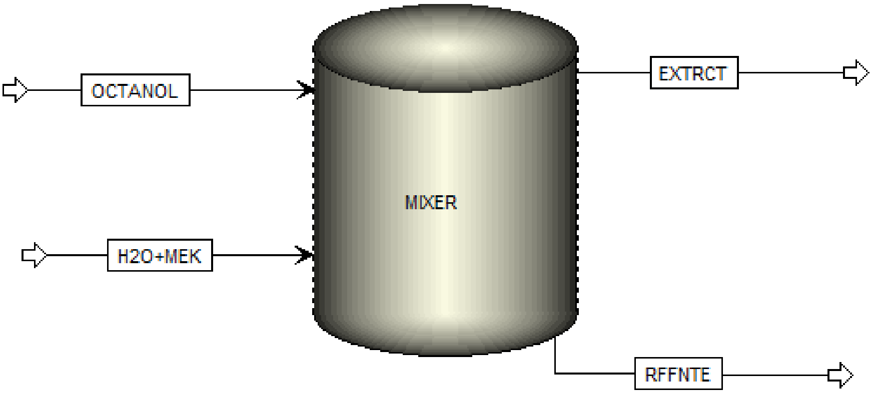
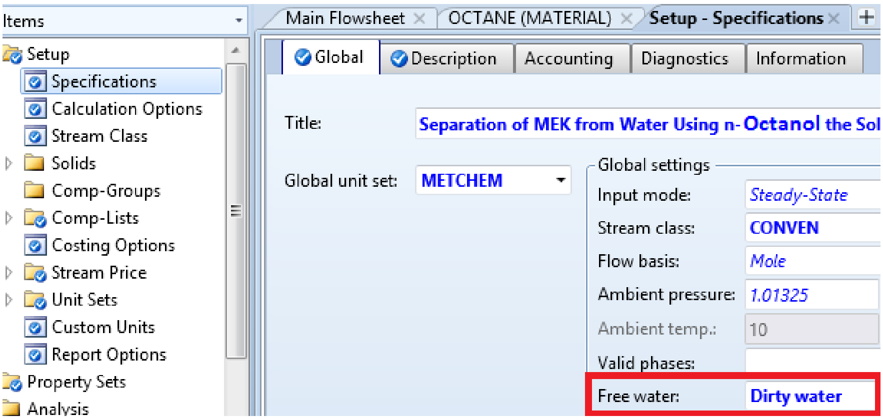


Figure 5.4 A mixer that mimics a single-stage extraction unit for the sake of separating MEK from water using *n*-octanol as the solvent.

Since we expect that trace amounts of both *n*-octanol and MEK remain persistent in water stream, then we will use dirty water for free water choice in “**Navigation**” pane, under “**Setup**” folder | “**Specifications**” sheet | “**Global**” tab window, as shown in Figure 5.5.



Title: Separation of MEK from Water Using n-Octanol the Sol

Global unit set: METCHEM

Input mode: Steady-State

Stream class: CONVEN

Flow basis: Mole

Ambient pressure: 1.01325

Ambient temp.: 10

Valid phases:

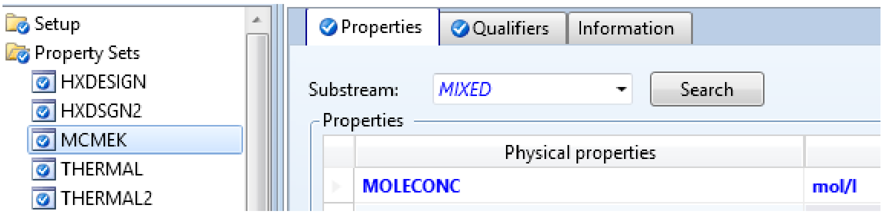
Free water: Dirty water

Figure 5.5 Selection of “**Free water**” mode as “*Dirty water*” for having some dispersed organics in water phase.

We have deliberately chosen water and *n*-octanol as the two immiscible solvents to be used in extraction process simply because there is an abundant literature about the partition coefficient of many organic species between *n*-octanol and water. For example, Sangster [1] reported values of the 10-based logarithmic partition coefficient (log P) of simple organic compounds. The partition coefficient P is defined as $P = (X^{\text{oct}}/X^{\text{H2O}})$, where P represents the dimensionless ratio of the solubility of a given solute species in *n*-octanol to that in water phase at equilibrium conditions (both are saturated phases) in terms of pressure, temperature, and form of solute species (i.e., monomer vs. dimer). For MEK (2-butanone), the recommended value for log P is 0.29 ± 0.05. Let us carry out a sensitivity analysis using the three models and see which one gives realistic results in light of the given experimental data.

5.3 DEFINING NEW PROPERTY SETS

In “**Navigation**” pane under “**Property Sets**” folder, let us define one new property set: “**MCMEK**” that stands for the molar concentration of MEK in a liquid mixture. We see in the next section how such a term is assigned to raffinate and extract streams. Figure 5.6 shows the definition of “**MCMEK**”.



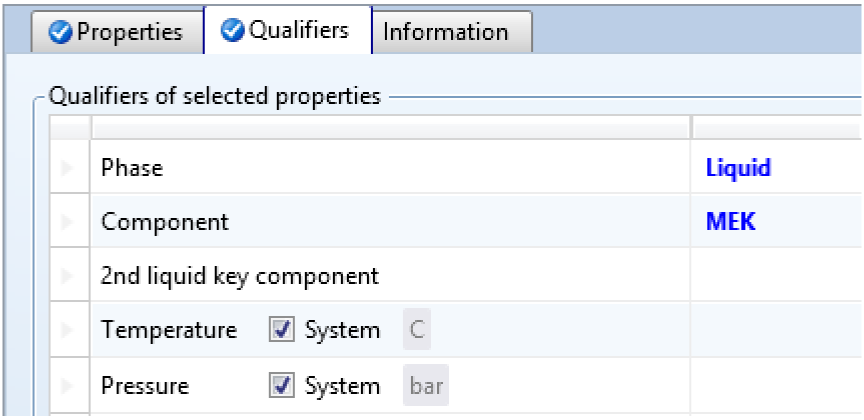
Substream: *MIXED*

Properties

	Physical properties	
	MOLECONC	**mol/l**

Figure 5.6 “**MCMEK**” is defined as the molar concentration of MEK in a liquid mixture.

On the other hand, Figure 5.7 shows the qualifier (the phase to which this property is assigned) of the selected property.



Qualifiers of selected properties

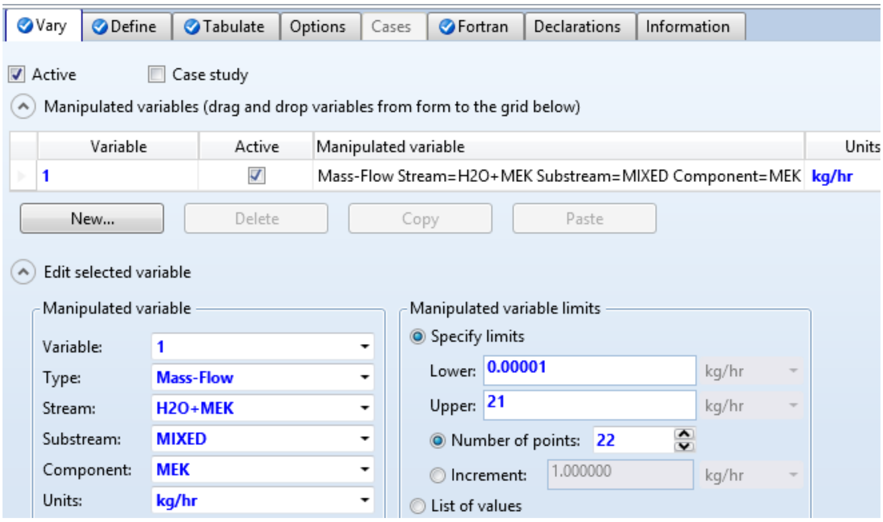
Phase	**Liquid**
Component	**MEK**
2nd liquid key component	
Temperature ☑ System C	
Pressure ☑ System bar	

Figure 5.7 Defining the qualifier (the phase to which the property is associated) of the selected property.

5.4 THE PROPERTY METHOD VALIDATION VERSUS EXPERIMENTAL DATA USING SENSITIVITY ANALYSIS

In “**Navigation**” pane, go to “**Model Analysis Tools**” | “**Sensitivity**”. At the end of the form, click on the “**New**” button and choose a name for this sensitivity. The default name is “**S-1**”. When you have done this, the “**Vary**” tab window should look like that in Figure 5.8.

Given that the maximum solubility of MEK in water at 20°C is 22.5 wt%, according to the National Institute for Occupational Safety and Health (US CDC) data [2], which



☑ Active ☐ Case study

Manipulated variables (drag and drop variables from form to the grid below)

Variable	Active	Manipulated variable	Units
1	☑	Mass-Flow Stream=H2O+MEK Substream=MIXED Component=MEK	kg/hr

Edit selected variable

Manipulated variable

Variable: 1
Type: Mass-Flow
Stream: H2O+MEK
Substream: MIXED
Component: MEK
Units: kg/hr

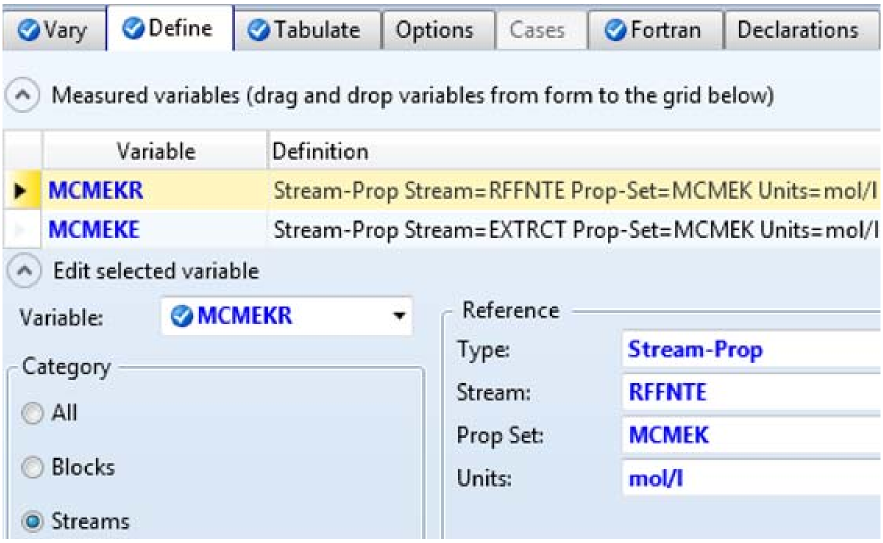
Manipulated variable limits

● Specify limits
Lower: 0.00001 kg/hr
Upper: 21 kg/hr
● Number of points: 22
○ Increment: 1.000000 kg/hr
○ List of values

Figure 5.8 The mass flow rate of MEK in "**H2O+MEK**" stream is to be varied from 0.00001 to 21 kg/h.

amounts almost to 21.8 kg/75 kg of water, we would like to vary MEK flow rate in "**H2O+MEK**" feed stream from almost zero up to the maximum solubility of MEK in water, that is, 21 kg/h as shown in the "**Vary**" tab window. The solubility of MEK in water decreases with temperature; hence, we restricted the upper limit to 21 kg/h.

Figure 5.9 shows the "**Define**" tab window where two flowsheet variables are defined as the molar concentration of MEK in raffinate ("**RFFNTE**") and extract ("**EXTRCT**") streams.



Measured variables (drag and drop variables from form to the grid below)

Variable	Definition
MCMEKR	Stream-Prop Stream=RFFNTE Prop-Set=MCMEK Units=mol/l
MCMEKE	Stream-Prop Stream=EXTRCT Prop-Set=MCMEK Units=mol/l

Edit selected variable

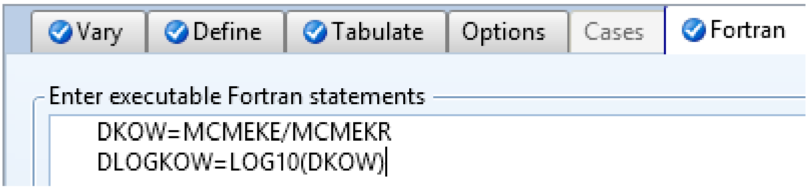
Variable: MCMEKR

Category
○ All
○ Blocks
● Streams

Reference
Type: Stream-Prop
Stream: RFFNTE
Prop Set: MCMEK
Units: mol/l

Figure 5.9 Defining two flowsheet variables "**MCMEKR**" and "**MCMEKE**" that stand for the molar concentration of MEK in raffinate and extract streams, respectively.

We will go to the "**Fortran**" tab window and define the partition coefficient ($P = K_{OW}$) as "**DKOW**" and its base-10, logarithmic mean value ($\log_{10} P = \log_{10} K_{OW}$) as "**DLOGKOW**". Both terms are prefixed by "D" to make them double not integer values, according to FORTRAN language coding. The "**Fortran**" tab window is shown in Figure 5.10. Notice that for the single-stage storage tank, the upper phase (i.e., "**EXTRCT**") represents the organic phase and the lower phase ("**RFFNTE**") represents the aqueous phase. You can verify such phases via looking at the simulation results and see which one is rich in what.

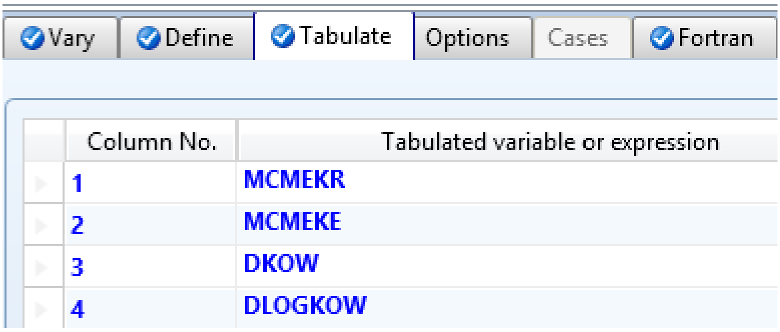


Enter executable Fortran statements

```
DKOW=MCMEKE/MCMEKR
DLOGKOW=LOG10(DKOW)
```

Figure 5.10 In "**Fortran**" tab window, we define P (or, K_{OW}) and $\log_{10} P$ (or, $\log_{10} K_{OW}$) as "**DKOW**" and "**DLOGKOW**", respectively. Both terms are prefixed by "D" to make them double not integer values.

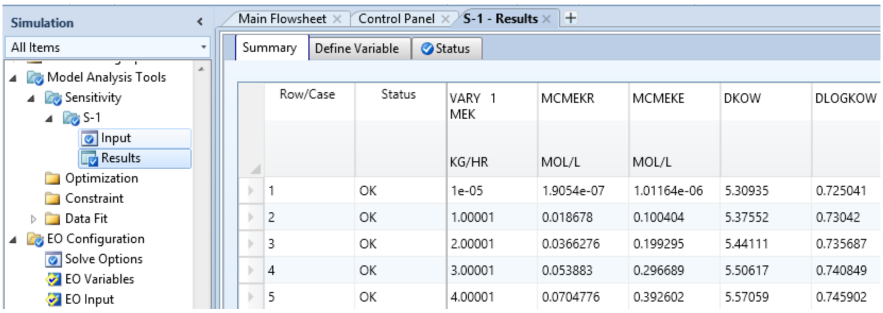
Finally, the "**Tabulate**" tab window is the place for presenting the data column-wise as shown in Figure 5.11.



Column No.	Tabulated variable or expression
1	MCMEKR
2	MCMEKE
3	DKOW
4	DLOGKOW

Figure 5.11 The "**Tabulate**" tab window for column-wise data presentation.

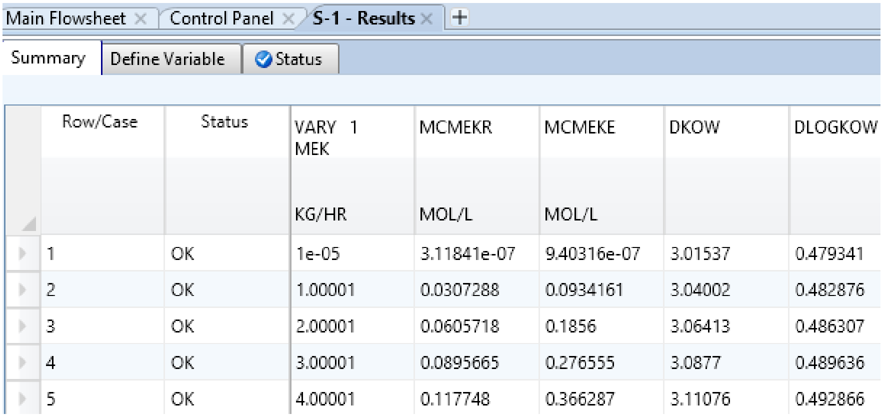
Reset and run the show. Figure 5.12 shows the sensitivity analysis results using "**NRTL**" property model. Notice that even at such very low concentrations of MEK (i.e., 0.00001 kg/h MEK flow rate), "**NRTL**" model predicts a value of 0.725, which is higher than the equilibrium value of 0.29.



Row/Case	Status	VARY 1 MEK KG/HR	MCMEKR MOL/L	MCMEKE MOL/L	DKOW	DLOGKOW
1	OK	1e-05	1.9054e-07	1.01164e-06	5.30935	0.725041
2	OK	1.00001	0.018678	0.100404	5.37552	0.73042
3	OK	2.00001	0.0366276	0.199295	5.44111	0.735687
4	OK	3.00001	0.053883	0.296689	5.50617	0.740849
5	OK	4.00001	0.0704776	0.392602	5.57059	0.745902

Figure 5.12 “**NRTL**” property method simulation results where the lowest $\log_{10} P$ value is 0.725 for 0.00001 kg/h MEK flow rate and this value lies above the equilibrium value of 0.29.

In the second property method test, we change the property method to “**UNIFAC**” by temporarily switching to “**Properties**” environment, reinitializing the simulation, and running the show. Switch back to “**Simulation**” environment, reset, and run the show. Figure 5.13 shows the sensitivity analysis results using “**UNIFAC**” property method. Here, at low MEK concentration, the $\log_{10} P$ value is 0.479, which is closer to the equilibrium value of 0.29 than “**NRTL**”-based value.

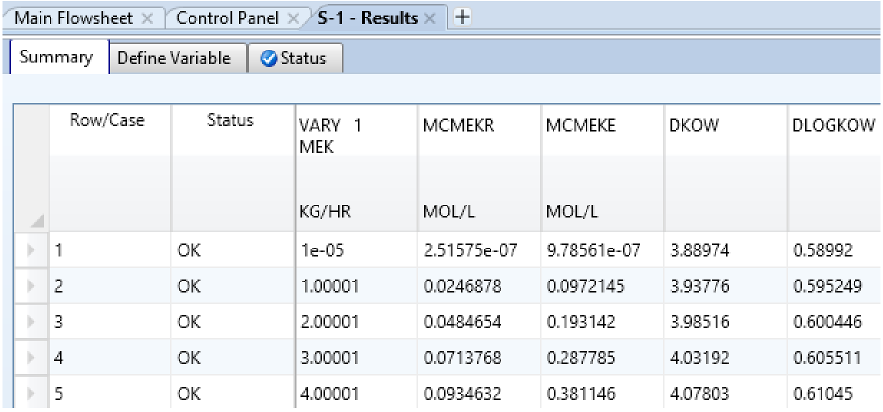


Row/Case	Status	VARY 1 MEK KG/HR	MCMEKR MOL/L	MCMEKE MOL/L	DKOW	DLOGKOW
1	OK	1e-05	3.11841e-07	9.40316e-07	3.01537	0.479341
2	OK	1.00001	0.0307288	0.0934161	3.04002	0.482876
3	OK	2.00001	0.0605718	0.1856	3.06413	0.486307
4	OK	3.00001	0.0895665	0.276555	3.0877	0.489636
5	OK	4.00001	0.117748	0.366287	3.11076	0.492866

Figure 5.13 “**UNIFAC**” property method simulation results where the lowest $\log_{10} P$ value is 0.479 for 0.00001 kg/h MEK flow rate and this value is still above the equilibrium value of 0.29.

In the third property method test, let us change the property method to “**UNIQUAC**” by temporarily switching to “**Properties**” environment, reinitializing the simulation, making sure that the option: “*Estimate missing parameters by UNIFAC*” is selected under “**Methods**” | “**Parameters**” | “**Binary Interaction**” | “**UNIQ-1**” sheet, and running the show. Notice that the missing MEK–octanol binary interaction parameters will be estimated by “**UNIFAC**” method similar to “**NRTL**” case that was shown earlier in Figure 5.1.

Switch back to “**Simulation**” environment, reset, and run the show. Figure 5.14 shows the sensitivity analysis results using “**UNIQUAC**” property method. With “**UNIQUAC**” method, the lowest $\log_{10} P$ value is 0.5899 at very low MEK concentrations, which is still higher than the equilibrium value of 0.29.



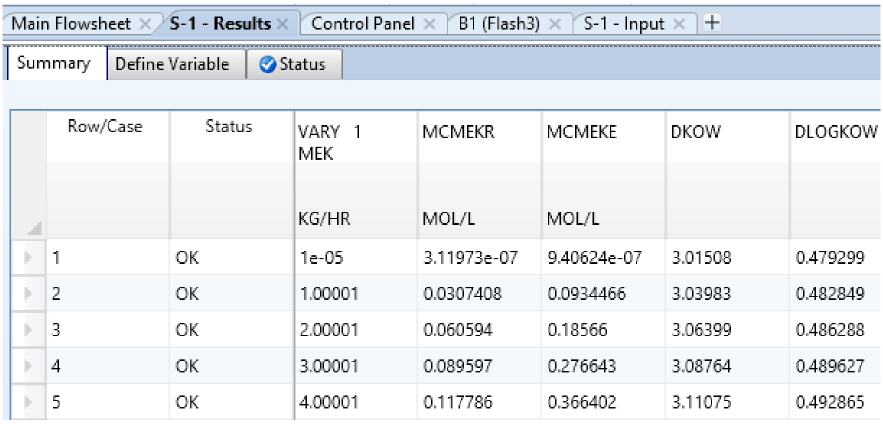
Row/Case	Status	VARY 1 MEK KG/HR	MCMEKR MOL/L	MCMEKE MOL/L	DKOW	DLOGKOW
1	OK	1e-05	2.51575e-07	9.78561e-07	3.88974	0.58992
2	OK	1.00001	0.0246878	0.0972145	3.93776	0.595249
3	OK	2.00001	0.0484654	0.193142	3.98516	0.600446
4	OK	3.00001	0.0713768	0.287785	4.03192	0.605511
5	OK	4.00001	0.0934632	0.381146	4.07803	0.61045

Figure 5.14 “UNIQUAC” property model simulation results where the lowest $\log_{10} P$ value of 0.5899 is accomplished at 0.00001 kg/h of MEK flow rate.

It turns out that “**UNIFAC**” property method gives the smallest difference between experimental and predicted data. Hence, it will be recommended as the property method for extraction of MEK from water using *n*-octanol.

NOTE #1: *“**UNIFAC**” property method turns out to be the most adequate for describing the H2O–MEK–n-octanol extraction system. As pointed out earlier, there exists a property method that will be the most adequate for a given chemical system at a given T and P and it is the design engineer’s duty to seek such a proper model in light of being contrasted* versus *the available experimental data . On the contrary, “**WILSON**” property method failed to partition MEK between the two phases, which practically ended up with huge values of DLOGKOW (test results are not shown here). In fact, the molar concentration value of MEK in “**EXTRCT**” stream (i.e., “**MCMEKE**”) could not be calculated by “**WILSON**” property method, unlike the other three activity-coefficient-based methods.*

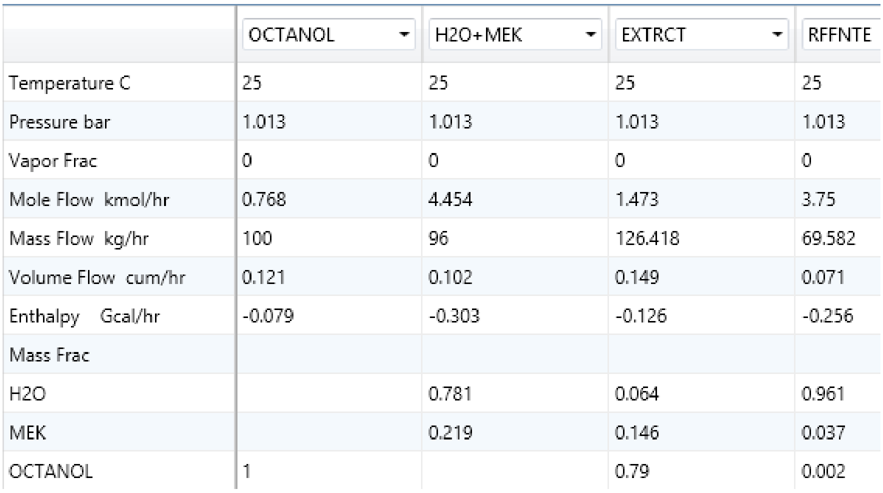
It is worth mentioning here that if the “**Flash3**” type separator is used instead of the mixing tank, the results will be essentially the same. Figure 5.15 shows the sensitivity analysis results upon using the “**Flash3**” type separator for “**UNIFAC**” property method case. Both models assume that if we contact “**H2O+MEK**” with “**OCTANOL**” stream, allow a thorough mixing, and a sufficient time for settling or phase separation, then an equilibrium condition will take place between raffinate (“**RFFNTE**”) and extract (“**EXTRCT**”) leaving streams.



Row/Case	Status	VARY 1 MEK KG/HR	MCMEKR MOL/L	MCMEKE MOL/L	DKOW	DLOGKOW
1	OK	1e-05	3.11973e-07	9.40624e-07	3.01508	0.479299
2	OK	1.00001	0.0307408	0.0934466	3.03983	0.482849
3	OK	2.00001	0.060594	0.18566	3.06399	0.486288
4	OK	3.00001	0.089597	0.276643	3.08764	0.489627
5	OK	4.00001	0.117786	0.366402	3.11075	0.492865

Figure 5.15 "**UNIFAC**" property method simulation results using the "**Flash3**" type separator model are the same as those of the mixing tank model (Figure 5.13).

Figure 5.16 shows the mass fraction of streams entering into or leaving out a single-stage extraction (flash drum) unit using "**UNIFAC**" property method. Notice that the extract stream is very poor in water and, on the contrary, raffinate stream is very rich in water. The outlet vapor stream for the flash drum is zero. Moreover, MEK is more relaxed in octanol than in water environment. In simple words, the extraction process is like the process of migration where people are encouraged (or forced in many cases) to leave their countries and go to a new country (i.e., a new heaven, hopefully).



	OCTANOL	H2O+MEK	EXTRCT	RFFNTE
Temperature C	25	25	25	25
Pressure bar	1.013	1.013	1.013	1.013
Vapor Frac	0	0	0	0
Mole Flow kmol/hr	0.768	4.454	1.473	3.75
Mass Flow kg/hr	100	96	126.418	69.582
Volume Flow cum/hr	0.121	0.102	0.149	0.071
Enthalpy Gcal/hr	-0.079	-0.303	-0.126	-0.256
Mass Frac				
H2O		0.781	0.064	0.961
MEK		0.219	0.146	0.037
OCTANOL	1		0.79	0.002

Figure 5.16 The composition of streams using a single-stage extraction (flash drum) unit as described by "**UNIFAC**" property method.

5.5 A MULTISTAGE EXTRACTION COLUMN

Under “**Properties**” environment, set the property model to “**UNIFAC**”. Under “**Estimation**” folder | “**Setup**” sheet, select “*Estimate all missing parameters*” option. Click “**Reset**” followed by “**Next**” button. Once the properties analysis is completed successfully, switch to “**Simulation**” environment. We will run the same problem, but this time we will choose “**Extract**” column from “**Columns**” tab in “**Model Palette**”. Basically, replace the single-stage mixer by the multistage “**Extract**” type column and your simulation flowsheet will be similar to that shown in Figure 5.17.

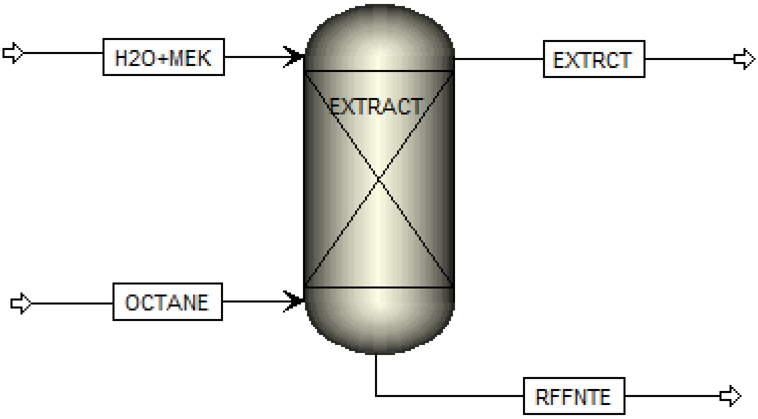
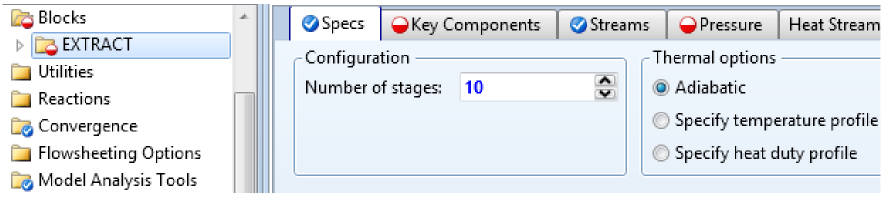


Figure 5.17 Replacement of the single-stage mixer by the multistage extraction column.

Clicking on “**Next**” button will bring the user to “**Setup**” sheet for “**EXTRACT**” column (the fourth icon from left under “**Columns**” tab in “**Model Palette**”). The first sheet is “**Specs**” where the user decides on the number of theoretical stages and selects the thermal option, as shown in Figure 5.18. We will choose an adiabatic extractor with 10 stages.



Configuration

Number of stages: 10

Thermal options

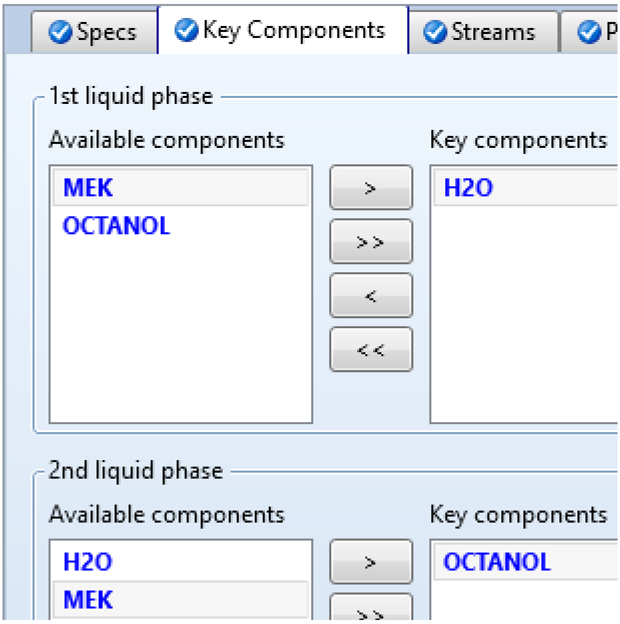
● Adiabatic

○ Specify temperature profile

○ Specify heat duty profile

Figure 5.18 The “**Specs**” tab window where the number of theoretical stages and the selection of thermal option are defined.

After you are done with “**Specs**” tab sheet, go to “**Key Components**” sheet where you need to specify the key component for both “**RFFNTE**” and “**EXTRCT**” streams as shown in Figure 5.19. Use this sheet to specify the key components used to identify the



1st liquid phase

Available components: MEK, OCTANOL

Key components: H2O

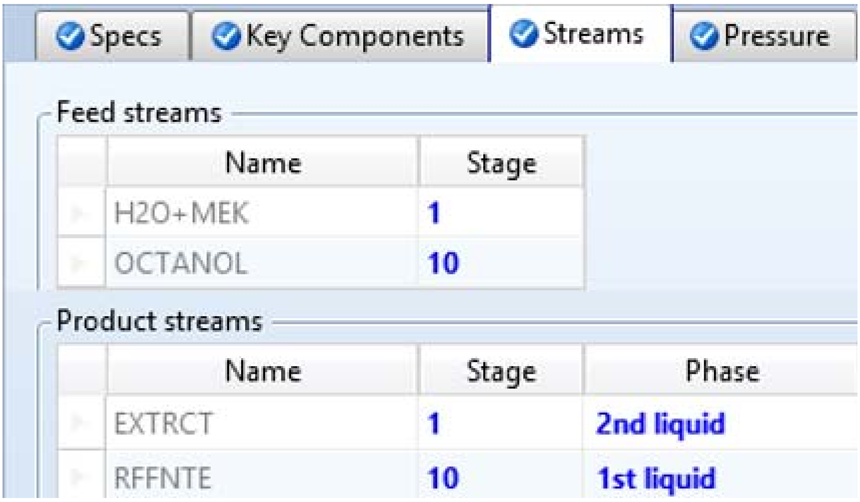
2nd liquid phase

Available components: H2O, MEK

Key components: OCTANOL

Figure 5.19 Selection of two key components one for the “**1st liquid phase**” and another for the “**2nd liquid phase**”.

first and second liquid phases. You must identify the key components in each phase to help the phase-splitting algorithm deal with the wide range of compositions in extractors, which may include only first liquid in the top feed and only second liquid in the bottom feed. It is the concentrations of these key components, not density, which identifies the phases. The first liquid phase flows from the first stage (top) down to the last stage (bottom). The second flows in the opposite direction. *“**Extract**” column model can treat the first liquid phase as either the solvent/extract or feed/raffinate phase*. Here, we have the first liquid as feed/raffinate phase. H_2O component was chosen for the “**1st liquid phase**” and octanol component for the “**2nd liquid phase**”. If you are confused for the first time, go to “**Streams**” tab and Aspen Plus will automatically assign the two liquid phases for the two outlet streams. As shown in “**Streams**” sheet in Figure 5.20, the “**1st liquid phase**” stands for raffinate outlet stream and “**2nd liquid phase**” for extract outlet stream. In Figure 5.19, notice that MEK component can be moved to the right side to be the second key component defining the second liquid phase without altering the final simulation results in terms of flow rates and compositions.



Feed streams

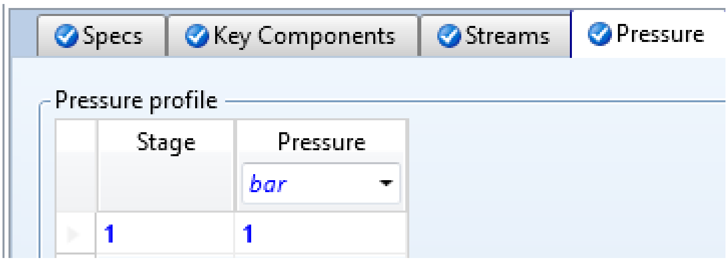
Name	Stage
H2O+MEK	1
OCTANOL	10

Product streams

Name	Stage	Phase
EXTRCT	1	2nd liquid
RFFNTE	10	1st liquid

Figure 5.20 The **Streams** tab window deciphers what the “**1st liquid phase**” and the “**2nd liquid phase**” are all about.

In the “**Pressure**” tab window, you need to define, at least, the value of pressure at one stage. This is shown in Figure 5.21.

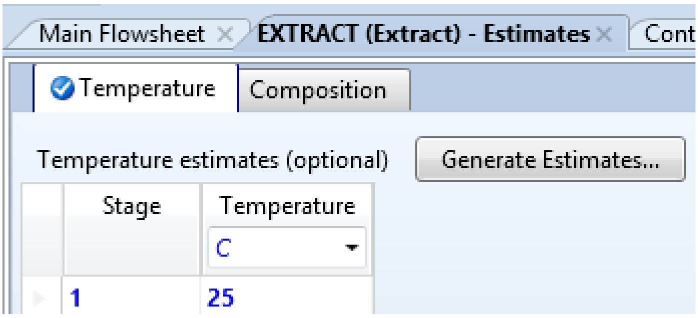


Pressure profile

Stage	Pressure bar
1	1

Figure 5.21 Defining the pressure profile within the extraction column for, at least, one stage.

Clicking on “**Next**” button will bring you to “**Estimates**” sheet, which is the final step where the temperature profile within the extraction column must be defined. Again, you need to specify, at least, the temperature at one stage, as shown in Figure 5.22.

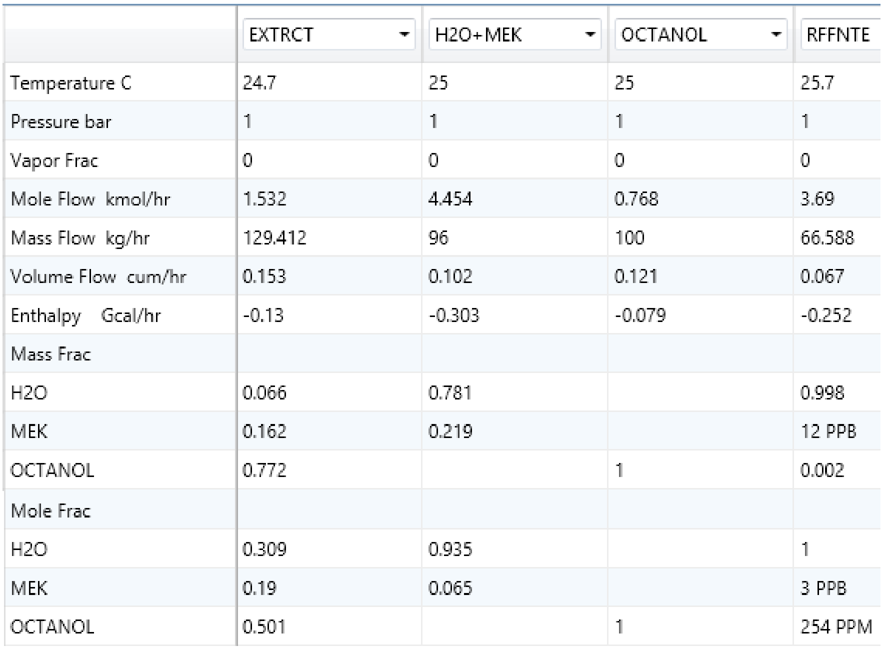


Temperature estimates (optional)

Stage	Temperature C
1	25

Figure 5.22 Defining the temperature profile within the extraction column, at least, at one stage.

Reinitialize and run the show. Figure 5.23 shows the stream results as part of simulation results. The raffinate ("**RFFNTE**") stream is extra pure water (i.e., trace amounts of MEK and *n*-octanol). On the other hand, the extract ("**EXTRCT**") stream is mainly *n*-octanol and MEK. The latter stream will need further purification to split it into almost pure *n*-octanol and pure MEK. This is left as a Homework/Classwork Problem 5.1 for the user to try using "**RadFrac**" distillation column.



	EXTRCT	H2O+MEK	OCTANOL	RFFNTE
Temperature C	24.7	25	25	25.7
Pressure bar	1	1	1	1
Vapor Frac	0	0	0	0
Mole Flow kmol/hr	1.532	4.454	0.768	3.69
Mass Flow kg/hr	129.412	96	100	66.588
Volume Flow cum/hr	0.153	0.102	0.121	0.067
Enthalpy Gcal/hr	-0.13	-0.303	-0.079	-0.252
Mass Frac				
H2O	0.066	0.781		0.998
MEK	0.162	0.219		12 PPB
OCTANOL	0.772		1	0.002
Mole Frac				
H2O	0.309	0.935		1
MEK	0.19	0.065		3 PPB
OCTANOL	0.501		1	254 PPM

Figure 5.23 The estimated properties of the multistage extraction column outlet streams.

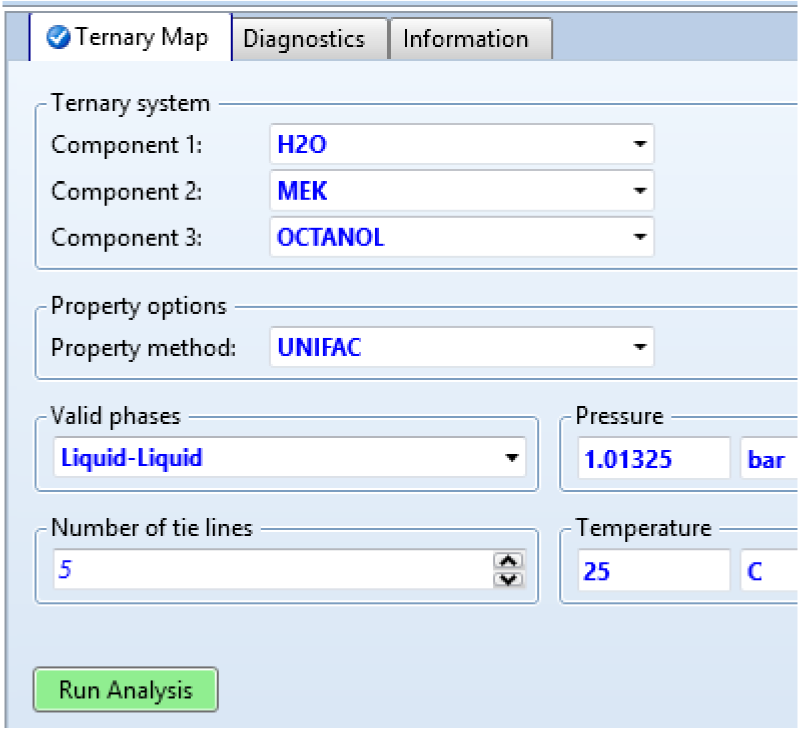
NOTE #2: *The user may raise a question: what about if we directly use distillation to split MEK from water without the necessity of using two units composed of extraction followed later by distillation?*

The answer is simply we can and the right choice will be judged by minimizing the total annual cost to be paid for each configuration. Of course, the total annual cost is the sum of the annual operating and annual fixed cost. In addition, the presence of an azeotrope at a certain composition will restrict using distillation; instead, extraction is one alternative that can be used to circumvent the azeotrope condition. If an azeotrope test is carried out, you will notice that an azeotrope exists between MEK and water at 1.0 atm, $T = 73.64°C$, and $X_{MEK} = 0.6925$ mole fraction (or $x_{MEK} = 0.9001$ mass fraction). This azeotropic condition is shown as a standalone blue square at the right side of the triangle in Figure 5.25. This means that if we use atmospheric distillation for our feed mixture with $X_{MEK} = 0.065$ ($x_{MEK} = 0.219$), the top distillate will have at most 0.9 mass fraction of MEK (the rest will be water); hence, we cannot end up with almost a pure stream of MEK as it is typical in distillation processes to end up with almost pure streams.

We also did it here for the sake of learning how to use the extraction model in Aspen Plus.

5.6 THE TRIANGLE DIAGRAM

Finally, under “**Properties**” environment, click on “**Home**” ribbon | “**Analysis**” group | “**Ternary Diag**” button to open up the “**Ternary Map**” tab form to select the three components, the temperature, and the pressure, as shown in Figure 5.24. Notice that in “**Navigation**” pane, a subfolder named “**TERDI-1**” is automatically created under “**Analysis**” folder.



Component 1: H2O
Component 2: MEK
Component 3: OCTANOL
Property method: UNIFAC
Valid phases: Liquid-Liquid
Pressure: 1.01325 bar
Number of tie lines: 5
Temperature: 25 C

Figure 5.24 The "**Ternary Map**" tab form where the user decides on the three components, *T*, and *P*.

Click on "**Run Analysis**" button and the ternary map for the ternary mixture will pop up as shown in Figure 5.25. Each vertex of the triangle represents the 100% pure substance; the top represents MEK, the right-bottom water, and the left-bottom octanol. On the other hand, each side of the triangle represents the binary mixture; for example, the right side is for water–MEK mixture. Anywhere inside the triangle, we will have a ternary mixture made of three components. The region (denoted by Aspen Plus as phase envelope) applicable for extraction processes resides at the bottom-right region of the triangle. To read the composition for a given point using the ternary diagram of three compositional scales, let us consider the point with a large red circle shown in Figure 5.25. Draw three lines issuing from the same spot and each of which is drawn parallel to one side of the triangle and ends at one compositional scale. For the encircled spot, the mole fraction for water reads about 0.40; for MEK 0.45; and for octanol 0.15. This can also be seen while being under "**Properties**" environment in "**Navigation**" pane at "**Analysis**" | "**TERDI-1**" | "**Results**" sheet, as shown in Figure 5.26.

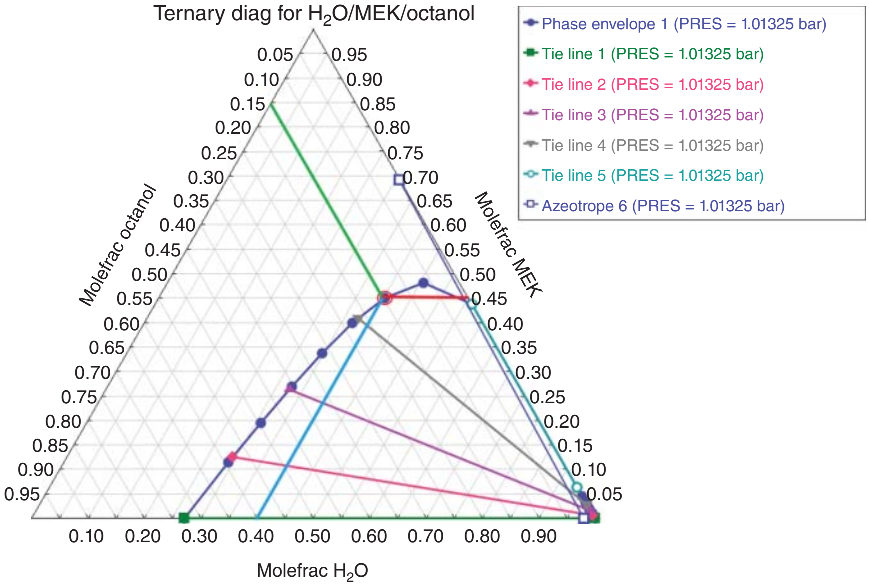
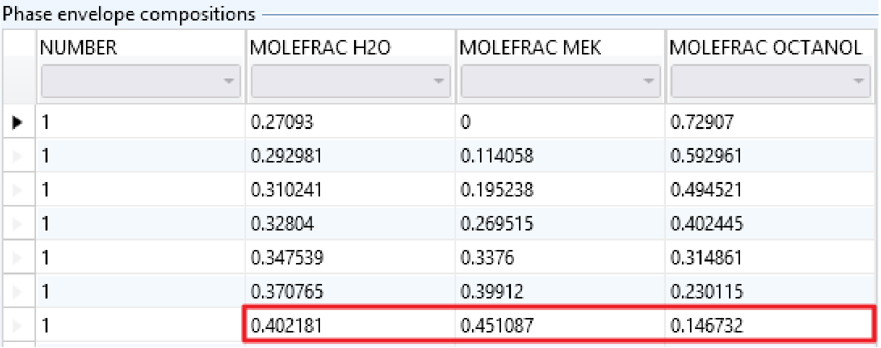


Figure 5.25 The triangle diagram showing the location of the operable region for extraction processes. The blue standalone square on the right side represents an azeotropic condition for the binary mixture of MEK and water. *See Plate section for color representation of this figure.*



Phase envelope compositions

	NUMBER	MOLEFRAC H2O	MOLEFRAC MEK	MOLEFRAC OCTANOL
▶	1	0.27093	0	0.72907
	1	0.292981	0.114058	0.592961
	1	0.310241	0.195238	0.494521
	1	0.32804	0.269515	0.402445
	1	0.347539	0.3376	0.314861
	1	0.370765	0.39912	0.230115
	1	0.402181	0.451087	0.146732

Figure 5.26 The composition of the spot within the large red circle is also shown in “**Analysis**” | “**TERDI-1**” | “**Results**” sheet.

NOTE #3: *There exists a mutual solubility between water and MEK at low and high mole fraction of water. See Stephenson [3]. These two mutual solubility points represent the two endpoints of the turquoise-line that exactly lies on the right side of the triangle shown in Figure 5.25.*

REFERENCES

[1] Sangster, J. (1989) Octanol–water partition coefficients of simple organic compounds. *Journal of Physical and Chemical Reference Data*, **18** (3), 1111–1227.

[2] http://www.cdc.gov/niosh/ipcsneng/neng0179.html (accessed March 30, 2016).

[3] Stephenson, R.M. (1992) Mutual solubilities: water–ketones, water–ethers, and water–gasoline–alcohols. *Journal of Chemical Engineering Data*, **37** (1), 80–95.

HOMEWORK/CLASSWORK 5.1 (SEPARATION OF MEK FROM OCTANOL)

Given the extract ("**EXTRCT**") outlet stream, design a "**RadFrac**" distillation column that will handle the separation of MEK–1-octanol mixture into two streams, one pure in 1-octanol and another very rich in MEK. Water, in addition to being condensed as "**COND-H2O**" stream, is present in trace amounts and will be part of the top stream as shown in Figure 5.27. The property model is "**UNIFAC**".

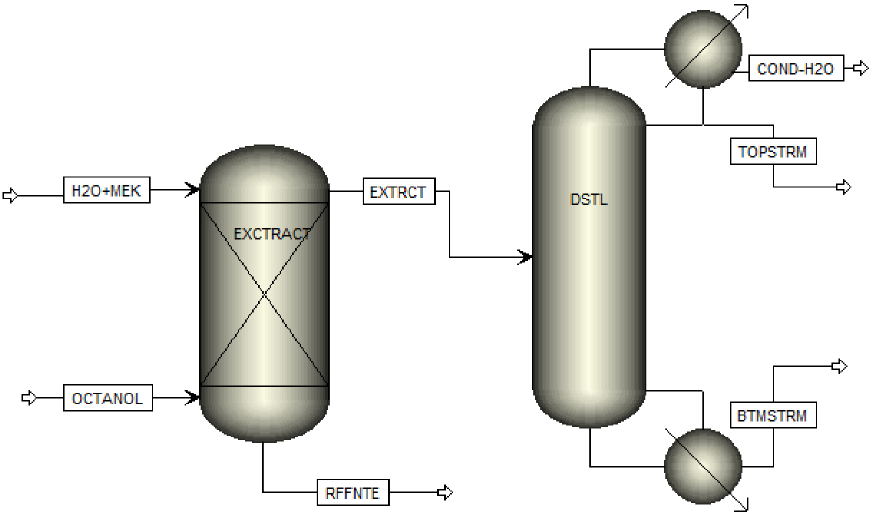
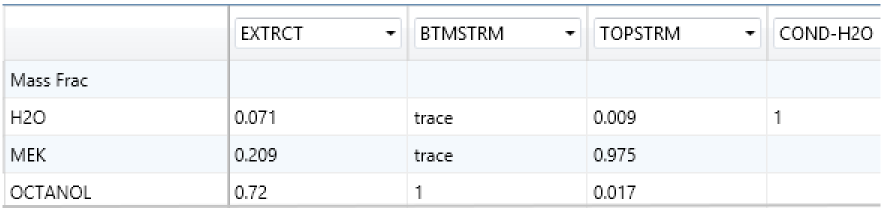


Figure 5.27 The addition of "**RadFrac**" distillation column to the existing flowsheet to split "**EXTRCT**" stream into MEK and *n*-octanol streams.

Your results should be more or less similar to those shown in Figure 5.28.



	EXTRCT	BTMSTRM	TOPSTRM	COND-H2O
Mass Frac				
H2O	0.071	trace	0.009	1
MEK	0.209	trace	0.975	
OCTANOL	0.72	1	0.017	

Figure 5.28 Separation of "**EXTRCT**" mixture stream into three pure streams.

HOMEWORK/CLASSWORK 5.2 (SEPARATION OF MEK FROM WATER USING OCTANE)

Repeat the same task in Homework/Classwork 5.1 but replace 1-octanol by 1-octane, as shown in Figure 5.29.

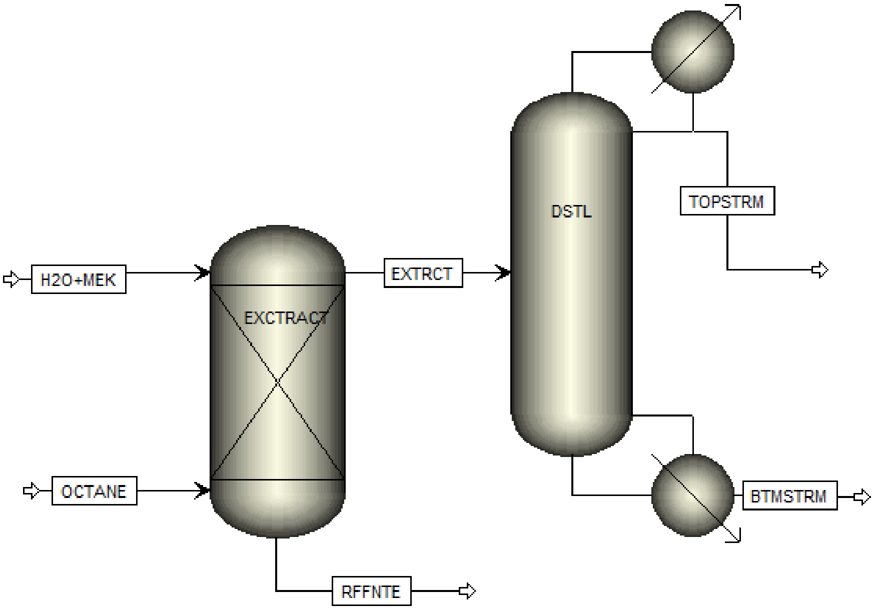
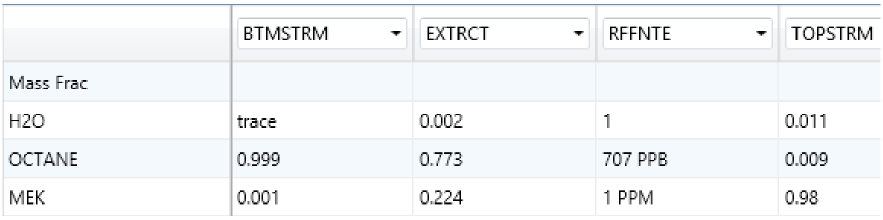


Figure 5.29 The process flowsheet for separating MEK from water using 1-octane.

All input data are the same except for 1-octanol being replaced by 1-octane. The property method can be any activity coefficients based method. Figure 5.30 shows stream results using "**UNIQUAC**" as the property method. In brief, your task is to separate MEK from water using 1-octane while ending up with almost pure streams of water, MEK, and octane.



	BTMSTRM	EXTRCT	RFFNTE	TOPSTRM
Mass Frac				
H2O	trace	0.002	1	0.011
OCTANE	0.999	0.773	707 PPB	0.009
MEK	0.001	0.224	1 PPM	0.98

Figure 5.30 Stream results for MEK–water separation using 1-octane. The property method used is "**UNIQUAC**".

HOMEWORK/CLASSWORK 5.3 (SEPARATION OF ACETIC ACID FROM WATER USING ISOPROPYL BUTYL ETHER)

A 1000 kg/h of acetic acid–water mixture with 45 wt% acetic acid will be extracted using pure isopropyl butyl ether (IPBE) as the solvent. The residual concentration of acetic acid has to be about 9 wt% or less and that of IPBE 0.3 wt% via using a multistep counter flow extraction column operating at 20°C. Design an extraction column that can handle the job by determining the required solvent flow rate (kg/h) and the number of stages. In addition to the default "**NRTL**" property method and based on the given process and type of components being handled, use the "**Property Method Selection Assistant**" to assist you in finding the most adequate property method. The process flowsheet is shown in Figure 5.31. Show the ternary diagram, based on either liquid–liquid or vapor–liquid–liquid phase equilibrium, for the three-component mixture at 1 atm and 25°C for LLE case or 1 atm only for VLLE case. Notice that not all recommended methods may perform well in converging to a reasonable solution or even be able to predict the ternary diagram for the given three-component solution. Moreover, elevate the maximum number of iterations to 50 instead of 25, under "**Convergence**" subfolder. This problem serves as a good example in demonstrating the discrepancy in predicting flow and fluid stream properties between one recommended property method and another.

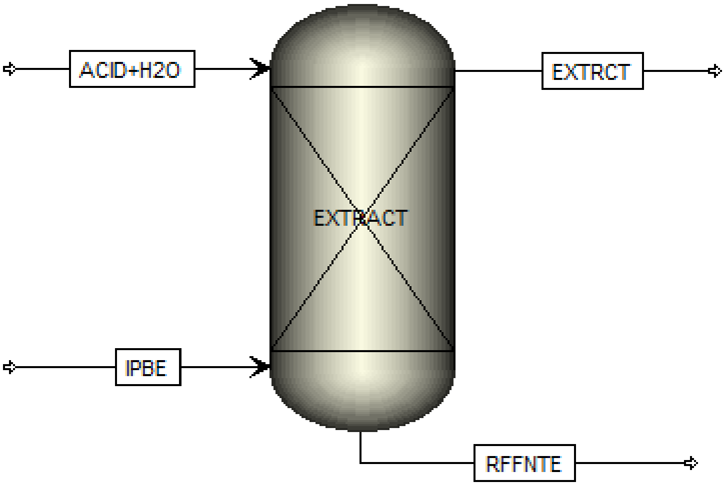


Figure 5.31 The process flowsheet for the extraction of acetic acid from water using isopropyl butyl ether (IPBE).

HOMEWORK/CLASSWORK 5.4 (SEPARATION OF ACETONE FROM WATER USING TRICHLOROETHANE)

A 1000 kg/h of acetone–water mixture with 40 wt% acetone will be extracted using pure 1,1,2-trichloroethane (TCE) as the solvent. The residual concentration of acetone has to be about 0.2 wt% and that of TCE 0.5 wt% via using a multistep counter flow extraction column operating at 20°C. Design an extraction column that can handle the job by determining the required solvent flow rate (kg/h) and the number of stages. The property method is set to default, that is, "**NRTL**". The process flowsheet is shown in Figure 5.32. Show the ternary diagram, based on liquid–liquid phase equilibrium, for the three-component mixture at 1 atm and 25°C.

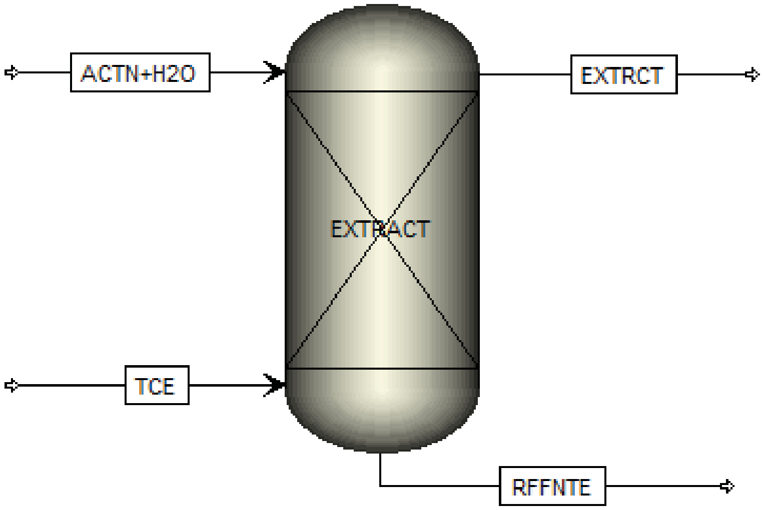


Figure 5.32 The process flowsheet for extraction of acetone from water using pure 1,1,2-trichloroethane (TCE).

HOMEWORK/CLASSWORK 5.5 (SEPARATION OF PROPIONIC ACID FROM WATER USING MEK)

A 1000 kg/h of propionic acid–water mixture with 40 wt% propionic acid will be extracted using methyl ethyl ketone (MEK) as the solvent. The residual concentration of propionic acid has to be almost 0.0 wt% and that of MEK 6 wt% via using a multistep counter flow extraction column operating at 20°C. Design an extraction column that can handle the job by determining the required solvent flow rate (kg/h) and the number of stages. In addition to the default "**NRTL**" property method and based on the given process and type of components being handled, use the "**Property Method Selection Assistant**" to assist you in finding the most adequate property method. The process flowsheet is shown in Figure 5.33. Show the ternary diagram, based on either liquid–liquid or vapor–liquid–liquid

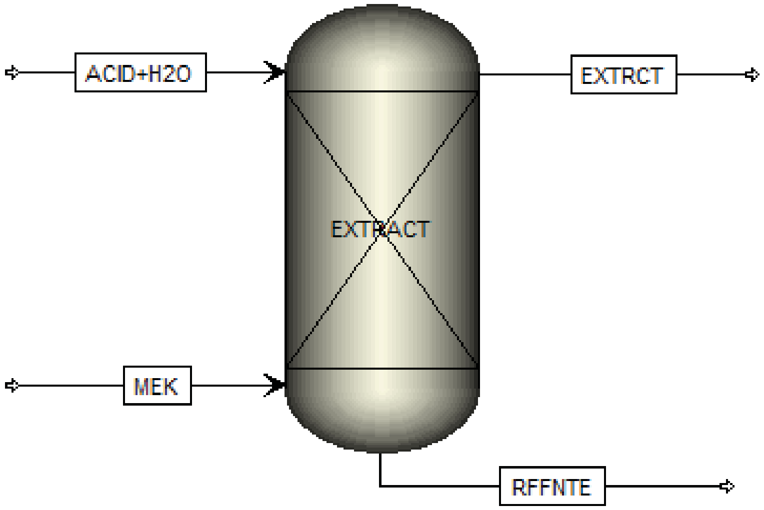


Figure 5.33 The process flowsheet for extraction of propionic acid from water using pure methyl ethyl ketone (MEK).

phase equilibrium, for the three-component mixture at 1 atm and 25°C for LLE case or 1 atm only for VLLE case. Notice that not all recommended methods may perform well in converging to a reasonable solution or even be able to predict the ternary diagram for the given three-component solution. Moreover, elevate the maximum number of iterations to 50 instead of 25, under "**Convergence**" subfolder. This problem serves as another good example in demonstrating the discrepancy in predicting flow and fluid stream properties between one recommended property method and another.

6

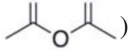
REACTORS WITH SIMPLE REACTION KINETIC FORMS

6.1 PROBLEM DESCRIPTION

This chapter deals with chemical reactor design. The problem was taken from Fogler [1]. The problem was stated and solved in Example 8.5, under two reactor conditions: an adiabatic plug-flow reactor (PFR) and a PFR with a constant cooling temperature.

NOTE #1: *This chapter only covers reactions with simple kinetics (i.e., what is called "**POWERLAW**" type reaction in Aspen Plus terminology). Complex kinetics type of reactions (i.e., what is called "**LHHW**" type reaction in Aspen Plus terminology) will be the battlefield of CHAPTER 7. I split Aspen Plus reaction engineering applications into two chapters so that the student does not get overwhelmed or clotted by the versatile features of Aspen Plus being applied to chemical reaction engineering (or reactor design).*

6.2 DEFINING REACTION RATE CONSTANT TO ASPEN PLUS® ENVIRONMENT

In a treatment of the design of an acetic anhydride () manufacturing facility, it is stated that one of the key steps is the vapor-phase cracking of acetone to ketene and methane:

$$CH_3COCH_3 \rightarrow CH_2CO + CH_4 \tag{6.1}$$

Aspen Plus®: Chemical Engineering Applications, First Edition. Kamal I.M. Al-Malah.

Companion Website: www.wiley.com/go/Al-Malah/AspenPlusApplications

It is further stated that this reaction is first order with respect to acetone and that the specific reaction rate can be expressed by

$$\ln k = 34.34 - 34{,}222\,/\,T \tag{6.2}$$

In this design, it is desired to feed 7850 kg of acetone per hour to a tubular reactor. If the reactor is adiabatic, the feed is pure acetone, the inlet temperature is 1035 K, and the pressure is 162 kPa (1.6 atm), what will be the tubular reactor volume needed to achieve 20% conversion?

Acetic anhydride is prepared by the reaction of ethenone (ketene) with acetic acid at 45–55°C and low pressure (0.05–0.2 bar).

$$\mathrm{H_2C = C = O\ +\ CH_3COOH\ \rightarrow (CH_3CO)_2O}\ \ (\Delta H = -63\ \mathrm{kJ/mol}) \tag{6.3}$$

There are two different ways by which we can define the reaction rate constant to Aspen Plus environment. We arrange Equation 6.2 in these two forms: one form contains a reference temperature, T_o, and another does not. However, both forms are equivalent. Take the exponent value for both sides of Equation 6.2 and we have

$$k = e^{34.34\,-\frac{34{,}222}{T}} = e^{34.34}e^{-\frac{34{,}222}{T}} = e^{34.34} \times e^{-\frac{34{,}222 \times R}{R \times T}} = 8.1973 \times 10^{14} \times e^{-\frac{284{,}521.7}{R \times T}} \tag{6.4}$$

Alternatively, T_o can be arbitrarily chosen and k^* will be calculated accordingly. Let us use $T_o = 1000$ K. We have

$$k = k^* e^{-\frac{E}{R}\left(\frac{1}{T}-\frac{1}{T_o}\right)} = k^* e^{-\frac{E}{R}\left(\frac{1}{T}-\frac{1}{1000}\right)} = k^* \times e^{-\frac{E}{R}\left(\frac{1}{T}\right)} \times e^{\frac{E}{R}\left(\frac{1}{1000}\right)} \tag{6.5}$$

Equate both expressions of k, we have

$$k = e^{34.34}e^{-\frac{34{,}222}{T}} = k^* e^{-\frac{E}{R}\left(\frac{1}{T}\right)} e^{\frac{E}{R}\left(\frac{1}{1000}\right)} \tag{6.6}$$

First, equate the exponent terms, on both sides, which contain *1/T* term to calculate E:

$$\begin{aligned} -\frac{34{,}222}{T} &= -\frac{E}{R}\left(\frac{1}{T}\right) \Rightarrow \frac{E}{R} = 34{,}222 \Rightarrow E = R \times 34{,}222 = 8.314 \times 34{,}222 \\ &= 284{,}521.7\mathrm{J/mol} \end{aligned} \tag{6.7}$$

Notice that E is the same as that in Equation 6.4. Second, substitute the value of E from Equation 6.7 into Equation 6.6 and equate constants on both sides of Equation 6.6.

$$e^{34.34} = k^* e^{\frac{E}{R}\left(\frac{1}{1000}\right)} = k^* e^{\frac{284{,}521.7}{8.314}\left(\frac{1}{1000}\right)} = k^* e^{34.222} \Rightarrow k^* = e^{34.34-34.222} = e^{0.118} = 1.125 \tag{6.8}$$

Notice that k^* is calculated in terms of $T_o = 1000$ K. However, E is fixed for a given reaction and does not depend on T_o.

Equation 6.5 becomes

$$k = k^* e^{-\frac{E}{R}\left(\frac{1}{T}-\frac{1}{T_o}\right)} = 1.125 e^{-\frac{284{,}521.7}{\mathrm{R}}\left(\frac{1}{T}-\frac{1}{1000}\right)} \tag{6.9}$$

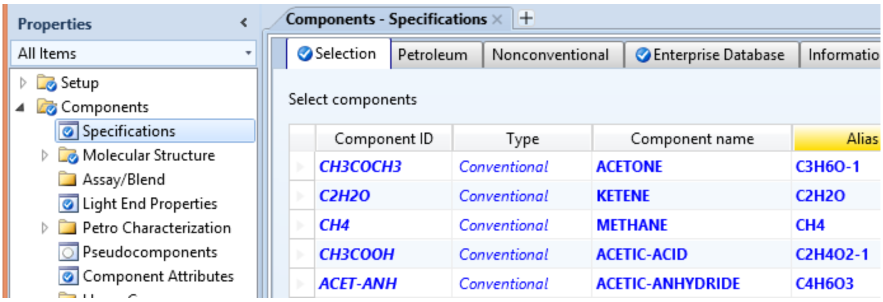
where k is in reciprocal seconds (for a 1st–order reaction) and T is in Kelvin.

In general, the rate constant k can be expressed in either form, Equation 6.4 or 6.9, depending on the chemical reaction engineering textbook being used.

6.3 ENTERING COMPONENTS AND METHOD OF PROPERTY

Using “**Specialty Chemicals with Metric Units**” template, create an Aspen Plus project. Under “**Properties**” environment, in “**Navigation**” pane, go to “**Setup**” | “**Global**” sheet and enter the title: “*Production of Acetic Anhydride*”.

In “**Navigation**” pane, click on “**Components**” folder, and you will be faced by “**Selection**” tab window. Use “**Find**” button, shown at the bottom of “**Selection**” tab window, to search for components by name or chemical formula. Add the following components: ACETONE (CH_3COCH_3), KETENE (C_2H_2O), METHANE (CH_4), ACETIC-ACID (CH_3COOH), and ACETIC-ANHYDRIDE (ACET-ANH) as shown in Figure 6.1.

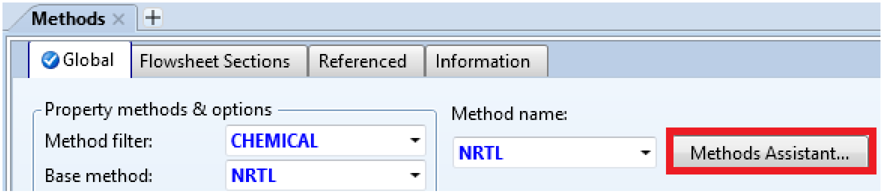


Select components

Component ID	Type	Component name	Alias
CH3COCH3	Conventional	ACETONE	C3H6O-1
C2H2O	Conventional	KETENE	C2H2O
CH4	Conventional	METHANE	CH4
CH3COOH	Conventional	ACETIC-ACID	C2H4O2-1
ACET-ANH	Conventional	ACETIC-ANHYDRIDE	C4H6O3

Figure 6.1 Entering reactants and products of the reactions involved in the synthesis of acetic anhydride.

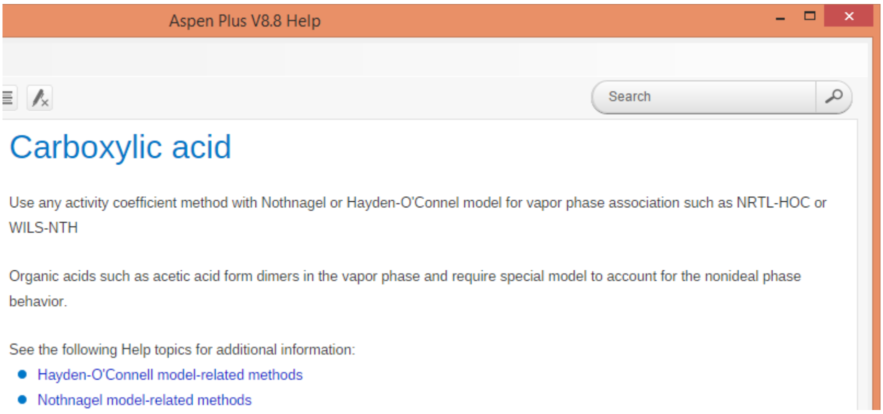
Go to “**Methods**” folder | “**Global**” sheet and use the “**Property Method Selection Assistant**” wizard by clicking on the “**Methods Assistant** … ” button shown in Figure 6.2.



Method filter: CHEMICAL
Base method: NRTL
Method name: NRTL

Figure 6.2 Clicking on the “**Methods Assistant** … ” button, will invoke the “**Property Method Selection Assistant**” wizard.

Select “**Specify process type**”; followed by selecting the type of process to be “**Chemical**”; and finally clicking “**Carboxylic acids**” as a subset of “**Chemical**” processes. This will guide you to either “**NRTL-HOC**” or “**WILS-NTH**” as shown in Figure 6.3.



Carboxylic acid

Use any activity coefficient method with Nothnagel or Hayden-O'Connel model for vapor phase association such as NRTL-HOC or WILS-NTH

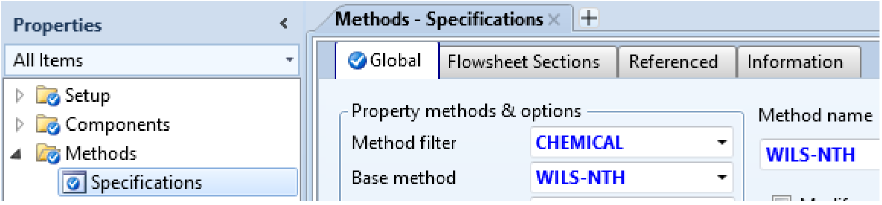
Organic acids such as acetic acid form dimers in the vapor phase and require special model to account for the nonideal phase behavior.

See the following Help topics for additional information:

- Hayden-O'Connell model-related methods
- Nothnagel model-related methods

Figure 6.3 The property method selection assistant will recommend either “**NRTL-HOC**” or “**WILS-NTH**” for the subcategory: “**Chemical**” | “**Carboxylic acids**”.

You can choose either one; so, in “**Global**” tab window, from the “**Method name**” pull-down menu select “**WILS-NTH**” as shown in Figure 6.4.



Method filter: CHEMICAL
Base method: WILS-NTH
Method name: WILS-NTH

Figure 6.4 Following the recommendation by the “**Property Method Selection Assistant**” wizard, the property method is set to “**WILS-NTH**”.

Under “**Methods**” | “**Parameters**” | “**Binary Interaction**” | “**WILSON-1**” sheet be sure that the “***Estimate missing parameters by UNIFAC***” option is checked. Click “**Reset**” followed by “**Next**” button to run the simulation and assure that properties analysis completed successfully.

NOTE #2: *“**Control Panel**” shows a warning as follows:*

```
*    WARNING IN PHYSICAL PROPERTY SYSTEM
     PROP-NAME WILSON FOR COMPONENT PAIR CH3COCH3 AND C2H2O
     CANNOT BE ESTIMATED USING THE UNIFAC METHOD AS SPECIFIED
     BECAUSE OF MISSING INPUT PARAMETERS:
          STRUCTUR, GMUFR, GMUFQ
```

*Such a warning can be ignored given the fact that the pairwise interaction parameters are already calculated by UNIFAC method and are shown in “**Parameters**” | “**Binary Interaction**” | “**WILSON-1**” sheet with the source as R-PCES. Moreover, even* *if we define the structure of ketene under “**Components**” | “**Molecular Structure**” via the built-in Aspen Plus Molecule Editor, the warning will persist.*

*To remove this persisting warning to propagate to “Simulation” environment, deselect the option “Estimate missing parameters by UNIFAC” after the pairwise interaction parameters are all calculated and are shown in “**Parameters**” | “**Binary Interaction**” | “**WILSON-1**” sheet, and rerun the simulation under “**Properties**” environment for the second time you will notice that the nagging warning will disappear and the “**Properties Analysis/Setup Complete**” pop-up window will tell the user that properties analysis successfully completed. Nevertheless, a warning like this can be ignored*

```
WARNING IN PHYSICAL PROPERTY SYSTEM
   FUNCTIONAL GROUP GENERATION FOR THE UNIFAC METHOD CANNOT BE COM-
  PLETED
   FOR COMPONENT C2H2O.  THE FOLLOWING ATOMS WERE NOT MATCHED:
   C 1  C 2  O 3
```

6.4 THE RIGOROUS PLUG-FLOW REACTOR (RPLUG)

At the start, the flowsheet consists of one inlet stream, a plug-flow reactor (“**PFR**”), and one product stream. It should resemble Figure 6.5. This can be done by adding the “**RPlug**” reactor found under “**Reactors**” tab in “**Model Palette**”.

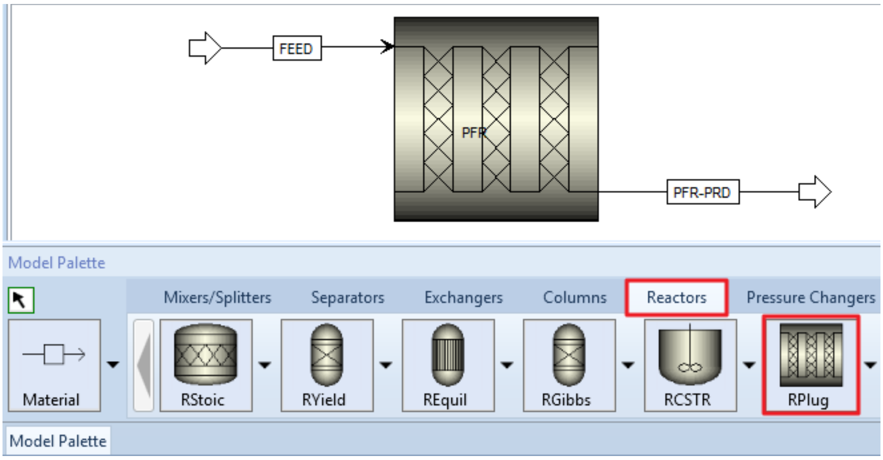


Figure 6.5 The addition of “**PFR**” block to the flowsheet using the “**RPlug**” reactor under “**Reactors**” tab in “**Model Palette**”.

Table 6.1 shows a brief description about each reactor model found under “**Reactors**” tab.

TABLE 6.1 Different reactor models are found in Aspen Plus under "Reactors" tab in "Model Palette".

Model	Description	Purpose	Use
Rstoic	Stoichiometric reactor	Stoichiometric reactor with specified reaction extent or conversion	Reaction kinetics is unknown or unimportant but its stoichiometry and extent are given
RYield	Yield reactor	Reactor with specified yield	Reaction stoichiometry and kinetics are unknown or unimportant but yield distribution is known
REquil	Equilibrium reactor	Chemical and phase equilibrium by stoichiometric calculations	Single- and two-phase chemical equilibrium and simultaneous phase equilibrium. The user must specify the reaction stoichiometry and the reactor conditions. If no additional specifications are given, "**REquil**" model will assume that the reactions will reach equilibrium
RGibbs	Equilibrium reactor	Chemical and phase equilibrium by Gibbs free energy minimization, subject to atom balance constraints	Chemical and/or simultaneous phase and chemical equilibrium. Solid phase equilibrium may be included. This model does not require reaction stoichiometry; however, the user must specify the reactor temperature and pressure, or pressure and enthalpy. See Homework/Classwork 9.4 (The Selectivity of Parallel Reactions)
RCSTR	Continuous stirred-tank reactor	Continuous stirred-tank reactor	One-, two-, or three-phase stirred-tank reactor with reaction taking place in the vapor or liquid
RPlug	Plug-flow reactor	Plug-flow reactor	One-, two-, or three-phase plug-flow reactor with reaction taking place in the vapor or liquid
RBatch	Batch reactor	Batch or semi-batch reactor	Batch and semibatch reactor with known reaction kinetics

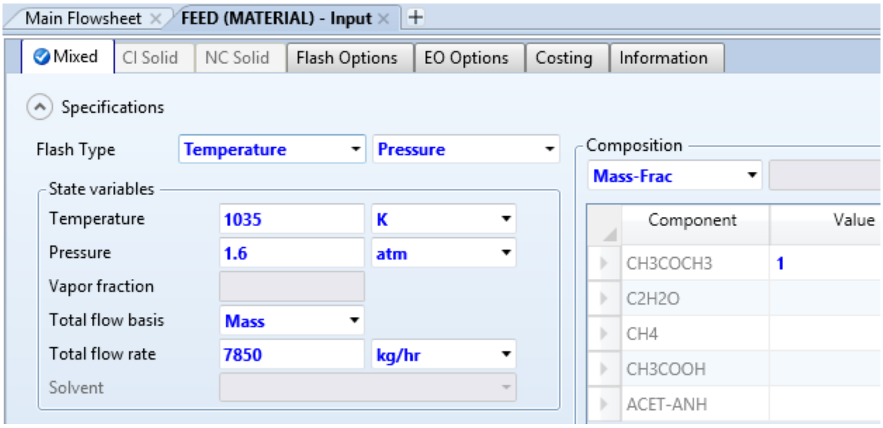
Click on "**Next**" button, and Aspen Plus will bring the user to entering feed stream properties

Temperature: 1035 K (change units if necessary)

Pressure: 1.6 atm (change units if necessary)

Total flow: Change to Mass kg/h

For the total mass flow rate of "**FEED**" stream, type 7850. Leave ketene and methane at zero (no mass flow in the feed stream). For "**Composition**" drop-down menu, use "*Mass-Frac*" and enter 1.0 for acetone (CH_3COCH_3). See Figure 6.6.



Flash Type: Temperature, Pressure

Temperature	1035	K
Pressure	1.6	atm
Vapor fraction		
Total flow basis	Mass	
Total flow rate	7850	kg/hr
Solvent		

Composition: Mass-Frac

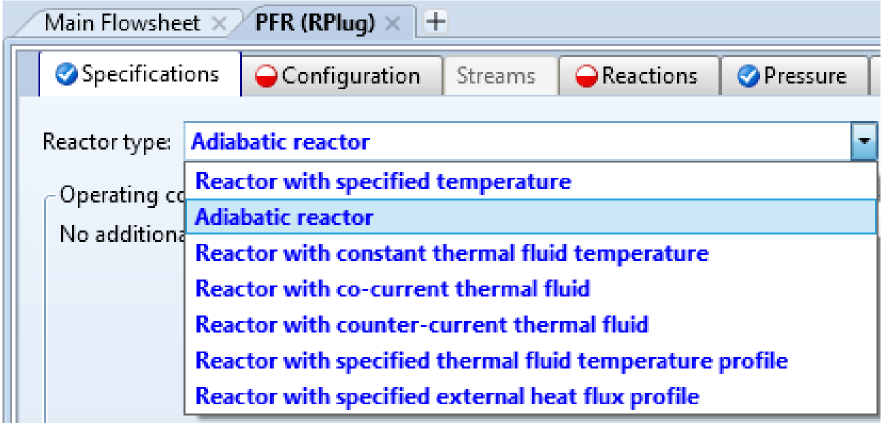
Component	Value
CH3COCH3	1
C2H2O	
CH4	
CH3COOH	
ACET-ANH	

Figure 6.6 Entering feed stream properties in terms of flow, P, T, and composition.

Click on “**Next**” button.

6.5 REACTOR AND REACTION SPECIFICATIONS FOR RPLUG (PFR)

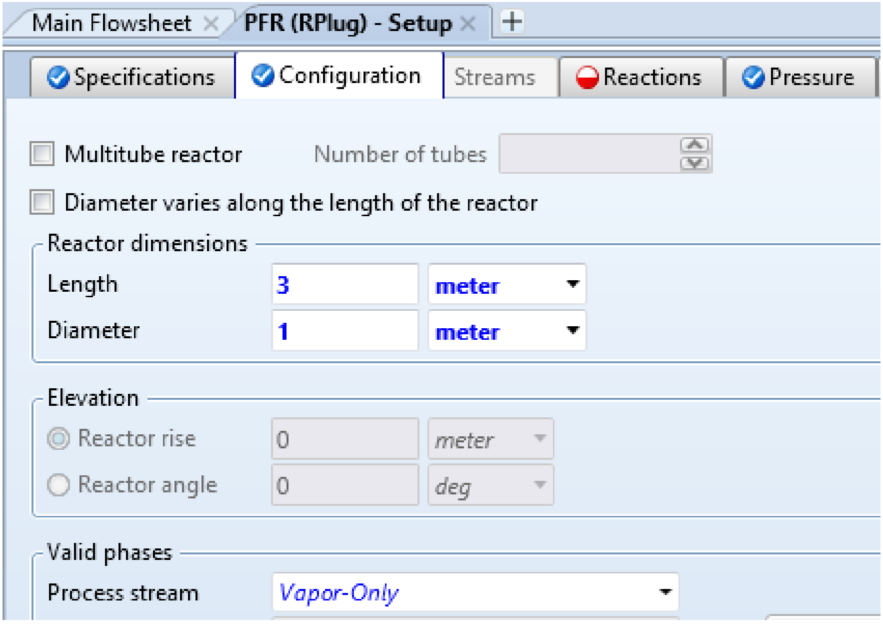
“**Reactor type**”: “*Adiabatic reactor*”, as shown in Figure 6.7.



Reactor type: Adiabatic reactor

Figure 6.7 Under “**Specifications**” tab, choose the type of plug-flow reactor (PFR).

Move to “**Configuration**” tab and enter specifications as shown in Figure 6.8.



☐ Multitube reactor Number of tubes

☐ Diameter varies along the length of the reactor

Reactor dimensions

Length 3 meter

Diameter 1 meter

Elevation

◉ Reactor rise 0 meter

○ Reactor angle 0 deg

Valid phases

Process stream Vapor-Only

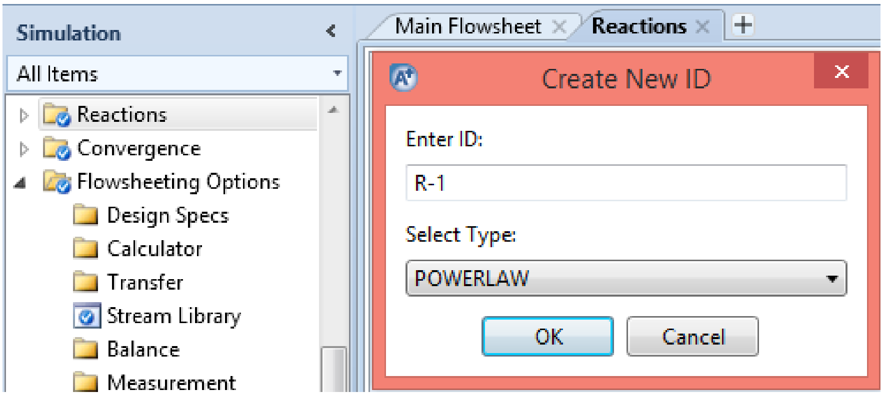
Figure 6.8 “**PFR**” is chosen as a single-tube reactor (*i.e.* a cylinder with length 3.0 and diameter 1 m). The “**Process stream**” is “*Vapor-Only*” based on the given pressure and temperature.

On the other hand, the user may choose, however, a multitube reactor, for instance, 1000 tubes of length 2.5 meters and inside diameter (ID) of 0.9 inches.

<u>**NOTE #3:**</u> *If the inlet pressure value is left “0”, under the “**Pressure**” tab shown in Figure* 6.8, *then we will instruct Aspen Plus to let the inlet pressure be equal to the feed stream pressure.*

If you click on “**Reactions**” tab, you will notice that you need to associate a reaction set to “**PFR**” block; however, since we did not define any reaction yet, the available reaction sets side will be empty.

Click on “**Next**” button to create the reaction set as shown in Figure 6.9, which will be added later to the “**Reactions**” tab here. Figure 6.9 shows that we created “**R-1**” reaction set with “**POWERLAW**” type. The reason for describing “**R-1**” as a reaction set is simply because it may contain more than one reaction. Here, we have only one reaction as given by Equation 6.1.



Create New ID

Enter ID: R-1

Select Type: POWERLAW

Figure 6.9 The reaction type is "**POWERLAW**" with an ID: "**R-1**".

Figure 6.10 shows the "**Stoichiometry**" tab window where we need to define the reaction stoichiometry.

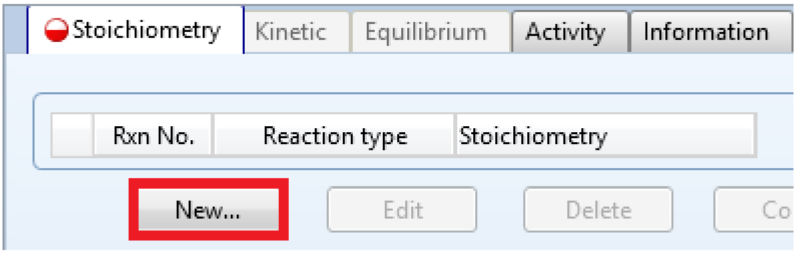
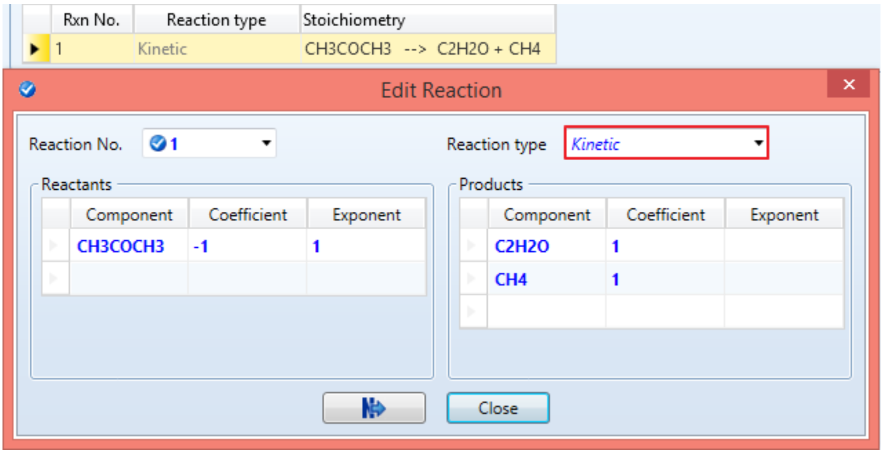


Figure 6.10 The reaction set "**R-1**" is still undefined for Aspen Plus.

Click on "**New** … " button and the "**Edit Reaction**" window will pop up where the user will be required to define the reaction equation, its type whether kinetic or equilibrium, and the reaction order (*i.e.*, exponent) if it is of kinetic type, as shown in Figure 6.11.



Rxn No.	Reaction type	Stoichiometry
1	Kinetic	CH3COCH3 --> C2H2O + CH4

Reaction No. 1

Reaction type Kinetic

Reactants

Component	Coefficient	Exponent
CH3COCH3	-1	1

Products

Component	Coefficient	Exponent
C2H2O	1	
CH4	1	

Figure 6.11 The "**Edit Reaction**" window where the user defines the reaction equation and whether or not it is of "*Kinetic*" type. Here, it means that the reaction is first order with respect to acetone (CH_3COCH_3).

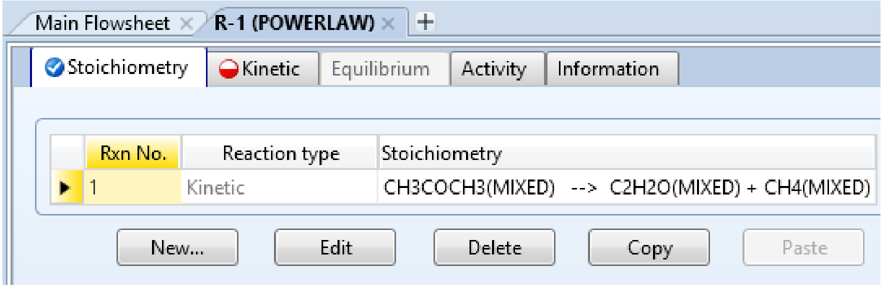
Under "**Reaction type**", select "*Kinetic*".

Under "**Reactants**", select acetone (CH_3COCH_3) from the components pull-down menu and set the "**Coefficient**" to −*1* and the "**Exponent**" to *1*.

Under "**Products**", select ketene and methane and set both coefficients to *1*.

Click on "**Next**" button or "**Close**" button shown at the bottom of the "**Edit Reaction**" window.

Figure 6.12 shows that the reaction stoichiometry is defined; however, the kinetic parameters are not yet defined.



Rxn No.	Reaction type	Stoichiometry
1	Kinetic	CH3COCH3(MIXED) --> C2H2O(MIXED) + CH4(MIXED)

Figure 6.12 The reaction stoichiometry (*i.e.*, equation) is already defined but the kinetic parameters are not.

NOTE #4: *Based on Aspen Plus built-in help, here is how to enter kinetic parameters for a reaction:*

If To is specified, then the general law expression will be

$$r = k(T/T_o)^n e^{(-E/R)\left[\frac{1}{T}-\frac{1}{T_o}\right]} \prod_{i=1}^{N} C_i^{\alpha_i} \tag{6.10}$$

On the other hand if T_o is not specified, the general law expression will reduce to

$$r = k(T)^n e^{(-E/R)\left[\frac{1}{T}\right]} \prod_{i=1}^{N} C_i^{\alpha_i} \tag{6.11}$$

*The rate is expressed in kmol/(s · basis) where the basis is either m^3 for "**Rate Basis:** Reac (vol)", or kilogram catalyst for "**Rate Basis:** Cat (wt)".*

The reactor volume or catalyst weight is determined by specifications in the reactor where the reaction is used.

Next, click on the "**Kinetic**" tab where the user needs to input the kinetic parameters.

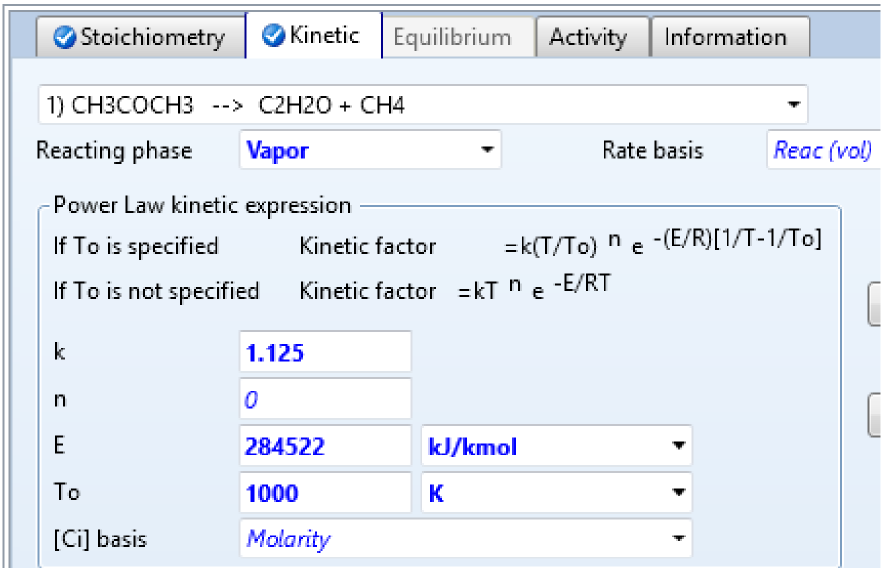
Change "**Reacting phase**" to "*Vapor*". The "**Rate basis**" will be left as "*Reac(vol)*".

Enter *1.125* for ***k*** (*i.e.*, *k** in Eq. 6.9)

Enter *1000* K for $\mathbf{T_o}$

Enter the activation energy **E** of the Arrhenius equation, E = 284,521.7 J/mol (Eq. 6.4 or Eq. 6.7). Notice **E** is also equal to 284,521.7 kJ/kmol.

Figure 6.13 shows the "**Kinetic**" tab window, after inputting the required data.



1) CH3COCH3 --> C2H2O + CH4

Reacting phase: Vapor

Rate basis: Reac (vol)

If To is specified Kinetic factor $=k(T/To)^{n}\ e^{-(E/R)[1/T-1/To]}$

If To is not specified Kinetic factor $=kT^{n}\ e^{-E/RT}$

k: 1.125

n: 0

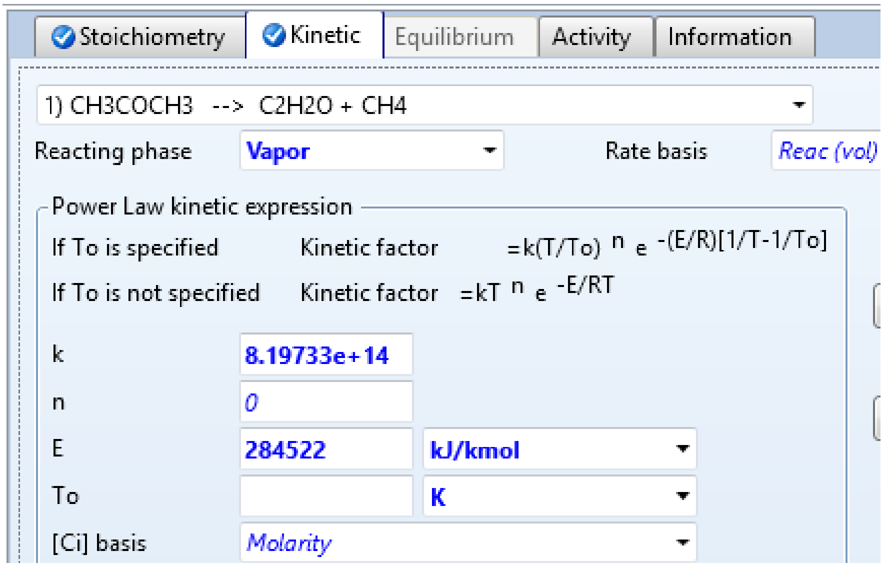
E: 284522 kJ/kmol

To: 1000 K

[Ci] basis: Molarity

Figure 6.13 The reaction phase and the kinetic parameters are defined in "**Kinetic**" tab window, based on Equation 6.9 and in light of Equation 6.10.

Alternatively, the user may attempt to enter the kinetic data based on Equation 6.4, as shown in Figure 6.14.



1) CH3COCH3 --> C2H2O + CH4

Reacting phase: Vapor

Rate basis: Reac (vol)

Power Law kinetic expression

If To is specified: Kinetic factor $=k(T/T_o)^{n}\, e^{-(E/R)[1/T-1/T_o]}$

If To is not specified: Kinetic factor $=kT^{n}\, e^{-E/RT}$

k: 8.19733e+14

n: 0

E: 284522 kJ/kmol

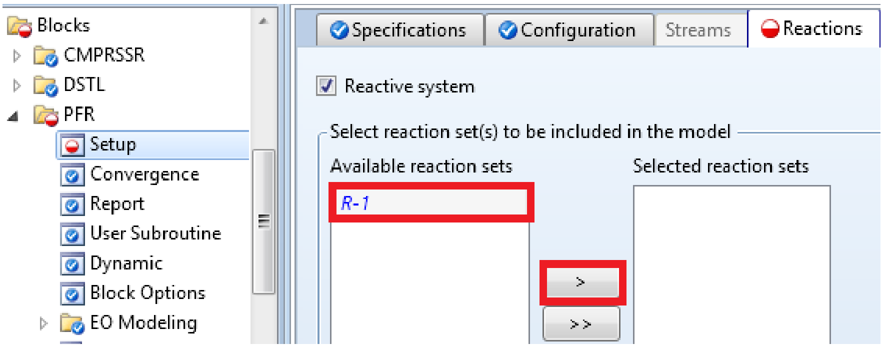
To: K

[Ci] basis: Molarity

Figure 6.14 The reaction phase and the kinetic parameters are defined in "**Kinetic**" tab window, based on Equation 6.4 and in light of Equation 6.11.

Notice that in Figure 6.8 "**PFR**" block still lacks some information (*i.e.*, a half-filled red circle).

Click on "**Next**" button and Aspen Plus will move to the "**Setup**" window of "**PFR**" block as shown in Figure 6.15.



☑ Reactive system

Select reaction set(s) to be included in the model

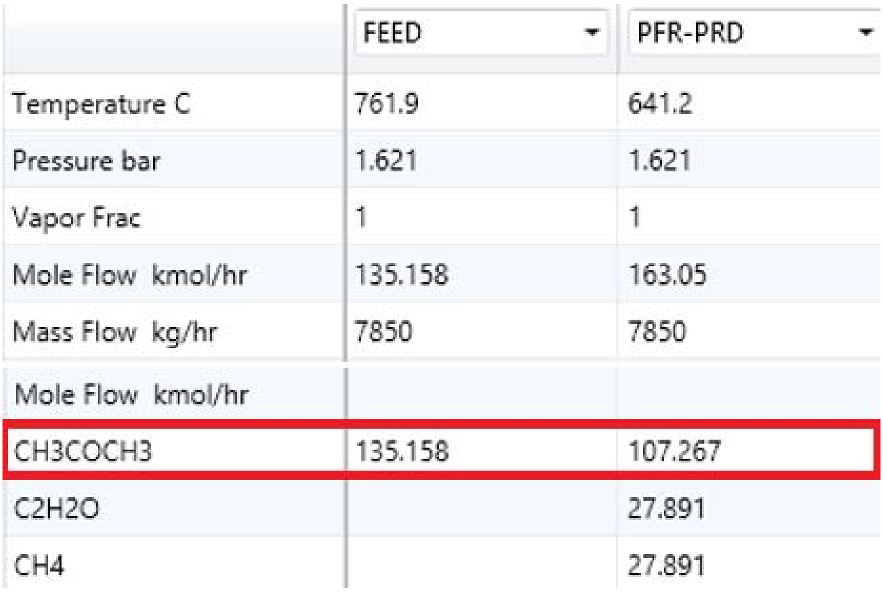
Available reaction sets: R-1

Selected reaction sets:

Figure 6.15 The user needs to highlight "**R-1**" set on the left side and then to move it to the right side *via* the first top arrow.

6.6 RUNNING THE SIMULATION (PFR ONLY)

Click on "**Next**" and "**OK**" buttons. When the simulation is complete, go to "**Blocks**" | "**PFR**" | "**Stream Results**". Figure 6.16 shows the stream properties from and to "**PFR**" block.



	FEED	PFR-PRD
Temperature C	761.9	641.2
Pressure bar	1.621	1.621
Vapor Frac	1	1
Mole Flow kmol/hr	135.158	163.05
Mass Flow kg/hr	7850	7850
Mole Flow kmol/hr		
CH3COCH3	135.158	107.267
C2H2O		27.891
CH4		27.891

Figure 6.16 The stream results of PFR. The conversion, X, can be calculated as (27.89)/135.16 = 0.206.

Check the conversion (X = moles reacted/moles fed). Does $X = 20\%$? If $X < 20\%$, you must increase the length of "**PFR**". If $X > 20\%$, you must decrease the length of "**PFR**". For our case, it is found that $X = (27.89)/135.16 = 0.206$ (20.6%). Luckily, the tube length is satisfactory.

EXERCISE 6.1

Utilizing the results shown in Figure 6.16, answer the following questions:

- Given that the PFR is adiabatically operated and the product stream temperature (641.2°C) is less than that of the feed stream (761.9°C), what will be the heat of reaction, endothermic or exothermic?
- Unlike the total mass flow rate (7850 kg/h) that remains unchanged, why is the total molar flow rate of the product stream (163.05 kmol/h) is greater than that of the feed stream (135.158 kmol/h)?
- What is the molecular weight of the pure feed stream?
- What is the average molecular weight of the product stream?

6.7 COMPRESSOR (CMPRSSR) AND RADFRAC RECTIFYING COLUMN (RECTIF)

On the other hand, if we look at the outlet composition of the reactor product stream (**PFR-PRD**), we will find that it contains an excessive amount of acetone, which means that we need to separate acetone from the products ketene and methane prior to sending ketene to the second reactor that will be installed later. So, we have to add an absorption tower that will basically split acetone from ketene and methane. Figure 6.17 shows the addition of two pieces of equipment: the first is the gas compressor and the second is "**RadFrac**" type absorption tower (rectifier). The rectifier is basically the upper half of a distillation tower with a condenser and no reboiler.

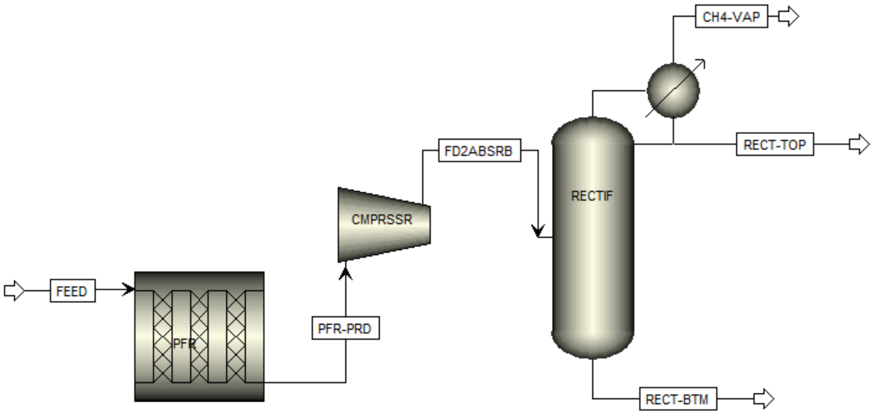
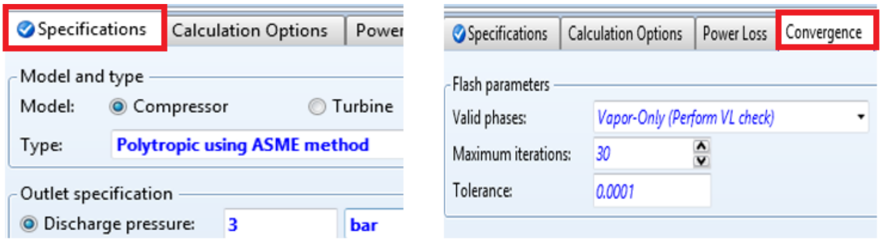


Figure 6.17 For the sake of purification, a compressor and absorption tower (rectifier) will be installed prior to introducing the product stream to the second reactor that will be installed at a later stage.

Figure 6.18 shows that the discharge pressure for the compressor is 3 bar and the convergence condition is such that we have vapor only while performing vapor–liquid (VL) check. Of course, an error will be issued if a two-phase system coexists within the compressor.



Model and type

Model: ● Compressor ○ Turbine

Type: Polytropic using ASME method

Outlet specification

● Discharge pressure: 3 bar

Flash parameters

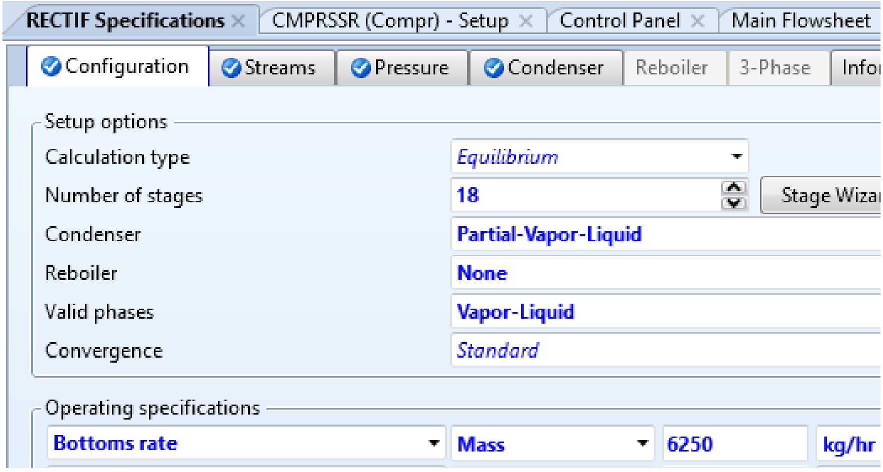
Valid phases: Vapor-Only (Perform VL check)

Maximum iterations: 30

Tolerance: 0.0001

Figure 6.18 Specifications for the compressor; "**Polytropic using ASME method**" type is chosen and a discharge pressure of 3 bar is assigned (*left*) and a restriction for the presence of vapor phase only (*right*).

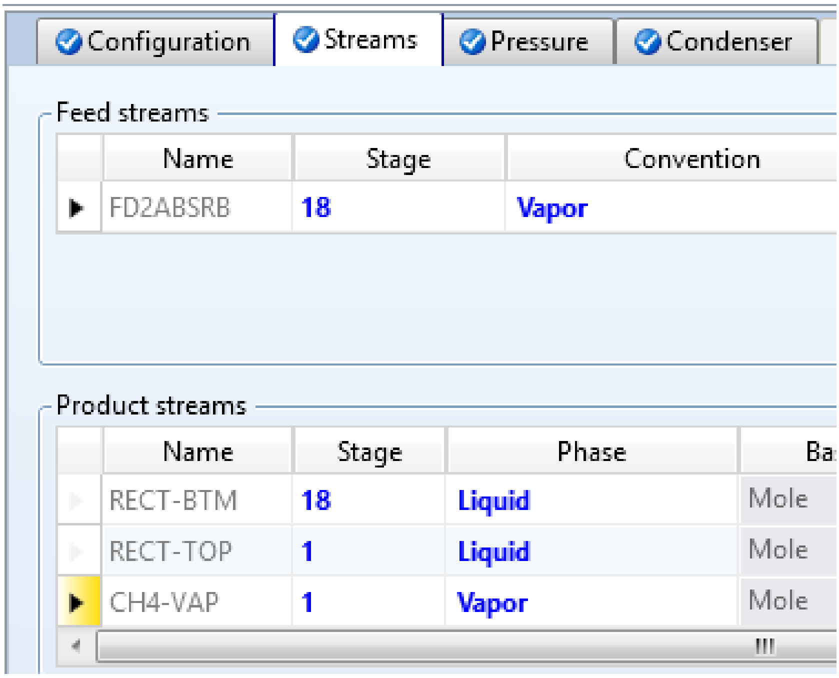
On the other hand, Figure 6.19 shows “**RECTIF**” | “**Specifications**” | “**Setup**” | “**Configuration**” tab window. The user must specify the number of stages, reboiler type (if any), condenser type, and one of “**Operating specifications**”, such as “*Bottoms rate*”. It is to be mentioned here that a bottoms mass flow rate of 6250 kg/h is a matter of trial-and-error approach because it affects the composition of both the top and bottom streams. Obviously, the value has to be somewhere between zero and that of the feed stream entering the tower.



Calculation type: Equilibrium
Number of stages: 18
Condenser: Partial-Vapor-Liquid
Reboiler: None
Valid phases: Vapor-Liquid
Convergence: Standard
Bottoms rate: Mass 6250 kg/hr

Figure 6.19 The “**Configuration**” tab window for the “**Setup**” sheet for the absorption column named “**RECTIF**”. The number of stages; condenser type; reboiler type (if any); and one of “**Operating specifications**”, such as “*Bottoms rate*”, are to be entered here.

Click on “**Next**” button and Aspen Plus will move to the “**Streams**” tab window as shown in Figure 6.20. Here, the location of the feed stream (or feed tray) must be defined with respect to the top tray (#1). Notice that the location of the feed tray is way down at the bottom of the rectifier. This makes sense as we need not have a reboiler; the feed stream will be available as the vapor phase throughout the entire rectifying column.



Feed streams

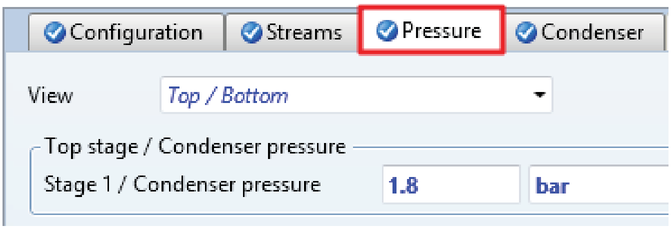
	Name	Stage	Convention
▶	FD2ABSRB	18	Vapor

Product streams

	Name	Stage	Phase	Ba
	RECT-BTM	18	Liquid	Mole
	RECT-TOP	1	Liquid	Mole
▶	CH4-VAP	1	Vapor	Mole

Figure 6.20 The location of feed tray from the first top tray (#1) is made *via* "**Streams**" tab window. The vapor feed will be introduced at the bottom; hence, there is no need for reboiler in a rectifying column.

Click on "**Next**" button and you will be prompted by "**Pressure**" tab window as shown in Figure 6.21. Here, the pressure at the top stage (condenser stage) must be defined. Enter *1.8 bar* for the condenser pressure.



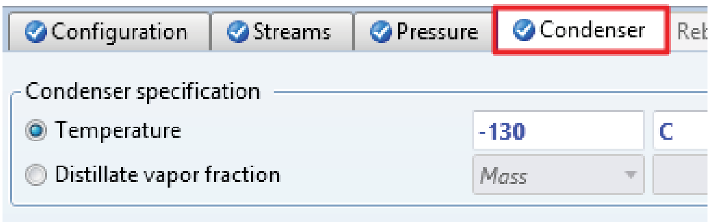
View: Top / Bottom

Top stage / Condenser pressure

Stage 1 / Condenser pressure: 1.8 bar

Figure 6.21 The "**Pressure**" tab window is used to define the pressure profile throughout the column.

Click on "**Next**" button and you will be prompted by "**Condenser**" tab window as shown in Figure 6.22. Here, the temperature of the condenser must be defined. Alternatively, the distillate vapor fraction can be defined. Enter $-130°C$ for the condenser temperature.



Condenser specification

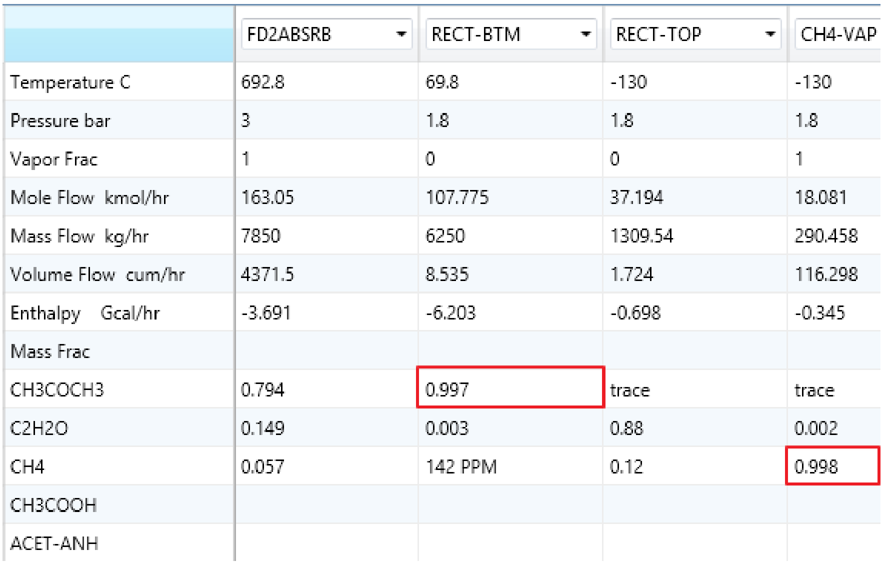
● Temperature -130 C

○ Distillate vapor fraction Mass

Figure 6.22 The "**Condenser**" tab window is used to define the condenser temperature.

6.8 RUNNING THE SIMULATION (PFR + CMPRSSR + RECTIF)

Click on "**Reset**" followed by "**Next**" and by "**OK**" button to allow Aspen Plus to do the calculations on your behalf. Figure 6.23 shows a portion of the results, which pertains to the absorption column. As you can see that the bottom (**RECT-BTM**) stream is 99.7 wt% acetone and the top (**RECT-TOP**) stream is mainly composed of methane and ketene. The acetone stream will be recycled to the inlet of PFR. Moreover, the vapor portion of the top stream is 99.8 wt% methane gas, which can be combined with another stream and be sent to a storage facility for methane. Here, we have a partial condenser (see Figure 6.19), which means not all of the rising vapor up the column will be condensed; a small portion will remain as is and the rest will be condensed and split into the top liquid (distillate) and returning (*i.e.*, reflux) stream.



	FD2ABSRB	RECT-BTM	RECT-TOP	CH4-VAP
Temperature C	692.8	69.8	-130	-130
Pressure bar	3	1.8	1.8	1.8
Vapor Frac	1	0	0	1
Mole Flow kmol/hr	163.05	107.775	37.194	18.081
Mass Flow kg/hr	7850	6250	1309.54	290.458
Volume Flow cum/hr	4371.5	8.535	1.724	116.298
Enthalpy Gcal/hr	-3.691	-6.203	-0.698	-0.345
Mass Frac				
CH3COCH3	0.794	0.997	trace	trace
C2H2O	0.149	0.003	0.88	0.002
CH4	0.057	142 PPM	0.12	0.998
CH3COOH				
ACET-ANH				

Figure 6.23 The simulation results indicate that "**RECTIF**" tower managed to isolate acetone from the other two components methane and ketene.

EXERCISE 6.2

Carry out pure component analysis. Under "**Properties**" environment, click on "**Home**" ribbon | "**Analysis**" tab | "**Pure**" button and select the thermodynamic property to be "**PL**", which represents the vapor pressure of a pure component as a function of temperature. Select the temperature range between 0 and 100°C and the phase to be liquid to analyze the vapor pressure of the three components acetone, ketene, and methane. Sort them in descending order with respect to volatility. Verify that acetone is the least volatile.

6.9 RadFrac DISTILLATION COLUMN (DSTL)

As was done in the previous step, the top "**RECT-TOP**" stream will be sent to another "**RadFrac**" type distillation tower where methane will be separated from ketene, as shown in Figure 6.24.

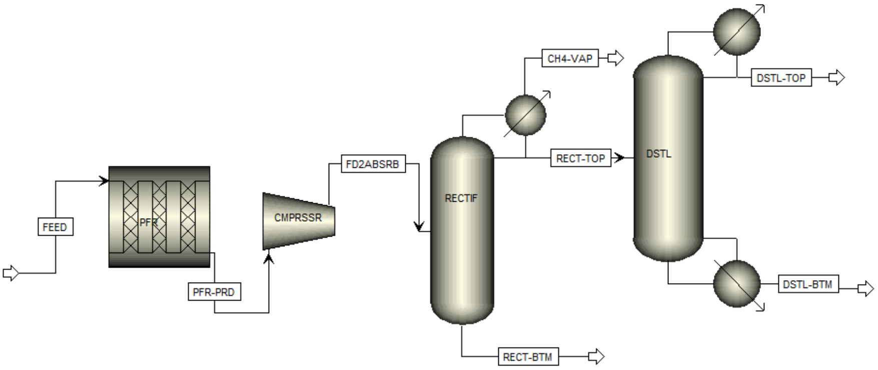
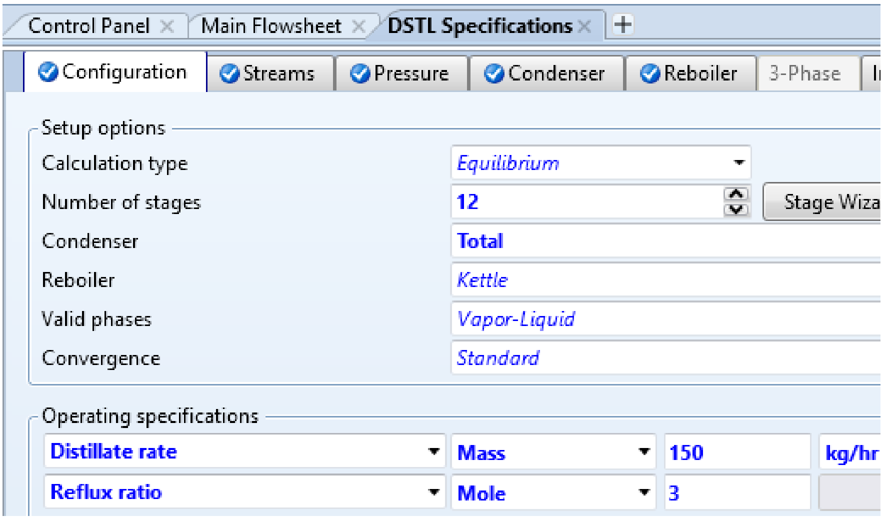


Figure 6.24 The addition of "**RadFrac**" type distillation tower to separate methane from ketene.

Figures 6.25–6.27 show the specifications of the "**RadFrac**" type distillation column (**DSTL**).



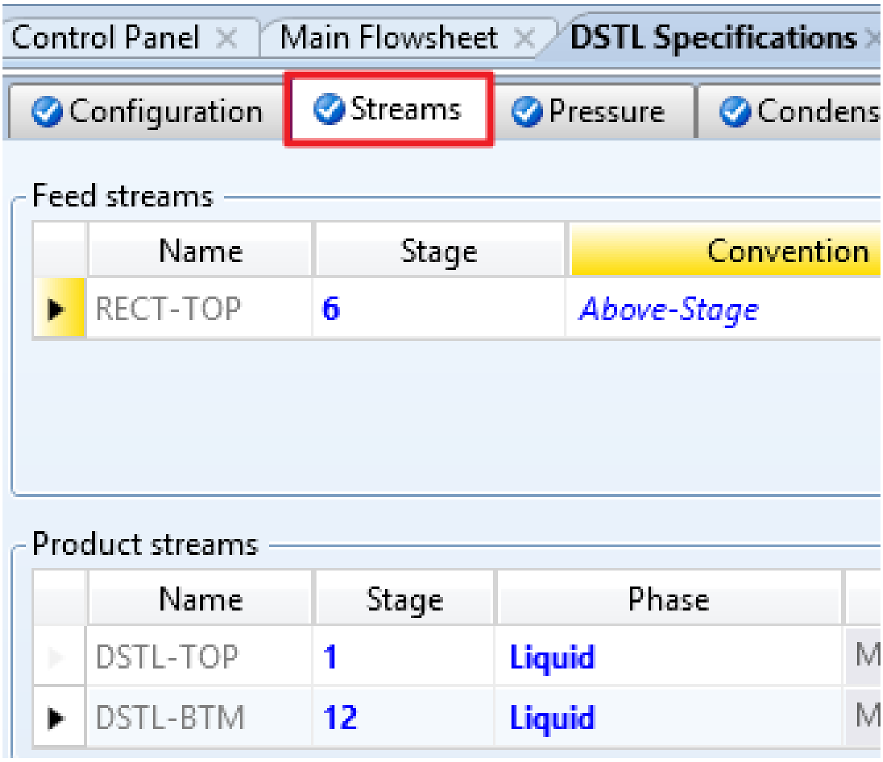
Setup options

Calculation type: Equilibrium
Number of stages: 12
Condenser: Total
Reboiler: Kettle
Valid phases: Vapor-Liquid
Convergence: Standard

Operating specifications

Distillate rate	Mass	150	kg/hr
Reflux ratio	Mole	3	

Figure 6.25 In "**Configuration**" tab window, condenser and reboiler type, # of stages, and two operating specifications are defined.



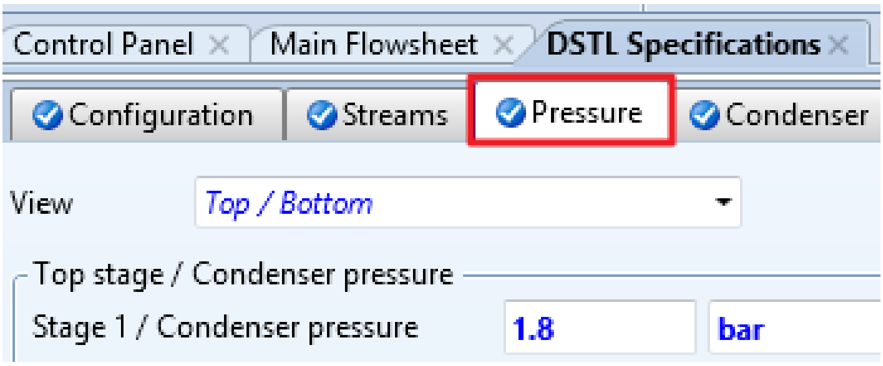
Feed streams

Name	Stage	Convention
RECT-TOP	6	Above-Stage

Product streams

Name	Stage	Phase	
DSTL-TOP	1	Liquid	M
DSTL-BTM	12	Liquid	M

Figure 6.26 Location of the feed tray (#6 from the top) for "**DSTL**" column.



View: Top / Bottom

Top stage / Condenser pressure

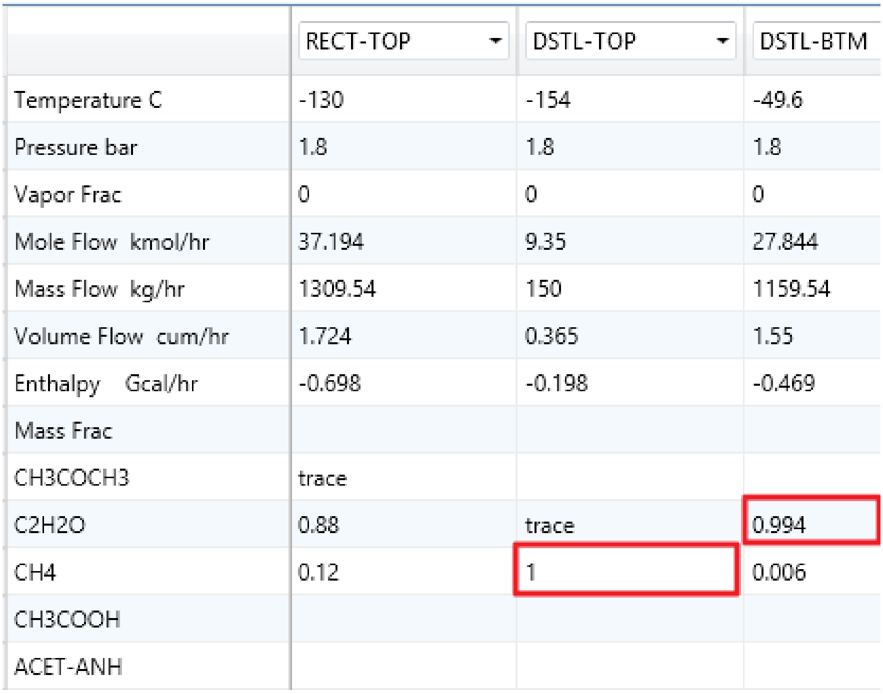
Stage 1 / Condenser pressure: 1.8 bar

Figure 6.27 Pressure profile of "**DSTL**" column.

6.10 RUNNING THE SIMULATION (PFR + CMPRSSR + RECTIF + DSTL)

Reinitialize, click on "**OK**" button twice, click on (**Next**) button, and on "**OK**" button. See "**Control Panel**" if there is an error or serious warning regarding the process simulation.

Figure 6.28 shows a portion of the results, which pertains to the recently added piece of equipment (*i.e.*, "**DSTL**").



	RECT-TOP	DSTL-TOP	DSTL-BTM
Temperature C	-130	-154	-49.6
Pressure bar	1.8	1.8	1.8
Vapor Frac	0	0	0
Mole Flow kmol/hr	37.194	9.35	27.844
Mass Flow kg/hr	1309.54	150	1159.54
Volume Flow cum/hr	1.724	0.365	1.55
Enthalpy Gcal/hr	-0.698	-0.198	-0.469
Mass Frac			
CH3COCH3	trace		
C2H2O	0.88	trace	0.994
CH4	0.12	1	0.006
CH3COOH			
ACET-ANH			

Figure 6.28 The "**RadFrac**" type distillation column ("**DSTL**") successfully separated the methane/ketene mixture ("**RECT-TOP**") into two extra pure streams: "**DSTL-TOP**" ($Y_{CH4} = 1.0$) and "**DSTL-BTM**" ($Y_{CH2CO} = 0.994$).

Of course, methane can be used either as a precursor for other chemical industries or as a fuel (*i.e.*, source of energy). On the other hand, ketene will be finally sent to the second reactor where it reacts with acetic acid to form acetic anhydride.

6.11 REACTOR AND REACTION SPECIFICATIONS FOR RCSTR

Figure 6.29 shows that a rigorous CSTR (“**RCSTR**”) is added for carrying out the second reaction, that is, reaction of ketene with acetic acid to form acetic anhydride. In addition, acetic acid (“**ACETACID**”) stream is also added to the inlet of the new reactor.

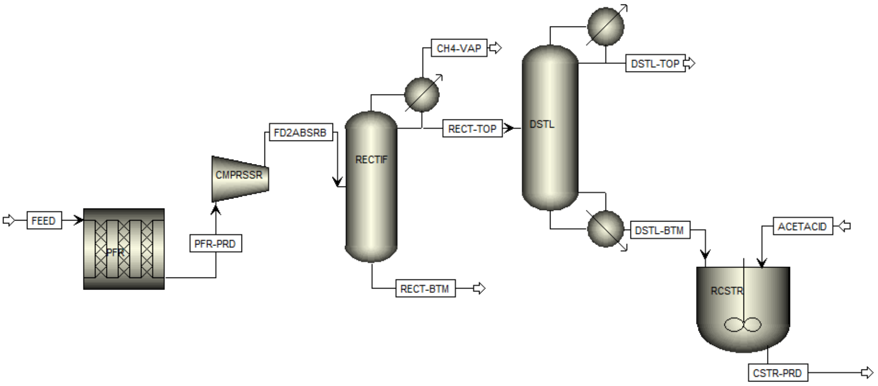
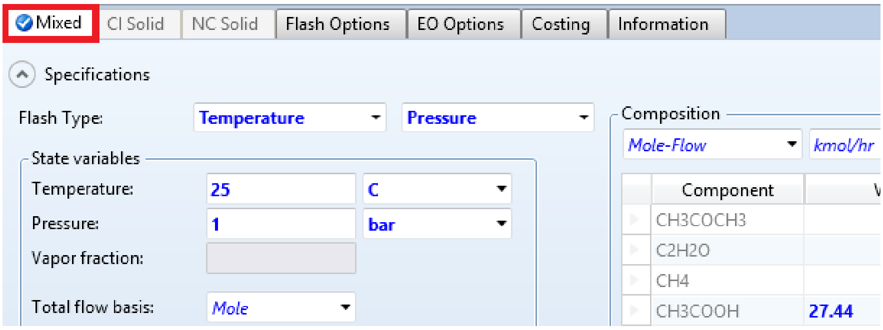


Figure 6.29 Addition of a Rigorous CSTR (“**RCSTR**”) for the sake of carrying out the second reaction, that is, reaction of ketene with acetic acid to form acetic anhydride.

Click on “**NEXT**” button and Aspen Plus will bring you to the input form of “**ACETACID**” stream. Here, the molar flow rate (kmol/h) of acetic acid will be equal to that of ketene present in “**DST-BTM**” stream. Figure 6.30 shows the “**Mixed**” tab input form of “**ACETACID**” stream.



Flash Type: Temperature Pressure

State variables

Temperature: 25 C

Pressure: 1 bar

Vapor fraction:

Total flow basis: Mole

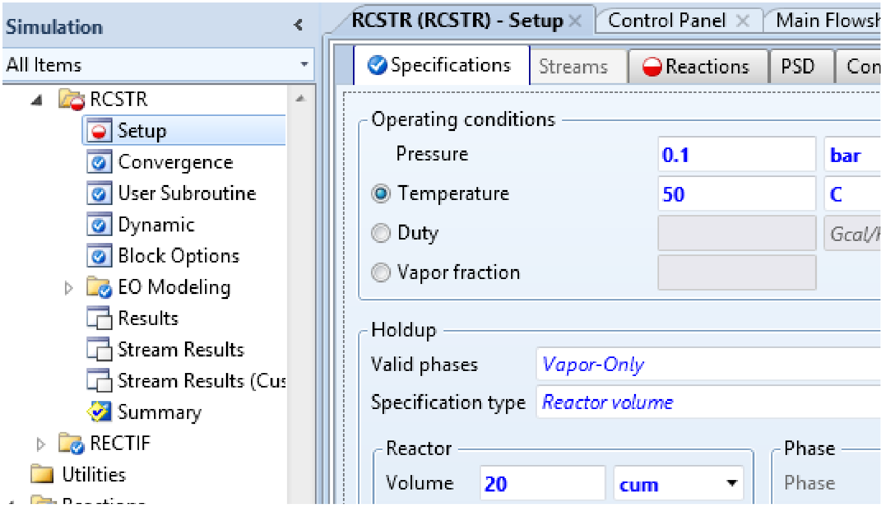
Composition

Mole-Flow kmol/hr

Component	V
CH3COCH3	
C2H2O	
CH4	
CH3COOH	27.44

Figure 6.30 Entering stream properties *via* “**Mixed**” tab window under “**Input**” sheet of “**ACETACID**” stream.

Click on “**Next**” button and Aspen Plus will bring you to “**RCSTR**” | “**Setup**” window. Figure 6.31 shows that a temperature of 50°C and a pressure of 0.1 bar were entered for the reactor condition. As a result of very low pressure, the reaction will be carried out in vapor phase (see Exercise 6.3). Twenty cubic meter is assumed as the reactor volume.



Operating conditions

Pressure 0.1 bar

● Temperature 50 C

○ Duty Gcal/

○ Vapor fraction

Holdup

Valid phases *Vapor-Only*

Specification type *Reactor volume*

Reactor

Volume 20 cum

Phase

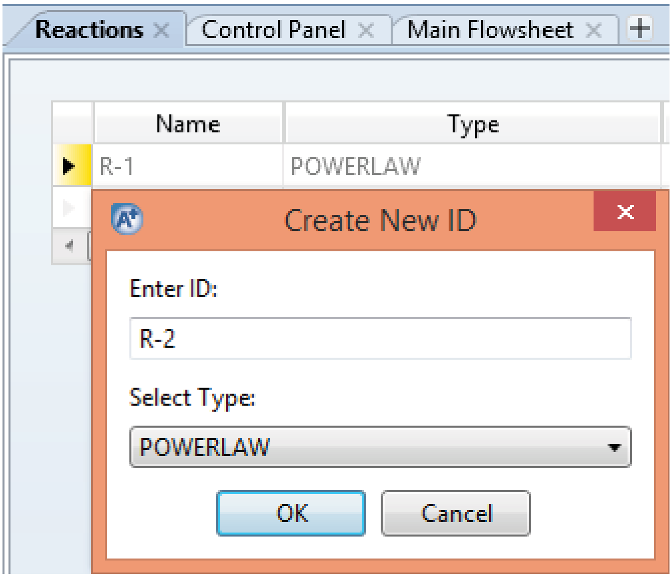
Phase

Figure 6.31 The reactor conditions in terms of pressure, temperature, reaction phase, and reactor volume.

Now, it is time for defining the type of reaction in this reactor. Since we do not have the reaction kinetics (the rate constant, activation energy, and reaction order), then we will assume that the reaction attains equilibrium. If the reaction kinetic data is available, then the reaction type must be converted from equilibrium to kinetic so that reaction products will be better estimated.

For equilibrium reactions, ASPEN can predict or calculate equilibrium data. Let us go and define the reaction first, and then get back to “**Reactions**” tab under “**RCSTR**” | “**Setup**” window (shown as a half-filled red circle in Figure 6.31). Go to “**Reactions**” folder in “**Navigation**” pane so that we can define a new reaction that will account for the conversion of acetic acid and ketene into acetic anhydride. The “**Reactions**” window has already “**R-1**” reaction set.

As we have dealt with the previous reaction “**R-1**” set, click on the “**New …** ” button and you will be prompted by a window similar to that shown in Figure 6.32.



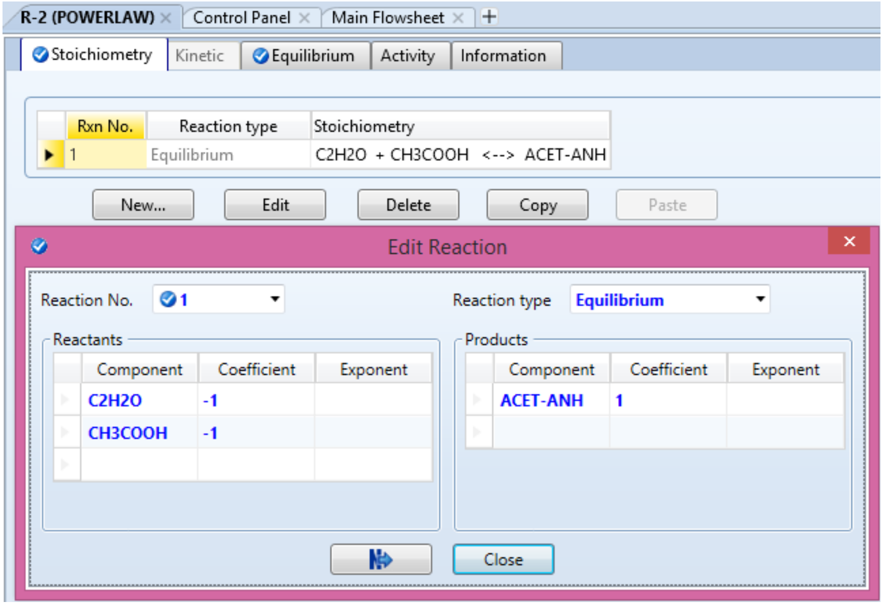
Name	Type
R-1	POWERLAW

Enter ID: R-2

Select Type: POWERLAW

Figure 6.32 The new reaction is given the ID of "***R-2***" and it is of type "**POWERLAW**".

Click on "**OK**" button shown in Figure 6.32 and Aspen Plus will revert to "**Stoichiometry**" tab window where we need to define the stoichiometry of the equilibrium reaction. Click on "**New …** " button at the bottom of the "**Stoichiometry**" tab window, the "**Edit Reaction**" window will pop-up as shown in Figure 6.33, where we enter the stoichiometry of each reacting species, whether it is reactant or product, and the reaction type.



Rxn No.	Reaction type	Stoichiometry
1	Equilibrium	C2H2O + CH3COOH <--> ACET-ANH

Reaction No. 1

Reaction type Equilibrium

Reactants

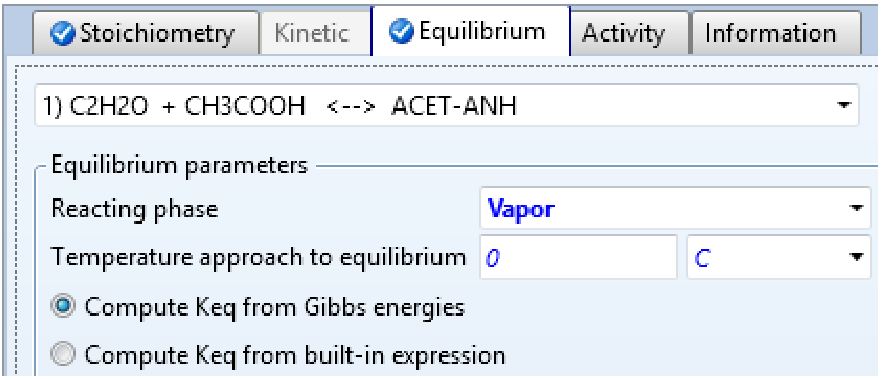
Component	Coefficient	Exponent
C2H2O	-1	
CH3COOH	-1	

Products

Component	Coefficient	Exponent
ACET-ANH	1	

Figure 6.33 Enter -1 for reactant coefficient and $+1$ for product coefficient and choose "**Reaction type**" as "*Equilibrium*".

Click on “**N→**” button at the bottom of the “**Edit Reaction**” window and Aspen Plus will bring you back to reaction **R-2** window. Click on “**Equilibrium**” tab and its window will show up as in Figure 6.34. Select the reacting phase as vapor and select the first choice. If *Keq* = *f(T)* is given, then you may go with the second option.



1) C2H2O + CH3COOH <--> ACET-ANH

Reacting phase: Vapor

Temperature approach to equilibrium: 0 C

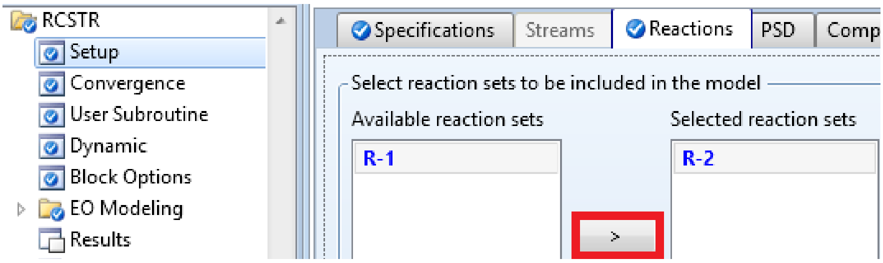
● Compute Keq from Gibbs energies

○ Compute Keq from built-in expression

Figure 6.34 In “**Equilibrium**” tab window, choose the reaction phase to be “*Vapor*” and select the first choice (i.e., ● Compute Keq from Gibbs energies).

You will notice that everything is now defined for Aspen Plus except for “**RCSTR**” block where we need to associate “**R-2**” reaction set with “**RCSTR**” block.

Click on “**Next→**” button and Aspen Plus will bring you to “**RCSTR**” block as shown in Figure 6.35. Highlight **R-2** from the “**Available reaction sets**” and move it to the “**Selected reaction sets**” side.



Available reaction sets: R-1

Selected reaction sets: R-2

Figure 6.35 Association of “**RCSTR**” with “**R-2**” reaction set.

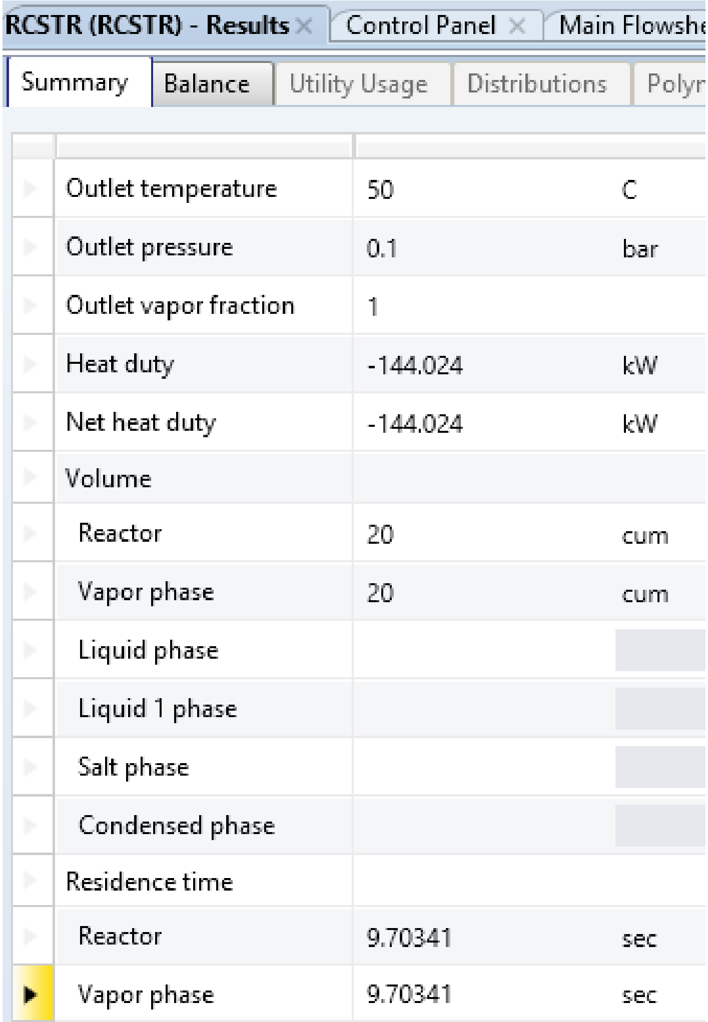
After selecting “**R-2**” reaction set, the blue checkmark will replace the half-filled red circle.

6.12 RUNNING THE SIMULATION (PFR + CMPRSSR + RECTIF + DSTL + RCSTR)

Aspen Plus is ready to start the simulation. Click on “**Reset**” followed by “**Next→**” button and Aspen Plus will start the process of simultaneously solving the set of steady-state total mass-balance, component mass-balance, and energy-balance equations around each block, augmented by all thermodynamic and equation of state relationships.

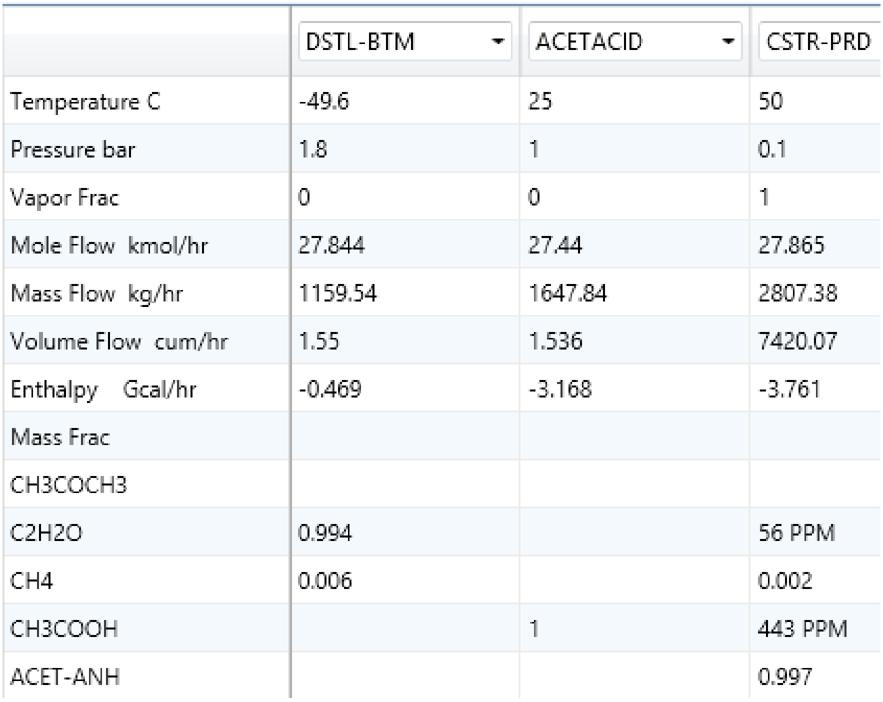
Check “**Control Panel**” to see if there is any error or serious warning.

Figures 6.36 and 6.37 show the simulation results pertaining to “**RCSTR**” block.



Outlet temperature	50	C
Outlet pressure	0.1	bar
Outlet vapor fraction	1	
Heat duty	-144.024	kW
Net heat duty	-144.024	kW
Volume		
Reactor	20	cum
Vapor phase	20	cum
Liquid phase		
Liquid 1 phase		
Salt phase		
Condensed phase		
Residence time		
Reactor	9.70341	sec
Vapor phase	9.70341	sec

Figure 6.36 The heat duty, the reactor volume, and the residence time for “**RCSTR**” block. A reactor volume of 20 m^3 is needed with a residence time of 9.7 s and the heat of reaction is exothermic.



	DSTL-BTM	ACETACID	CSTR-PRD
Temperature C	-49.6	25	50
Pressure bar	1.8	1	0.1
Vapor Frac	0	0	1
Mole Flow kmol/hr	27.844	27.44	27.865
Mass Flow kg/hr	1159.54	1647.84	2807.38
Volume Flow cum/hr	1.55	1.536	7420.07
Enthalpy Gcal/hr	-0.469	-3.168	-3.761
Mass Frac			
CH3COCH3			
C2H2O	0.994		56 PPM
CH4	0.006		0.002
CH3COOH		1	443 PPM
ACET-ANH			0.997

Figure 6.37 The inlet and outlet streams of "**RCSTR**" block plus their properties in terms of flow rate, *P*, *T*, and composition.

Finally, notice that the mass fraction of acetic anhydride in the product stream is 0.997 with trace amounts of other chemical species.

EXERCISE 6.3

Under "**Properties**" environment, go to "**Home**" ribbon | "**Analysis**" tab | and click on "**Mixture Analysis**" (Mixture) button and create a mixture analysis case study. Verify that that an equimolar mixture of ketene and acetic acid at 50°C and 0.1 bar ("**RCSTR**" condition) will be in the vapor phase not in the liquid phase. Use the property set "**TXPORT**" to tell whether or not we have a vapor mixture at the given conditions of *P* and *T*.

6.13 SENSITIVITY ANALYSIS: THE REACTOR'S OPTIMUM OPERATING CONDITIONS

At the end of this chapter, we show an example to demonstrate the parametric plot for one dependent variable as a function of two independent variables. The advantage is to see how the dependent variable changes as a function of both independent variables; hence, we will have the chance to see the function topology in terms of minimum and maximum points.

Methanol is widely used as an industrial feedstock and may become an alternative energy resource. It is mainly produced from a mixture of carbon monoxide, carbon dioxide, and hydrogen under high pressure and temperature using Cu/ZnO-based catalysts. Synthesis of methanol involves three main reactions [2]:

$$CO + 2H_2 \Longleftrightarrow CH_3OH \tag{6.12}$$

$$CO_2 + 3H_2 \Longleftrightarrow CH_3OH + H_2O \tag{6.13}$$

$$CO + H_2O \Longleftrightarrow CO_2 + H_2 \tag{6.14}$$

We will test the synthesis of methanol under equilibrium conditions using the rigorous CSTR (**RCSTR**) model. The pressure can vary between 15 and 75 bar and temperature between 450 and 550 K.

The feed stream enters the reactor at 500 K and 50 bar with 1/3 mole fraction equally for CO, CO_2, and H_2. The total molar flow rate can be set 99 kmol/h. The same reactor conditions are assumed as those of the feed in terms of P and T. The reactor volume is assumed 5 m^3. The goal is to maximize the selectivity of methanol production. To achieve this, we will carry out the following steps:

1. Choose "**Chemicals with Metric Units**" template to create a steady-state flowsheet as shown in Figure 6.38. As the pressure is higher than 10 bar, the property model can be "**PSRK**" with "**Free-water method**" set to "*STEAMNBS*", under "**Methods**" | "**Specifications**" | "**Global**" sheet.

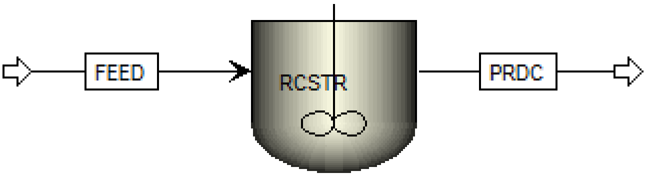
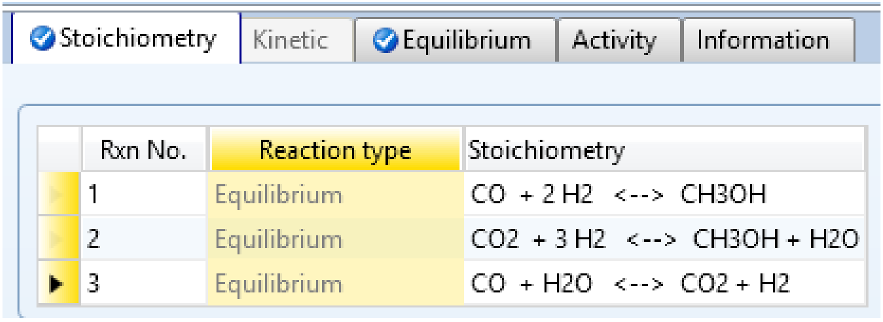


Figure 6.38 Testing methanol synthesis via the rigorous-CSTR (**RCSTR**) model.

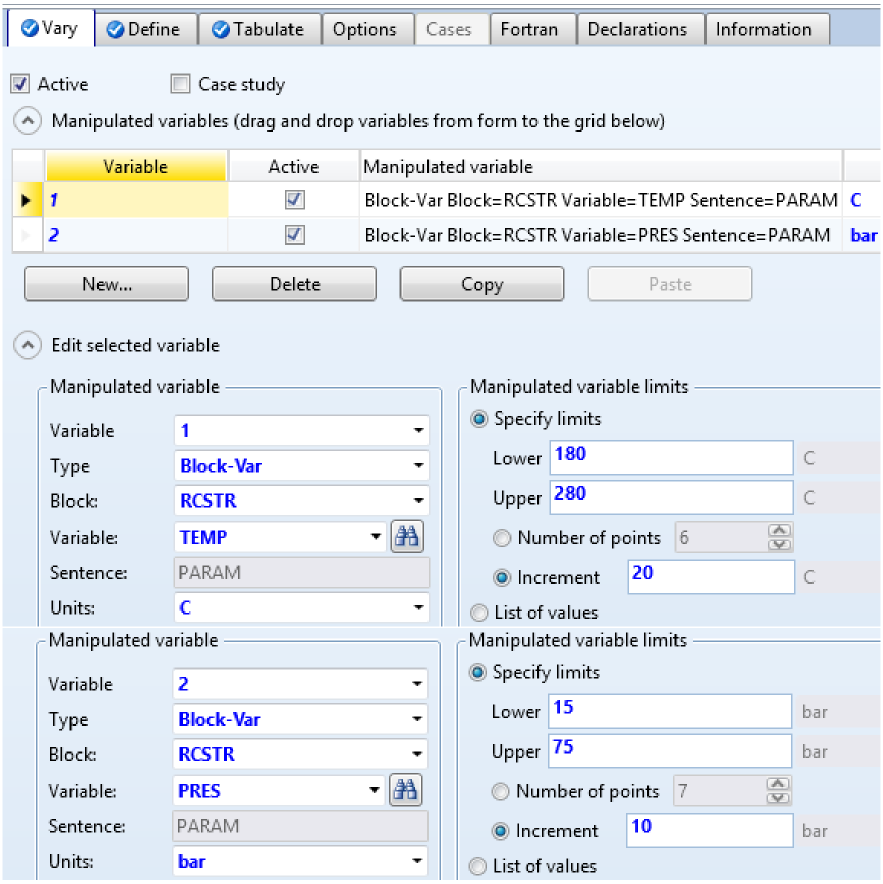
2. Add the five components: CO, CO_2, H_2, H_2O, and CH_3OH.
3. Under “**Properties**” environment, go to “**Estimation**” | “**Input**” | “**Setup**” sheet and be sure that the “*Estimate all missing parameters*” option is affirmed. Click “**Reset**” followed by “**Next**” button to run the simulation and assure that properties analysis completed successfully. Switch to “**Simulation**” environment.
4. Define three “**POWERLAW**” type equilibrium reactions as shown in Figure 6.39.



Rxn No.	Reaction type	Stoichiometry
1	Equilibrium	CO + 2 H2 <--> CH3OH
2	Equilibrium	CO2 + 3 H2 <--> CH3OH + H2O
3	Equilibrium	CO + H2O <--> CO2 + H2

Figure 6.39 Defining the three equilibrium reactions involved in methanol synthesis.

5. In “**Navigation**” pane and under “**Model Analysis Tools**” folder | “**Sensitivity**” subfolder, create “**S-1**” set. In “**Vary**” tab window, vary both *T* and *P* as block (“**RCSTR**”) variables between 180 and 280°C with an increment of 20°C for *T* and between 15 and 75 bar with an increment of 10 bar for *P*, as shown in Figure 6.40 for “**RCSTR**” T & P variable. In “**Define**” tab window, define the sensitivity variable as the mole fraction of methanol (**MFMETH**) in the product (**PRDC**) stream. In “**Tabulate**” tab window, tabulate “**MFMETH**”.



☑ Active ☐ Case study

Manipulated variables (drag and drop variables from form to the grid below)

Variable	Active	Manipulated variable	
1	☑	Block-Var Block=RCSTR Variable=TEMP Sentence=PARAM	C
2	☑	Block-Var Block=RCSTR Variable=PRES Sentence=PARAM	bar

Edit selected variable

Manipulated variable

Variable: 1
Type: Block-Var
Block: RCSTR
Variable: TEMP
Sentence: PARAM
Units: C

Manipulated variable limits

● Specify limits
Lower: 180 C
Upper: 280 C
○ Number of points: 6
● Increment: 20 C
○ List of values

Manipulated variable

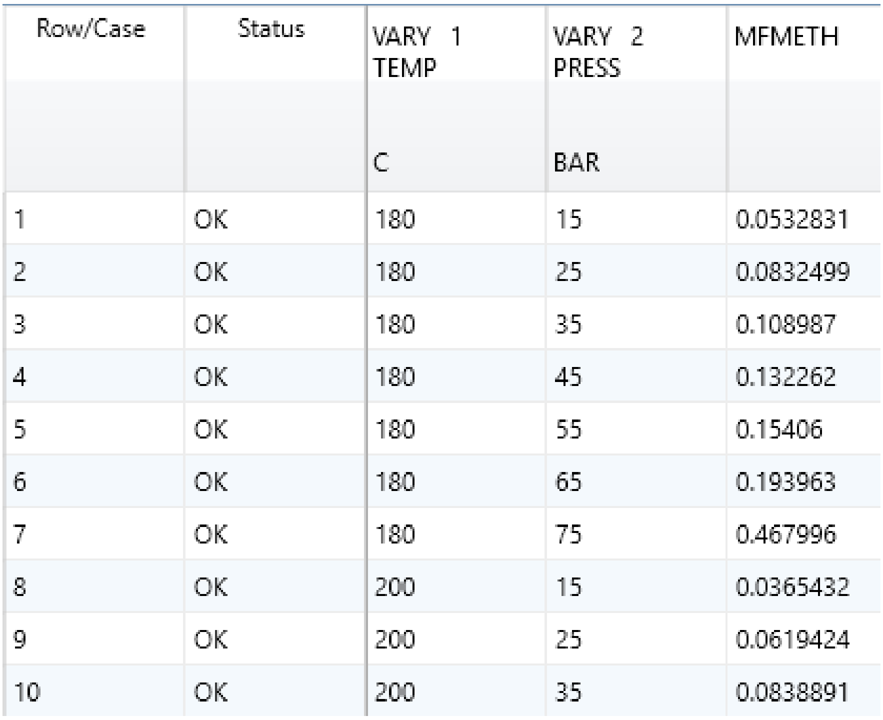
Variable: 2
Type: Block-Var
Block: RCSTR
Variable: PRES
Sentence: PARAM
Units: bar

Manipulated variable limits

● Specify limits
Lower: 15 bar
Upper: 75 bar
○ Number of points: 7
● Increment: 10 bar
○ List of values

Figure 6.40 *T* & *P* of the reactor will be varied to see how they affect the reaction performance.

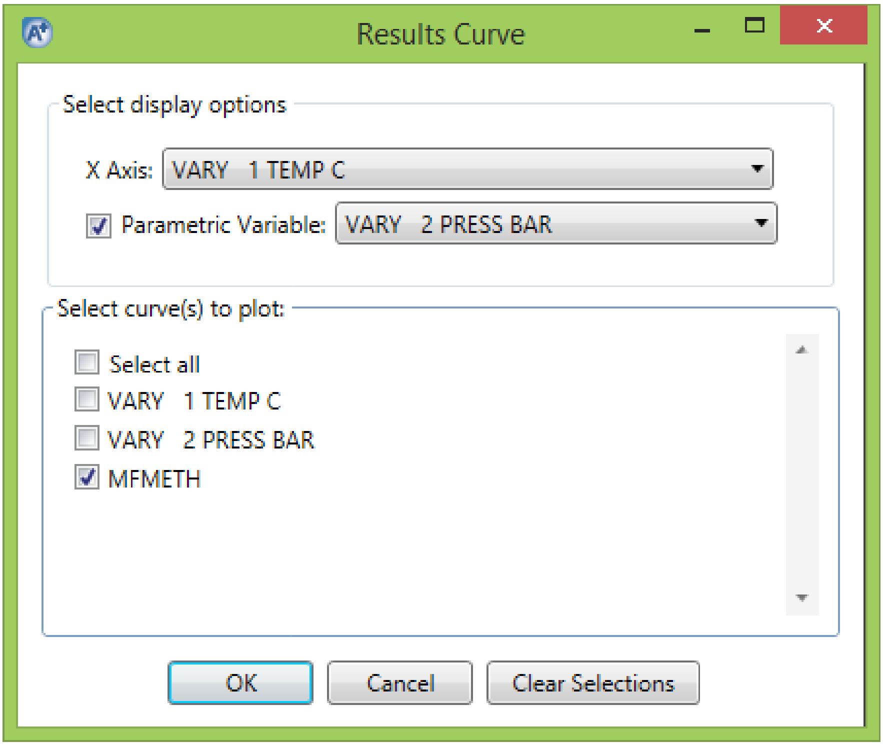
6. Reinitialize and run the show. The Sensitivity (**S-1**) results are shown in Figure 6.41.



Row/Case	Status	VARY 1 TEMP C	VARY 2 PRESS BAR	MFMETH
1	OK	180	15	0.0532831
2	OK	180	25	0.0832499
3	OK	180	35	0.108987
4	OK	180	45	0.132262
5	OK	180	55	0.15406
6	OK	180	65	0.193963
7	OK	180	75	0.467996
8	OK	200	15	0.0365432
9	OK	200	25	0.0619424
10	OK	200	35	0.0838891

Figure 6.41 A portion of sensitivity analysis results where both *T* and *P* are varied to see their effects on **MFMETH**.

7. While the "**S-1**" summary of results window (*i.e.*, Figure 6.41) is active, click on "**Home**" ribbon **|** "**Plot**" group **|** "**Results Curve**" button and the "**Results Curve**" window will show up, as shown in Figure 6.42. Select *T* as X-Axis, *P* as the parametric variable, and **MFMETH** as the dependent variable (*i.e.*, Y-Axis).



Results Curve

Select display options

X Axis: VARY 1 TEMP C

☑ Parametric Variable: VARY 2 PRESS BAR

Select curve(s) to plot:

☐ Select all
☐ VARY 1 TEMP C
☐ VARY 2 PRESS BAR
☑ MFMETH

Figure 6.42 The “**Results Curve**” window where the user decides on X, Y, and the parametric variable.

8. Click on “**OK**” button and finally the “**Sensitivity Results Curve**” plot will show up as in Figure 6.43, which shows **MFMETH** = *f(P,T)*. **MFMETH** is maximum at high *P* and low *T*.

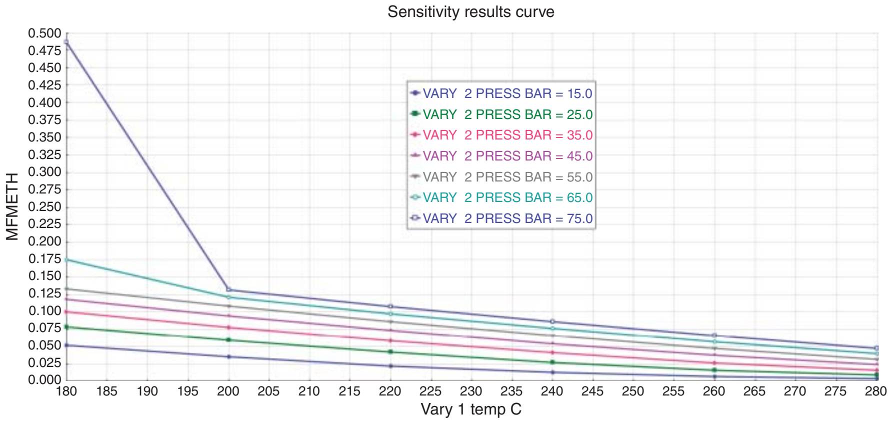
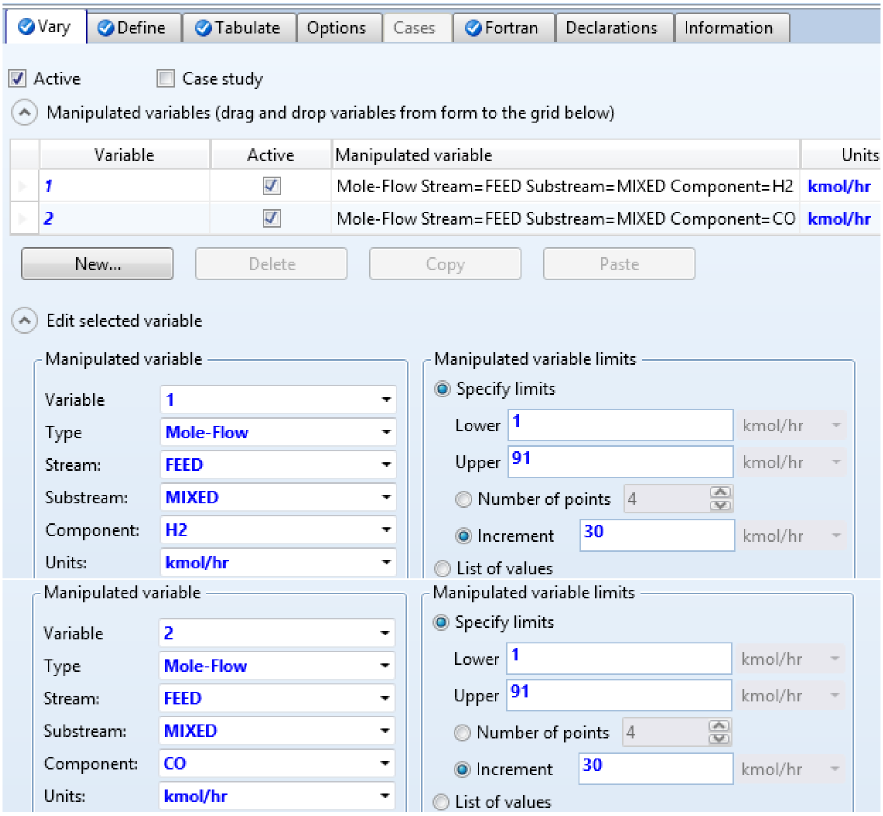


Figure 6.43 The effect of **RCSTR** operating conditions *P* and *T* on **MFMETH** (*i.e.*, conversion).

9. Change "**RCSTR**" P and T to 75 bar and 180°C (453 K), respectively. In "**Navigation**" pane and under "**Model Analysis Tools**" | "**Sensitivity**" | "**S-1**" sheet, right-click on "**S-1**" and select **Deactivate** command from the shortcut context menu. This means that "**S-1**" analysis will not be included in simulation as we have already made use of it and changed "**RCSTR**" conditions to high P and low T to maximize the mole fraction of methanol (**MFMETH**) in the product stream.
10. Define a new sensitivity set "**S-2**". Figure 6.44 shows "**Vary**" tab window. The first variable (Variable no. 1) that accounts for H_2 molar flow rate in **FEED** stream between 1 and 91 kmol/h with an increment of 30 kmol/h. The second variable (Variable no. 2) will be CO molar flow rate in **FEED** stream between 1 and 91 kmol/h with an increment of 30 kmol/h. On the other hand, CO_2 will not be changed as we say here that **MFMETH** in **PRDC** stream is a function of four linearly independent variables: $Y_{CH3OH} = f(P, T, Y_{H2}, Y_{CO})$. We have already found the best values of P and T that will maximize Y_{CH3OH}. Y_{CO2} is dependent on Y_{H2} and Y_{CO}, as the summation adds up to one.



☑ Active ☐ Case study

Manipulated variables (drag and drop variables from form to the grid below)

Variable	Active	Manipulated variable	Units
1	☑	Mole-Flow Stream=FEED Substream=MIXED Component=H2	kmol/hr
2	☑	Mole-Flow Stream=FEED Substream=MIXED Component=CO	kmol/hr

Edit selected variable

Manipulated variable

Variable: 1
Type: Mole-Flow
Stream: FEED
Substream: MIXED
Component: H2
Units: kmol/hr

Manipulated variable limits

● Specify limits
Lower: 1 kmol/hr
Upper: 91 kmol/hr
○ Number of points: 4
● Increment: 30 kmol/hr
○ List of values

Manipulated variable

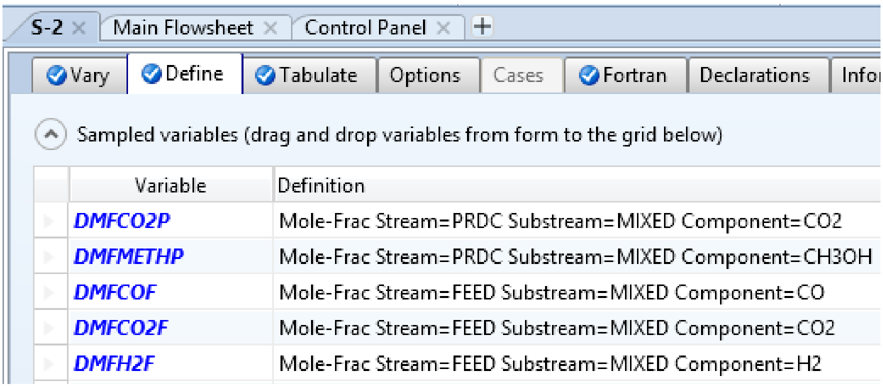
Variable: 2
Type: Mole-Flow
Stream: FEED
Substream: MIXED
Component: CO
Units: kmol/hr

Manipulated variable limits

● Specify limits
Lower: 1 kmol/hr
Upper: 91 kmol/hr
○ Number of points: 4
● Increment: 30 kmol/hr
○ List of values

Figure 6.44 The feed molar flow rate of H_2 and CO will be varied to see how they affect the reaction performance.

11. Figure 6.45 shows the “**Define**” tab window, which includes the composition of feed and product stream. The variables are prefixed by “**D**”, as in **FORTRAN** code, to treat all variables as real or double not integer (with prefix “**M**”).



Sampled variables (drag and drop variables from form to the grid below)

Variable	Definition
DMFCO2P	Mole-Frac Stream=PRDC Substream=MIXED Component=CO2
DMFMETHP	Mole-Frac Stream=PRDC Substream=MIXED Component=CH3OH
DMFCOF	Mole-Frac Stream=FEED Substream=MIXED Component=CO
DMFCO2F	Mole-Frac Stream=FEED Substream=MIXED Component=CO2
DMFH2F	Mole-Frac Stream=FEED Substream=MIXED Component=H2

Figure 6.45 The “**Define**” tab window, which includes the composition of feed and product stream. The variables are prefixed by “**D**”, in compliance with **FORTRAN** code, to treat all variables as double not integer (prefix “**M**”).

12. Under “**Fortran**” tab, define the following three variables:

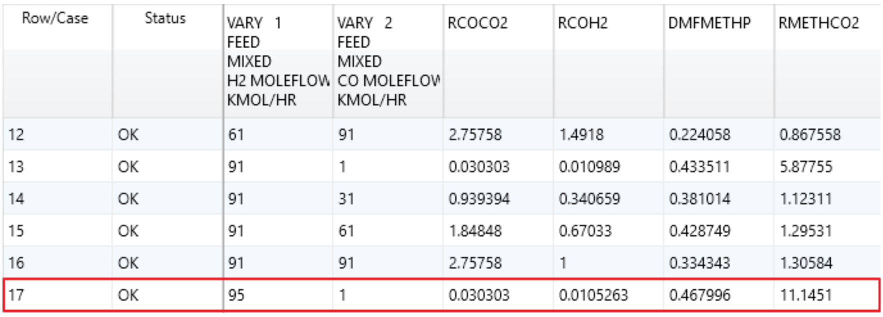
    RCOCO2 = DMFCOF/DMFCO2F

    RCOH2 = DMFCOF/DMFH2F

    RMETHCO2 = DMFMETHP/DMFCO2P

    The first represents $(Y_{CO}/Y_{CO2})_{FEED}$; the second $(Y_{CO}/Y_{H2})_{FEED}$; and the third $(Y_{CH3OH}/Y_{CO2})_{PRDC}$. Again, we have only two linearly independent ratios out of three, which describe the composition of **FEED** stream. The higher the value of the third term (**RMETHCO2**), the higher will be the selectivity of CH_3OH over CO_2 (the undesired side product *via* the third reaction).

13. Under **Tabulate** tab, include the following set of variables:
    1. **RCOCO2**
    2. **RCOH2**
    3. **DMFMETHP**
    4. **RMETHCO2**
14. Reinitialize and run the show.
15. Figure 6.46 shows the values of **DMFMETHP** and **RMETHCO2** in **PRD** stream as a function the molar feed ratios **RCOCO2** and **RCOH2**. The maximum yield and selectivity occurs at **RCOCO2** = 0.0303 and **RCOH2** = 0.0105. The feed composition will be



Row/Case	Status	VARY 1 FEED MIXED H2 MOLEFLOW KMOL/HR	VARY 2 FEED MIXED CO MOLEFLOW KMOL/HR	RCOCO2	RCOH2	DMFMETHP	RMETHCO2
12	OK	61	91	2.75758	1.4918	0.224058	0.867558
13	OK	91	1	0.030303	0.010989	0.433511	5.87755
14	OK	91	31	0.939394	0.340659	0.381014	1.12311
15	OK	91	61	1.84848	0.67033	0.428749	1.29531
16	OK	91	91	2.75758	1	0.334343	1.30584
17	OK	95	1	0.030303	0.0105263	0.467996	11.1451

Figure 6.46 The sensitivity analysis results showing the best feed molar ratios where both the yield and selectivity are maximum.

$$\mathrm{Y}_{\mathrm{H_2}} = 95/(95+1+33) = 0.7364;\ \mathrm{Y}_{\mathrm{CO}} = 1/(95+1+33) = 0.0078;$$
$$\mathrm{Y}_{\mathrm{CO_2}} = 33/(95+1+33) = 0.2558$$

Also, from the given molar feed ratios, evaluated at the maximum yield and selectivity

$$\sum_{i=1}^{N} Y_i = 1:\quad Y_{\mathrm{CO}} + Y_{\mathrm{CO_2}} + Y_{\mathrm{H_2}} = 1 = Y_{\mathrm{CO}} + (1/\mathbf{RCOCO2}) \times Y_{\mathrm{CO}} + (1/\mathbf{RCOH2}) \times Y_{\mathrm{CO}} = [Y_{\mathrm{CO}} + (33.00) \times Y_{\mathrm{CO}} + (95.00) \times Y_{\mathrm{CO}}] = 1 \rightarrow Y_{\mathrm{CO}} = 1/129 = 0.0078.$$

In doing so, we have optimized the reactor performance in terms of P, T through "**S-1**" analysis and feed molar composition through "**S-2**" analysis, where both analyses when combined will give the maximum yield and selectivity. Consequently and based on "**S-2**" analysis, the best feed molar composition will be 73.64 mol% H_2; 25.58 mol% CO_2; and 0.78 mol% CO.

REFERENCES

[1] Fogler, H.S. (2006) Elements of Chemical Reaction Engineering, 4th edn, Pearson Education, Inc., New Jersey.

[2] Lim, H.W., Park, M., Kang, S. *et al.* (2009) Modeling of the kinetics for methanol synthesis using Cu/ZnO/Al_2O_3/ZrO_2 catalyst: Influence of carbon dioxide during hydrogenation. *Industrial and Engineering Chemistry Research*, **48** (23), 10448–10455.

[3] Hangx, G., Kwant, G., Maessen, H., *et al.* (2001) Reaction Kinetics of the Esterification of Ethanol and Acetic Acid Towards Ethyl Acetate, Intelligent Column Internals for Reactive Separations (INTINT), Deliverable 22, 2001.

HOMEWORK/CLASSWORK 6.1 (HYDROGEN PEROXIDE SHELF-LIFE)

Hydrogen peroxide 3 wt% solution (active ingredient: H_2O_2) is an antiseptic oral debriding agent, which can be used as a first aid to help prevent the risk of infection in minor cuts, scrapes, and burns. Moreover, it helps in the removal of phlegm, mucus, or other secretions associated with occasional sore mouth; however, it must be externally used.

Consider the decomposition of H_2O_2:

$$2H_2O_{2(aq)} \xrightarrow{k} 2H_2O + O_{2(g)} \tag{6.15}$$

With Arrhenius kinetics:

$$k = 4.80 \times 10^8 e^{(-78{,}683.7/RT)} \tag{6.16}$$

where k has unit of s^{-1} and the reaction order is one with respect to H_2O_2. Let us analyze how the concentration of H_2O_2 will drop with time if we keep the bottle both at room temperature (25°C) and inside the household refrigerator (5°C). To simulate the bottle, we will use **RBATCH** model where we allow the reaction to take place and we will stop the reaction when the conversion reaches 90%, or the mass fraction of H_2O_2 drops from 0.03 to 0.003. The time will be reported by Aspen Plus simulator. To achieve this goal, carry out the following steps:

1. Choose "**Specialty Chemicals with Metric Units**" template to create the process flowsheet. The default property model will be "**NRTL**".
2. Add the three components: H_2O, O_2, and H_2O_2.
3. In "**Navigation**" pane, select O_2 as Henry component by creating "**HC-1**" set under "**Components**" | "**Henry Comps**".
4. Select "**HC-1**" from the drop- down list in "**Methods**" | "**Specifications**" | "**Global**" tab window.
5. Go to "**Methods**" | "**Parameters**" | "**Binary Interaction**" | "**NRTL-1**" sheet and be sure that the "*Estimate missing parameters by UNIFAC*" option is selected. Click "**Reset**" followed by "**Next**" button to run the simulation and assure that properties analysis completed successfully. See NOTE #2 for: *WARNING IN PHYSICAL PROPERTY SYSTEM*.
6. Switch to "**Simulation**" environment.
7. From the "**Model Palette**", under "**Reactors**" tab, select "**RBATCH**" and add it to your open project. Add two streams one for the batch at time zero and another for the product at the end of the batch time. Your flowsheet should be similar to that shown in Figure 6.47.

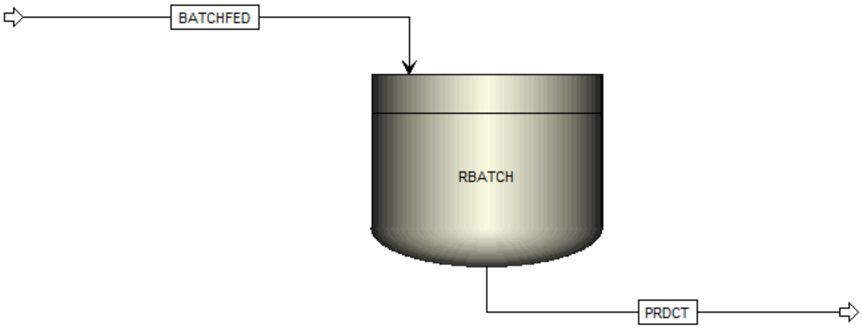
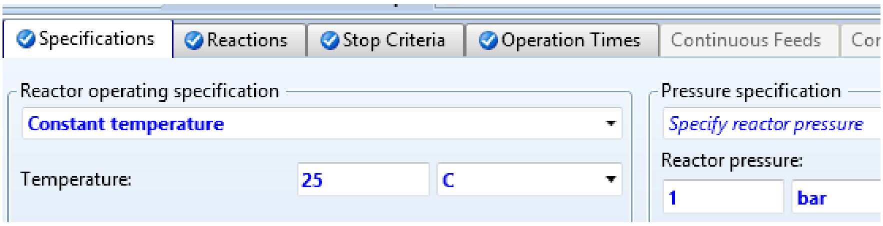


Figure 6.47 Visualization of H_2O_2 bottle as "**RBATCH**" type reactor.

8. The "**BATCHFED**" stream has 97 kg/h H_2O and 3 kg/h H_2O_2 at 1 bar and 25°C.
9. The simulation will be carried out twice: first, at room temperature (25°C) and 1 bar, and the second, at household refrigerator temperature (5°C) and 1 bar. This will demonstrate the effect of temperature on the shelf-life of the peroxide within the bottle if we keep it outside or inside the refrigerator, respectively.
10. In "**Navigation**" pane, under "**Reactions**" folder, define the aforementioned reaction (Eq. 6.15) named **R-1** as kinetic type and enter the kinetic parameters (Eq. 6.16) in "**Kinetic**" tab window. Notice that the reaction phase is liquid and [Ci] basis is molarity.
11. In "**Blocks**" | "**RBATCH**" | "**Setup**" | "**Specifications**" tab window, enter the data as shown in Figure 6.48.

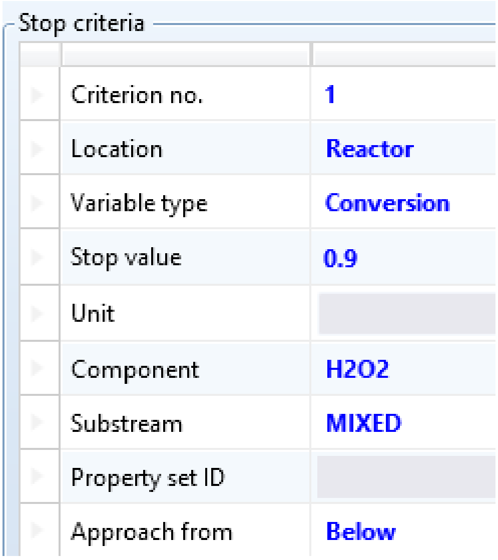


Reactor operating specification
Constant temperature
Temperature: 25 C

Pressure specification
Specify reactor pressure
Reactor pressure:
1 bar

Figure 6.48 "**RBATCH**" reactor specifications (constant *P* & *T*).

12. In "**Reactions**" tab window, associate "**R-1**" with "**RBATCH**" reactor.
13. In "**Stop Criteria**" tab window, enter the data as shown in Figure 6.49.

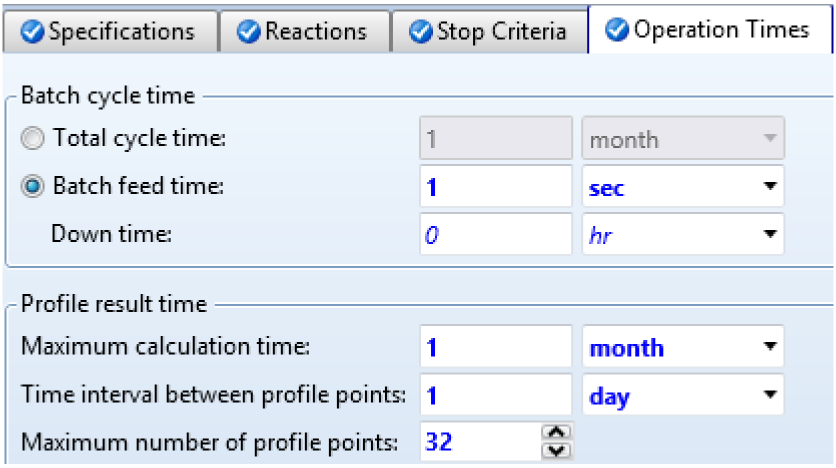


Stop criteria

Criterion no.	1
Location	Reactor
Variable type	Conversion
Stop value	0.9
Unit	
Component	H2O2
Substream	MIXED
Property set ID	
Approach from	Below

Figure 6.49 The stop criteria to stop the reaction and report the batch time whenever H_2O_2 conversion of 0.9 is reached.

14. In "**Operation Times**" tab window, enter the data as shown in Figure 6.50.



Batch cycle time

○ Total cycle time: 1 month

● Batch feed time: 1 sec

Down time: 0 hr

Profile result time

Maximum calculation time: 1 month

Time interval between profile points: 1 day

Maximum number of profile points: 32

Figure 6.50 The batch feed time for H_2O_2 bottle will be very short and no need for down time, unlike the real batch reactors where they require loading/unloading time.

15. Reinitialize and run the show.
16. Report the reaction time (in hours or days) under "**RBATCH**" | "**Results**" | "**Summary**" tab form until the mass fraction of H_2O_2 drops to 0.003 from the initial value 0.03.

17. For the second run, that is, the batch reactor temperature will be 5°C not 25°C. Report the reaction time in hours or days. Compare both values. Do you recommend keeping the bottle of H_2O_2 solution inside the room (25°C) or inside the refrigerator (5°C)?

HOMEWORK/CLASSWORK 6.2 (ESTERIFICATION PROCESS)

Consider the reaction between ethanol and acetic acid to produce ethyl acetate and water, or what is called esterification process (Figure 6.51):

$$CH_3CH_2OH + CH_3COOH \leftrightarrow CH_3COOCH_3CH_2 + H_2O \tag{6.17}$$

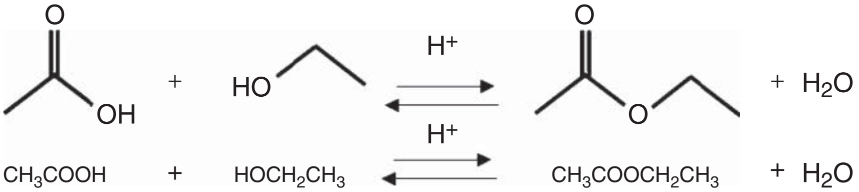


Figure 6.51 A schematic symbolizes the reaction between acetic acid and ethanol to produce ethyl acetate (an ester) and water (the esterification process).

The following kinetic data were quoted from Hangx *et al.* [3]. Purolite CT179 was used as a catalyst, which is a porous cation exchange resin, containing sulfonic acid groups. The particle diameter was 0.6–1.4 mm. The typical porosity is assumed to be 0.5.

Using such a catalyst, it was found that the reaction is first order with respect to ethanol and 1.5th order with respect to acetic acid. The reaction rate constant is described by Arrhenius kinetics for both forward and backward directions:

$$r_f = k_1 x_{\mathrm{ETOH}} x_{\mathrm{ACOH}}^{1.5} = \left(4.24 \times 10^3 (\mathrm{kmol/kg\,cat} \cdot \mathrm{s}) \times e^{-\frac{48{,}300}{RT}}\right) x_{\mathrm{ETOH}} x_{\mathrm{ACOH}}^{1.5} \tag{6.18}$$

$$r_b = k_2 x_{\mathrm{ETOAC}} x_{\mathrm{H2O}} = \left(4.55 \times 10^5 (\mathrm{kmol/kg\,cat} \cdot \mathrm{s}) \times \mathrm{e}^{-\frac{66{,}200}{RT}}\right) x_{\mathrm{ETOAC}} x_{\mathrm{H2O}} \tag{6.19}$$

where x represents the mole fraction of a given component. Remember that, according to Aspen Plus built-in help, the reaction rate must be expressed as kmol/kg cat · s (see Eqs. 6.10 and 6.11). The authors reported the value as mol/kg catalyst · s; that is why we have to adjust the basis.

Since the lowest normal boiling point is 77.1°C for ethyl acetate (**ETOAC**), we can run the reaction at 1 atm. and a temperature less than 77.1°C. Alternatively, we can elevate the pressure inside the reactor, which will grant us the luxury to increase the temperature above 77.1°C. Execute the following steps:

1. Choose "**Chemicals with Metric Units**" template to create the process flowsheet. The default property model will be "**NRTL**".
2. Add the four components, shown in Figure 6.51, to components list.

3. Go to “**Methods**” | “**Parameters**” | “**Binary Interaction**” | “**NRTL-1**” sheet and be sure that the “*Estimate missing parameters by UNIFAC*” option is selected. Click “**Reset**” followed by “**Next**” button to run the simulation and assure that properties analysis completed successfully. Switch to “**Simulation**” environment.
4. From the “**Model Palette**”, under “**Reactors**” tab, select “**RCSTR**” and add it to your open project. Add two streams one for the feed and another for the product. Your flowsheet should be similar to that shown in Figure 6.52.

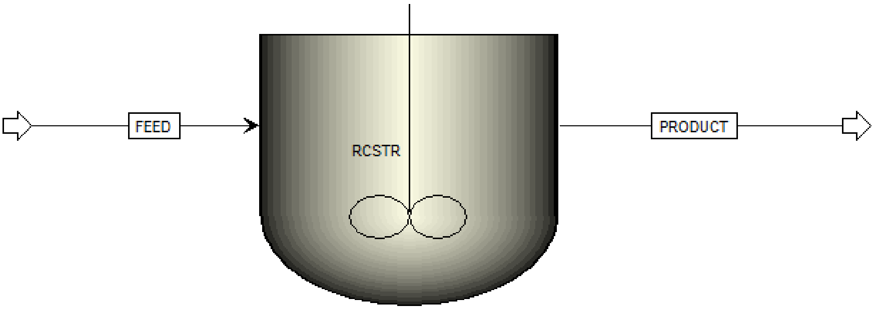
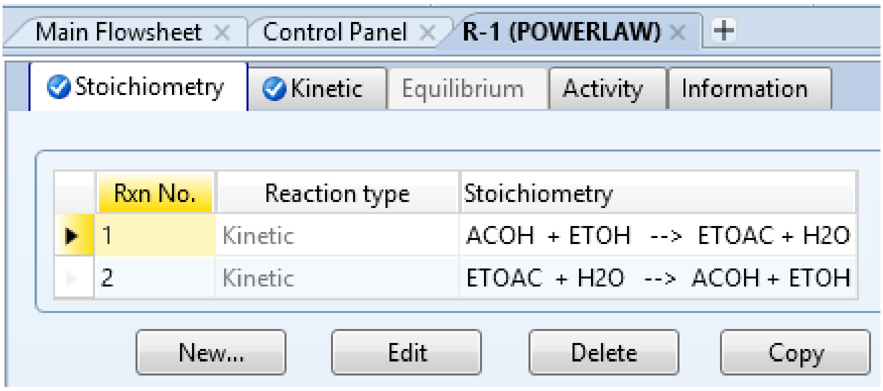


Figure 6.52 The flowsheet for ethyl acetate production using “**RCSTR**” type reactor.

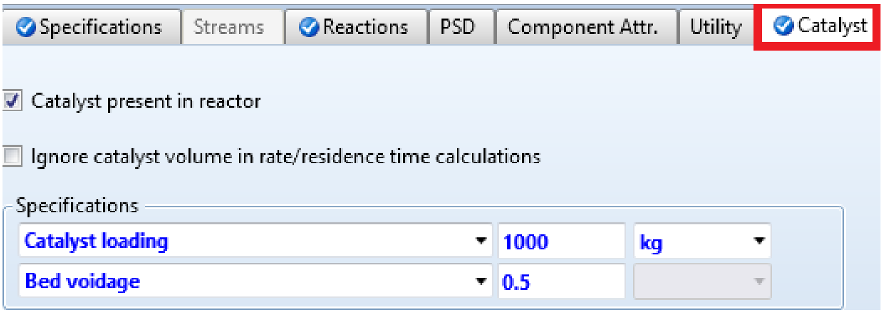
5. Set the feed stream at 2 atm. and 100°C with a flow rate of 50 kmol/h for each of “**ACOH**” and “**ETOH**” reactant.
6. Define the forward and backward reactions given by Equations (6.17), (6.18), and (6.19). The type of reaction is “*POWERLAW*” with “*Kinetic*” type, as shown in Figure 6.53. Notice that reaction #1 stands for the forward and #2 for the backward direction.



Rxn No.	Reaction type	Stoichiometry
1	Kinetic	ACOH + ETOH --> ETOAC + H2O
2	Kinetic	ETOAC + H2O --> ACOH + ETOH

Figure 6.53 “**R-1**” reaction set is resolved into two kinetic reactions the forward and backward direction.

7. In **Kinetic** tab window, enter the Arrhenius kinetic parameters, the rate basis (*i.e.*, Cat (wt)), the reacting phase, and [Ci] basis as mole fraction for both the forward and backward reactions.
8. In "**Blocks**" | "**RCSTR**" | "**Setup**" | "**Specifications**" tab window, enter 2 atm for pressure; 100°C for temperature; the valid phase as liquid only; and 1 h as the residence time.
9. In "**Blocks**" | "**RCSTR**" | "**Setup**" | "**Reactions**" tab window, associate "**R-1**" with "**RCSTR**".
10. In "**Blocks**" | "**RCSTR**" | "**Setup**" | "**Catalyst**" tab window, select the catalyst attributes as shown in Figure 6.54.



☑ Catalyst present in reactor

☐ Ignore catalyst volume in rate/residence time calculations

Specifications

Catalyst loading 1000 kg

Bed voidage 0.5

Figure 6.54 Entering catalyst attributes as the reaction rate is expressed per unit mass of a catalyst not volume of a reactor as is the case with homogeneous reactions.

11. Reinitialize and run the show. Check for any simulation errors or warnings. Report the reactor volume for the given residence time and the composition of the product stream.

12. Carry out a sensitivity test via varying the reactor temperature between 50 and 130°C with an increment of 5°C and via defining the dependent variable as the mole fraction of ethyl acetate in the product stream. Plot the mole fraction of ethyl acetate as a function of temperature and see the optimum reactor temperature that gives the maximum amount of ethyl acetate.

HOMEWORK/CLASSWORK 6.3 (LIQUID-PHASE ISOMERIZATION OF *n*-BUTANE)

Normal butane, *n*-C_4H_{10}, is to be reversibly isomerized to isobutane, *i*-C_4H_{10}, in a plug-flow reactor (PFR). Isobutane is a valuable product that is used in the manufacture of gasoline additives. The reaction is to be carried out adiabatically in the liquid phase under high pressure ($P = 20$ bar) using essentially trace amounts of a liquid catalyst. Calculate the PFR and CSTR volumes necessary to process 163 kmol/h at 70% conversion of a feed mixture made of 90 mol% *n*-butane and 10 mol% *i*-pentane (2-methyl-butane), which is considered an inert. The feed enters at 330 K and 20 bar.

The kinetic data were quoted from Fogler [1] and were modified to suit Aspen Plus basis for entering the kinetic parameters and concentration.

$$n\text{-C}_4\text{H}_{10} \leftrightarrow i\text{-C}_4\text{H}_{10} \tag{6.20}$$

Equation 6.20 can be resolved into forward and backward steps:

$$n\text{-C}_4\text{H}_{10} \overset{\text{k}_1}{\Rightarrow} i\text{-C}_4\text{H}_{10} \tag{6.21}$$

$$-r_{n-\text{C}_4} = \text{k}_1\text{C}_{n-\text{C}_4} \tag{6.22}$$

$$k_1 = 2.94 \times 10^7(\text{s}^{-1}) \times e^{\left(-\frac{65{,}300}{8.314*T}\right)} \tag{6.23}$$

$$i\text{-C}_4\text{H}_{10} \overset{\text{k}_2}{\Rightarrow} n\text{-C}_4\text{H}_{10} \tag{6.24}$$

$$-r_{i-\text{C}4} = k_2\text{C}_{i-\text{C}_4} \tag{6.25}$$

$$k_2 = 1.176 \times 10^8(\text{s}^{-1}) \times e^{\left(-\frac{72{,}200}{8.314*T}\right)} \tag{6.26}$$

1. Choose “**Chemicals with Metric Units**” template to create the process flowsheet. Set the default property model to be “**PENG-ROB**” for having a hydrocarbon system.
2. Add the three components – *n*-butane, isobutene, and 2-methyl-butane – to components list.
3. Click on “**Reset**” followed by “**Next**” button to run the simulation and assure that properties analysis completed successfully. Switch to “**Simulation**” environment.
4. From the “**Model Palette**”, under “**Reactors**” tab, select “**RPlug**” and add it to your open project. Add two streams one for the feed and another for the product. Your flowsheet should be similar to that shown in Figure 6.55.

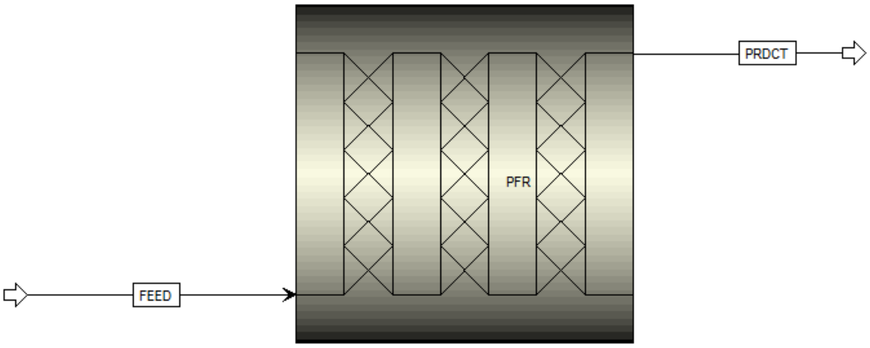


Figure 6.55 The flowsheet for *n*-butane isomerization using “**RPlug**” type reactor.

5. Enter the feed stream properties as indicated in the problem statement.
6. For the reactor volume requirement, enter *3* m for length and *1.1* m for diameter, which will give a 2.6 m^3 single cylindrical tube, and select *Liquid-only* for "**Valid phases**".
7. Define two "**POWERLAW**" reaction sets that represent the set of equations given by Equations 6.21–6.26. Assure that the reaction medium is liquid; the rate basis is reactor volume; and concentration basis is molarity.
8. Associate the reaction set, which contains both reactions, to "**PFR**" block.
9. Reset, run the show, and check for error or serious warning *via* "**Control Panel**".
10. Report the conversion of *n*-C_4 into *i*-C_4. Is the number close to 0.7 as reported by Fogler [1] for a PFR with a volume of 2.6 m^3?
11. Repeat the previous steps but this time for "**RCSTR**" block. For the same volume requirement (*i.e.*, reactor volume = 2.6 m^3), calculate the conversion at the exit of such a CSTR.
12. What will be the CSTR volume (expressed in m^3) needed to achieve 70% conversion?
13. Which reactor type do you recommend for the liquid-phase *n*-C_4 isomerization?

7

REACTORS WITH COMPLEX (NON-CONVENTIONAL) REACTION KINETIC FORMS

7.1 PROBLEM DESCRIPTION

The kinetic data of the following set of reactions were excerpted from Bussche and Froment [1]. Keep in mind, however, the following points:

- The kinetic data are rewritten here in a format that matches how they should be entered into Aspen Plus® reaction kinetic sheets (see next section).
- The rate constants and equilibrium constants, which were obtained via curve-fitting and were reported in table 2 of the same reference, are converted here to match the basis of Aspen Plus. For the reaction rate constant, the basis is *kmol/(kg cat·s·Pa)* for an overall first-order reaction in terms of reacting species and will be, of course, *kmol/(kg cat·s·Pa*^{2}) for an overall second-order kinetics given that the basis for [*Ci*] is the partial pressure expressed in *Pa* not in bar, as indicated in Aspen Plus built-in help.

Consider the conversion of carbon dioxide and hydrogen into methanol according to the following set of reactions:

$$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O \tag{7.1}$$

$$r_{CH_3OH}(\text{kmol/kg cat}\cdot\text{s}) = \frac{1.07\times10^{-13}\times e^{(4{,}413.76/T)}\left(K_{f1}\times P_{CO_2}\times P_{H_2} - K_{b1}\times\frac{P_{CH_3OH}\times P_{H_2O}}{P_H^2}\right)}{(1+K_1\times(P_{H_2O}/P_{H_2})+K_2P_{H_2}^{0.5}+K_3P_{H_2O})^3} \tag{7.2}$$

Aspen Plus®: Chemical Engineering Applications, First Edition. Kamal I.M. Al-Malah.

Companion Website: www.wiley.com/go/Al-Malah/AspenPlusApplications

$$r_{CH_3OH}(\text{kmol/kg cat} \cdot \text{s}) = \frac{1.07 \times 10^{-13} \times e^{(4{,}413.76/T)} \left(P_{CO_2} \times P_{H_2} - 3.9084 \times 10^{20} \times e^{(-7{,}059.726/T)} \times \frac{P_{CH_3OH} \times P_{H_2O}}{P_H^2}\right)}{(1 + 3{,}453.38 \times (P_{H_2O}/P_{H_2}) + 1.578 \times 10^{-3} \times e^{(2{,}068.44/T)} \times P_{H_2}^{0.5} + 6.62 \times 10^{-16} \times e^{(14{,}928.915/T)} P_{H_2O})^3} \tag{7.3a}$$

Alternatively,

$$r_{CH_3OH}(\text{kmol/kg cat} \cdot \text{s}) = \frac{\left(1.07 \times 10^{-13} \times e^{(4{,}413.76/T)} \times P_{CO_2} \times P_{H_2} - 4.182 \times 10^{7} \times e^{(-2{,}645.966/T)} \times \frac{P_{CH_3OH} \times P_{H_2O}}{P_H^2}\right)}{(1 + 3{,}453.38 \times (P_{H_2O}/P_{H_2}) + 1.578 \times 10^{-3} \times e^{(2{,}068.44/T)} \times P_{H_2}^{0.5} + 6.62 \times 10^{-16} \times e^{(14{,}928.915/T)} P_{H_2O})^3} \tag{7.3b}$$

$$CO_2 + H_2 \leftrightarrow CO + H_2O \tag{7.4}$$

$$r_{CO}(\text{kmol/kg cat} \cdot \text{s}) = \frac{122 \times e^{(-(11{,}398.244/T))} \left(K_{f2} \times P_{CO_2} - K_{b2} \times \frac{P_{CO} \times P_{H_2O}}{P_{H_2}}\right)}{(1 + K_1 \times (P_{H_2O}/\mathrm{P}_{H_2}) + K_2 P_{H_2}^{0.5} + K_3 P_{H_2O})^1} \tag{7.5}$$

$$r_{CO}(\text{kmol/kg cat} \cdot \text{s}) = \frac{122 \times e^{(-(11{,}398.244/T))} \left(P_{CO_2} - 0.009354 \times e^{(4773.259/T)} \times \frac{P_{CO} \times P_{H_2O}}{P_{H_2}}\right)}{(1 + 3453.38 \times (P_{H_2O}/P_{H_2}) + 1.578 \times 10^{-3} \times e^{(2068.44/T)} \times P_{H_2}^{0.5} + 6.62 \times 10^{-16} \times e^{(14{,}928.915/T)} P_{H_2O})^1} \tag{7.6a}$$

Alternatively,

$$r_{CO}(\text{kmol/kg cat} \cdot \text{s}) = \frac{\left(122 \times e^{(-(11{,}398.24/T))} \times P_{CO_2} - 1.1412 \times e^{(-(6624.98/T))} \times \frac{P_{CO} \times P_{H_2O}}{P_{H_2}}\right)}{(1 + 3453.4 \times (P_{H_2O}/P_{H_2}) + 1.578 \times 10^{-3} \times e^{(2068.4/T)} \times P_{H_2}^{0.5} + 6.62 \times 10^{-16} \times e^{(14{,}928.9/T)} P_{H_2O})^1} \tag{7.6b}$$

Both reactions are solid-catalyzed exothermic reactions; their kinetic forms, as given by Equations 7.2 and 7.5, obey what is called Langmuir–Hinshelwood–Hougen–Watson (**LHHW**) form.

It is worth mentioning here that the first reaction (Eq. 7.1) describes the conversion of CO_2 and H_2 into methanol (desired product), in the presence of a solid catalyst, at the same time the water–gas shift reaction (Eq. 7.4) goes in parallel with the first reaction, which results in undesired products. This solid catalyst is usually silver or metal oxide.

Moreover, both forms of each Equations 7.3 and 7.6 were tested using Aspen Plus simulator. It was found that using Equations 7.3a and 7.6a ended up with either simulation error or non-sense results for selecting a different basis for feed stream composition. On the other hand, using Equations 7.3b and 7.6a ended up with reasonable results for selecting a different basis for feed stream composition.

In my judgment, one may conclude that this has to deal with the fact that Aspen Plus expects from the user to express the kinetic factor with a positive activation energy. If we look at Equation 7.3a as it stands, we will notice that the activation energy has to be negative in order to have a positive exponential argument (the term outside the numerator bracket is called the kinetic factor). On the other hand, if the driving force expression (anything within the big two brackets of the numerator) does contain a positive exponential argument (e.g., the first term of the driving force expression in Eq. 7.3b), it can be then swallowed by Aspen Plus, because LHHW model tolerates having both negative and positive exponential arguments within the driving force expression as well as within the adsorption term (the denominator in any previous equation). Hence, we will use Equations 7.3b and 7.6b, where the kinetic factor is merged into the driving force expression, ending up with a kinetic factor equal to unity.

NOTE #1: *The bracketed term in the denominator of equations 7.3 and 7.6 is called the adsorption term that accounts for the key role of a catalyst in providing the platform for the negotiating parties (reacting species) so that they can sit together and interact (proximity effect), like each other (activation complex), go inside exclusive private rooms (micro-pores and channels) and wait a while for having babies (products) as a result of the new relationships (chemical bonds), and finally the end of the love session where the new born babies (products) will leave the platform and play faraway in the yard. That explains why the kinetics is a bit cumbersome compared with the casual relationships (conventional kinetics) shown in Chapter 6. The additional terms appearing in the denominator account for competitive adsorption of species, other than* CO_2*, such as* H_2O *and* H_2 *in this case, where such adsorbing species will retard the conversion of* CO_2 *into* CH_3OH*. This is simply because they will occupy vacant seats (sites) on the surface of the catalyst, which will otherwise be occupied by* CO_2 *molecules. Notice that the bracketed term in the denominator of Equation 7.3 is raised to the power three (i.e., for methanol production), indicating that the competitive adsorption (or inhibition effect) is more pronounced on methanol production than on the water–gas shift reaction (Eq. 7.6). In social context, there are many lovers waiting on the list to be seated (adsorbed). They wait someone to leave (desorb) his/her seat. Notice that the overall reaction rate (i.e., speed) is not only governed by intrinsic kinetics of the reaction (i.e., motivation of reacting species) but also by mass transfer from and to catalyst sites. That is why we have to take into account the two-way journey both from and to hosting catalyst sites. This is the end of the love boat journey.*

In principle, we would like to maximize the first (desired) reaction and minimize the second (undesired) reaction. This can be achieved via maximizing the selectivity, which can be defined in different forms; here is one:

$$\text{Selectivity} = \frac{\text{Desired product}}{\text{Undesired product}} = \frac{(\text{CH}_3\text{OH})}{(\text{CO})} \tag{7.7}$$

7.2 NON-CONVENTIONAL KINETICS: LHHW TYPE REACTION

In Chapter 6, we dealt with **"POWERLAW"** type (i.e., a simple kinetic expression) reaction. In this chapter, we show how to handle a complex kinetic type of reactions.

For rate-controlled reactions, Aspen Plus provides a built-in **Langmuir–Hinshelwood–Hougen–Watson (LHHW)** expression for calculating the rate of reaction.

The general **LHHW** expression is

$$r = \frac{\text{(kinetic factor)(driving force expression)}}{\text{(adsorption term)}} \tag{7.8}$$

where

Kinetic factor:

$$k^{*}\left(\frac{T}{T_{\mathrm{o}}}\right)^{n} e^{-\frac{E}{R}\left(\frac{1}{T}-\frac{1}{T_{\mathrm{o}}}\right)} \text{ or } k^{*}e^{-\frac{E}{R}\left(\frac{1}{T}\right)} \tag{7.9}$$

Driving force expression:

$$\mathrm{k}_1 \prod_{i=1}^{N} C_i^{\alpha_\mathrm{i}} - \mathrm{k}_2 \prod_{j=1}^{N} C_j^{\beta_j} \tag{7.10}$$

Adsorption term:

$$\left(\sum_{i=1}^{M} K_i \left(\prod_{j=1}^{N} C_j^{\nu_j}\right)\right)^{m} \tag{7.11}$$

The concentration terms C_i and C_j depend on the concentration basis you select:

[Ci] basis	Concentration term C
Molarity	Component molar concentration (kmol/m^3)
Molality	Component molality (mol/kg H_2O)
Mole fraction	Component mole fraction
Mass fraction	Component mass fraction
Partial pressure	Component partial pressure (N/m^2)
Mass concentration	Component mass concentration (kg/m^3)

7.3 GENERAL EXPRESSIONS FOR SPECIFYING LHHW TYPE REACTION IN ASPEN PLUS

Consider a reaction: $\mathbf{W + X \leftrightarrow Y + Z}$

In the general case, the rate expression is

$$\text{Rate} = \frac{k^{*}e^{-\frac{E}{R}\left(\frac{1}{T}\right)}\left\{k_f[W][X] - k_b[Y][Z]\right\}}{\text{Adsorption expression}} \tag{7.12a}$$

Remember that the first term in the numerator can be inserted inside the bracelets and Equation 7.12a then becomes

$$\text{Rate} = \frac{\left\{k_f k^{*}e^{-\frac{E}{R}\left(\frac{1}{T}\right)}[W][X] - k_b k^{*}e^{-\frac{E}{R}\left(\frac{1}{T}\right)}[Y][Z]\right\}}{\text{Adsorption expression}} = \frac{\left\{k_f^{*}[W][X] - k_b^{*}[Y][Z]\right\}}{\text{Adsorption expression}} \tag{7.12b}$$

7.3.1 The "Driving Force" for the Non-reversible (Irreversible) Case

If the reaction is **non-reversible (or irreversible)**, the kinetic constants can be combined into the main constant *k* with its temperature dependency specified by *E*. The reduced rate expression of Equation 7.12a becomes

$$\text{Rate} = \frac{k^{*}e^{-\frac{E}{R}\left(\frac{1}{T}\right)}\{[W][X]\}}{\text{Adsorption expression}} = \frac{k^{*}e^{-\frac{E}{R}\left(\frac{1}{T}\right)}\{1\times[W][X]-0\times[Y][Z]\}}{\text{Adsorption expression}} \tag{7.13}$$

where $k_f = 1$ and $k_b = 0$ in Equation 7.12a.

To specify this in Aspen Plus, here is the outline for the irreversible case:

- Create a reaction set of **"LHHW"** type from the drop-down list.
- Define the reactants and products based on the given reaction stoichiometry, such as equations 7.1 and 7.4.
- Enter values for *k* and *E* on the "**Kinetic**" sheet.
- Click on the "**Driving Force**" button in the "**Kinetic**" sheet. In LHHW reaction set, for "*Term 1*" enter $\mathbf{A} = \mathbf{0}$ (i.e., $k_f = 1$ and $\mathbf{A} = \ln(k_f) = ln(1) = 0$) and concentration exponent equal to whatever the power each reactant is raised to (e.g., both [W] and [X] are each raised to power **1** in Equation 7.13).
- Set "**Enter term**" (found in "**Driving Force Expression**" window) entry to "*Term 2*", and enter a large negative value for **A** (i.e., $k_b = 0$ and$\text{A} = \ln(k_b) = \ln(0) = -\infty$). NOTE: There is no need to enter exponents for products [Y] and [Z] as k_b is already zero for the irreversible case.

7.3.2 The "Driving Force" for the Reversible Case

For **reversible reactions**, the rate expression can be written as

$$\text{Rate} = \frac{\left\{k_f[W][X] - k_b[Y][Z]\right\}}{\text{Adsorption expression}} \tag{7.14}$$

To specify this in Aspen Plus, here is the outline for the reversible case:

- Create reaction set of **"LHHW"** type from the drop-down list.
- Define the reactants and products based on the given reaction stoichiometry, such as Equations 7.1 and 7.4.
- Enter values for $k = 1$ and $E = 0$ on the "**Kinetic**" sheet.
- Click on "**Driving Force**" button in the "**Kinetic**" sheet. In LHHW reaction set, for "*Term 1*" enter concentration exponent equal to whatever the power each reactant is raised to (e.g., both [W] and [X] are each raised to power **1** in Equation 7.14).
- For k_f in "*Term 1*", A, B, C, and D parameters are entered according to one of the following equations:

$$\ln(k_f) = A + \frac{B}{T} + C\ln(T) + DT \tag{7.15}$$

Alternatively,

$$k_f = \exp(A)\exp\left(\frac{B}{T}\right)T^C\exp(DT) \tag{7.16}$$

- Set "**Enter term**" (found in "**Driving Force Expression**" window) entry to "*Term 2*", and enter concentration exponent equal to whatever the power each product is raised to (e.g., both [Y] and [Z] are each raised to power **1** in Equation 7.14).

For k_b in "**Term 2**", A, B, C, and D parameters are entered according to one of the following equations:

$$\ln(k_b) = A + \frac{B}{T} + C\ln(T) + DT \tag{7.17}$$

Alternatively,

$$k_b = \exp(A)\exp\left(\frac{B}{T}\right)T^C\exp(DT) \tag{7.18}$$

7.3.3 The "Adsorption Expression"

The "**Adsorption Expression**" in **LHHW** reactions depends on the assumed adsorption mechanism. Expressions for various mechanisms can be found in Perry's *Chemical Engineers' Handbook* [2]. Suppose the mechanism is given by

$$\text{Adsorption} = \left\{1 + K_w[W] + K_X[X] + K_Y[Y] + K_z[Z]\right\}^n \tag{7.19}$$

To enter this adsorption expression in Aspen Plus, under "**Kinetic**" tab, click on "**Adsorption**" button and "**Adsorption Expression**" window will pop up. Set "**Adsorption expression exponent**" to **n** and define five terms. For the concentration exponent, enter as shown in Table 7.1:

TABLE 7.1 The concentration exponent for each component is assigned based on the power each component concentration is raised to as it appears in the adsorption term (i.e., Eq. 7.19)

Component	Term no. 1	Term no. 2	Term no. 3	Term no. 4	Term no. 5
W	0	**1**	0	0	0
X	0	0	**1**	0	0
Y	0	0	0	**1**	0
Z	0	0	0	0	**1**

For the adsorption constants, enter **A** = 0 (i.e., $A = \ln(1) = 0$) for "**Term no. 1**", and enter temperature-dependent expressions in the other terms for the corresponding **K**'s; again, similar to the forms shown in Equations 7.15 or 7.16. Usually **C** and **D** will be **0**.

7.4 THE PROPERTY METHOD: "SRK"

NOTE #2: *Since methanol production takes place at a pressure greater than 10 bar, then using the* ***Property Method Selection Assistant****, it is recommended to use an equation of state, such as "****SR-POLAR****", "****SRK****", and "****PSRK****". "****SRK****" was selected.*

Choose "**Chemicals with Metric Units**" template to create a steady-state flow sheet. The default property model will be "**NRTL**". However, as mentioned in **NOTE #2**, "**NRTL**" will be replaced by "**SRK**". Moreover, in "**Methods**" | "**Specifications**" | "**Global**" tab window set the “**Free-water method**” to “*STEAMNBS*”. Give a title for the project and add the five components: CO, CO_2, H_2, H_2O, and CH_3OH.

Under “**Properties**” environment, go to “**Methods**” | “**Parameters**” | “**Binary Interaction**” | “**SRKKIJ -1**” sheet and ensure that the “*Estimate missing parameters by UNIFAC*” option is selected. Click on “**Reset**” followed by “**Next**” button to run the simulation and assure that properties analysis completed successfully. Switch to “**Simulation**” environment.

7.5 RPLUG FLOWSHEET FOR METHANOL PRODUCTION

In general, a multitubular non-adiabatic packed-bed reactor, with the heat transfer fluid flowing on the shell side, is used. Let us add one “**RPLUG**” block and hook one feed and one product stream to it, as shown in Figure 7.1.

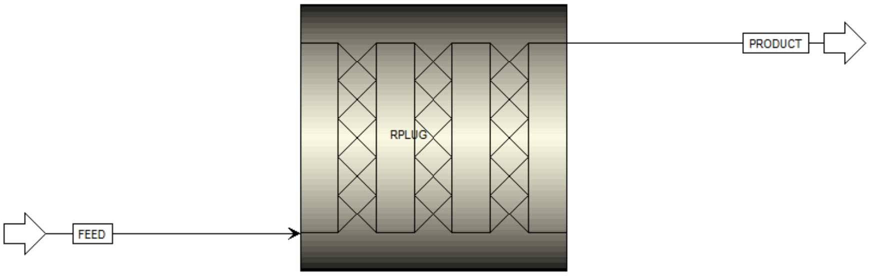
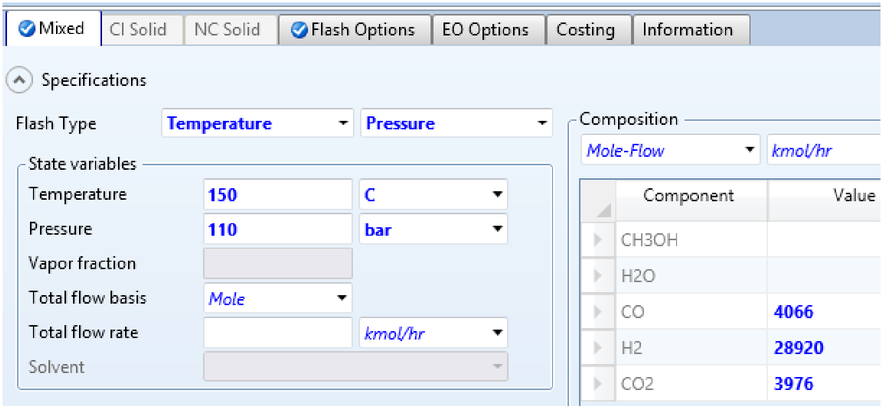


Figure 7.1 A simple flowsheet for methanol production using rigorous-PLUG (**RPLUG**).

7.6 ENTERING INPUT PARAMETERS

Click on “**Next→**” button where you will be gliding at “**FEED**” stream specifications; enter the input parameters (in terms of *T*, *P*, flow rate, and composition) as shown in Figure 7.2. Such numbers were quoted from [3].



Specifications

Flash Type: Temperature | Pressure

State variables

Temperature	150	C
Pressure	110	bar
Vapor fraction		
Total flow basis	Mole	
Total flow rate		kmol/hr
Solvent		

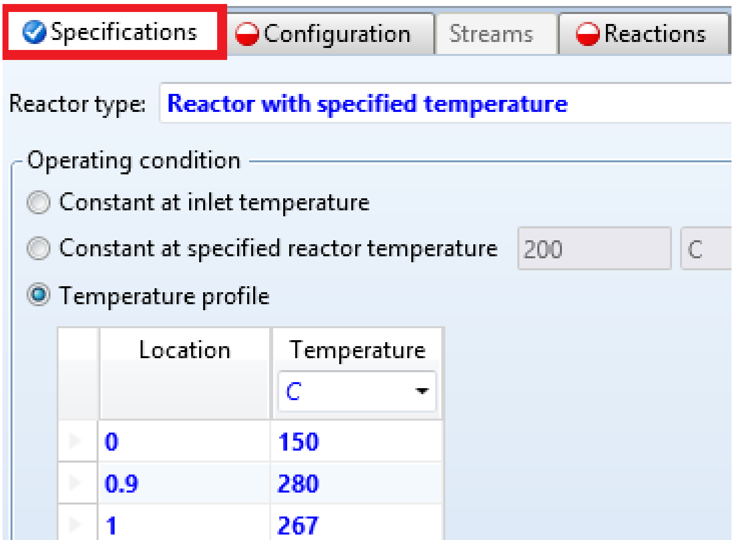
Composition

Mole-Flow | kmol/hr

Component	Value
CH3OH	
H2O	
CO	4066
H2	28920
CO2	3976

Figure 7.2 The feed stream properties in terms of *T*, *P*, flow rate, and composition.

Figure 7.3 shows **RPLUG** specifications in terms of *heat transfer mode and temperature profile.* Again, numbers were taken from [3]. However, it will be left as an exercise for the user to try other numbers as well as other configurations of heat transfer and temperature profile.



Reactor type: Reactor with specified temperature

Operating condition

○ Constant at inlet temperature

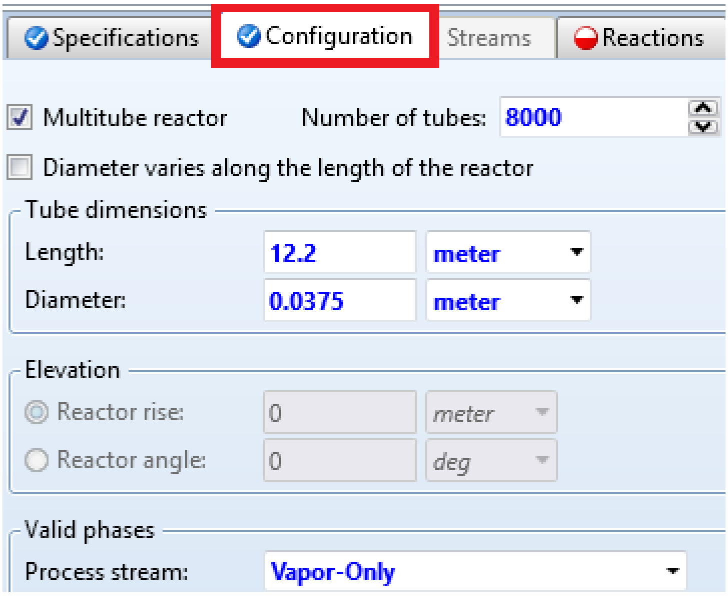
○ Constant at specified reactor temperature 200 C

● Temperature profile

Location	Temperature C
0	150
0.9	280
1	267

Figure 7.3 "**RPLUG**" specifications in terms of heat transfer and temperature profile.

Click on "**Next→**" button or directly go to "**Configuration**" tab so that we can enter reactor dimensions as shown in Figure 7.4.



☑ Multitube reactor Number of tubes: 8000

☐ Diameter varies along the length of the reactor

Tube dimensions

Length: 12.2 meter

Diameter: 0.0375 meter

Elevation

○ Reactor rise: 0 meter

○ Reactor angle: 0 deg

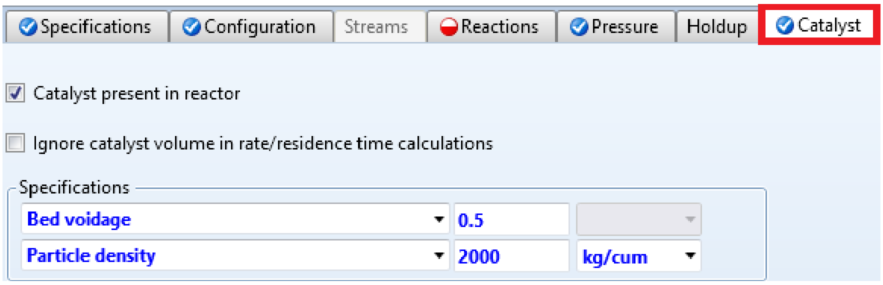
Valid phases

Process stream: Vapor-Only

Figure 7.4 Reactor dimensions in "**Configuration**" tab window.

The combination of number of tubes, the pipe diameter, and its length, will be merely judged by the ability of Aspen Plus to converge to a “reasonable” solution without having any simulation errors. Of course, we have to assume reasonable values for length and diameter. We have the choice to use a multitube reactor or a single-tube reactor but with a different pipe length and diameter for each case. Luyben [3] data were used for the sake of comparison; nevertheless, this does not prevent the user from trying other geometrical configurations, as well.

We will leave the “**Reactions**” tab for a while and go to “**Catalyst**” tab window where we define the catalyst properties. Figure 7.5 shows the properties of catalyst in terms of its particle density and bed voidage. Alternatively, the catalyst loading could be entered instead of one of the aforementioned properties.



☑ Catalyst present in reactor

☐ Ignore catalyst volume in rate/residence time calculations

Specifications

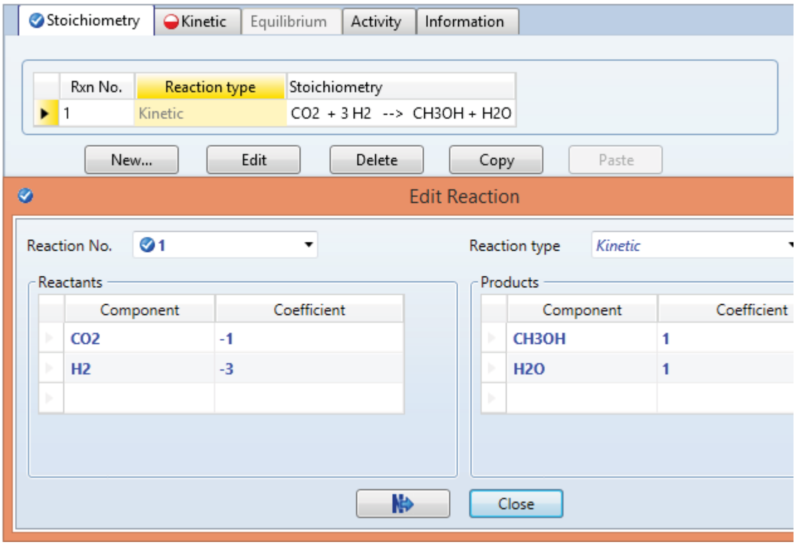
Bed voidage	0.5	
Particle density	2000	kg/cum

Figure 7.5 Defining the catalyst properties in terms of its particle density and bed voidage, in “**Catalyst**” tab window.

7.7 DEFINING METHANOL PRODUCTION REACTIONS AS LHHW TYPE

Notice that the “**Reactions**” tab (see Figure 7.5) is labeled by a half-filled red circle, indicating that we must associate a reaction set to the reactor. Both Equations 7.1 and 7.4 will be defined as **“LHHW”** type. Go to “**Reactions**” folder; click on “**New** … ” button, and the “**Create New ID**” window will pop-up. Choose the default ID (**R-1**) and select “*LHHW*” for the reaction type. Click on “**OK**” button and Aspen Plus will bring you to “**Stoichiometry**” tab window. At the bottom of “**Stoichiometry**” tab window, click on “**New** … ” button and the “**Edit Reaction**” window will show up where you need to plug in the stoichiometric data as shown in Figure 7.6. Unlike the case for a simple kinetic expression, used in Chapter 6, the exponents will be defined later in “**Driving Force Expression**” window.

Click on “**Close**” or “**Next**” button at the bottom of the **Edit Reaction** window (Figure 7.6). Go to “**Kinetic**” tab window where you need to enter the kinetic data for



Rxn No.	Reaction type	Stoichiometry
1	Kinetic	CO2 + 3 H2 --> CH3OH + H2O

Reaction No. 1
Reaction type Kinetic

Reactants

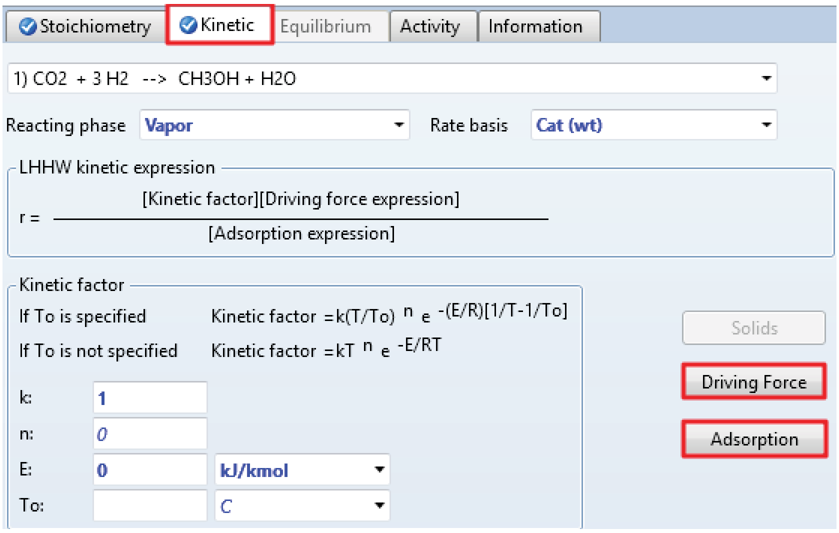
Component	Coefficient
CO2	-1
H2	-3

Products

Component	Coefficient
CH3OH	1
H2O	1

Figure 7.6 Defining the coefficients for reacting species of **"LHHW"** type reaction in "**R-1**" set (Eq. 7.1). The exponents will be defined later in "**Driving Force Expression**" window.

the first reaction (Eq. 7.3b). Enter the data as shown in Figure 7.7. The kinetic factor will reduce to unity as we merge it into the driving force expression.



1) CO2 + 3 H2 --> CH3OH + H2O
Reacting phase Vapor
Rate basis Cat (wt)

LHHW kinetic expression

$$r = \frac{\text{[Kinetic factor][Driving force expression]}}{\text{[Adsorption expression]}}$$

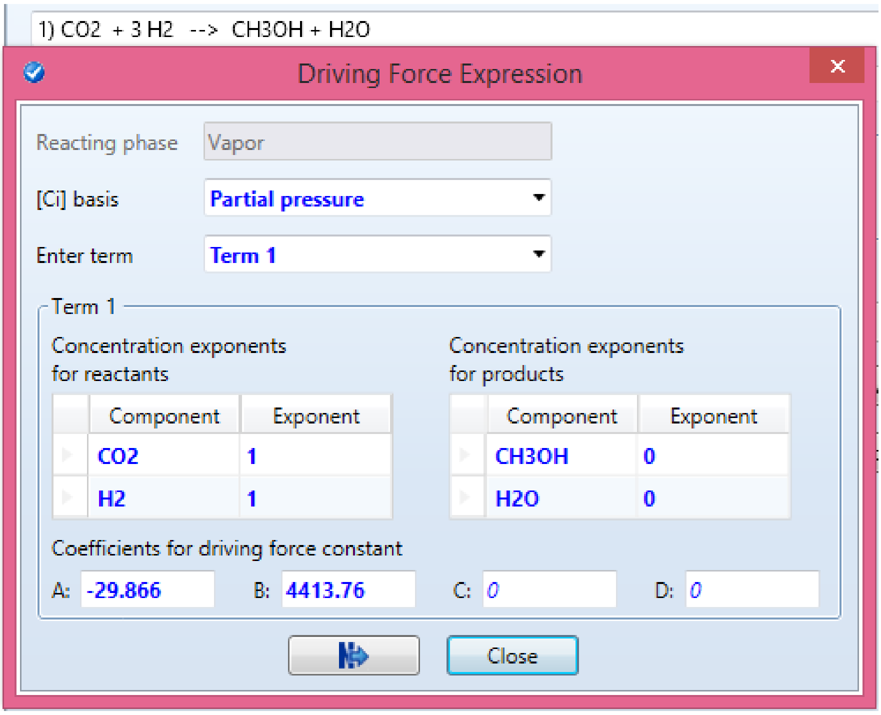
Kinetic factor
If To is specified Kinetic factor $= k(T/To)^{n} e^{-(E/R)[1/T-1/To]}$
If To is not specified Kinetic factor $= kT^{n} e^{-E/RT}$

k: 1
n: 0
E: 0 kJ/kmol
To: C

Figure 7.7 The reacting phase is vapor, rate basis is catalyst weight, $k = 1$, and $E = 0$, as given by Equation 7.3b.

Based on Equation 7.3b form, the driving force expression is represented by the reversible case (Eq. 7.14), where $k_f = 1.07 \times 10^{-13} \times e^{(4413.76/T)}$ and $k_b = 4.182 \times 10^{7} \times e^{(-(2645.966/T))}$. Click on "**Driving Force**" button (shown in Figure 7.7) and the "**Driving**

Force Expression" window will show up as shown in Figure 7.8. Enter [Ci] basis, which is the partial pressure of component in the gas-phase. From the drop-down list, select "*Term1*" first and fill the concentration exponent for each component involved in the forward direction and leave the exponent for others empty or make it zero.



1) CO2 + 3 H2 --> CH3OH + H2O

Driving Force Expression

Reacting phase: Vapor

[Ci] basis: Partial pressure

Enter term: Term 1

Term 1

Concentration exponents for reactants	
Component	Exponent
CO2	1
H2	1

Concentration exponents for products	
Component	Exponent
CH3OH	0
H2O	0

Coefficients for driving force constant

A: -29.866 B: 4413.76 C: 0 D: 0

Figure 7.8 The driving force term in Equation 7.3b represents a reversible case (Eq. 7.14). "**Term 1**" is defined here for the forward direction, with given **A** and **B** coefficient for the driving force constant.

For "**Term 1**": $A + \frac{B}{T} = \ln(1.07 \times 10^{-13} \times e^{(4413.76/T)}) \Rightarrow \boldsymbol{A} = -29.866; \boldsymbol{B} = 4413.76.$

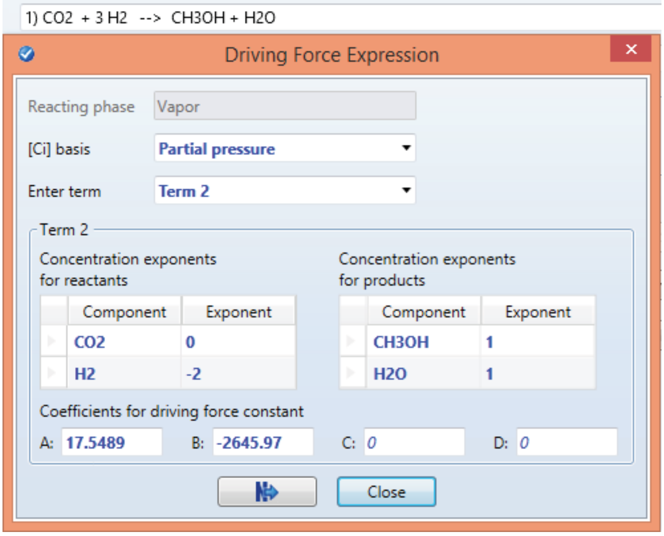
While the "**Driving Force Expression**" window is still active, select "*Term 2*", instead of "*Term1*", and fill the concentration exponent for each component involved in the backward direction. For CO_2, you may enter zero for the exponent or leave it empty.

For "**Term 2**": $A + \frac{B}{T} = \ln\left(4.182 \times 10^{7} \times e^{\left(\frac{-2645.966}{T}\right)}\right) \Rightarrow \boldsymbol{A} = 17.5489; \boldsymbol{B} = -2645.97.$

Figure 7.9 shows the "**Driving Force Expression**" window for "**Term 2**".

Click on "**Adsorption**" button (see Figure 7.7) and the "**Adsorption Expression**" window will show up as shown in Figure 7.10. The bracketed term in the denominator of Equation 7.3b is raised to power 3; hence, the "**Adsorption expression exponent**" is set to *3*. Table 7.1 will reduce to Table 7.2 (see below), simply because the denominator of Equation 7.3b, which represents the adsorption term, can be put in a form similar to that of Adsorption $= \{1 + K_w[W] + K_X[X] + K_Y[Y] + K_z[Z]\}^n$7.19:

$$\{1(H_2)^0(H_2O)^0 + K_{H_2O/H_2}(H_2)^{-1}(H_2O)^1 + K_{H_2}(H_2)^{0.5}(H_2O)^0 + K_{H_2O}[H_2]^0[H_2O]^1\}^3 \tag{7.20}$$



1) CO2 + 3 H2 --> CH3OH + H2O

Reacting phase: Vapor

[Ci] basis: Partial pressure

Enter term: Term 2

Term 2

Concentration exponents for reactants

Component	Exponent
CO2	0
H2	-2

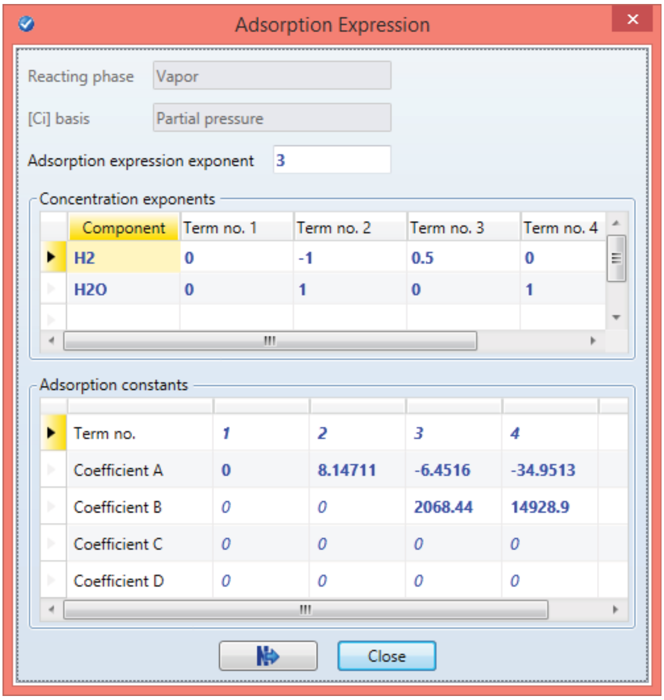
Concentration exponents for products

Component	Exponent
CH3OH	1
H2O	1

Coefficients for driving force constant

A: 17.5489 B: -2645.97 C: 0 D: 0

Figure 7.9 The driving force term in Equation 7.3b represents a reversible case (Eq. 7.14). "**Term 2**" is defined here for the backward direction, with given **A** and **B** coefficient for the driving force constant.



Reacting phase: Vapor

[Ci] basis: Partial pressure

Adsorption expression exponent: 3

Concentration exponents

Component	Term no. 1	Term no. 2	Term no. 3	Term no. 4
H2	0	-1	0.5	0
H2O	0	1	0	1

Adsorption constants

Term no.	1	2	3	4
Coefficient A	0	8.14711	-6.4516	-34.9513
Coefficient B	0	0	2068.44	14928.9
Coefficient C	0	0	0	0
Coefficient D	0	0	0	0

Figure 7.10 The "**Adsorption Expression**" window where the concentration exponents are concluded by matching, term by term, the adsorption term (i.e., denominator of Eq. 7.3b) with Equation 7.20 The adsorption coefficients A, B, C, and D for "**Term no. 1**" up to "**Term no. 4**" are evaluated by taking the logarithmic value of each term found in the denominator of Equation 7.3b.

TABLE 7.2 The concentration exponent, as explained by Equation 7.20, for H_2 and H_2O as the only components appearing in the denominator of Equation 7.3.

Component	Term no. 1	Term no. 2	Term no. 3	Term no. 4
H_2	0	**−1**	**0.5**	0
H_2O	0	**1**	0	**1**

This explains why the exponent is 0 for both components in "**Term no. 1**"; −1 for H_2 and 1 for H_2O in "**Term no. 2**"; 0.5 for H_2 and 0 for H_2O in "**Term no. 3**"; and finally 0 for H_2 and 1 for H_2O in "**Term no. 4**".

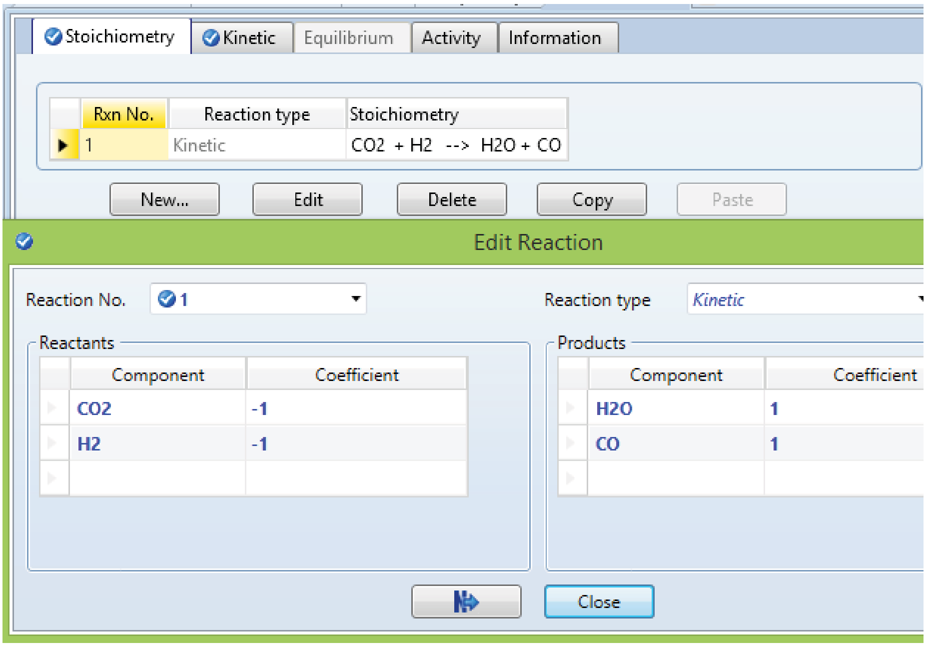
For "**Term no. 1**": $A = \ln(1) = 0$; $B = C = D = 0$.

For "**Term no. 2**": $A = \ln(3453.38) = 8.1471087$; $B = C = D = 0$.

For "**Term no. 3**": $A + \frac{B}{T} = \ln(1.578 \times 10^{-3} \times e^{(2068.44/T)}) = -6.4516 + \frac{2068.44}{T} \rightarrow A = -6.4516;\ B = 2068.44;\ C = D = 0.$

For "**Term no. 4**": $A + \frac{B}{T} = \ln(6.62 \times 10^{-16} \times e^{(14\,928.915/T)}) = -34.9513 + \frac{14\,928.915}{T} \rightarrow A = -34.9513;\ B = 14{,}928.915;\ C = D = 0.$

Let us define the second reaction (Eq. 7.4) also as "**LHHW**" type. Go to "**Reactions**" folder; click on "**New …**" button, and the "**Create New ID**" window will pop-up. Choose the default ID (**R-2**) and select "*LHHW*" for the reaction type. Click on "**OK**" button and Aspen Plus will bring you to "**Stoichiometry**" tab window. At the bottom of "**Stoichiometry**" tab window, click on "**New …**" button and the "**Edit Reaction**" window will show up where you need to plug in the stoichiometric data (coefficients only) as shown in Figure 7.11. The exponents will be defined later in "**Driving Force Expression**" window.



Rxn No.	Reaction type	Stoichiometry
1	Kinetic	CO2 + H2 --> H2O + CO

Reaction No. 1

Reaction type Kinetic

Reactants

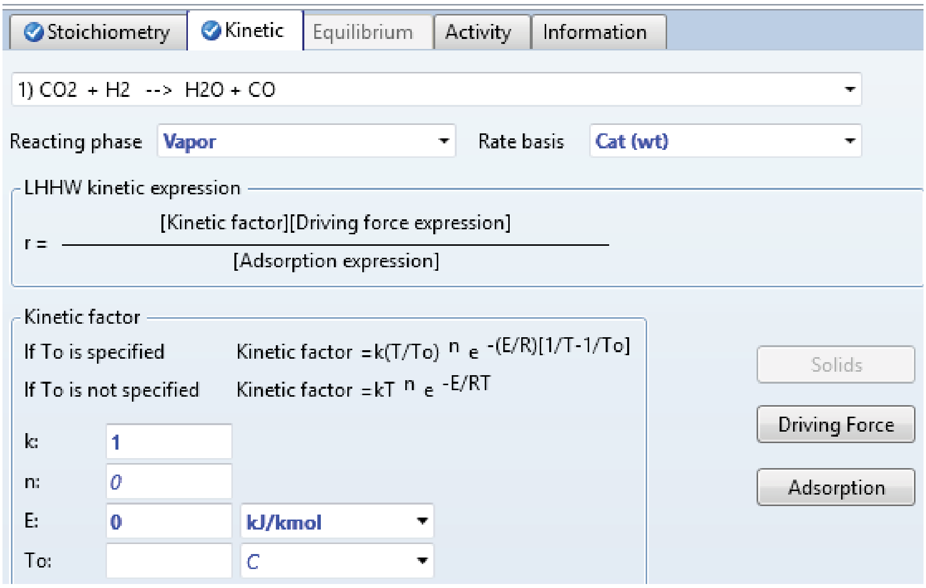
Component	Coefficient
CO2	-1
H2	-1

Products

Component	Coefficient
H2O	1
CO	1

Figure 7.11 Defining the coefficients only for reacting species of "**LHHW**" type reaction in "**R-2**" set (Eq. 7.4). The exponents will be later defined in "**Driving Force Expression**" window.

Click on “**Close**” or “**Next**” button at the bottom of the “**Edit Reaction**” window. Go to “**Kinetic**” tab window where you need to enter the kinetic data for the second reaction (Eq. 7.4). Enter the data as shown in Figure 7.12. Again, the kinetic factor will reduce to unity as we merge it into the driving force expression.



1) CO2 + H2 --> H2O + CO

Reacting phase: Vapor

Rate basis: Cat (wt)

LHHW kinetic expression

$$r = \frac{[\text{Kinetic factor}][\text{Driving force expression}]}{[\text{Adsorption expression}]}$$

Kinetic factor

If To is specified: Kinetic factor $= k(T/To)^{n} e^{-(E/R)[1/T-1/To]}$

If To is not specified: Kinetic factor $= kT^{n} e^{-E/RT}$

k: 1

n: 0

E: 0 kJ/kmol

To: C

Figure 7.12 The reacting phase is vapor, rate basis is catalyst weight, $k = 1$, and $E = 0$, as given by Equation 7.6b

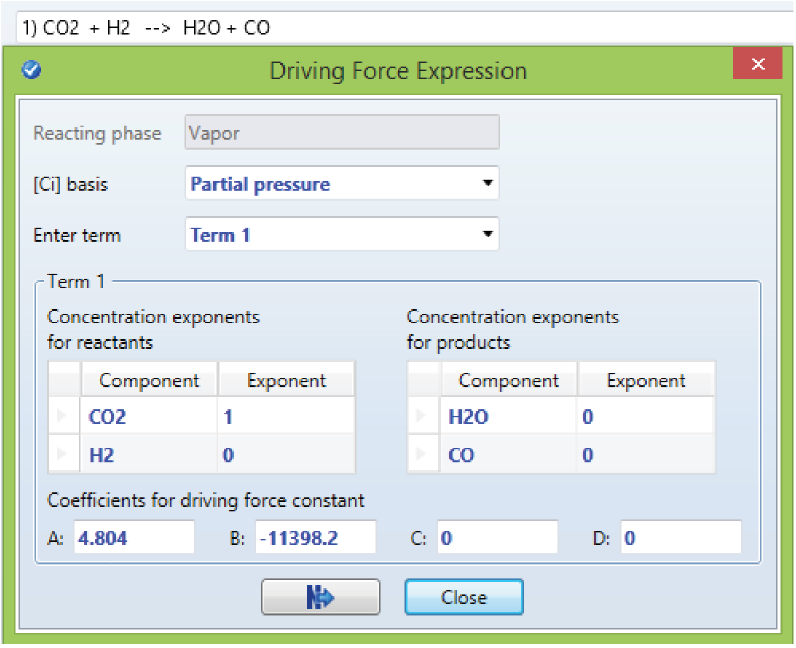
Based on Equation 7.6b form, the driving force expression is represented by a reversible case (Eq. 7.14), where $k_f = 122 \times e^{(-11,398.24/T)}$ and $k_b = 1.1412 \times e^{(-6624.98/T)}$. Click on “**Driving Force**” button (shown in Figure 7.12) and the “**Driving Force Expression**” window will show up as shown in Figure 7.13. Enter [Ci] basis, which is the partial pressure of component in the given gas phase. Select “**Term1**” first and fill the concentration exponent for each component involved in the forward direction and leave the exponent for others empty or make it zero.

For **“Term 1”:** $A + \frac{B}{T} = \ln(122 \times e^{(-(11,398.24/T))}) \Rightarrow \boldsymbol{A} = 4.804; \boldsymbol{B} = -11,398.24$.

While the “**Driving Force Expression**” window is still active, select “**Term 2**”, instead of “**Term1**”, and fill the concentration exponent for each component involved in the backward direction. For CO_2, you may enter zero for the exponent or leave it empty.

For **“Term 2”:** $A + \frac{B}{T} = \ln(1.1412 \times e^{(-6624.98/T)}) = 0.13208 + \frac{-6624.98}{T}$. This implies that $\mathbf{A} = 0.13208$ and $\boldsymbol{B} = -6624.98$.

Figure 7.14 shows the “**Driving Force Expression**” window for “**Term 2**”.



1) CO2 + H2 --> H2O + CO

Reacting phase: Vapor

[Ci] basis: Partial pressure

Enter term: Term 1

Term 1

Concentration exponents for reactants

Component	Exponent
CO2	1
H2	0

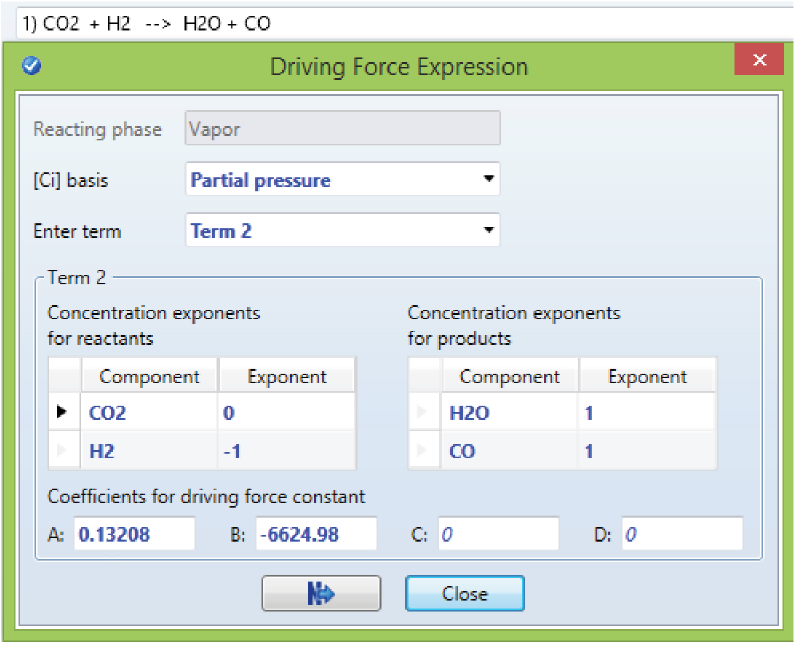
Concentration exponents for products

Component	Exponent
H2O	0
CO	0

Coefficients for driving force constant

A: 4.804 B: -11398.2 C: 0 D: 0

Figure 7.13 The driving force term in Equation 7.6b represents a reversible case (Eq. 7.14). "**Term 1**" is defined here for the forward direction, with given **A** and **B** coefficient for the driving force.



1) CO2 + H2 --> H2O + CO

Reacting phase: Vapor

[Ci] basis: Partial pressure

Enter term: Term 2

Term 2

Concentration exponents for reactants

Component	Exponent
CO2	0
H2	-1

Concentration exponents for products

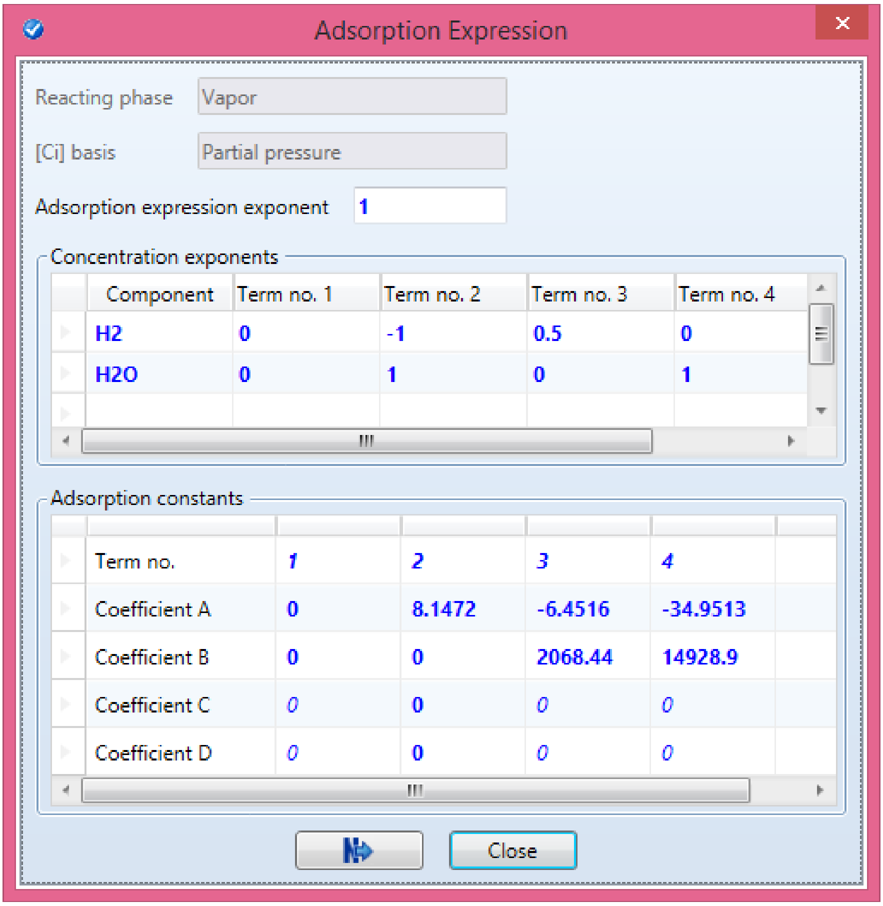
Component	Exponent
H2O	1
CO	1

Coefficients for driving force constant

A: 0.13208 B: -6624.98 C: 0 D: 0

Figure 7.14 The driving force term in Equation 7.6b represents a reversible case (Eq. 7.14). "**Term 2**" is defined here for the backward direction, with given **A** and **B** coefficient for the driving force constant.

Click on “**Adsorption**” button (see Figure 7.12) and the “**Adsorption Expression**” window will show up as shown in Figure 7.15. The bracketed term in the denominator of Equation 7.6b is raised to power 1; hence, the “**Adsorption expression exponent**” is equal to *1*. Notice that other entries for the “**Adsorption Expression**” window are exactly the same as those shown in Figure 7.10, for the first reactor. This is simply because, the bracketed term appearing in the denominator of Equation 7.3b is identically the same as that in the denominator of Equation 7.6b.



Reacting phase: Vapor
[Ci] basis: Partial pressure
Adsorption expression exponent: 1

Concentration exponents

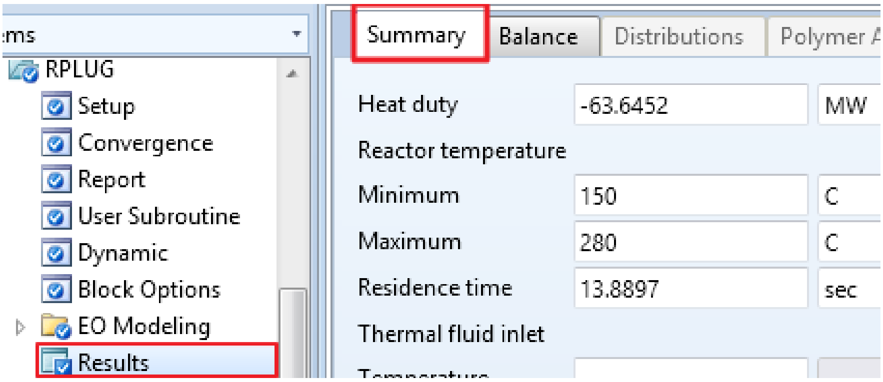
Component	Term no. 1	Term no. 2	Term no. 3	Term no. 4
H2	0	-1	0.5	0
H2O	0	1	0	1

Adsorption constants

Term no.	1	2	3	4
Coefficient A	0	8.1472	-6.4516	-34.9513
Coefficient B	0	0	2068.44	14928.9
Coefficient C	0	0	0	0
Coefficient D	0	0	0	0

Figure 7.15 The “**Adsorption Expression**” window for the second reaction, where the entries are the same as those used in Figure 7.10; except for the adsorption expression exponent where it is set to *1* here, instead of *3*.

After defining both reactions, associate them to “**RPLUG**” block under “**Reactions**” tab. The simulator is now ready via noticing that life is blue like the sky and ocean and no red (hell) signs are present. Click on “**Reset**” followed by “**Next**” button to run the show and watch for any simulation error/warning. Figure 7.16 shows summary results for “**RPLUG**” block where it shows a relatively very large heat duty, indicating the presence of highly exothermic reactions. To verify which direction is exothermic for a given reversible



Heat duty -63.6452 MW
Reactor temperature
Minimum 150 C
Maximum 280 C
Residence time 13.8897 sec
Thermal fluid inlet

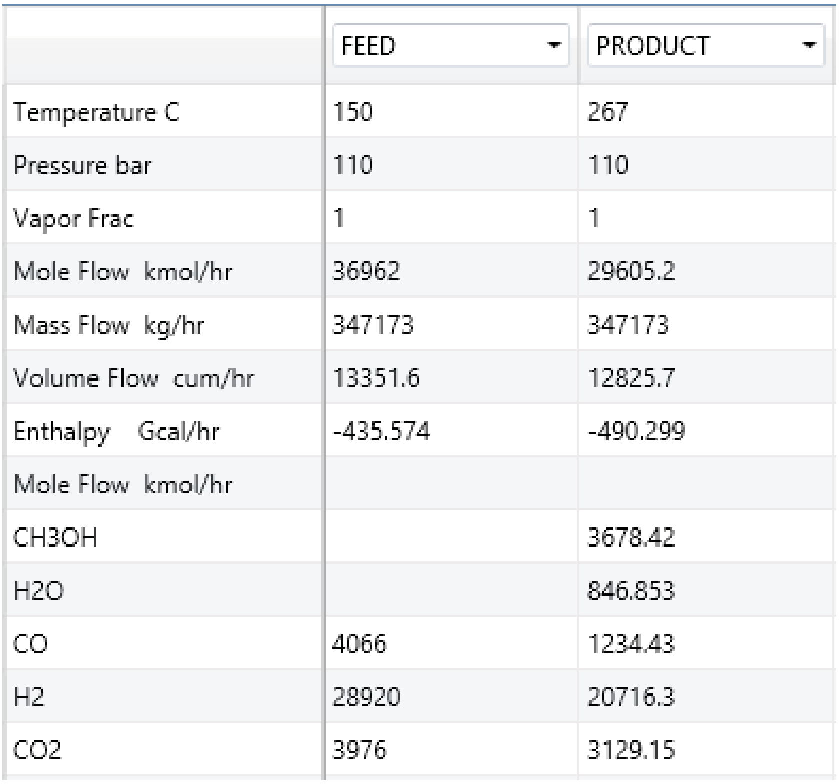
Figure 7.16 Reactor summary results for "**RPLUG**" block with a highly exothermic heat duty.

reaction, select one reaction at a time in the reactor unit, reinitialize, and rerun the show. Performing such a procedure will reveal to us that the first reaction is exothermic in the forward reaction (i.e., formation of methanol), whereas the second reaction is exothermic in the backward direction (i.e., consumption of CO and H_2O). The molar flow rate of each component in the feed and in the product stream, as shown in Figure 7.17, will tell us that the first reaction went in the forward direction (i.e., in favor of methanol formation) and the second reaction in the backward direction (i.e., in favor of CO consumption); hence, it explains why CO flow rate in the product stream is less than that in the feed stream.

Figure 7.17 shows stream results summary for the reactor inlet and outlet streams, where methanol is present in the product stream. For the sake of comparison, Luyben's data [3] for the product stream were 1468, 21,673, and 3292 kmol/h for CO, H_2, and CO_2, respectively. The data here are 1234, 20,716, and 3129 kmol/h for CO, H_2, and CO_2, respectively. The difference in results in my judgment is due to: first, the kinetic model being used; for example, the adsorption term in our case is made of four terms but in Luyben's case the first two terms were only incorporated (see table 11.1 on page 190 [3]); second, the thermodynamic property method used in simulation; and third, the version of Aspen Plus itself.

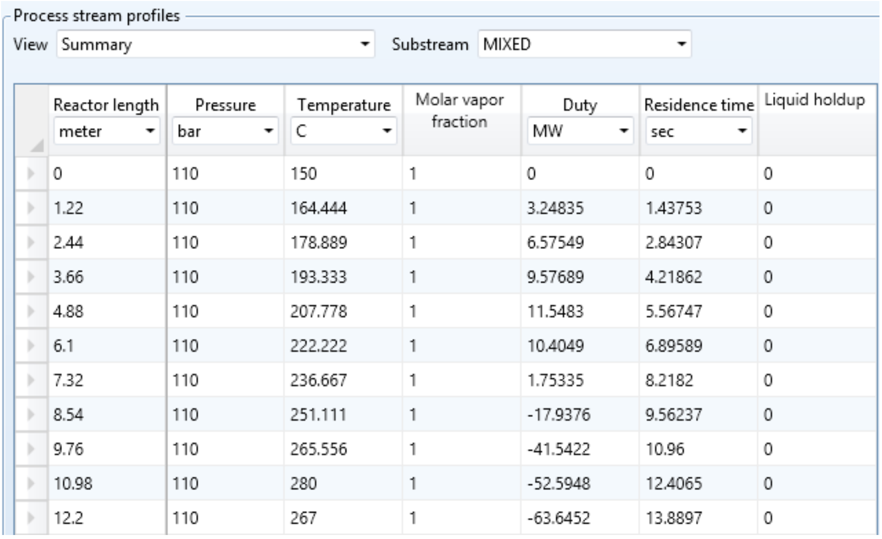
A useful source of information about a plug-flow reactor performance is provided by Aspen Plus via what is called the reactor profile. Go to "**Blocks**" | "**RPLUG**" | "**Profiles**" and select "**Process Stream**" tab window, if it is not already selected by Aspen Plus, where it shows properties, such as pressure, temperature, residence time, molar vapor fraction, and molar composition as function of either reactor length or residence time. Figure 7.18 shows such reacting medium properties as a function of both reactor length and residence time. You can at this stage ("**Process Stream**" tab window is active), make use of the "**Plot**" group, found in "**Home**" ribbon, and choose any combination of x and y variables to generate $y = f(x)$ or generate a parametric plot where you show $y = f(x)$ evaluated at different z values, where z is the parametric variable.

You may wish to see the molar composition for each component as a function of the reactor length via selecting "*Molar composition*" option from the drop-down list of the "**View**" item shown in Figure 7.18. Figure 7.19 shows the molar composition profile in the axial direction. Again, you may wish to generate a profile plot making use of "**Plot**" group found in "**Home**" ribbon, while the "**Process Stream**" tab window is active.



	FEED	PRODUCT
Temperature C	150	267
Pressure bar	110	110
Vapor Frac	1	1
Mole Flow kmol/hr	36962	29605.2
Mass Flow kg/hr	347173	347173
Volume Flow cum/hr	13351.6	12825.7
Enthalpy Gcal/hr	-435.574	-490.299
Mole Flow kmol/hr		
CH3OH		3678.42
H2O		846.853
CO	4066	1234.43
H2	28920	20716.3
CO2	3976	3129.15

Figure 7.17 Stream results summary for the inlet and outlet stream of the plug-flow reactor. Methanol is present in the product stream.

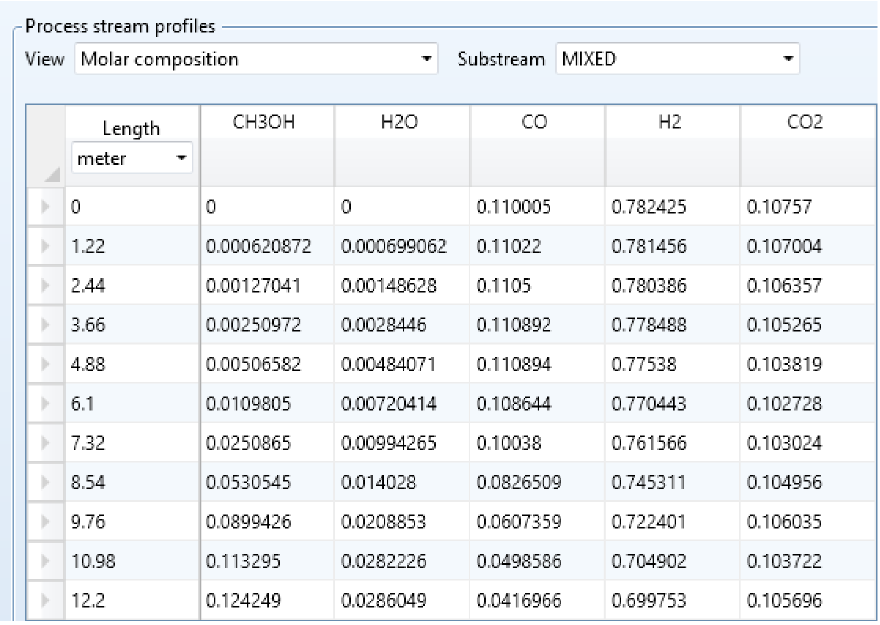


Process stream profiles

View Summary Substream MIXED

Reactor length meter	Pressure bar	Temperature C	Molar vapor fraction	Duty MW	Residence time sec	Liquid holdup
0	110	150	1	0	0	0
1.22	110	164.444	1	3.24835	1.43753	0
2.44	110	178.889	1	6.57549	2.84307	0
3.66	110	193.333	1	9.57689	4.21862	0
4.88	110	207.778	1	11.5483	5.56747	0
6.1	110	222.222	1	10.4049	6.89589	0
7.32	110	236.667	1	1.75335	8.2182	0
8.54	110	251.111	1	-17.9376	9.56237	0
9.76	110	265.556	1	-41.5422	10.96	0
10.98	110	280	1	-52.5948	12.4065	0
12.2	110	267	1	-63.6452	13.8897	0

Figure 7.18 Reacting medium properties, such as pressure, temperature, molar vapor fraction (for a potential phase change), and heat duty, as function of either reactor length (or residence time), are available via the reactor profile sheet.



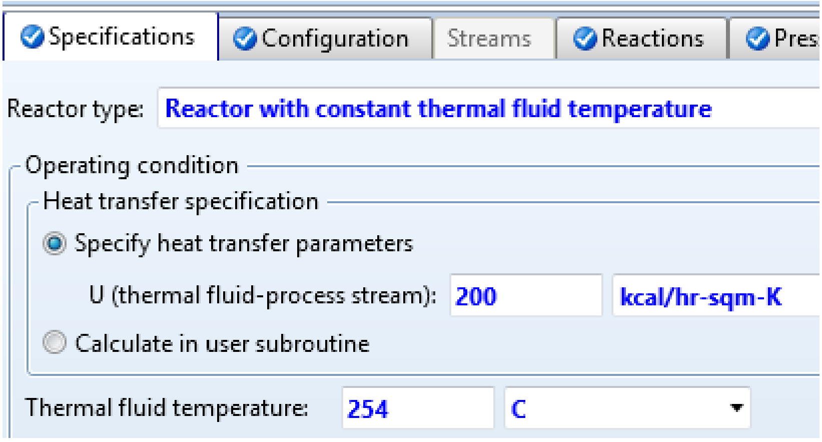
Process stream profiles

View: Molar composition Substream: MIXED

Length meter	CH3OH	H2O	CO	H2	CO2
0	0	0	0.110005	0.782425	0.10757
1.22	0.000620872	0.000699062	0.11022	0.781456	0.107004
2.44	0.00127041	0.00148628	0.1105	0.780386	0.106357
3.66	0.00250972	0.0028446	0.110892	0.778488	0.105265
4.88	0.00506582	0.00484071	0.110894	0.77538	0.103819
6.1	0.0109805	0.00720414	0.108644	0.770443	0.102728
7.32	0.0250865	0.00994265	0.10038	0.761566	0.103024
8.54	0.0530545	0.014028	0.0826509	0.745311	0.104956
9.76	0.0899426	0.0208853	0.0607359	0.722401	0.106035
10.98	0.113295	0.0282226	0.0498586	0.704902	0.103722
12.2	0.124249	0.0286049	0.0416966	0.699753	0.105696

Figure 7.19 The molar composition profile for reactants and products as a function reactor length (i.e., the axial direction).

It is worth mentioning that instead of using *Reactor with specified temperature* option as shown in Figure 7.3, one may also attempt to use "*Reactor with constant thermal fluid temperature*" option with a specified overall heat transfer coefficient between the tube and shell sides of the reactor (also as a heat exchanger), as shown in Figure 7.20 and obtain another convergent solution (i.e., no simulation error/warning).



Reactor type: Reactor with constant thermal fluid temperature

Operating condition

Heat transfer specification

● Specify heat transfer parameters

U (thermal fluid-process stream): 200 kcal/hr-sqm-K

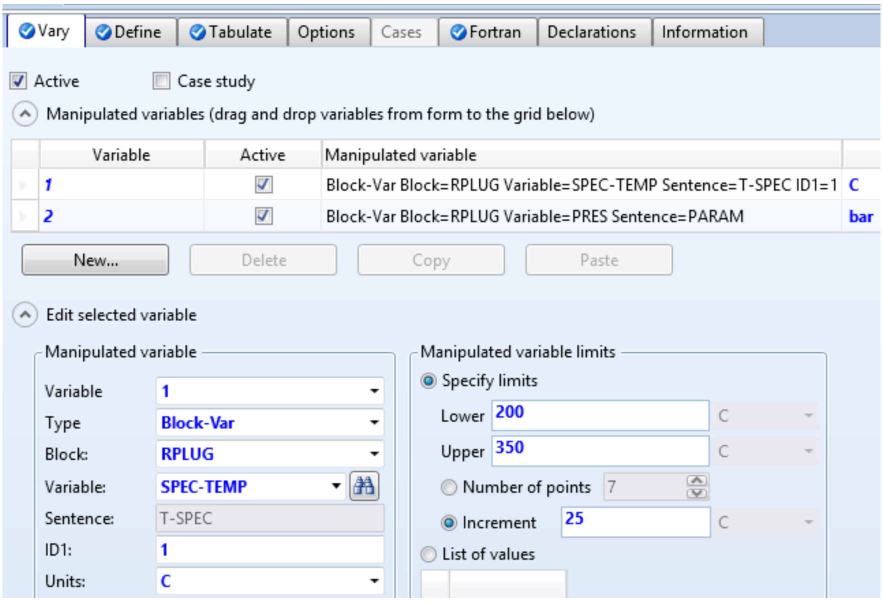
○ Calculate in user subroutine

Thermal fluid temperature: 254 C

Figure 7.20 Another configuration for "**PFR**" where "*Reactor with constant thermal fluid temperature*" option is selected with a specified overall heat transfer coefficient between the tube and shell sides of the reactor (also as a heat exchanger).

7.8 SENSITIVITY ANALYSIS: EFFECT OF TEMPERATURE AND PRESSURE ON SELECTIVITY

Create “**S-1**” set under “**Model Analysis Tools**” | “**Sensitivity**” subfolder. Figure 7.21 shows the first manipulated variable, that is, the specified temperature of the reactor at which the gas-phase reaction takes place.



☑ Active ☐ Case study

Manipulated variables (drag and drop variables from form to the grid below)

Variable	Active	Manipulated variable	
1	☑	Block-Var Block=RPLUG Variable=SPEC-TEMP Sentence=T-SPEC ID1=1	C
2	☑	Block-Var Block=RPLUG Variable=PRES Sentence=PARAM	bar

Edit selected variable

Manipulated variable

Variable: 1
Type: Block-Var
Block: RPLUG
Variable: SPEC-TEMP
Sentence: T-SPEC
ID1: 1
Units: C

Manipulated variable limits

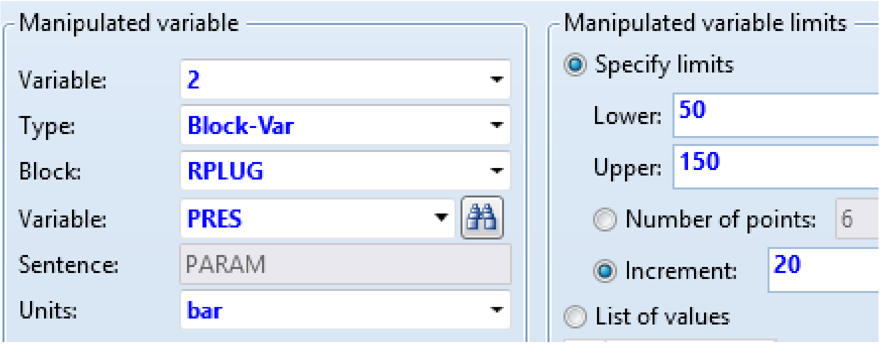
● Specify limits
Lower: 200 C
Upper: 350 C
○ Number of points: 7
● Increment: 25 C
○ List of values

Figure 7.21 The temperature of the gas-phase reactor is to be manipulated, as the first variable, to see the maximum selectivity of methanol production as given by Equation 7.7 for the two parallel reactions.

One important point here is that you have to keep the “**Reactor type**” (under “**Specifications**” tab as shown in Figure 7.3) to “*Reactor with specified temperature*” and select the second (*Constant at specified reactor temperature*) or third (Temperature profile) subchoice. If you try other modes of “**Reactor type**”, then an error message will show up as in the following statement:

```
"ERROR WHILE CHECKING INPUT SPECIFICATIONS FOR VARIED VARIABLE IN
      SENSITIVITY BLOCK: "S-1"
      NO "T-SPEC" SENTENCE WAS ENTERED IN THE REFERENCED
      PARAGRAPH. VARIABLE DEFINITION IGNORED".
```

On the other hand, Figure 7.22 shows the second manipulated variable, that is, the specified pressure of the reactor at which the gas-phase reaction takes place.



Manipulated variable

Variable: 2

Type: Block-Var

Block: RPLUG

Variable: PRES

Sentence: PARAM

Units: bar

Manipulated variable limits

● Specify limits

Lower: 50

Upper: 150

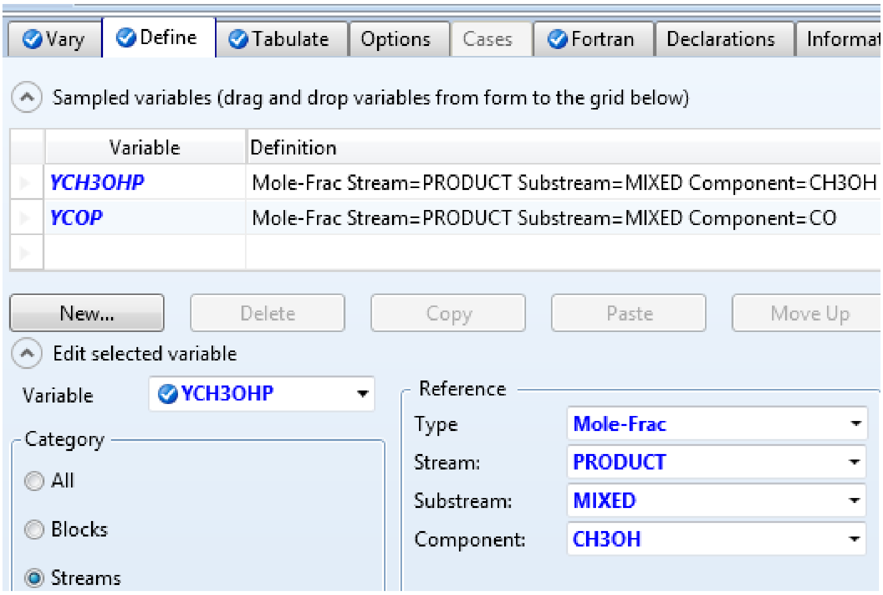
○ Number of points: 6

● Increment: 20

○ List of values

Figure 7.22 The pressure of the gas-phase reactor is to be manipulated, as the second variable, to see the maximum selectivity of methanol production as given by Equation 7.7 for the two parallel reactions.

We will define the mole fraction of CH_3OH and CO in the product stream. Figure 7.23 shows the definition of two variables: “**YCH3OHP**” the mole fraction of methanol and “**YCOP**” the mole fraction of CO in the product stream.



Sampled variables (drag and drop variables from form to the grid below)

Variable	Definition
YCH3OHP	Mole-Frac Stream=PRODUCT Substream=MIXED Component=CH3OH
YCOP	Mole-Frac Stream=PRODUCT Substream=MIXED Component=CO

Edit selected variable

Variable: YCH3OHP

Category

○ All

○ Blocks

● Streams

Reference

Type: Mole-Frac

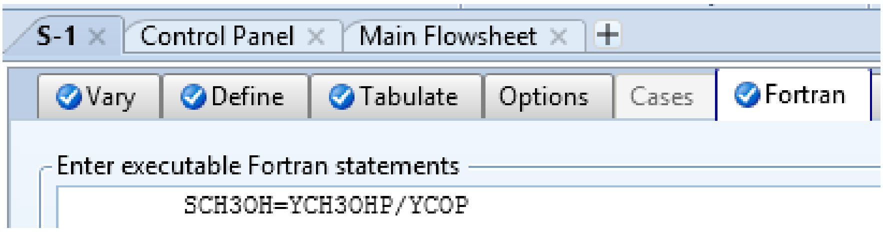
Stream: PRODUCT

Substream: MIXED

Component: CH3OH

Figure 7.23 Defining two “**Sensitivity**” variables: “**YCH3OHP**” the mole fraction of methanol and “**YCOP**” the mole fraction of CO in the product stream.

In “**Fortran**” tab window, we define the selectivity of methanol, “**SCH3OH**”, as the mole fraction ratio of CH_3OH to CO, as shown in Figure 7.24.

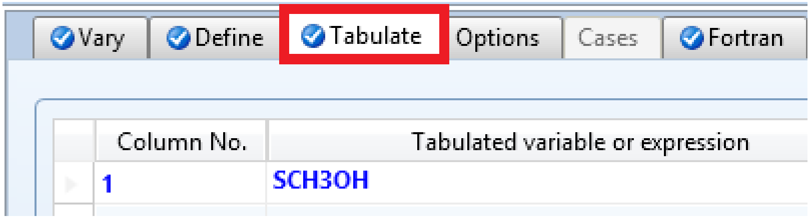


Enter executable Fortran statements

```
SCH3OH=YCH3OHP/YCOP
```

Figure 7.24 Defining the selectivity by "**SCH3OH**" as the mole fraction (or molar ratio) of the desired over the undesired product for the two parallel reactions.

In "**Tabulate**" tab window, we tabulate the variable "**SCH3OH**" as column number 1 in sensitivity analysis results, as shown in Figure 7.25.



Column No.	Tabulated variable or expression
1	SCH3OH

Figure 7.25 Tabulating "**SCH3OH**" as column number 1 in sensitivity analysis results.

Reinitialize and run the show. Go to "**Model Analysis Tools**" | "**Sensitivity**" | "**S-1**" | "**Results**" | "**Summary**" tab window, then from **Plot** group found in "**Home**" ribbon, click on "**Results Curve**" button and "**Results Curve**" window will pop-up. Select *X*, *Y*, and the parametric variable, click on "**OK**" button at the bottom of the given window, and a plot will be generated as shown in Figure 7.26. For the given feed composition, it is found that the maximum value of methanol selectivity occurs at $T = 250°C$ and $P = 150\,bar$.

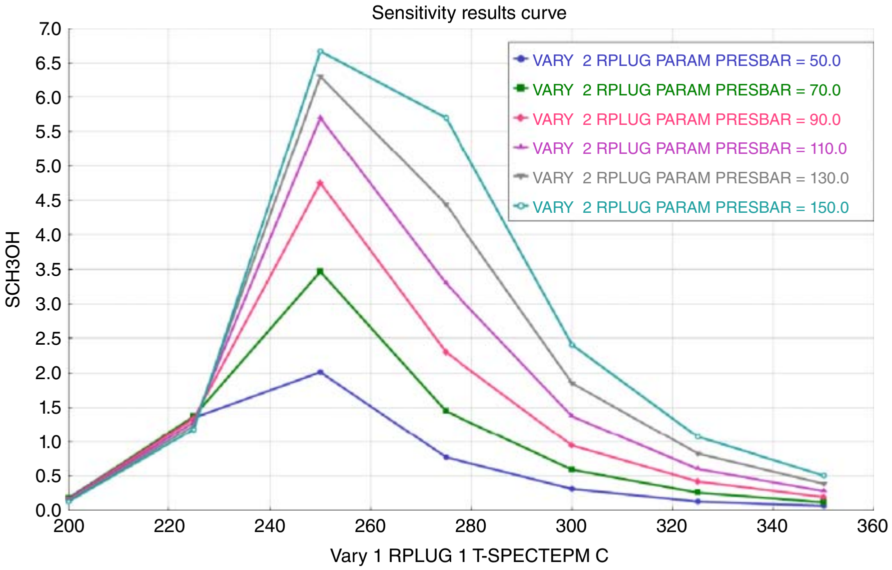


Figure 7.26 For the given feed molar flow rate and composition, it is found that the maximum methanol selectivity occurs at *T = 250°C* and *P = 150 bar*.

NOTE #3: *For the given feed molar flow rate and composition, the overall reactor heat duty for the combined reactions is negative, which means the exothermic heat will heat up the reactor medium if the reactor is not cooled down in proportion with the amount of generated heat. So, a constant-temperature reactor means in this regard that we have a steady-state energy balance such that the amount of heat generated is equal to the amount of heat exchanged with the cooling medium on the shell side.*

At last, an optimization analysis was carried out and the optimum temperature was found to be 278.5°C as we increase the pressure up to 350 bars. Of course, this does not mean that the reactor should be run at such a high pressure value, because the cost of compression and of the material of construction (i.e., more material thickness to withstand high pressure) will be soaring with increasing pressure. Hence, there should be an optimum economic value that will dictate where to draw the limit for the maximum applied pressure. One last note regards running the optimization analysis while the sensitivity analysis is in the deactivated mode. Do not run them at one time as you will get simulation errors because of different manipulated ranges for pressure and temperature of the reactor. To activate/deactivate a case study, right-click and select activate/deactivate submenu item from the context menu.

REFERENCES

[1] Vanden Bussche, K.M. and Froment, G.F. (1996) A steady-state kinetic model for methanol synthesis and the water gas shift reaction on a commercial Cu/ZnO/Al_2O_3 catalyst. *Journal of Catalysis*, **161**, 1–10.

[2] Perry, R.H. and Green, D.W. (1997) *Perry's Chemical Engineers' Handbook*, 7th edn Table 7.2 and 7.3, page 7.12 Reaction Kinetics, McGraw Hill, New Jersey, USA.

[3] Luyben, W.L. (2011) *Principles and Case Studies of Simultaneous Design*, John Wiley & Sons, Inc., New Jersey.

[4] http://www.scribd.com/doc/92000117/LHHW-Kinetics (accessed April 15, 2016).

[5] Dittmeyer, R., Höllein, V., Quicker, P. *et al.* (1999) Factors controlling the performance of catalytic dehydrogenation of ethylbenzene in palladium composite membrane reactors. *Chemical Engineering Science*, **54**, 1431–1439.

[6] Abbasi, R., Wu, L., Wanke, S.E., and Hayes, R.E. (2012) Kinetics of methane combustion over Pt and Pt–Pd catalysts. *Chemical Engineering Research and Design*, **90**, 1930–1942.

[7] Felder, R.M. and Rousseau, R.W. (eds) (2005) *Elementary Principles of Chemical Processes*, 3rd edn, John Wiley & Sons, Inc., Hoboken.

HOMEWORK/CLASSWORK 7.1 (GAS-PHASE OXIDATION OF CHLOROFORM)

Consider the following gas-phase reaction [4]:

$$2CHCl_3 + 2H_2O + O_2 \rightarrow 2CO_2 + 6HCl \tag{7.21}$$

$$\begin{aligned} r\ (\text{kmol/m}^3 \cdot \text{s}) &= \frac{kC_{CH_3Cl}}{1 + K_{HCl}C_{Hcl} + K_{CHCl_3}C_{CHCl_3}} \\ &= \frac{3.72 \times 10^5 \times e^{(-(21\,700/RT))}(1 \times C_{CH_3Cl} - 0)}{(1 + 5.97 \times 10^3 \times e^{(2440/RT)}C_{HCl} + 1.23 \times 10^3 \times e^{(5330/RT)}C_{CHCl_3})} \end{aligned} \tag{7.22}$$

where $k\ (s^{-1})$, C_{CH_3Cl} (mol/l), and C_{HCl} (mol/l) Notice that (mol/L) = ($kmol/m^3$).

Carry out the following steps:

1. Choose "**Chemicals with Metric Units**" template to create a steady-state flow sheet. Set the property model to "**UNIFAC**". Notice that for "**UNIFAC**" property method, there is no need to worry about estimating the pairwise, binary interaction parameters.
2. Give a title for the project and add the five components: $CHCl_3$, H_2O, O_2, CO_2, and HCl.
3. Click "**Reset**" followed by "**Next**" button to run the simulation and assure that properties analysis completed successfully. Switch to "**Simulation**" environment.
4. Set up a steady-state flowsheet with "**RPLUG**" block and attach one feed and one product stream, as shown in Figure 7.27.

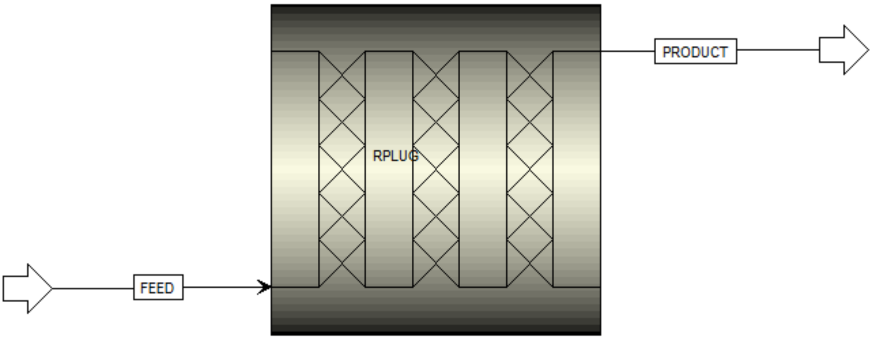


Figure 7.27 A schematic for conversion of chloroform into hydrogen chloride, using "**RPLUG**" type reactor.

5. For the feed stream, enter $T = 100°C$; $P = 1\ atm$; 40 kmol/h of $CHCl_3$; 40 kmol/h of H_2O; and 20 kmol/h of O_2.
6. In reactor "**Specifications**" tab window, choose *Reactor with specified temperature* and select the "**Operating condition**" to be "**Constant at specified reactor temperature**" = *100°C*.
7. In reactor "**Configuration**" tab window, choose a single tube with length 2 m; and the diameter 1.5 inches.
8. In the "**Reaction**" folder, create a reaction set "**R-1**" that defines Equation 7.21 as "**LHHW**" type. Enter kinetic parameters: the "**Reacting phase**" as *Vapor* and "**Rate basis**" as *Cat (wt)*. In the "**Driving Force Expression**" window, enter **[Ci] basis** as *Molarity*, for the forward reaction (i.e., "**Term no. 1**"), under "**Concentration exponents for reactants**", enter *1* for $CHCl_3$, and substitute for "**Coefficients for driving force constant**": **A**, **B**, **C**, & **D**, based on Equation 7.22. In the same window, repeat the latter step for the backward direction (i.e., "**Term no. 2**") in light of Equation 7.22.
9. In the "**Adsorption Expression**" window, substitute for the "**Adsorption expression exponent**", fill in the "**Concentration exponents**" matrix for HCl and $CHCl_3$ components, based on Equation 7.22, and the "**Adsorption constants**": **A**, **B**, **C**, and **D** for each term (i.e., "**Term no. 1**" up to "**Term no. 3**"). See Equation 7.20 and Figure 7.10 for the sake of comparison.
10. Associate "**R-1**" reaction set with "**R-PLUG**", under "**Reactions**" tab of **RPLUG** | "**Setup**" sheet.
11. For "**Pressure**" tab, you may set the pressure at the reactor inlet to be 1 bar for process stream with 0 pressure drop.
12. For "**Catalyst**" tab, select "**Catalyst present in the reactor**" and set the "**Particle density**" to $2000\ kg/m^3$ and "**Bed voidage**" to *0.5*.
13. Reinitialize and run the show. Watch out for simulation errors/warnings.
14. Report the reactor heat duty and product stream flow rate and composition.
15. Carry out sensitivity analysis to see the effect of pressure and temperature on the mole fraction of *HCl* in product stream. T range = [100–250]°C and P range = [0.5–6] bar. Show a parametric plot for Y_{HCl} as $f(T,P)$. What is your conclusion about the optimum pressure and temperature?

HOMEWORK/CLASSWORK 7.2 (FORMATION OF STYRENE FROM ETHYLBENZENE)

The kinetic data are quoted from Reference [5]. Consider the dehydrogenation of ethylbenzene into styrene:

$$C_8H_{10} \leftrightarrow C_8H_8 + H_2 \tag{7.23}$$

$$-r_1\,(\text{kmol/kg cat}\cdot\text{s}) = \left(K_f \times P_{C_8H_{10}} - K_b \times P_{C_8H_8} \times P_{H_2} / \left(1 + K_{C_8H_8}P_{C_8H_8}\right)^1\right)$$

$$-r_1\,(\text{kmol/kg cat}\cdot\text{s}) = \left(2.3496 \times e^{(-(158\,600/RT))} \times P_{C_8H_{10}} - 3.7594 \times 10^{-12} \times e^{(-(34\,339/RT))} \times P_{C_8H_8} \times P_{H_2} \Big/ \left(1 + 1.3 \times 10^{-4} P_{C_8H_8}\right)^1\right) \tag{7.24}$$

In addition, there are two additional reactions that take place in parallel:

$$C_8H_{10} \rightarrow C_6H_6 + CH_2CH_2 \tag{7.25}$$

$$-r_2\,(\text{kmol/kg cat}\cdot\text{s}) = k_{f2} \times P_{C_8H_{10}} = 1.37606 \times 10^{-6} \times e^{(-(114\,200/RT))} \tag{7.26}$$

$$C_8H_{10} + H_2 \rightarrow C_7H_8 + CH_4 \tag{7.27}$$

$$-r_3\,(\text{kmol/kg cat}\cdot\text{s}) = k_{f3} \times P_{C_8H_{10}} = 47.4107 \times e^{(-(208\,000/RT))} \tag{7.28}$$

Carry out the following steps:

1. Choose “**Chemicals with Metric Units**” template to create a steady-state flow sheet. Set the property model to “**PENG-ROB**”. Notice that for “**PENG-ROB**” property method, there is no need to worry about estimating the pairwise, binary interaction parameters.
2. Give a title for the project and add the eight components: benzene, ethylbenzene, styrene, ethylene, methane, toluene, hydrogen, and water.
3. Click “**Reset**” followed by “**Next**” button to run the simulation and assure that properties analysis completed successfully. Switch to “**Simulation**” environment.
4. Set up a steady-state flowsheet with “**RPLUG**” type reactor and attach one feed and one product stream, similar to that shown in Figure 7.27.
5. For the feed stream, enter *T = 600°C*; *P = 1.50 atm*; total molar flow rate 60 kmol/h of ethylbenzene, (i.e., mole fraction of C_8H_{10} is 1.0).
6. In the reactor “**Specifications**” tab, choose the “**Reactor type**” as “*Reactor with specified temperature*” and the “**Operating condition**” as “*Constant at specified reactor temperature*” = 600°C.
7. In the reactor “**Configuration**” tab, choose the single-tube case; the length 5 m and the diameter 5 m. The valid phase is vapor only.
8. In the “**Reaction**” folder, create a reaction set “**R-1**” that defines Equation 7.23 as “**LHHW**” type. Enter kinetic parameters: the “**Reacting phase**” as “*Vapor*” and “**Rate basis**” as “*Cat (wt)*”. In the “**Driving Force Expression**” window, enter “**[Ci] basis**” as “*Partial pressure*”, for the forward reaction (i.e., “**Term no. 1**”), under “**Concentration**

exponents for reactants", enter *1* for C_8H_{10}, and substitute for "**Coefficients for driving force constant**": **A**, **B**, **C**, and **D**, based on Equation 7.24. In the same window, repeat the latter step for the backward direction (i.e., "**Term no. 2**") in light of Equation 7.24.

9. In the "**Adsorption Expression**" window, substitute for the "**Adsorption expression exponent**", fill in the "**Concentration exponents**" matrix for C_8H_8 component, based on Equation 7.24, and the "**Adsorption constants**": **A**, **B**, **C**, and **D** for both terms (i.e., **Term no. 1** and **Term no. 2**). See Equation 7.20 and Figure 7.10 for the sake of comparison.
10. Create a second reaction set "**R-2**" that defines Equation 7.25 as "**POWERLAW**" type. Enter the "**Reacting phase**" as "*Vapor*"; "**Rate basis**" as "*Cat (wt)*"; the kinetic parameters (*k* and *E*) in light of Equation 7.26; and "**[Ci] basis**" as "*Partial pressure*".
11. Create a third reaction set "**R-3**" that defines Equation 7.27 as "**POWERLAW**" type. Enter the "**Reacting phase**" as "*Vapor*"; "**Rate basis**" as "*Cat (wt)*"; the kinetic parameters (*k* and *E*) in light of Equation 7.28; and "**[Ci] basis**" as "*Partial pressure*".
12. Associate "**R-1**", "**R-2**", and "**R-3**" reaction sets with "**RPLUG**", under "**Reactions**" tab of "**RPLUG**" | "**Setup**" sheet.
13. In "**Pressure**" tab, you may set the pressure at the reactor inlet to be 1.5 atm for process stream and 0 pressure drop.
14. In "**Catalyst**" tab, select "**Catalyst present in the reactor**" and set the "**Catalyst loading**" to *28,000 kg* and "**Bed voidage**" to *0.445*.
15. Reinitialize and run the show. Watch out for simulation errors/warnings.
16. Report the reactor heat duty and product stream molar flow rate and molar composition.
17. Referring to Felder and Rousseau [7], the fractional conversion percent (**FCP**) is defined as $\left[(\text{Moles reacted/Moles fed})_{\text{limiting reactant}}\right] \times 100\%$.

$$\mathbf{FCP} = \left(\left(C_8H_{10\text{feed}} - C_8H_{10\text{product}}\right) \Big/ C_8H_{10\text{feed}}\right) \times 100\% \tag{7.29}$$

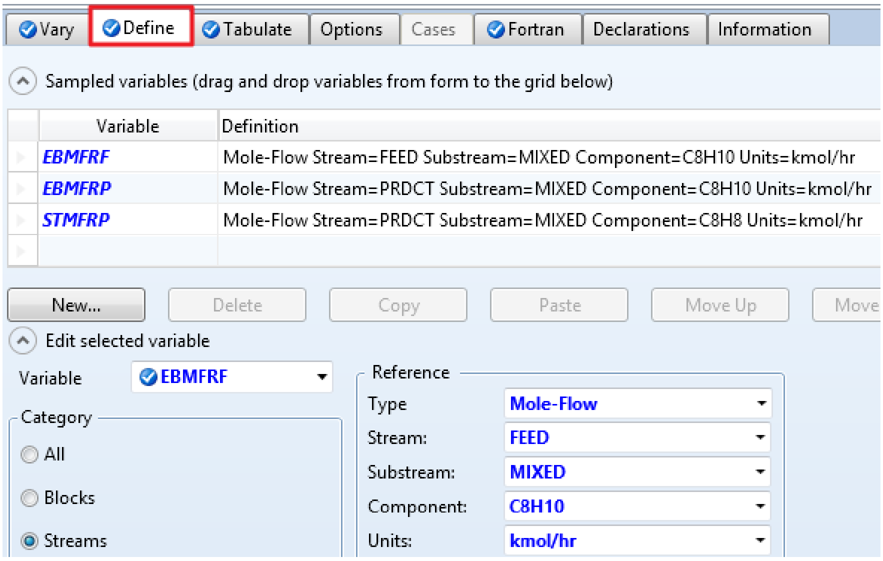
The yield percent (**YP**) as [(Moles of desired product formed)/(Moles that would have been formed if there were no side reactions and the reaction was complete)] × 100%.

$$\mathbf{YP} = \left(\left(C_8H_{8\text{product}}\right) \Big/ C_8H_{10\text{feed}}\right) \times 100\% \tag{7.30}$$

On a molar basis for both streams, report **FCP** for C_8H_{10} and **YP** for C_8H_8 (desired product). Notice that **FCP** gives information about the overall conversion of ethylbenzene (C_8H_{10}) into desired and undesired product, as well. On the other hand, **YP** gives information about the portion out of the overall reacting amount of C_8H_{10}, which is converted into the desired product (C_8H_8).

18. Change the feed stream as follows: *T* = *600°C*; *P* = *1.50 atm*; and total molar flow rate is 660 kmol/h of which 600 kmol/h is CH_4 and 60 kmol/h is ethylbenzene.
19. Reinitialize and rerun the show. Watch out for simulation errors/warnings.
20. Report **FCP** for C_8H_{10} and **YP** for C_8H_8 (desired product). Compare both values with those in step #17.

21. Using the latest feed stream properties listed in step #18, define a new sensitivity analysis “**S-1**” to see the effect of pressure and temperature on “**FCP**” and “**YP**” values.
22. In “**Vary**” tab window, vary the first “**RPLUG**” variable: “**SPEC-TEMP**” between 500 and 700°C with an increment of 25°C, and the second “**RPLUG**” variable: “**PRES**” between 1 and 5 bar with an increment of 1 bar.
23. In “**Define**” tab window, define the following three variables, as shown in Figure 7.28.
24. In “**Fortran**” tab window, define **FCP** and **YP** as a function of “**S-1**” defined variables, as shown in Figure 7.28:



Sampled variables (drag and drop variables from form to the grid below)

Variable	Definition
EBMFRF	Mole-Flow Stream=FEED Substream=MIXED Component=C8H10 Units=kmol/hr
EBMFRP	Mole-Flow Stream=PRDCT Substream=MIXED Component=C8H10 Units=kmol/hr
STMFRP	Mole-Flow Stream=PRDCT Substream=MIXED Component=C8H8 Units=kmol/hr

Edit selected variable

Variable: EBMFRF

Category
○ All
○ Blocks
● Streams

Reference
Type: Mole-Flow
Stream: FEED
Substream: MIXED
Component: C8H10
Units: kmol/hr

Figure 7.28 Defining three variables that represent the molar flow rate of C_8H_{10} in “**FEED**” stream; the molar flow rate of C_8H_{10} in “**PRDCT**” stream; and the molar flow rate of C_8H_8 in “**PRDCT**” stream.

FCP = ((EBMFRF-EBMFRP)/EBMFRF)*100.0
YP = (STMFRP/EBMFRF)*100.0

25. In “**Tabulate**” tab window, tabulate:
    FCP
    YP
26. Reinitialize and rerun the show. Watch out for simulation errors/warnings.
27. Generate a parametric plot for **FCP** and another for **YP**, as *f (T, P)*.
28. Draw your conclusion about the optimum *T* and *P* in terms of maximizing both **FCP** and **YP**.

HOMEWORK/CLASSWORK 7.3 (COMBUSTION OF METHANE OVER STEAM-AGED Pt–Pd CATALYST)

The kinetic data were quoted from Reference [6]. Consider the kinetics of methane combustion over steam-aged Pt–Pd catalyst while using steam to examine the inhibition effect of steam, produced during the combustion, on catalyst.

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \tag{7.31}$$

$$-r_{CH_4}\ (\text{kmol/kg cat}\cdot\text{s}) = \left(kC_{CH_4}/\left(1+K_{H_2O}C_{H_2O}\right)^1\right) = \frac{\left(k\times e^{(-(E/RT))}\times C_{CH_4}\right)}{\left(1+A_w\times e^{(\triangle H_{ads}/RT)}C_{H_2O}\right)^1} \tag{7.32}$$

We will consider the steam-aged Pt–Pd catalyst.

For temperature below 545°C, the kinetic parameters are [6]

k (s^{-1}): 1.81×10^3	E (kJ/mol): 72.6	A_w (m^3/kmol): 52.7	ΔH_{ads} (kJ/mol): 24.1

For temperature above 545°C, the kinetic parameters are [6]

k (s^{-1}): 8.01	E (kJ/mol): 35.7	A_w (m^3/kmol): 52.7	ΔH_{ads} (kJ/mol): 24.1

Notice that the kinetic parameters are adjusted such that they comply with Aspen Plus basis for entering kinetic parameters (see Chapter 6, NOTE #4).

Carry out the following steps:

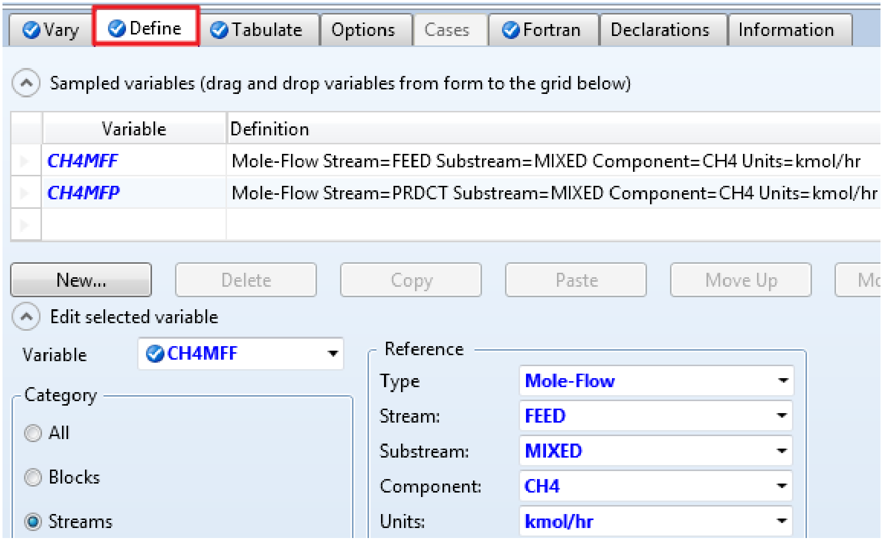
1. Choose "**Chemicals with Metric Units**" template to create a steady-state flow sheet. Set the property model to "**NRTL**".
2. Give a title for the project and add the five components: methane, oxygen, nitrogen, carbon dioxide, and water.
3. Under "**Properties**" environment, go to "**Methods**" | "**Parameters**" | "**Binary Interaction**" | "**NRTL -1**" sheet and be sure that the "*Estimate missing parameters by UNIFAC*" option is affirmed. Click on "**Reset**" followed by "**Next**" button to run the simulation and assure that properties analysis completed successfully. Switch to "**Simulation**" environment.
4. Set up a steady-state flowsheet with "**RPLUG**" type reactor and attach one feed and one product stream, similar to that shown in Figure 7.27.
5. For the feed stream, enter $T = 500°C$; $P = 5\ bar$; molar flow rate of 20 kmol/h for CH_4; 40 kmol/h for O_2; 160 kmol/h for N_2; and 10 kmol/h for water.
6. In the reactor "**Specifications**" tab window, choose the "**Reactor type**" as "*Reactor with specified temperature*" and the "**Operating condition**" as "*Constant at specified reactor temperature*" = 500°C.
7. In the reactor "**Configuration**" tab window, choose the single-tube case; the length 5 m and the diameter 1.5 m.

8. For the “**Reaction**” folder, create a reaction set “**R-1**” that defines Equation 7.31 as “**LHHW**” type. Enter kinetic parameters: the “**Reacting phase**” as “*Vapor*”; “**Rate basis**” as “*Cat (wt)*”; the rate constant, *k*; and the activation energy, *E*. In the “**Driving Force Expression**” window, enter “**[Ci] basis**” as “*Molarity*”; enter for the forward reaction (i.e., “**Term no. 1**”) the value of CH_4 as “**Concentration exponents for reactant**”; and fill in “**Coefficients for driving force constant**”: **A**, **B**, **C**, and **D**, based on Equation 7.32. In the last window, repeat the latter step for the backward direction (i.e., “**Term no. 2**”) in light of Equation 7.32.
9. In the “**Adsorption Expression**” window, fill in the “**Adsorption expression exponent**”; fill in the “**Concentration exponents**” matrix for H_2O component, based on Equation 7.32; and the “**Adsorption constants**”: **A**, **B**, **C**, and **D** for both terms (i.e., **Term no. 1** and **Term no. 2**). See Equation 7.20 and Figure 7.10 for the sake of comparison.
10. Associate “**R-1**” reaction set with “**RPLUG**”, under “**Reactions**” tab of “**RPLUG**” | “**Setup**” sheet.
11. In “**Pressure**” tab, you may set the pressure at the reactor inlet to be 5 bar for process stream and 0 pressure drop.
12. In “**Catalyst**” tab, select “**Catalyst present in the reactor**” and set the “**Particle density**” to *1000 kg/m*^{3} and “**Bed voidage**” to *0.35*.
13. Reinitialize and run the show. Watch out for simulation errors/serious warnings.
14. Report the reactor heat duty and product stream molar flow rate and molar composition.
15. Referring to Felder and Rousseau [7], the fractional conversion percent (**FCP**) is defined as [(Moles reacted/Moles fed) $_{\text{limiting reactant}}$] × 100%.

$$\mathbf{FCP} = \left(\left(CH_{4\text{feed}} - CH_{4\text{product}}\right) / CH_{4\text{feed}}\right) \times 100\% \tag{7.33}$$

16. Define a new sensitivity analysis “**S-1**” to see the effect of pressure and temperature on **FCP** value.
17. In “**Vary**” tab window, vary the first “**RPLUG**” variable: “**SPEC-TEMP**” between 400 and 540°C with an increment of 20°C, and the second “**RPLUG**” variable: “**PRES**” between 3 and 9 bar with an increment of 3 bar.
18. In “**Define**” tab window, define the following two variables, as shown in Figure 7.29.

19. In “**Fortran**” tab window, define **FCP** as a function of “**S-1**” defined variables, as shown in Figure 7.29:



Sampled variables (drag and drop variables from form to the grid below)

Variable	Definition
CH4MFF	Mole-Flow Stream=FEED Substream=MIXED Component=CH4 Units=kmol/hr
CH4MFP	Mole-Flow Stream=PRDCT Substream=MIXED Component=CH4 Units=kmol/hr

Variable: CH4MFF

Category: ● Streams

Type: Mole-Flow
Stream: FEED
Substream: MIXED
Component: CH4
Units: kmol/hr

Figure 7.29 Defining two variables that represent the molar flow rate of CH_4 both in “**FEED**” and “**PRDCT**” stream.

FCP = ((CH4MFF-CH4MFP)/CH4MFF)*100

20. In “**Tabulate**” tab window, tabulate:
    1 FCP
21. Reinitialize and rerun the show. Watch out for simulation errors/warnings.
22. Generate a parametric plot for **FCP** as *f (T, P)*.
23. Draw your conclusion about the optimum *T* and *P* in terms of maximizing **FCP**. Why does the effect of pressure on methane combustion reaction is practically insignificant, unlike the temperature effect.

8

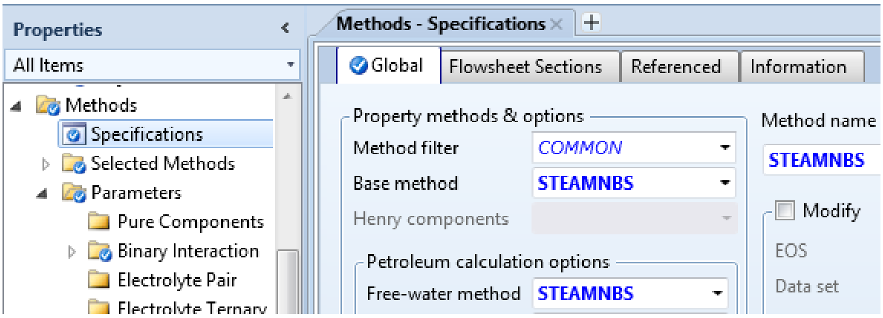
PRESSURE DROP, FRICTION FACTOR, ANPSH, AND CAVITATION

8.1 PROBLEM DESCRIPTION

To simulate a fluid flow setup, we consider the flow of water between two tanks that are 2 km apart, which are connected *via* pipes, valves, different fittings, and a pump to transport water from the first tank to the second.

8.2 THE PROPERTY METHOD: “STEAMNBS”

Aspen Plus has multiple unit operation options for simulating fluid transport problems, based on the complexity of the user’s application. Choose “**Specialty Chemicals with Metric Units**” template to create a steady-state flow sheet. Given the fact that the ASME steam tables are less accurate than the NBS/NRC steam tables, set the property method to “**STEAMNBS**”. The NBS/NRC steam tables are embedded, similar to any other equation of state, within the built-in “**Aspen Physical Property System**”. These steam tables can calculate any thermodynamic property of water. There are no parameter requirements. Figure 8.1 shows the “**Global**” tab window where the user decides on the property method.



Method filter: COMMON
Base method: STEAMNBS
Henry components:
Free-water method: STEAMNBS
Method name: STEAMNBS
☐ Modify

Figure 8.1 Selection of “**STEAMNBS**” as the property method for a water pumping system.

Aspen Plus®: Chemical Engineering Applications, First Edition. Kamal I.M. Al-Malah.

Companion Website: www.wiley.com/go/Al-Malah/AspenPlusApplications

Give a title for the project and add water as the only component. Click “**Reset**” followed by “**Next**” button to run the simulation and assure that properties’ analysis completed successfully. Switch to “**Simulation**” environment.

8.3 A WATER PUMPING FLOWSHEET

We will set up a steady-state flowsheet as shown in Figure 8.2.

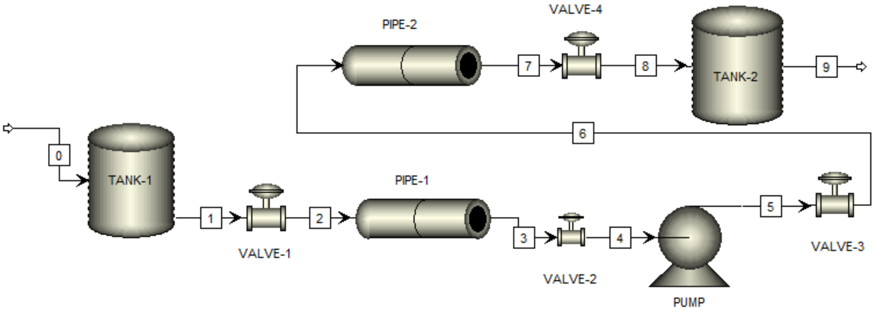


Figure 8.2 The flowsheet for water transport between two tanks that are 2 km apart.

In “**Model Palette**”, click on “**Pressure Changers**” tab. Under this tab, you will have many options that you can choose from for fluid flow purposes. Those unit operations can be used to model fluid flow processes. Pipes, pumps, and valves are chosen from such a category. On the other hand, the storage tank is chosen from the “**Mixers/Splitters**” tab under “**Mixer**” category.

Figure 8.2 shows that water is brought to “**TANK-1**” from an external source and it will be transported to “**TANK-2**” *via* means of connecting pipes, valves, fittings, and a pump. Moreover, “**TANK-1**” exists at a pressure of 2 atm where it suffices to push the liquid water until the entrance of the installed pump (installed at the midpoint between the two tanks). Water will continue its journey to “**TANK-2**” by the virtue of the pump work (i.e., compression).

Before we go into further specifications, let us decide on the optimum diameter for the pipe.

The optimum inside diameter (given in inch) for a turbulent flow is given [1] as

$$D_{i,\mathrm{opt}} = 3.9 \times q_{\mathrm{f}}^{0.46} \times \rho^{0.13} \tag{8.1}$$

In our case, we have $q_{\mathrm{f}} = 10\,\mathrm{m^3/h} = (353.146\,\mathrm{ft^3}/3600\,\mathrm{s}) = 0.098096\,\mathrm{ft^3/s}$

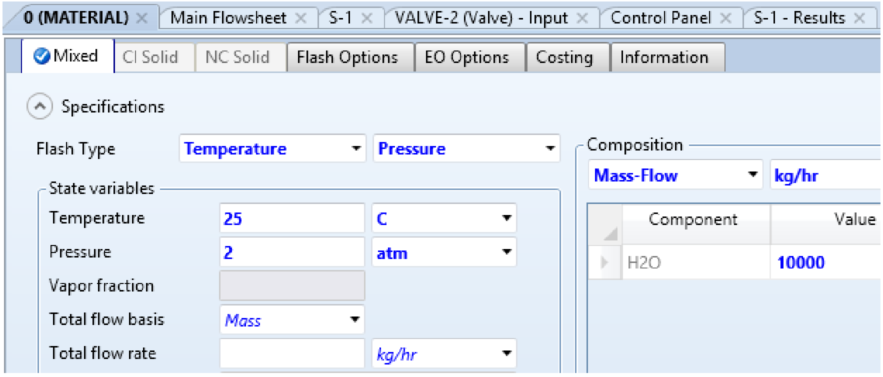
$$D_{i,\mathrm{opt}} = 3.9 \times 0.098096^{0.46} \times 62.3^{0.13} = 2.3'' \tag{8.2}$$

The closest nominal size will be 2.5″.

8.4 ENTERING PIPE, PUMP, AND FITTINGS SPECIFICATIONS

The following figures show specifications entered for the inlet stream and all blocks, starting upstream from "**0**" stream (inlet to "**Tank-1**") and going downstream to "**9**" stream ("**Tank-2**" outlet).

Figure 8.3 shows the input parameters for the inlet stream.



Flash Type: Temperature, Pressure

State variables

Temperature: 25 C

Pressure: 2 atm

Vapor fraction:

Total flow basis: Mass

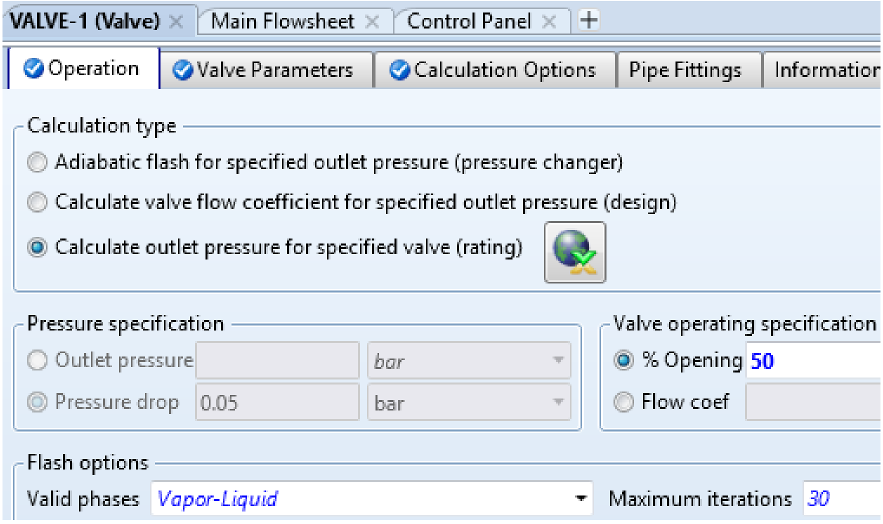
Total flow rate: kg/hr

Composition: Mass-Flow kg/hr

Component	Value
H2O	10000

Figure 8.3 Input parameters for the inlet "**0**" stream.

Figures 8.4 shows the options for calculating the outlet pressure and specification for percent valve opening pertaining to the first valve, that is, "**VALVE-1**" block.



Calculation type

○ Adiabatic flash for specified outlet pressure (pressure changer)

○ Calculate valve flow coefficient for specified outlet pressure (design)

● Calculate outlet pressure for specified valve (rating)

Pressure specification

○ Outlet pressure bar

○ Pressure drop 0.05 bar

Valve operating specification

● % Opening 50

○ Flow coef

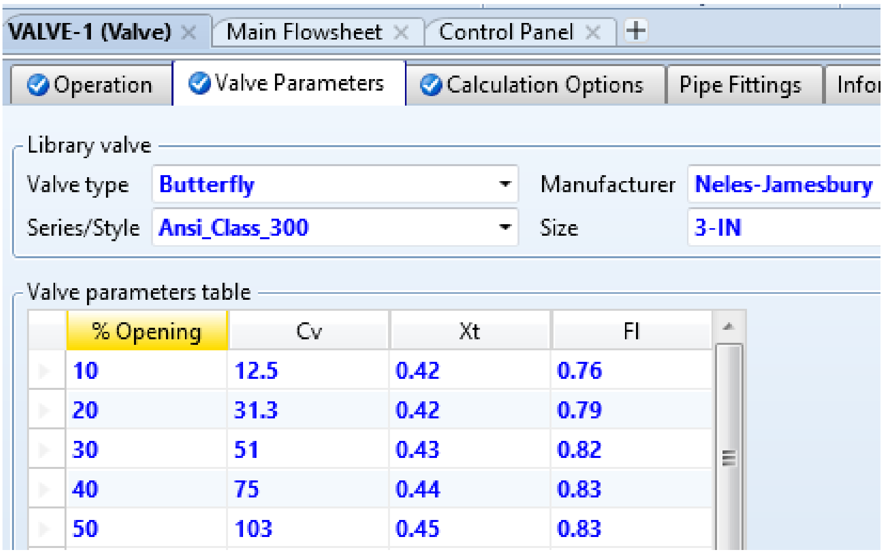
Flash options

Valid phases: Vapor-Liquid

Maximum iterations: 30

Figure 8.4 Specifications for "**VALVE-1**" block. The outlet pressure will be calculated for the specified valve (under "**Valve Parameters**" tab) and with a valve % opening of 50%.

Figure 8.5 shows “**Valve Parameters**” tab window where the user enters the valve type and its manufacturer. Notice that the butterfly type valve is used to regulate the flow rate of fluid *via* increasing or decreasing the opening area available for flow.



Library valve

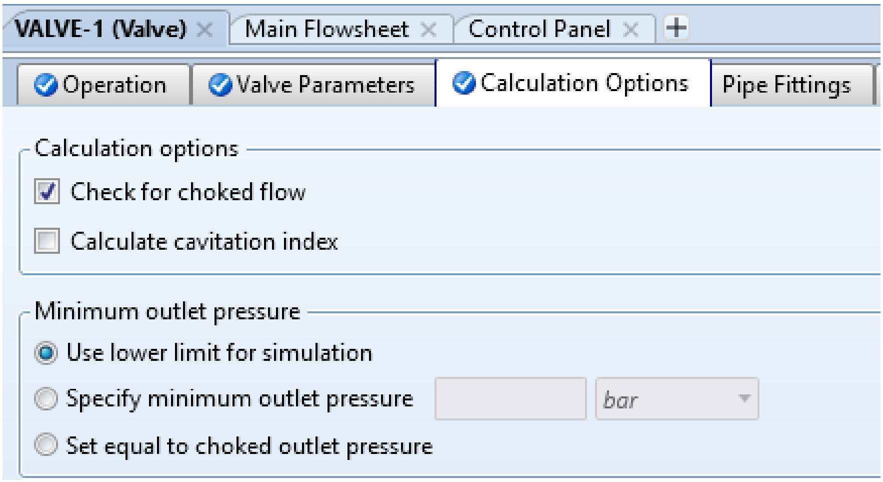
Valve type: Butterfly
Manufacturer: Neles-Jamesbury
Series/Style: Ansi_Class_300
Size: 3-IN

Valve parameters table

% Opening	Cv	Xt	Fl
10	12.5	0.42	0.76
20	31.3	0.42	0.79
30	51	0.43	0.82
40	75	0.44	0.83
50	103	0.45	0.83

Figure 8.5 In “**Valve Parameters**” tab window, the valve type is “*Butterfly*” and Aspen Plus provides specifications for “*Neles-Jamesbury*” manufacturer’s valve types, which facilitate the calculation of the outlet pressure valve.

Figure 8.6 shows “**Calculations Options**” tab window where Aspen Plus checks for the existence of choking condition. Notice that the choked flow for a compressible fluid, such as gases and vapors, is a limiting condition at which the choking occurs for an isentropic expansion condition (i.e., reduction in pressure below a certain critical value) such that the exit plane velocity is at sonic conditions or at a Mach number of 1 (velocity of sound



Calculation options

☑ Check for choked flow

☐ Calculate cavitation index

Minimum outlet pressure

● Use lower limit for simulation

○ Specify minimum outlet pressure bar

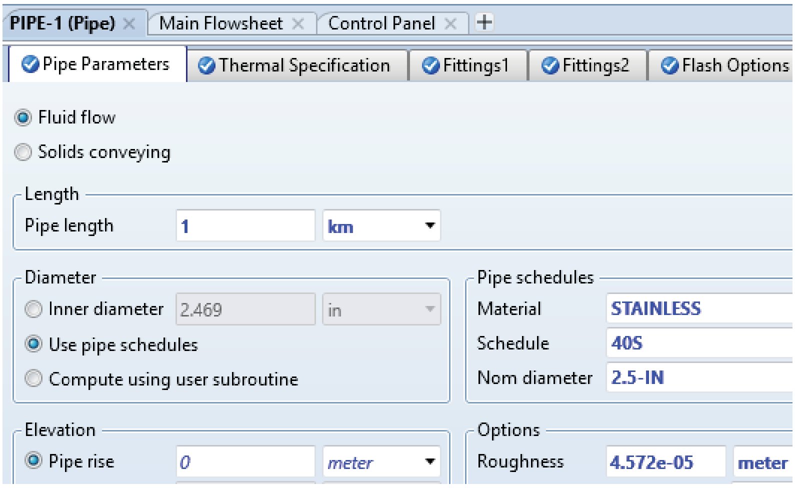
○ Set equal to choked outlet pressure

Figure 8.6 Checking for the occurrence of choked flow, which is a function of percent opening of the valve.

in an open air). At a choked flow condition, the mass flow rate is primarily dependent on the cross-sectional area of the hole, the upstream pressure, P_0, and weakly on the fluid temperature. The rate does not depend on the downstream pressure, at all.

On the other hand, for liquids, if the fluid is a liquid, a different type of limiting condition (also known as choked flow) occurs when the *venturi effect* acting on the liquid flow through the restriction decreases the liquid pressure to below that of the liquid vapor pressure at the prevailing liquid temperature. At such a point, the liquid will partially flash into bubbles of vapor (cavitation) and the subsequent collapse of the bubbles (implosion).

Figure 8.7 shows specifications for “**PIPE-1**” block, where its length is set to 1 km and diameter to 2.5″ nominal, with 40S schedule number, as estimated by Eq. (8.2).



● Fluid flow
○ Solids conveying

Length
Pipe length 1 km

Diameter
○ Inner diameter 2.469 in
● Use pipe schedules
○ Compute using user subroutine

Pipe schedules
Material STAINLESS
Schedule 40S
Nom diameter 2.5-IN

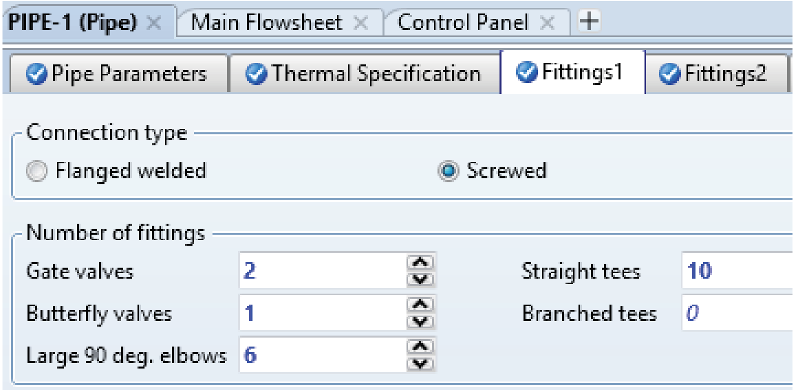
Elevation
● Pipe rise 0 meter

Options
Roughness 4.572e-05 meter

Figure 8.7 A pipe length of 1 km and nominal diameter of 2.5″, with 40S schedule #, is used for “**PIPE-1**” block.

In “**Thermal Specification**” tab window, select the “**Thermal specification type**” to be “*adiabatic*”.

In “**Fittings1**” tab window, the screwed connection type was selected as shown in Figure 8.8. The AWWA [2] states that “Isolating valves in the distribution system should



Connection type
○ Flanged welded ● Screwed

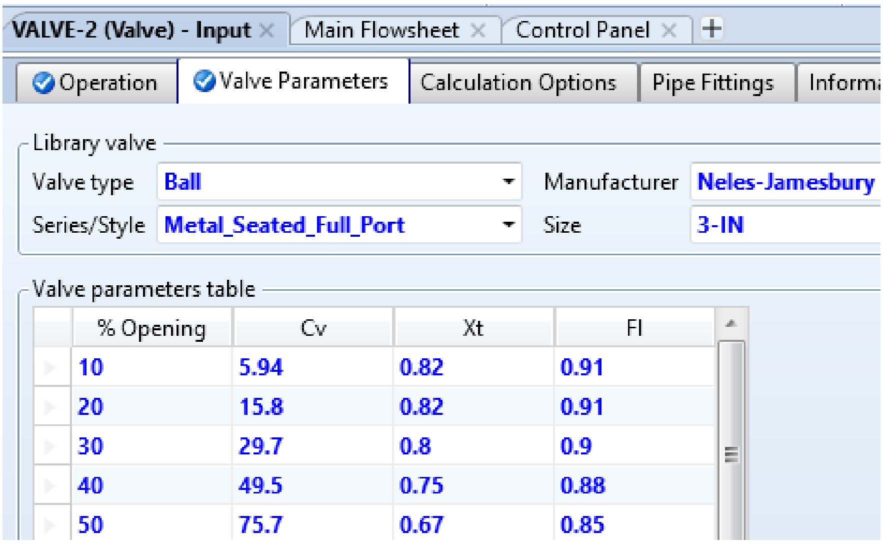
Number of fittings
Gate valves 2
Butterfly valves 1
Large 90 deg. elbows 6
Straight tees 10
Branched tees 0

Figure 8.8 Fittings number and types for “**PIPE-1**” block.

be located less than 500 ft apart (150 m) in business districts and less than 800 ft (240 m) apart in other parts of the system". Let us install three valves at 250, 500, and 750 m from the start of the pipe. We have already one valve just before and another just after the pipe. In addition, we have six 90°elbows and ten straight tees.

In general, screwed (threaded) ends, usually but not necessarily confined to pipe sizes of 150 mm or less, are widely used for bronze valves and to a lesser extent in iron and steel valves. On the other hand, flanged end valves are made in sizes from 150 mm upward. A flanged fitting is a type of connection used to join two or more pipes. Each of the pipes must be equipped with a flange, or raised ridge that runs around the outside perimeter of the pipe. Installers connect the two flanges *via* compression using bolts, clamps, or other fasteners. A flanged fitting may be used, however, in place of traditional threaded connectors, welding, or soldering. Some types of flanges are used in conjunction with welding or soldering to create a stronger pipe joint.

Figure 8.9 shows the "**Valve Parameters**" tab window for specifications of "**VALVE-2**" block where we use the "*Ball*" type instead of butterfly for the sake of knowing the different types of valve being used in industries. In "**Operation**" tab window, we use the same choice as that of "**VALVE-1**" block (see Figure 8.4). So does the case with "**Calculation Options**" tab window (see Figure 8.6).

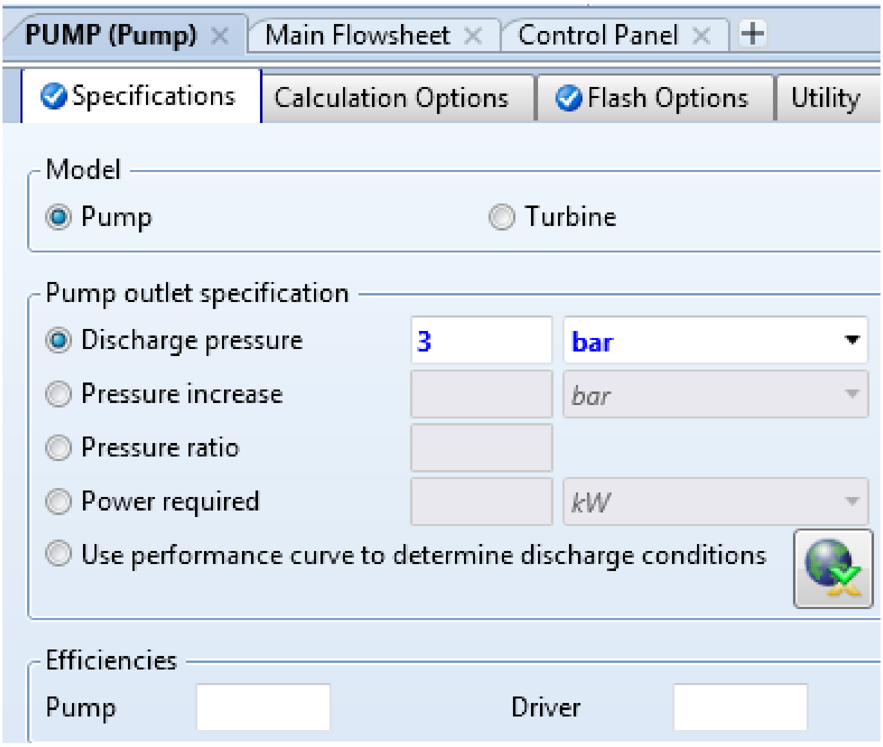


Valve type: Ball
Series/Style: Metal_Seated_Full_Port
Manufacturer: Neles-Jamesbury
Size: 3-IN

% Opening	Cv	Xt	Fl
10	5.94	0.82	0.91
20	15.8	0.82	0.91
30	29.7	0.8	0.9
40	49.5	0.75	0.88
50	75.7	0.67	0.85

Figure 8.9 For "**VALVE-2**" block, the ball type is used instead of the butterfly type.

Figure 8.10 shows the minimum specifications need to be entered by the user regarding the "**PUMP**" block. A discharge pressure of 3 bar is assumed to overcome friction along the road up to "**TANK-2**", in addition to the kinetic energy of the fluid itself upon discharging and the presence of elevation head. At the bottom of the "**Specifications**" tab window, Aspen Plus shows two blank boxes for the efficiency of the pump itself and for its driving motor as well. There is no need to enter them here because Aspen Plus will calculate the pump efficiency and the motor efficiency is usually assumed one, unless otherwise specified.



Model

● Pump ○ Turbine

Pump outlet specification

● Discharge pressure 3 bar

○ Pressure increase bar

○ Pressure ratio

○ Power required kW

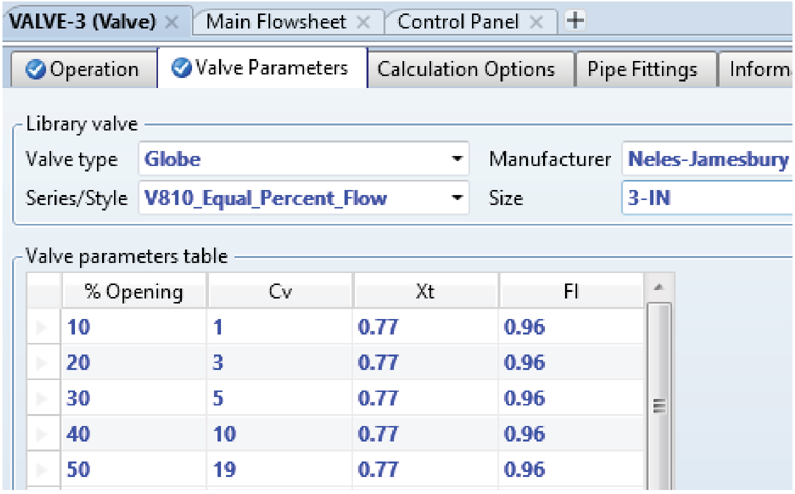
○ Use performance curve to determine discharge conditions

Efficiencies

Pump Driver

Figure 8.10 The minimum input specifications needed for the "**PUMP**" block. A discharge pressure of 3 bar is assumed to overcome downstream friction plus fluid discharging at the end-tank.

Figure 8.11 shows the specification for "**VALVE-3**" block where we use the globe type. In "**Operation**" tab window, we use the same choice as that of "**VALVE-1**" block (see



Library valve

Valve type: Globe

Manufacturer: Neles-Jamesbury

Series/Style: V810_Equal_Percent_Flow

Size: 3-IN

Valve parameters table

% Opening	Cv	Xt	Fl
10	1	0.77	0.96
20	3	0.77	0.96
30	5	0.77	0.96
40	10	0.77	0.96
50	19	0.77	0.96

Figure 8.11 For "**VALVE-3**" block, the "*Globe*" type is used with "*V810_Equal_Percent_Flow*" series/style.

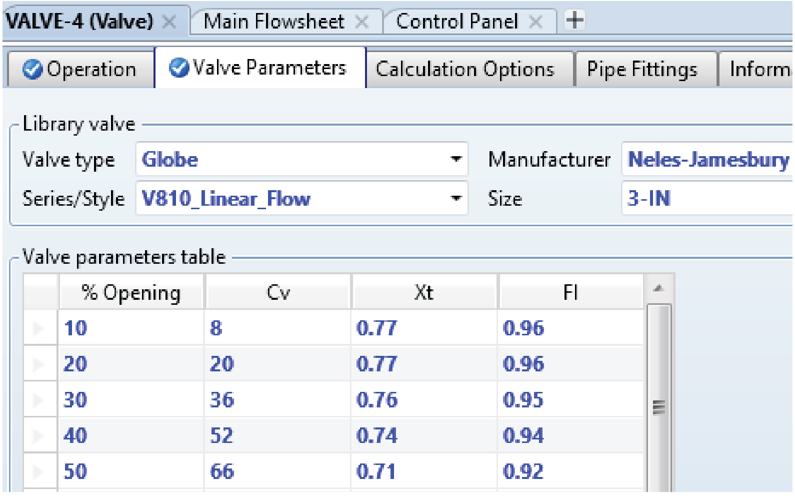
Figure 8.4). So is the case with “**Calculation Options**” tab window (see Figure 8.6). Notice that for a globe valve, the area available for flow is increased/decreased by raising/lowering the valve plug that is driven by a force of an actuator, which is normally connected to a control loop.

NOTE #1: *The “inherent characteristic” of a valve is the relationship between the flow rate through the valve and the travel of the closure of the valve stem as the stem is moved from the closed position to its rated travel with a “constant pressure drop across the valve”. Inherent valve characteristics are measured by the valve manufacturer in a test stand under a specified set of process conditions, particularly a constant differential pressure across the valve. The three most common valve characterizations are equal percentage, linear, and quick opening.*

On the other hand, the installed characteristic of a valve is the relationship between the flow rate through the valve and the travel of the closure of the valve stem as the stem is moved from the closed position to its designated travel under actual process conditions. In many process applications, the pressure drop across a valve varies with the flow. In these real instances, an equal percentage valve will act to linearize the process. The correct selection of valve characteristic to linearize the process gain will ease the tuning process and yield a robust system, from control point of view.

For “**PIPE-2**” block, the same specifications of “**PIPE-1**” block are used. Refer to “**PIPE-1**” block specifications, explained earlier.

Figure 8.12 shows the “**Valve Parameters**” tab window for specifications of “**VALVE-4**” block where we use the globe type valve. In “**Operation**” tab window, we use the same choice as that of “**VALVE-1**” block (see Figure 8.4). So is the case with “**Calculation Options**” tab window (see Figure 8.6).



Library valve

Valve type: Globe

Series/Style: V810_Linear_Flow

Manufacturer: Neles-Jamesbury

Size: 3-IN

Valve parameters table

% Opening	Cv	Xt	Fl
10	8	0.77	0.96
20	20	0.77	0.96
30	36	0.76	0.95
40	52	0.74	0.94
50	66	0.71	0.92

Figure 8.12 For “**VALVE-4**” block, the “*Globe*” type is used with “*V810_Linear_Flow*” series/style.

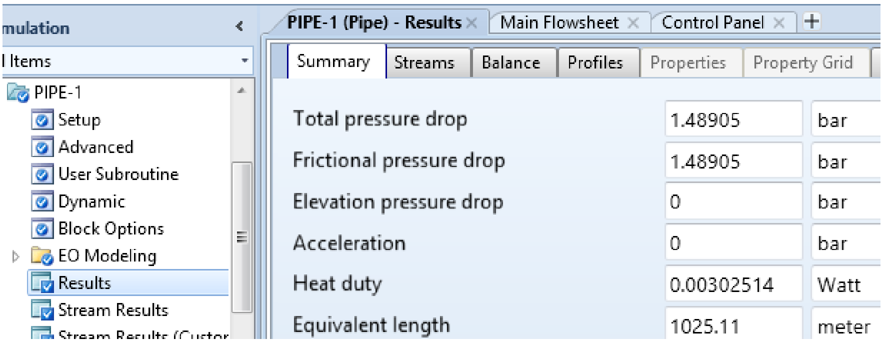
Finally, for “**TANK-2**” block, there will be no need to enter any input property; Aspen Plus will complete the missing information.

8.5 RESULTS: FRICTIONAL PRESSURE DROP, THE PUMP WORK, VALVE CHOKING, AND ANPSH VERSUS RNPSH

Reinitialize and run the show. See if there is any serious warning or error *via* the “**Control Panel**”.

Let us look at some simulation results and show where they can be accessed.

Figure 8.13 shows the results summary pertaining to “**PIPE-1**” block that is 1 km long. Notice here that there is a significant pressure drop due to friction along the pipe, in addition to the presence of 19 fitting objects (see Figure 8.8). That is why the pressure inside “**TANK-1**” is at 2 atm, which is sufficiently large to overcome all types of friction along fittings-augmented “**PIPE-1**” pipeline. Moreover, the reported equivalent length is 1025.11 m > 1000 m (original length). What does this mean? From fluid mechanics point of view, such an extra length of 25.11 m accounts for the resulting friction due to the presence of fitting objects in a manner equivalent to having a pipe of a total length equal to 1025.11 m but with no installed fitting objects.



Total pressure drop 1.48905 bar

Frictional pressure drop 1.48905 bar

Elevation pressure drop 0 bar

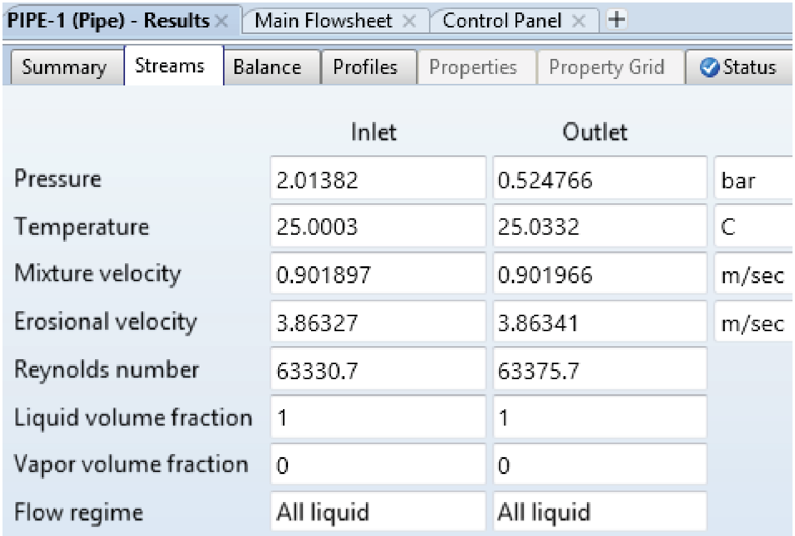
Acceleration 0 bar

Heat duty 0.00302514 Watt

Equivalent length 1025.11 meter

Figure 8.13 “**PIPE-1**” block result summary showing the friction pressure drop and the equivalent length.

Figure 8.14 shows the fluid and flow properties throughout the pipe itself. For example, you can see P, T, the mixture velocity (in this case liquid velocity as there is only one phase), and Reynolds number that tells we have a turbulent regime prevailing within the pipe.



	Inlet	Outlet	
Pressure	2.01382	0.524766	bar
Temperature	25.0003	25.0332	C
Mixture velocity	0.901897	0.901966	m/sec
Erosional velocity	3.86327	3.86341	m/sec
Reynolds number	63330.7	63375.7	
Liquid volume fraction	1	1	
Vapor volume fraction	0	0	
Flow regime	All liquid	All liquid	

Figure 8.14 The fluid and flow properties of liquid water flowing in the pipe itself under "**Streams**" tab.

EXERCISE 8.1

Why is there a pressure drop between the inlet and outlet condition? Why is there a minute temperature increase between the inlet and outlet condition?

If you click on "**Profiles**" tab, you will be able to see the pressure profile along the pipe. For example, while the "**Profile**" tab window is active, you may go to "**Home**" ribbon | "**Plot**" group and make use of the available buttons that can be clicked on to generate the corresponding plot. Figure 8.15 shows the pressure profile (or, pressure gradient) throughout

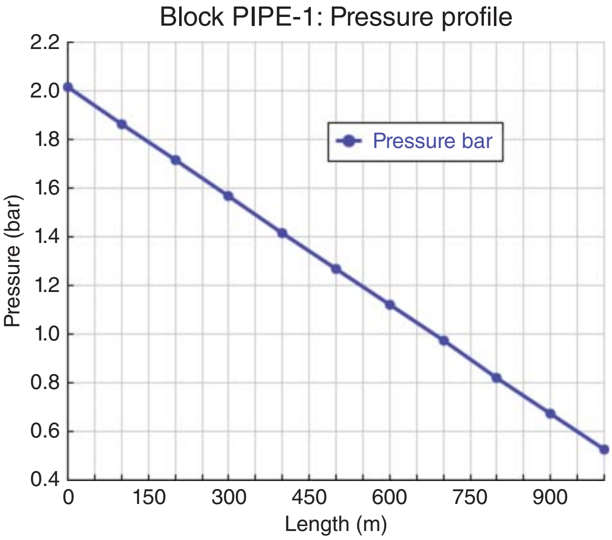
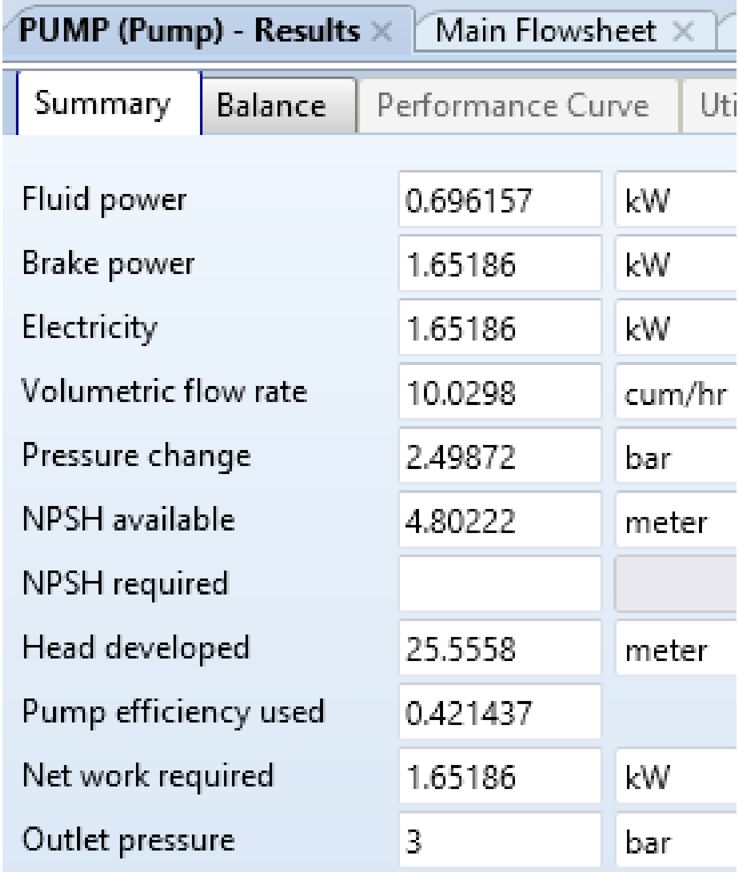


Figure 8.15 The pressure throughout the pipe decreases (i.e., pressure drop) with the axial distance as a result of energy dissipation due to friction.

"**PIPE-1**" pipeline. The slope of the line is negative (i.e., $\Delta P/\Delta X < 0$) simply because we have a friction that will result in a drop of pressure with increasing X along the pipe. If the pipe is frictionless, then we will have a constant pressure value along a horizontal pipe.

Figure 8.16 shows the results summary pertaining to the pump characteristics and performance. First, the fluid power is 0.69616 kW, which is equal to the brake power times the pump efficiency; that is 0.69616 kW = 1.65186 kW * 0.42144. This means that out of the input power supplied to the pump, only 42.14% is utilized to elevate the pressure of the fluid; the rest goes in the form of viscous dissipation (frictional heating as a result of moving fluid and pump rotor/blades). The brake power is equal to the supplied electricity as the motor efficiency is assumed one. The pressure change is about 2.5 bar, which is the difference in pressure between the inlet and outlet streams. The available net positive suction head (**ANPSH**) of the pump is 4.8 m. If **ANPSH** value is equal to or less than the required net positive suction head (**RNPSH**), the pump will then suffer from cavitation (see next section). Cavitation means formation of vapor bubbles at the inlet of the pump, which will travel with the liquid until they hit the solid boundaries (such as blades or vanes) where they burst (implode) or collapse causing a negative pressure pulse, or vibration. This

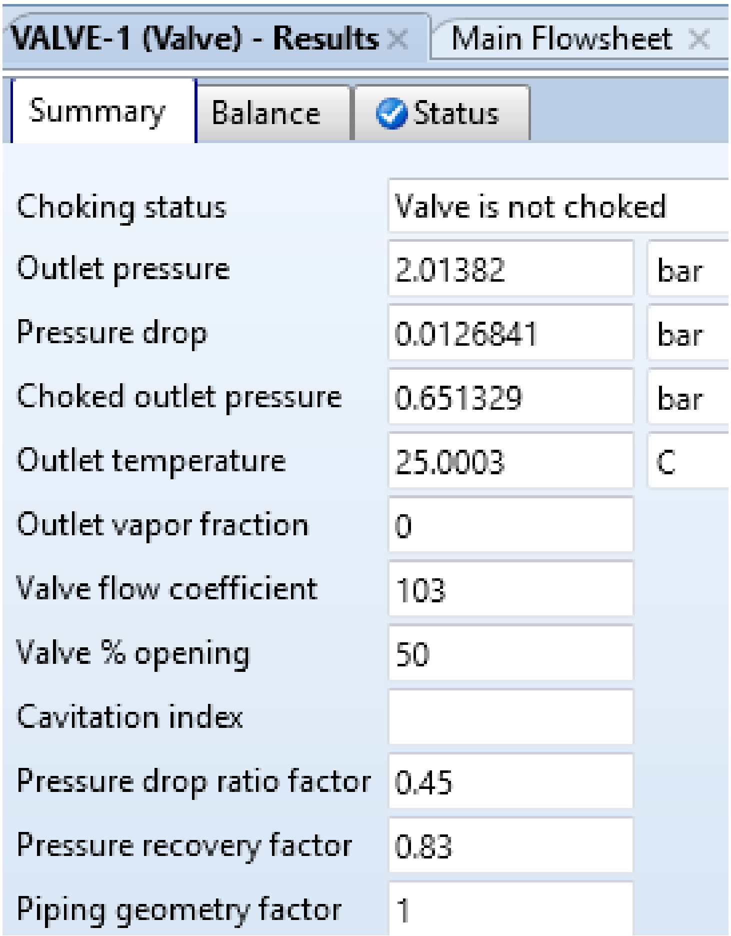


Fluid power	0.696157	kW
Brake power	1.65186	kW
Electricity	1.65186	kW
Volumetric flow rate	10.0298	cum/hr
Pressure change	2.49872	bar
NPSH available	4.80222	meter
NPSH required		
Head developed	25.5558	meter
Pump efficiency used	0.421437	
Net work required	1.65186	kW
Outlet pressure	3	bar

Figure 8.16 The pump characteristics and performance.

continuous cycle of formation and collapse of bubbles will cause an early wear and tear of the pump blades/vanes, in addition to the reduction in its pumping performance.

Figure 8.17 shows the summary of the first valve ("**VALVE-1**") results where again it shows if the reduction in pressure due to the reduction in flow area as a result of being semi-closed (i.e., valve % opening is 50%) may cause valve choking. The liquid flow through the restriction decreases the liquid pressure to below that of the liquid vapor pressure at the prevailing liquid temperature. At that point, the liquid will partially flash into vapor bubbles and the subsequent collapse of the bubbles (i.e., cavitation).

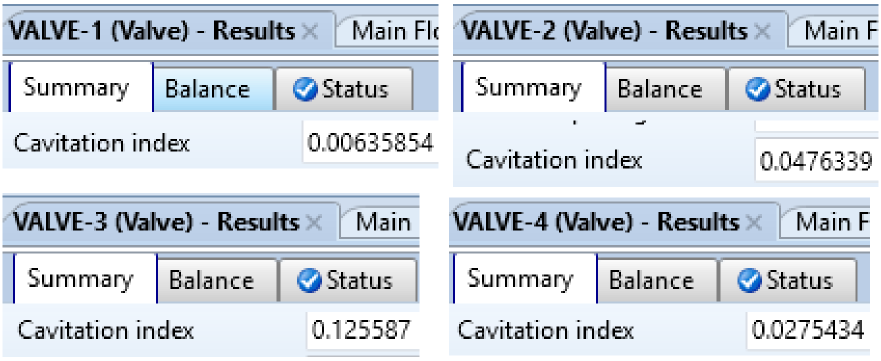


Choking status	Valve is not choked	
Outlet pressure	2.01382	bar
Pressure drop	0.0126841	bar
Choked outlet pressure	0.651329	bar
Outlet temperature	25.0003	C
Outlet vapor fraction	0	
Valve flow coefficient	103	
Valve % opening	50	
Cavitation index		
Pressure drop ratio factor	0.45	
Pressure recovery factor	0.83	
Piping geometry factor	1	

Figure 8.17 The valve status in terms of choking condition as a result of flow area restriction.

Cavitation is quite noisy and physically damages valves, pipes, and associated fitting objects. The outlet pressure is 2.014 bar that lies above the calculated choked outlet pressure of 0.651 bar.

If the "**Calculate cavitation index**" option is enabled in "**Calculation Options**" tab window (see Figure 8.6), Aspen Plus will provide a cavitation index for each of the four



Cavitation index 0.00635854

Cavitation index 0.0476339

Cavitation index 0.125587

Cavitation index 0.0275434

Figure 8.18 "**Valve-3**" is most vulnerable, among the four installed valves, to the choking condition.

valves as shown in Figure 8.18. The likelihood of cavitation in a valve is measured by the cavitation index. Aspen Plus calculates the cavitation index as

$$K_c = ((P_{in} - P_{out})/(P_{in} - P_v)) \tag{8.3}$$

where

K_C	Cavitation index
P_{in}	Inlet pressure
P_{out}	Outlet pressure
P_v	Vapor pressure at the given temperature

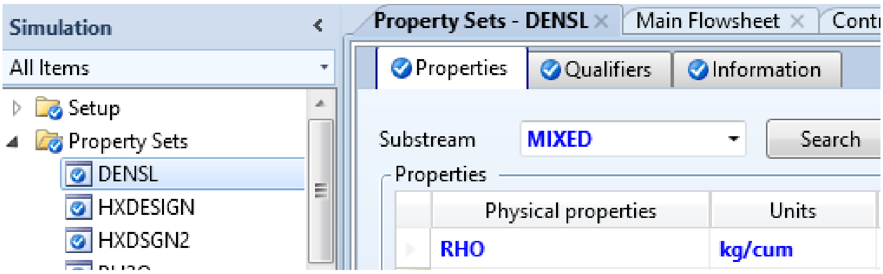
In principle, we should run our liquid flow system such that $0 \le K_c < 1$. If K_C is exactly one, then we will have cavitation (boiling or formation of gas bubbles) and the valve will choke. Obviously, if P_{out} drops below P_v, then we will end up with $K_C > 1$. This means that the process liquid will be converted into superheated vapor. This will make the situation even worse than cavitation condition. Notice that transport of vapor/gas is different from that of liquid in terms of used pieces of equipment as well as the extent of heat transfer, mass transfer, or both.

Finally, the pressure at the end of the journey (i.e., inside **TANK-2**) is 1.123 bar, which is larger than atmospheric so that it can discharge liquid water to an open (i.e., ventilated) tank.

NOTE #2: *The value of pressure inside* ***TANK-1*** *(or "****0****" inlet stream pressure) and of the discharge pressure of the pump ("****PUMP****") may be elevated in a manner to avoid the occurrence of cavitation anywhere along the pipeline system. Of course, the higher the pressure is, the better the condition will be in terms of avoiding cavitation; however, the operating cost will increase with increasing discharge pressure of the pump. Obviously, we need the minimum pressure/pumping requirement to assure the continuous and smooth flow from "****TANK-1****" to "****TANK-2****".*

8.6 MODEL ANALYSIS TOOLS: SENSITIVITY FOR THE ONSET OF CAVITATION OR VALVE CHOKING CONDITION

Before we move to "**Model Analysis Tools**", let us define two stream properties using "**Property Sets**" in "**Navigation**" pane. The first property will be the density of stream "**DENSL**" as shown in Figure 8.19. Under "**Qualifiers**" tab, select the phase to be "*liquid*". Notice here that the mixture property "**RHOMX**" must be used in case we have a liquid mixture, not a pure liquid as is the case here.

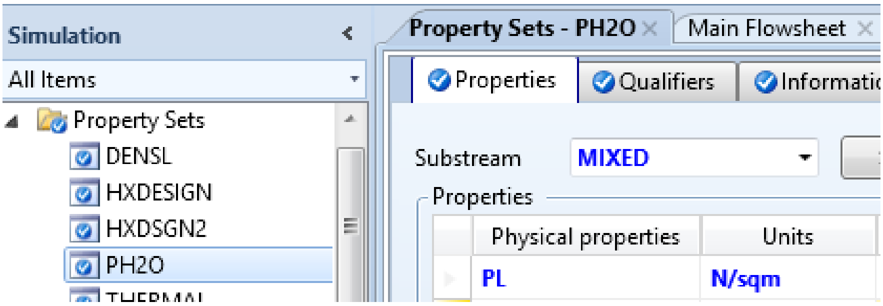


Substream: MIXED

Physical properties	Units
RHO	kg/cum

Figure 8.19 DENSL accounts for **RHO**, which is the density of a pure substance for a given stream.

The second property will be the vapor pressure of water at the given temperature as shown in Figure 8.20. Again, under "**Qualifiers**" tab, select the phase to be "*liquid*".



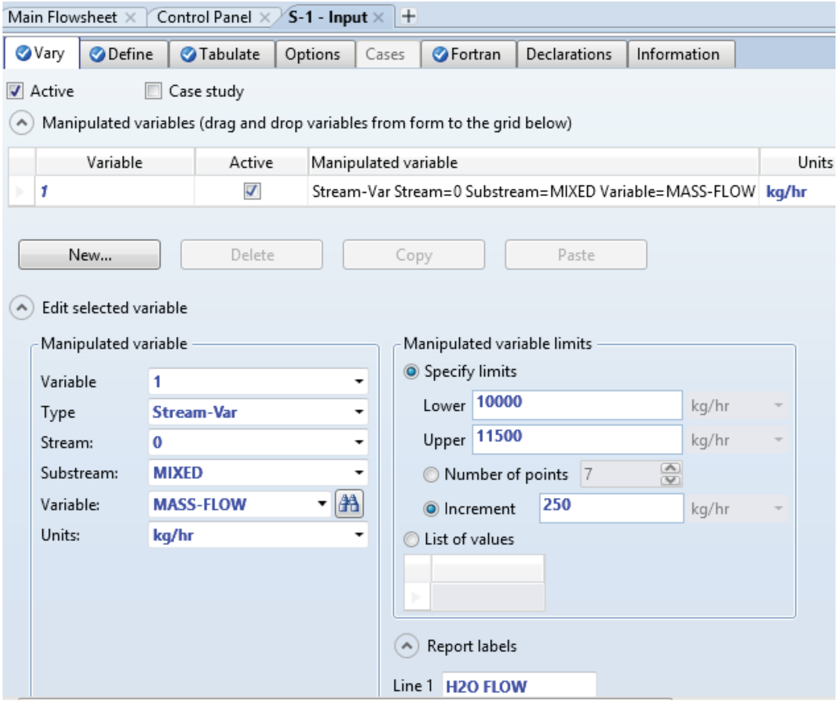
Substream: MIXED

Physical properties	Units
PL	N/sqm

Figure 8.20 "**PH2O**" accounts for "**PL**", which is the vapor pressure of water at the given temperature, for a given stream.

We would like to show here more useful calculations regarding the fluid and flow characteristics. In "**Navigation**" pane, under "**Model Analysis Tools**" folder, choose "**Sensitivity**" subfolder and click on "**New** … " button and "**Create New ID**" window will pop up with the default name "**S-1**". Click on "**OK**" button to accept the default name.

Figure 8.21 shows "**Vary**" tab window, where we define a range and increment for the mass flow rate of liquid water (i.e., **manipulated variable**). In other words, changing the mass flow rate of liquid water means changing Reynolds number, which, in turn, will affect the rest of Reynolds-dependent defined variables. Moreover, at the bottom of the window ("**Report labels**" section), the user may enter one word for each line so that it will describe the manipulated variable in the "**Results**" section.



☑ Active ☐ Case study

Manipulated variables (drag and drop variables from form to the grid below)

Variable	Active	Manipulated variable	Units
1	☑	Stream-Var Stream=0 Substream=MIXED Variable=MASS-FLOW	kg/hr

Manipulated variable

Variable: 1
Type: Stream-Var
Stream: 0
Substream: MIXED
Variable: MASS-FLOW
Units: kg/hr

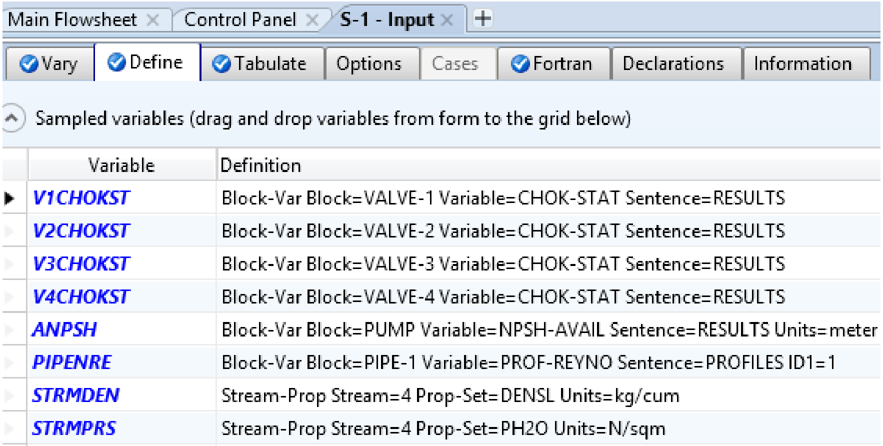
Manipulated variable limits

● Specify limits
Lower 10000 kg/hr
Upper 11500 kg/hr
○ Number of points 7
● Increment 250 kg/hr
○ List of values

Line 1 H2O FLOW

Figure 8.21 In “**Vary**” tab window, the user is required to define the manipulated variable, its range, and increment.

Figure 8.22 shows “**Define**” tab window, where we define a number of variables so that we can reference them either in “**Tabulate**” or in “**Fortran**” tab window. The variables defined here refer to a block-variable, stream-variable, or stream-property variable that refers to a previously defined property set. The defined variables will give us more insight on the nature of fluid and flow when we attempt to change the total mass flow rate of water being transported from “**TANK-1**” to “**TANK-2**”. “**V1CHOKST**” up to “**V4CHOKST**”



Sampled variables (drag and drop variables from form to the grid below)

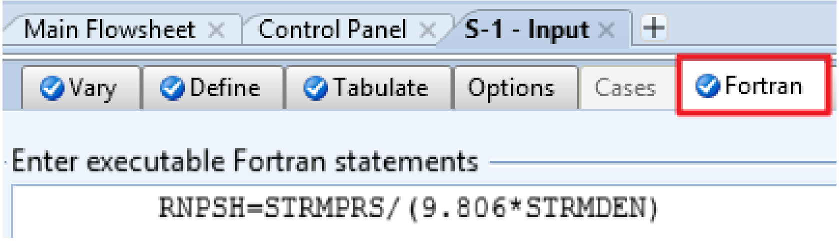
Variable	Definition
V1CHOKST	Block-Var Block=VALVE-1 Variable=CHOK-STAT Sentence=RESULTS
V2CHOKST	Block-Var Block=VALVE-2 Variable=CHOK-STAT Sentence=RESULTS
V3CHOKST	Block-Var Block=VALVE-3 Variable=CHOK-STAT Sentence=RESULTS
V4CHOKST	Block-Var Block=VALVE-4 Variable=CHOK-STAT Sentence=RESULTS
ANPSH	Block-Var Block=PUMP Variable=NPSH-AVAIL Sentence=RESULTS Units=meter
PIPENRE	Block-Var Block=PIPE-1 Variable=PROF-REYNO Sentence=PROFILES ID1=1
STRMDEN	Stream-Prop Stream=4 Prop-Set=DENSL Units=kg/cum
STRMPRS	Stream-Prop Stream=4 Prop-Set=PH2O Units=N/sqm

Figure 8.22 Defining a list of “**Sensitivity**” variables as block or stream property variable.

account for the choking status of valves 1 up to 4, respectively. “**ANPSH**” accounts for the available net positive suction head of the pump. “**PIPENRE**” accounts for Reynolds number in “**PIPE-1**”. “**STRMDEN**” accounts for the liquid density (kg/m^3) of stream “**4**”, entering the pump. Finally, “**STRMPRS**” accounts for the vapor pressure (Pa) of liquid water at the given temperature for stream “**4**” entering the pump.

We will go now to “**Fortran**” tab and be back later to “**Tabulate**” tab window. Figure 8.23 shows one line FORTRAN (**For**mula **Tran**slation) code that will evaluate the required net positive suction head (**RNPSH**).

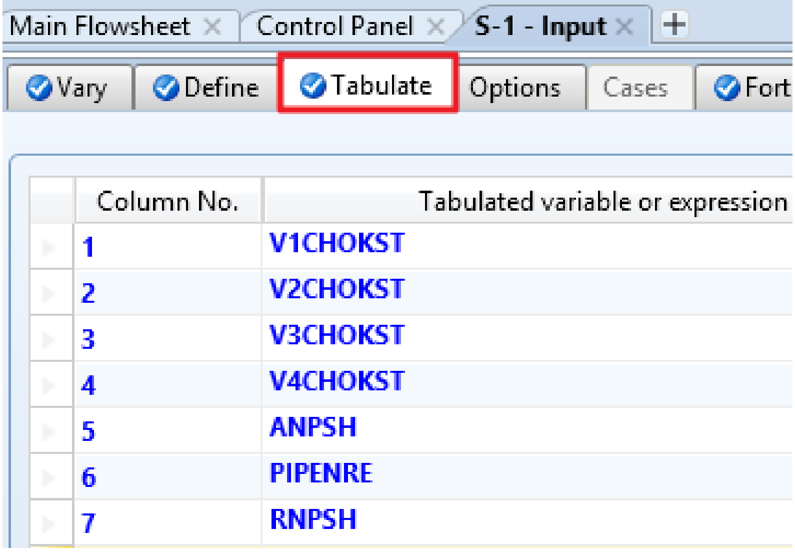
$$\text{RNPSH} = \frac{P^*_{\text{H}_2\text{O}}(T)}{\rho g}$$



```
RNPSH=STRMPRS/(9.806*STRMDEN)
```

Figure 8.23 “**Fortran**” tab window where one-line Fortran code is written to define “**RNPSH**” as a function of vapor pressure, the gravity constant, and the liquid water density.

Now, let us get back to “**Tabulate**” tab window where we decide what variables to present in the “**Results**” table. To import the list of variables, click on “**Fill Variables**” button at the bottom of “**Tabulate**” tab window. There is no need to keep “**STRMDEN**” and “**STRMPRS**” variable in the tabulated list; hence, highlight (right click on) the assigned number and select “**Delete Row**” submenu item from the context menu. On the other hand, manually enter “**RNPSH**” variable, which is defined in “**Fortran**” tab window. Figure 8.24



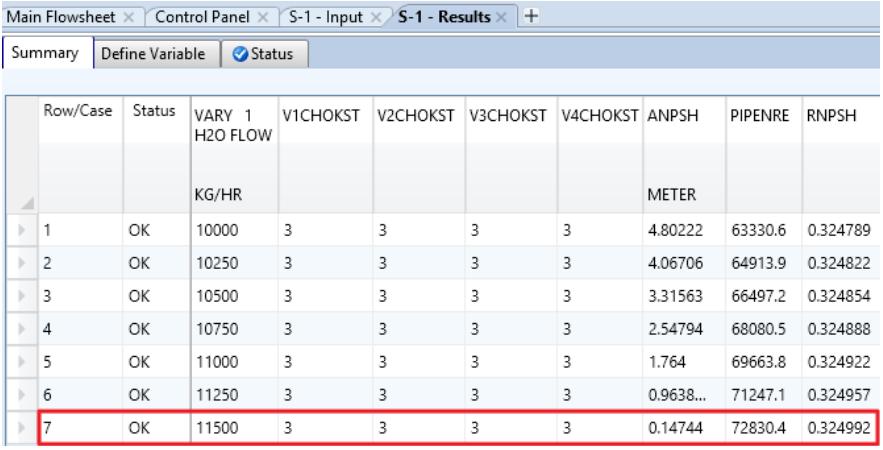
Column No.	Tabulated variable or expression
1	V1CHOKST
2	V2CHOKST
3	V3CHOKST
4	V4CHOKST
5	ANPSH
6	PIPENRE
7	RNPSH

Figure 8.24 In “**Tabulate**” tab window, the user decides what to present in the final “**Results**” table.

shows the rows that will appear as columns in “**S-1**” **Results**, after deleting “**STRMDEN**” and “**STRMPRS**” and adding “**RNPSH**” row.

Notice that the tabulated variables are either defined in “**Define**” or in “**Fortran**” tab window.

Reinitialize and run the show. Figure 8.25 shows the “**Summary**” tab sheet for tabulated columns in “**Model Analysis Tools**” | “**Sensitivity**” | “**S-1**” | “**Results**”. The number “*3*” for the valve status indicates that there is no choking condition. Although valves do not show any choking condition, nevertheless, the pump will suffer from cavitation at a water mass flow rate higher than or equal to 11,500 kg/h.

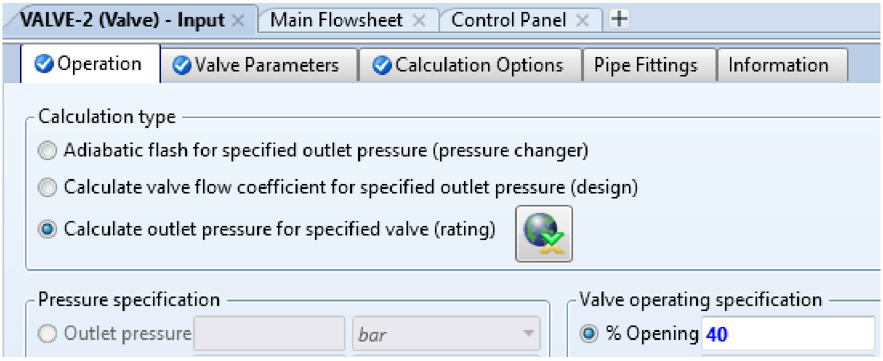


Row/Case	Status	VARY 1 H2O FLOW KG/HR	V1CHOKST	V2CHOKST	V3CHOKST	V4CHOKST	ANPSH METER	PIPENRE	RNPSH
1	OK	10000	3	3	3	3	4.80222	63330.6	0.324789
2	OK	10250	3	3	3	3	4.06706	64913.9	0.324822
3	OK	10500	3	3	3	3	3.31563	66497.2	0.324854
4	OK	10750	3	3	3	3	2.54794	68080.5	0.324888
5	OK	11000	3	3	3	3	1.764	69663.8	0.324922
6	OK	11250	3	3	3	3	0.9638...	71247.1	0.324957
7	OK	11500	3	3	3	3	0.14744	72830.4	0.324992

Figure 8.25 Values of “**S-1**” defined variables as a function of water flow rate (i.e., Reynolds number). $N_{Re} = 72{,}830$ is the minimum Reynolds number at which onset of cavitation occurs at the entrance of the pump.

Notice at a water flow rate of 11,500 kg/h ($N_{Re} = 72{,}830$) or above, **ANPSH** is less than **RNPSH**. Of course, *the higher the mass flow rate is, the worse will be the situation in terms of cavitation*. One can say that at the given operating pressure and temperature, a mass flow rate of 11,250 kg/h represents the critical value above which cavitation will occur. This means that the pump entrance is vulnerable to the phenomenon called cavitation. Cavitation means the formation of vapor (in this case water vapor) along with the liquid stream itself. Such vapor bubbles will burst at the vanes (impellers or blades) of the pump. In addition to the intermittent flow, the bursting of bubbles will cause an oscillation in pressure values and result in early wearing of pump blades. The valve choking status is fine with all four valves; there is no valve choking in any of them.

Let us impose more restriction on the fluid flow using "**VALVE-2**". Go to "**VALVE-2**" | "**Input**" | "**Operation**" tab window, change the percent opening from 50 to 40%, as shown in Figure 8.26.



Calculation type

○ Adiabatic flash for specified outlet pressure (pressure changer)

○ Calculate valve flow coefficient for specified outlet pressure (design)

● Calculate outlet pressure for specified valve (rating)

Pressure specification

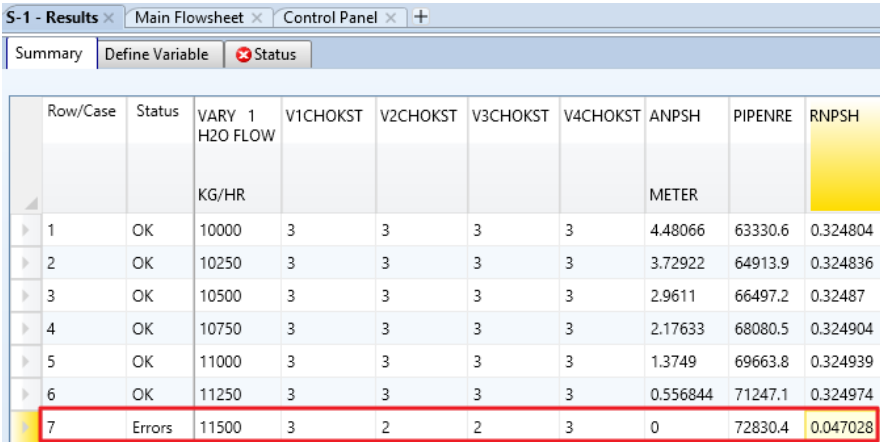
○ Outlet pressure bar

Valve operating specification

● % Opening 40

Figure 8.26 Imposing a more restriction on fluid flow by "**VALVE-2**" *via* reducing the percent opening to 40 instead of 50%.

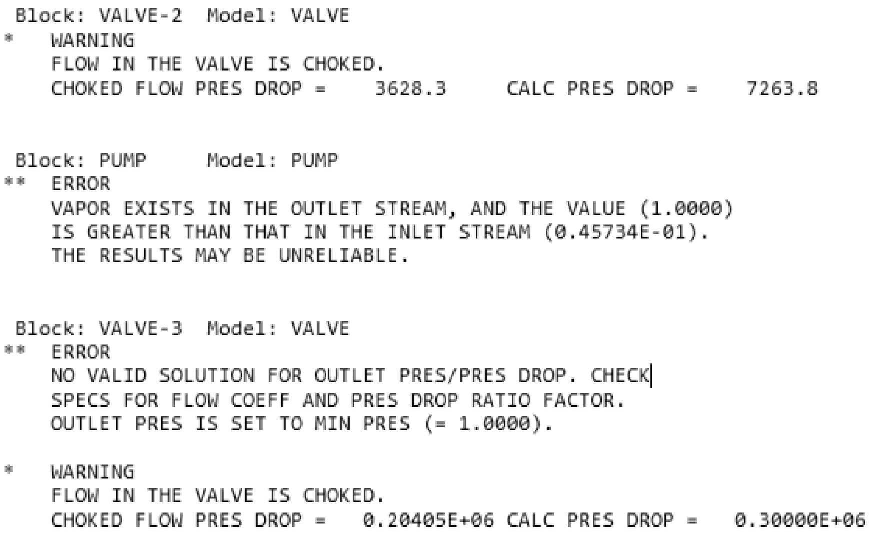
Reinitialize and run the show. Figure 8.27 shows the "**S-1**" sensitivity analysis results. Obviously, at last run, both "**VALVE-2**" and "**VALVE-3**" do suffer now from choking condition.



Row/Case	Status	VARY 1 H2O FLOW KG/HR	V1CHOKST	V2CHOKST	V3CHOKST	V4CHOKST	ANPSH METER	PIPENRE	RNPSH
1	OK	10000	3	3	3	3	4.48066	63330.6	0.324804
2	OK	10250	3	3	3	3	3.72922	64913.9	0.324836
3	OK	10500	3	3	3	3	2.9611	66497.2	0.32487
4	OK	10750	3	3	3	3	2.17633	68080.5	0.324904
5	OK	11000	3	3	3	3	1.3749	69663.8	0.324939
6	OK	11250	3	3	3	3	0.556844	71247.1	0.324974
7	Errors	11500	3	2	2	3	0	72830.4	0.047028

Figure 8.27 The choking status of both "**VALVE-2**" and "**VALVE-3**" has changed at the last run of sensitivity case study, indicating the occurrence of choking condition, whereas the first and fourth valve do not suffer from choking (i.e., cavitation).

Moreover, the "**Control Panel**" of Aspen Plus warns the user that there is a choking condition in "**VALVE-2**" and **VALVE-3** and pump cavitation, as shown in Figure 8.28.



```
 Block: VALVE-2  Model: VALVE
*   WARNING
    FLOW IN THE VALVE IS CHOKED.
    CHOKED FLOW PRES DROP =    3628.3     CALC PRES DROP =    7263.8


 Block: PUMP     Model: PUMP
**  ERROR
    VAPOR EXISTS IN THE OUTLET STREAM, AND THE VALUE (1.0000)
    IS GREATER THAN THAT IN THE INLET STREAM (0.45734E-01).
    THE RESULTS MAY BE UNRELIABLE.


 Block: VALVE-3  Model: VALVE
**  ERROR
    NO VALID SOLUTION FOR OUTLET PRES/PRES DROP. CHECK
    SPECS FOR FLOW COEFF AND PRES DROP RATIO FACTOR.
    OUTLET PRES IS SET TO MIN PRES (= 1.0000).

*   WARNING
    FLOW IN THE VALVE IS CHOKED.
    CHOKED FLOW PRES DROP =   0.20405E+06 CALC PRES DROP =   0.30000E+06
```

Figure 8.28 Aspen Plus “**Control Panel**” warns the user that the flow is choked in “**VALVE-2**” and “**VALVE-3**” and the pump also suffers from cavitation.

REFERENCES

[1] Peters and Timmerhaus (M. S. Peters and K. D. Timmerhaus) (1991) *Plant Design and Economics for Chemical Engineers*, 4 edn, McGraw-Hill, Inc., New York, USA, p. 496.

[2] AWWA (1986) *Introduction to Water Distribution*, American Water Works Association, Denver, Colo.

HOMEWORK/CLASSWORK 8.1 (PENTANE TRANSPORT)

Repeat the same task presented in the running tutorial of this chapter, but replace the *process fluid (water) by* ***n-pentane*** *(*C_5H_{12}*)*.

DO NOT FORGET TO CHANGE THE PROPERTY METHOD FROM “STEAMNBS” TO “NRTL”.

*Reset and run the simulation under “**Properties**” environment. Check “**Control Panel**” if there is any error or serious warning. Once the properties’ analysis successfully completes, switch to “**Simulation**” environment.*

*Change the pressure of “**0**” stream and the discharge pressure of “**PUMP**” such that you avoid the simulation errors (*i.e., *the problem of “negative absolute pressure and/or valve choking condition”). Check that you properly enter the “minimum” pressure requirement via reinitializing and rerunning the simulator. Assure that there are no simulation errors.*

a) The feed stream exists at temperature equal to 25°C. You need to assign a pressure value for both the feed stream and the pump exit stream (stream “**5**”). Carry out the sensitivity analysis by setting the mass flow rate range in "**Vary**" tab window (see Figure 8.21) between 9,000 and 10,000 kg/h with an increment of 100 kg/h. Report the critical mass flow rate for the onset of cavitation (i.e., **ANPSH≤RNPSH**).

b) Repeat part (a) but with a feed stream temperature equal to 36°C and see how increasing *T* will affect the minimum pressure requirement for the inlet ("**0**") stream and for pump exit stream. Keep the same mass flow rate range. Report the critical mass flow rate for the onset of cavitation (i.e., **ANPSH≤RNPSH**).

c) Repeat part (a) but with a feed stream temperature equal to 15°C and see how decreasing *T* will affect the minimum pressure requirement for the inlet ("**0**") stream and for pump exit stream. Keep the same mass flow rate range. Report the critical mass flow rate for the onset of cavitation (i.e., **ANPSH≤RNPSH**).

d) What is your conclusion about the minimum pressure requirement for the inlet ("**0**") stream and for the pump exit stream versus the operating temperature?

e) Alternatively, assign the minimum pressure requirement for the inlet ("**0**") stream and for the pump exit stream for all three cases ($T = 25$, 36, and 15°C) equal to that of the second case (i.e., $T = 36$°C). Notice here that in "**Vary**" tab window, the mass flow rate range will be different for each case. Report now the critical mass flow rate for each case (i.e., **ANPSH≤RNPSH**).

HOMEWORK/CLASSWORK 8.2 (GLYCEROL TRANSPORT)

Repeat the same task presented in the running tutorial of this chapter, but replace the process fluid *(water) by* ***glycerol****,* a highly viscous material. The temperature is 25°C.

DO NOT FORGET TO CHANGE THE PROPERTY METHOD FROM STEAMNBS TO NRTL.

*Reset and run the simulation under "**Properties**" environment. Check "**Control Panel**" if there is any error or serious warning. Once the properties' analysis successfully completes, switch to "**Simulation**" environment.*

a) Be sure that you successfully manage to run the show without having any simulation errors (i.e., the problem of negative absolute pressure and/or valve choking conditions). As you now deal with the liquid glycerol that has a viscosity three orders of magnitude larger than that of water at the same temperature, you should recall principles of fluid mechanics and assign the proper value for each of the following input parameters: the inner diameter of the pipe; the inlet stream ("**0**") pressure in; the discharge pressure of the pump; and the mass flow rate of glycerol. In other words, you should learn from this homework/classwork to answer the question: will the increase/decrease in any of the aforementioned input parameters make the flow system more/less vulnerable to negative absolute pressure and/or valve choking conditions?

b) After you reach the proper conditions in part (a), carry out the sensitivity analysis using the same list of variables in the running tutorial of this chapter (see Figure 8.22). Moreover, set the mass flow rate range in "**Vary**" tab window (see Figure 8.21) in a manner such that the upper limit just hits the condition where a simulation error starts showing up. This requires a sort of a trial-and-error approach to look for the critical mass flow rate where the simulator will not converge to a solution; that is, errors are issued by the simulator. For such a highly viscous material, does the problem have to deal with the cavitation (i.e., **ANPSH≤RNPSH**) or with something else?

HOMEWORK/CLASSWORK 8.3 (AIR COMPRESSION)

a) Choose "**Specialty Chemicals with Metric Units**" template to create a steady-state flow sheet. The property method will be set to "**PSRK**", because the applied pressure is above 10 bar. Moreover, the "**Free-water method**" should be set to "*STEAMNBS*", in "**Methods**" | "**Specifications**" |"**Global**" sheet. Reset and run the simulation in "**Properties**" environment. Check "**Control Panel**" if there is any error or serious warning. Once the properties' analysis successfully completes, switch to "**Simulation**" environment.

b) We plan to compress atmospheric air (room temperature and pressure for "**0**" inlet stream) to 50 bar at a rate of 10,000 kg/h using a multistage compressor with an interstage cooling and store the compressed air in a storage facility ("**TANK-1**") so that it can be used later, as shown in Figure 8.29.

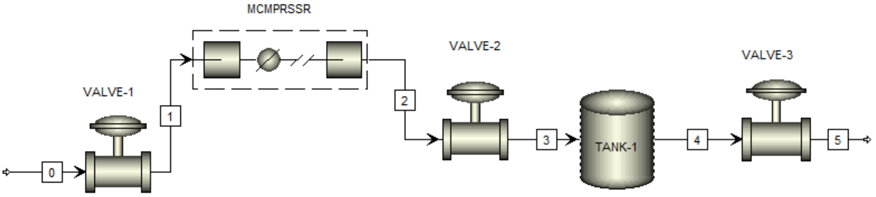


Figure 8.29 Compression and storage of air.

c) Use Equation 8.1 to find the optimum diameter and select the closest nominal pipe size.

d) For "**VALVE-1**" and "**VALVE-2**", the outlet pressure will be calculated with "**% Opening**" equal to "*50%*". Both are selected as "*Butterfly*" type, "*Neles-Jamesbury*" manufacturer, "*Ans_Class_300* series", and the size will be the closest nominal pipe size that you find in part (c).

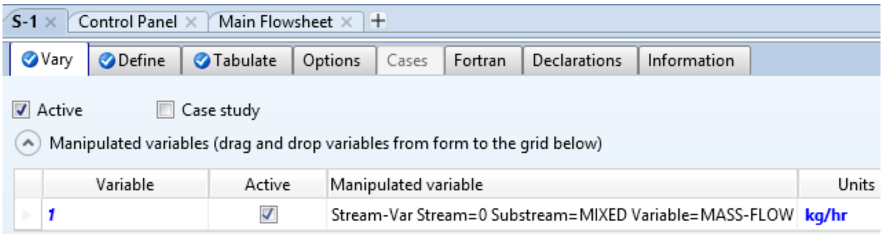
e) For "**VALVE-3**", the valve flow coefficient will be calculated for the specified outlet pressure: 10 bar. It is selected as "*Ball*" type, "*Neles-Jamesbury*" manufacturer, "*Metal_Seated_Full_Port*" series, and the size will be the closest nominal pipe size that you find in part (c).

f) For the multicompressor, four stages will be used with a fixed discharge pressure from last stage equal to 50 bar. For "**Cooler**" tab window, set the "*duty*" to be "*−0.34 Gcal/hr*" for each stage.

g) Be sure that you successfully manage to run the show without having any simulation errors (i.e., the problem of negative absolute pressure and/or valve choking conditions).

h) If you set the outlet pressure from "**VALVE-3**" to 3 instead of 10 bar, what will happen to the flow condition across the valve?

i) With an outlet pressure of 10 bar from "**VALVE-3**", carry out a sensitivity analysis (named "**S-1**") by defining the following manipulated variable in "**Vary**" tab window and as shown in Figure 8.30. Decide on the lower, upper, and the increment for the air mass flow rate.



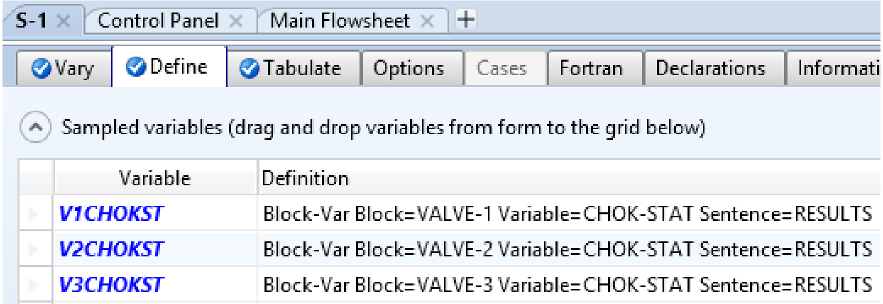
☑ Active ☐ Case study

Manipulated variables (drag and drop variables from form to the grid below)

Variable	Active	Manipulated variable	Units
1	☑	Stream-Var Stream=0 Substream=MIXED Variable=MASS-FLOW	kg/hr

Figure 8.30 The manipulated variable is defined in "**Vary**" tab window for "**S-1**" case study.

j) Define the list of variables shown in Figure 8.31.



Sampled variables (drag and drop variables from form to the grid below)

Variable	Definition
V1CHOKST	Block-Var Block=VALVE-1 Variable=CHOK-STAT Sentence=RESULTS
V2CHOKST	Block-Var Block=VALVE-2 Variable=CHOK-STAT Sentence=RESULTS
V3CHOKST	Block-Var Block=VALVE-3 Variable=CHOK-STAT Sentence=RESULTS

Figure 8.31 The defined variables that account for the choking status of the three valves.

k) You job is to find the upper limit that just hits the condition where a simulation error starts showing up. This requires a sort of a trial-and-error approach to look for the critical mass flow rate where the simulator will not converge to a solution; that is, errors are issued by the simulator. Which of the valves will exhibit choking a condition (or a choked flow), first?

l) Increase/decrease the percent opening of one of the valves and see how it affects the upper limit where a choking condition occurs.

9

THE OPTIMIZATION TOOL

9.1 PROBLEM DESCRIPTION: DEFINING THE OBJECTIVE FUNCTION

As quoted from Peters and Timmerhaus [1]: “Piping is a major item in the cost of chemical process plants. These costs in a fluid-process plant can run as high as 80% of the purchased equipment cost or 20% of the fixed capital investment”. The diameter of the pipe strongly influences the present value of the plant, through both the annual cost of electric power and the installation cost of the piping system (pipe, pumps, valves, etc.). We have used the equation given by Peter and Timmerhaus [1] in Chapter 8 (Eq. 8.1) to find the optimum pipe diameter under turbulent flow. In this chapter, we expand the work and give a more precise and detailed model on how to find the optimum diameter under turbulent condition. Genić *et al*. [2] gave a more detailed model and we present the set of equations here. The total annual pipe cost consists of two parameters: the annual fixed cost and the annual operational cost. The most economic pipe diameter will be the one that gives the lowest annual cost. In Genić *et al*.’s [2] approach, the cost of a pump is considered to be independent of the diameter D. The annual fixed cost ($/year) of a pipeline is given by

$$C_F = XD^xL(1 + F)(a + b) \tag{9.1}$$

where F is the factor that includes the cost of valves, fittings, and erection; a is the amortization or capital charge (annual); and b presents the maintenance costs (annual). D and L represent the pipe diameter (m) and length (m), respectively. According to 2015 prices, for carbon steel pipes $X = 124.6 \times (1.03)^{(2015-2008)} = 153.2$, $x = 1.472$, and $F = 6.5$. $a = b = 0.1$. Equation 9.1 becomes

$$C_F\,(\$/\text{year}) = 153.2 \times D^{1.472}L(1 + 6.5)(0.1 + 0.1) = 229.8 \times D^{1.472}L \tag{9.2}$$

Aspen Plus®: Chemical Engineering Applications, First Edition. Kamal I.M. Al-Malah.

Companion Website: www.wiley.com/go/Al-Malah/AspenPlusApplications

The annual operational cost of a pipeline is

$$C_{\mathrm{O}}(\$/\mathrm{year}) = 8 \times \frac{YC_{\mathrm{en}}(1+J)\xi L}{\pi^2 ED^5} \times \frac{\dot{m}^3}{\rho^2} \tag{9.3}$$

where

C_{en}: cost of pumping energy (0.072 \$/(kW·h));
E: the pump overall efficiency (dimensionless) = 0.5;
J: Ratio of minor pressure losses to friction pressure drop (dimensionless) = 0.5;
$\dot{m}$: the mass flow rate of an incompressible fluid (kg/s);
Y: the plant attainment (h/year) = 365 × 24 = 8760 h/year;
ξ: the friction factor (dimensionless) $= M\left(\frac{\varepsilon}{D}\right)^m = 0.11\left(\frac{\varepsilon}{D}\right)^{0.25}$;
ρ: The fluid density (kg/m^3).

Thus, Equation 9.3 becomes

$$\begin{aligned} C_{\mathrm{O}} &= 8 \times \frac{YC_{\mathrm{en}}(1+J)\xi L}{\pi^2 ED^5} \times \frac{\dot{m}^3}{\rho^2} = 8 \times \frac{8760 \times 0.072(1+0.5) \times 0.11(\varepsilon/D)^{0.25} L}{\pi^2 \times 0.5 \times D^5} \times \frac{\dot{m}^3}{\rho^2} \\ &= 168.71 \times \frac{(\varepsilon/D)^{0.25} L}{D^5} \times \frac{\dot{m}^3}{\rho^2} \end{aligned} \tag{9.4}$$

The total annual cost (\$/year) will be the sum of the annual fixed and operational cost:

$$C_{\mathrm{T}}(\$/\mathrm{year}) = C_{\mathrm{F}} + C_{\mathrm{O}} = 229.8 \times D^{1.472} L + 168.71 \times \frac{(\varepsilon/D)^{0.25} L}{D^5} \times \frac{\dot{m}^3}{\rho^2} \tag{9.5}$$

In order to show how to set up the objective function that should be either minimized or maximized, we use C_{T} as the objective function, which shall be minimized in this case.

NOTE #1: *The price factor X is time- and material-dependent adjustable parameter. The energy cost factor C_{en} is also a time-dependent adjustable parameter. Other factors can be scaled up or down in light of the type of chemical industry being handled.*

9.2 THE PROPERTY METHOD: “STEAMNBS”

Choose “**Specialty Chemicals with Metric Units**” template to create a steady-state flowsheet. Set the property method to “**STEAMNBS**”. See Section 8.2 for justification of “**STEAMNBS**” property method selection. Also, see Figure 8.1 for the “**Global**” tab window where the user enters the property method more than once.

Give a title for the project and add water as the only component. Click “**Reset**” followed by “**Next**” button to run the simulation and assure that properties’ analysis completed successfully. Switch to “**Simulation**” environment.

9.3 A FLOWSHEET FOR WATER TRANSPORT

Figure 9.1 shows that water is brought to "**TANK-1**" from an external source, and it will be transported to "**TANK-2**" via means of a pump and connecting pipe, which is 2000 m long.

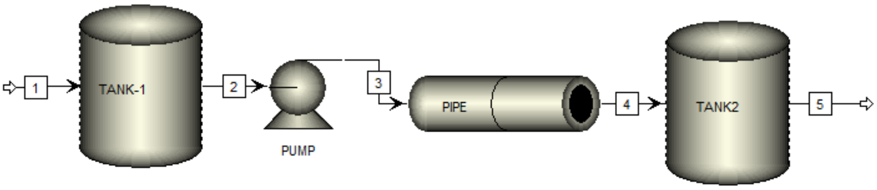
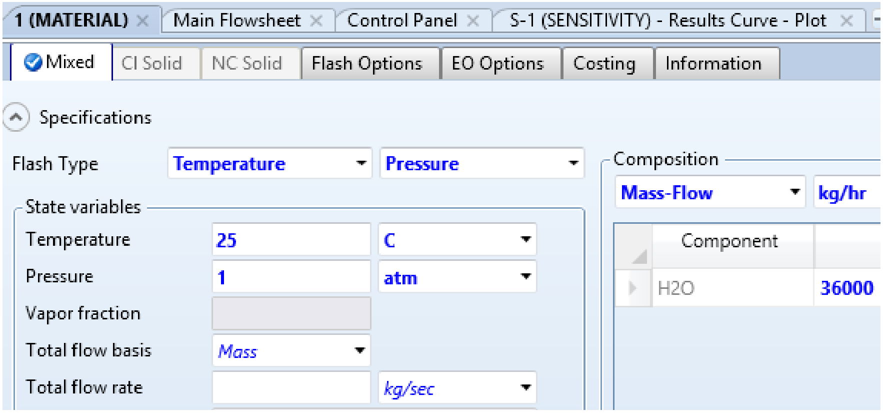


Figure 9.1 The flowsheet for water transport between two tanks that are 2000 m apart.

9.4 ENTERING STREAM, PUMP, AND PIPE SPECIFICATIONS

For components, enter "**WATER**" and choose "*STEAMNBS*" for the "**Property method**".

The following figures show specifications entered for the inlet stream, the first tank, the pump, and the pipe. Figure 9.2 shows P, T, and mass flow rate of water to the first tank.



Flash Type: Temperature, Pressure

State variables

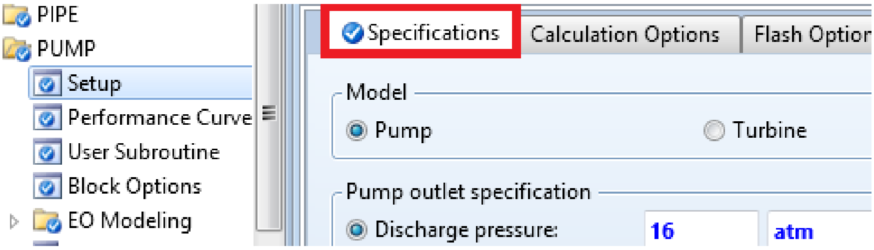
Temperature	25	C
Pressure	1	atm
Vapor fraction		
Total flow basis	Mass	
Total flow rate		kg/sec

Composition: Mass-Flow, kg/hr

Component	
H2O	36000

Figure 9.2 Input parameters for the inlet stream.

Figure 9.3 shows the specifications for the pump where the discharge pressure is assigned a value of 16 atm. Now this value should be adjusted in a way to avoid any sort of a simulation error, such as a negative absolute pressure, cavitation, or valve choking condition anywhere within the pipe or at the exit of the pipe. See Chapter 8 for such flow-related simulation errors.



Model

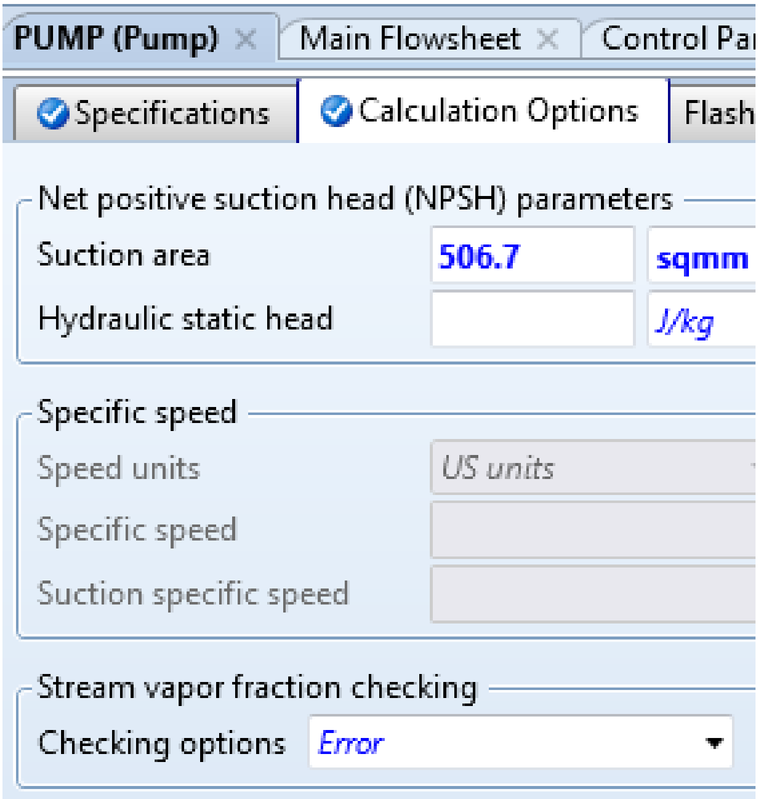
● Pump ○ Turbine

Pump outlet specification

● Discharge pressure: 16 atm

Figure 9.3 The discharge pressure is assigned a value of 16 atm to avoid any flow-related simulation errors, such as a negative absolute pressure, cavitation, or valve choking condition.

Figure 9.4 shows "**Calculation Options**" tab window for the pump, where we enter the suction area and select "**Checking options**" to be "*error*" for "**Stream vapor fraction checking**" item; the latter option means an error message will show up in "**Control Panel**" if vapor exists in the suction stream.



Net positive suction head (NPSH) parameters

Suction area 506.7 sqmm

Hydraulic static head J/kg

Specific speed

Speed units US units

Specific speed

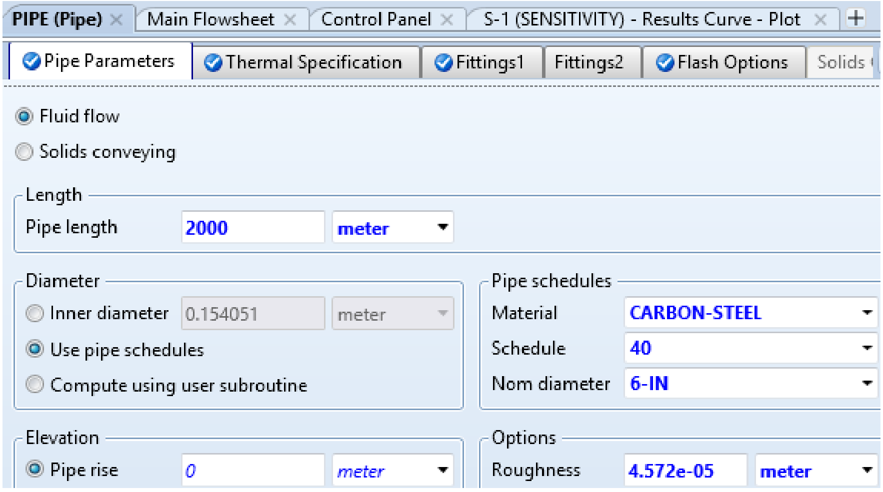
Suction specific speed

Stream vapor fraction checking

Checking options Error

Figure 9.4 In pump "**Calculation Options**" tab window, the "**Suction area**" and "**Checking options**" are specified.

Figure 9.5 shows the pipe parameters, such as the material of construction (i.e., carbon steel), its length, and its nominal diameter.



● Fluid flow
○ Solids conveying

Length
Pipe length 2000 meter

Diameter
○ Inner diameter 0.154051 meter
● Use pipe schedules
○ Compute using user subroutine

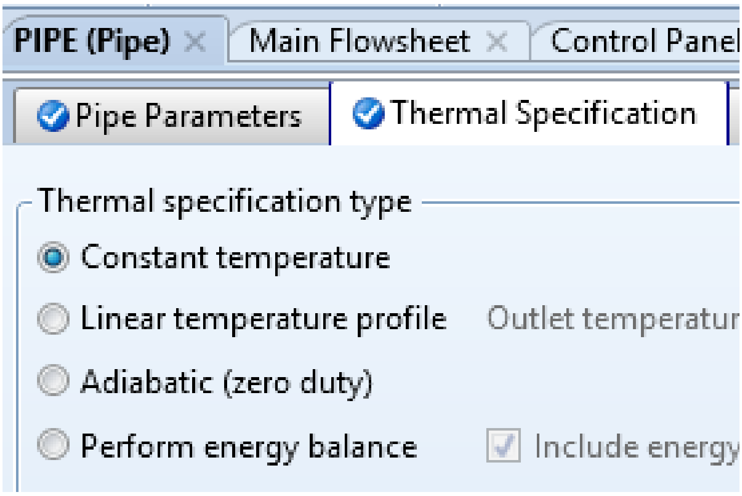
Pipe schedules
Material CARBON-STEEL
Schedule 40
Nom diameter 6-IN

Elevation
● Pipe rise 0 meter

Options
Roughness 4.572e-05 meter

Figure 9.5 Material of construction, length, and diameter for "**PIPE**" block.

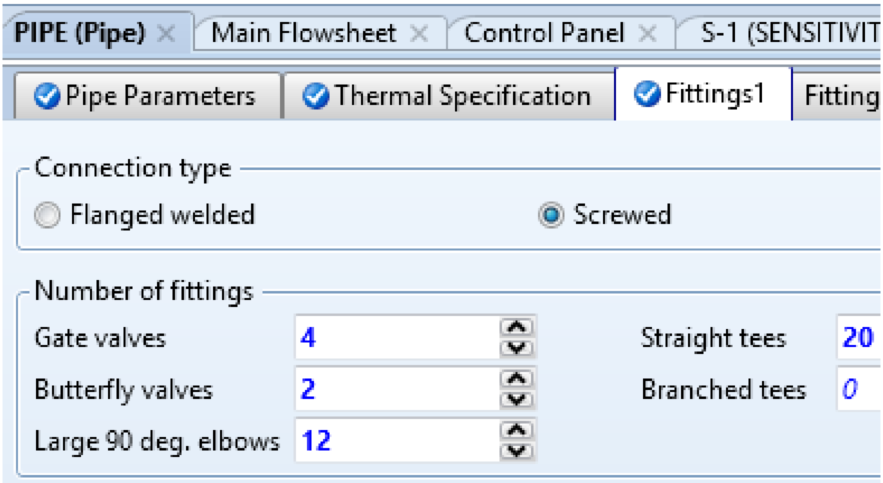
Figure 9.6 shows the thermal specification type. Here, a constant temperature profile is assumed.



Thermal specification type
● Constant temperature
○ Linear temperature profile Outlet temperatur
○ Adiabatic (zero duty)
○ Perform energy balance ☑ Include energy

Figure 9.6 "**Thermal Specification**" tab window for "**PIPE**" block. A constant temperature profile is selected.

Figure 9.7 shows the types of fittings installed on the pipe under "**Fittings1**" tab.



Connection type

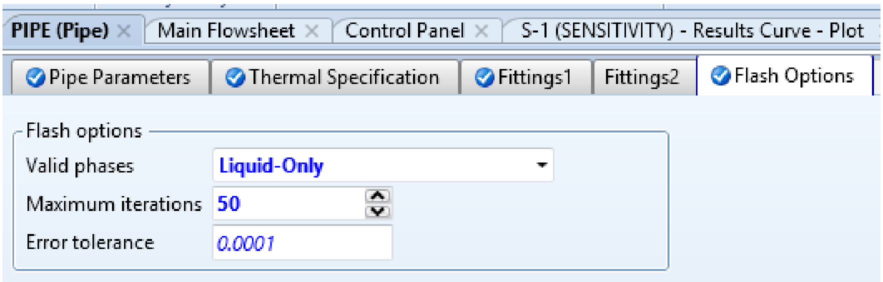
○ Flanged welded
● Screwed

Number of fittings

Gate valves 4
Butterfly valves 2
Large 90 deg. elbows 12
Straight tees 20
Branched tees 0

Figure 9.7 Different pipe fittings are installed along the pipeline.

To avoid redundant calculations and save Aspen Plus® and ourselves the extra headache of flash calculations, one single phase, that is, liquid phase is assumed throughout the entire pipe at room temperature and pressure, as shown in Figure 9.8.



Flash options

Valid phases Liquid-Only
Maximum iterations 50
Error tolerance 0.0001

Figure 9.8 For flash options, a single liquid phase is assumed prevailing within the pipe.

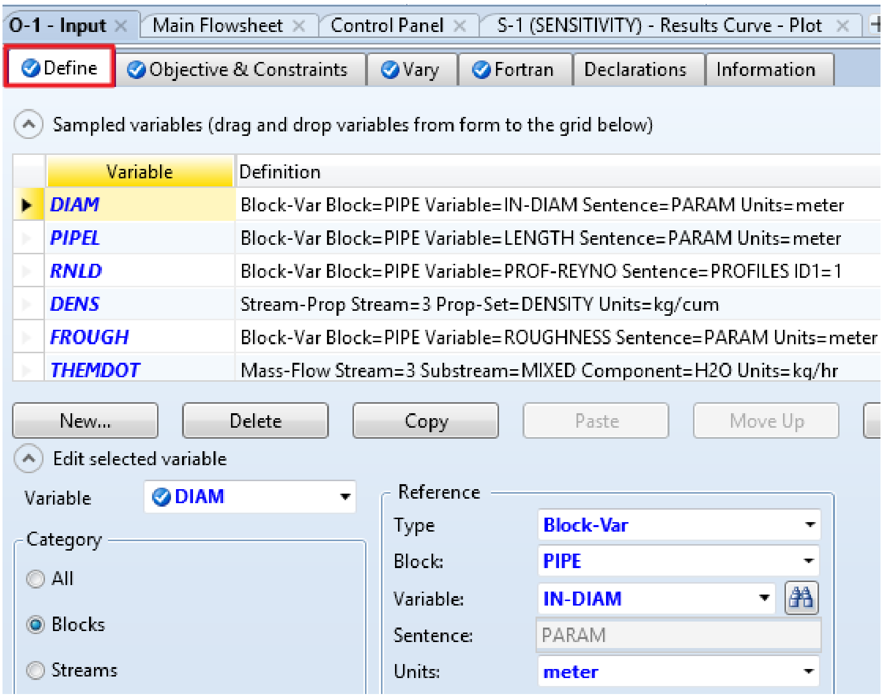
Reset and run the show. Check for any error or serious warning.

> **<u>NOTE #2:</u>** *Regarding the selection of a pipe diameter, we have chosen that to be 6 inches; however, the optimization tool that we plan to carry out in the next section will help us decide what the optimum diameter will be based on minimizing the objective function that accounts for the total annual cost.*

9.5 MODEL ANALYSIS TOOLS: THE OPTIMIZATION TOOL

You may run the simulator with the previous settings; however, we would like to show more useful calculations regarding the optimum pipe diameter. In "**Navigation**" pane, under “**Model Analysis Tools**” | “**Optimization**” subfolder, click on “**New …** ” button, and “**Create new ID**” window will pop up with the default name “**O-1**”. Click on “**OK**” button to accept the default name.

Here, we define a list of variables so that we can reference them in “**Fortran**” tab window. Figure 9.9 shows the list of defined variables. “**DIAM**” accounts for the inside pipe diameter (m); “**PIPEL**” for pipe length (m); “**RNLD**” for Reynolds number; “**DENS**” for a property set of the liquid density (kg/m^3) of stream “**3**”; “**FROUGH**” is the absolute roughness factor (m) of “**PIPE**” block; and “**THEMDOT**” is water mass flow rate in (kg/h). Notice that defining each of the previous variables is straightforward, except for “**DENS**” where the user has to define ahead a property set under “**Property Sets**” folder that is found in “**Navigation**” pane, as shown in Figure 9.10. Do not forget to select liquid phase under “**Qualifiers**” tab, as shown in Figure 9.10.

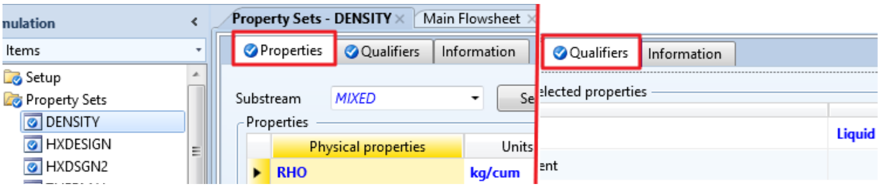


Variable	Definition
DIAM	Block-Var Block=PIPE Variable=IN-DIAM Sentence=PARAM Units=meter
PIPEL	Block-Var Block=PIPE Variable=LENGTH Sentence=PARAM Units=meter
RNLD	Block-Var Block=PIPE Variable=PROF-REYNO Sentence=PROFILES ID1=1
DENS	Stream-Prop Stream=3 Prop-Set=DENSITY Units=kg/cum
FROUGH	Block-Var Block=PIPE Variable=ROUGHNESS Sentence=PARAM Units=meter
THEMDOT	Mass-Flow Stream=3 Substream=MIXED Component=H2O Units=kg/hr

Variable: DIAM

Type: Block-Var
Block: PIPE
Variable: IN-DIAM
Sentence: PARAM
Units: meter

Figure 9.9 Defining a list of variables to be exploited later in “**Optimization**” tool under “**Fortran**” tab, where the objective function will be formulated.

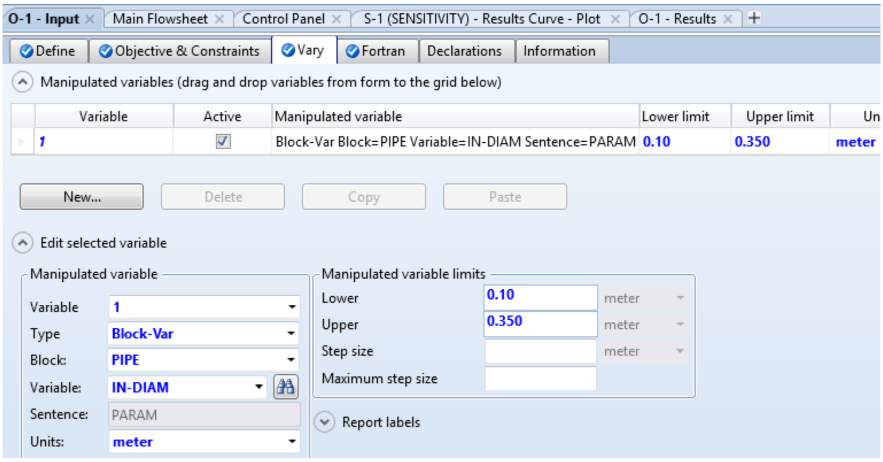


Substream: MIXED

Physical properties	Units
RHO	kg/cum

Figure 9.10 Defining a property set called “**DENSITY**” that accounts for the density of a pure liquid phase for a given stream. Here, we have only pure water.

Click “**Vary**” tab to define the range for this independent variable. Figure 9.11 shows “**Vary**” tab window, where a range is defined for the pipe diameter. The lower and upper limits of the manipulated variable can be adjusted in a manner to avoid simulation errors. For example, if you assign a very small value for the lower limit of a pipe diameter, then you try to push the fluid in a very narrow channel, which will result in a huge fluid velocity that decreases the static pressure of the fluid itself, according to Bernoulli’s equation, and results in cavitation or even a negative absolute pressure.



Manipulated variables (drag and drop variables from form to the grid below)

	Variable	Active	Manipulated variable	Lower limit	Upper limit	Un
	1	☑	Block-Var Block=PIPE Variable=IN-DIAM Sentence=PARAM	0.10	0.350	meter

Edit selected variable

Manipulated variable

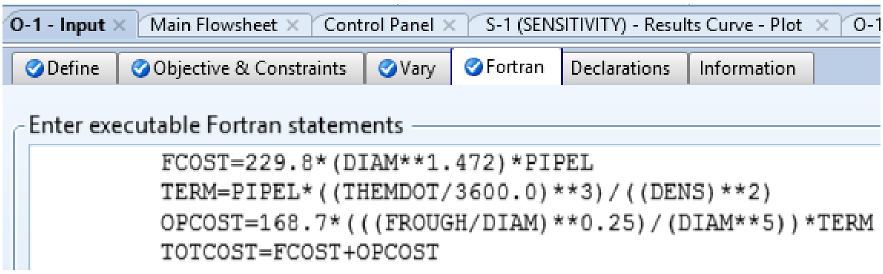
Variable 1
Type Block-Var
Block: PIPE
Variable: IN-DIAM
Sentence: PARAM
Units: meter

Manipulated variable limits

Lower 0.10 meter
Upper 0.350 meter
Step size meter
Maximum step size

Figure 9.11 The manipulated (independent) variable is entered in “**Vary**” tab window where the user is required to define the independent variable and its range.

We will go now to “**Fortran**” tab window and be back later to “**Objective & Constraints**” tab window. Figure 9.12 shows the set of executable FORTRAN commands or expressions that, upon execution, will evaluate the objective function (named “**TOTCOST**”), which is the summation of installed and operating cost (see Eq. 9.5). See **NOTE #4** later in this chapter explaining why we divided “**THEMDOT**” by *3600*.

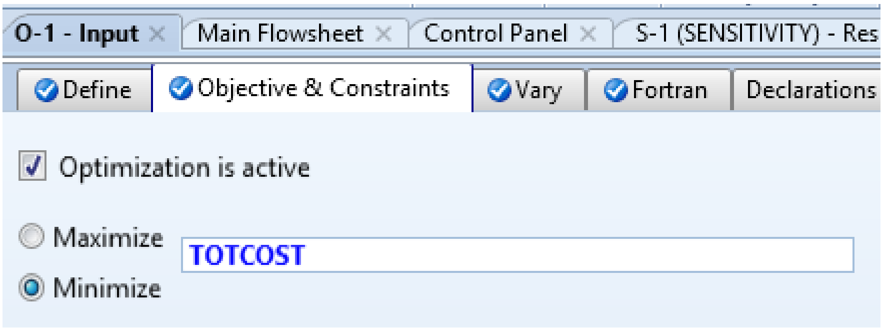


Enter executable Fortran statements

```
      FCOST=229.8*(DIAM**1.472)*PIPEL
      TERM=PIPEL*((THEMDOT/3600.0)**3)/((DENS)**2)
      OPCOST=168.7*(((FROUGH/DIAM)**0.25)/(DIAM**5))*TERM
      TOTCOST=FCOST+OPCOST
```

Figure 9.12 The set of FORTRAN commands written to evaluate the objective function (named “**TOTCOST**”), which is the summation of installed and operating cost (Eq. 9.5).

Now, let us get back to “**Objective & Constraints**” tab window where we decide what the objective function is and if there is any constraint imposed upon the objective function itself. Figure 9.13 shows the "**Objective & Constraints**" tab window. Here, the variable "**TOTCOST**", defined in "**Fortran**" tab window, will be the objective function to be minimized. There will be no constraints imposed on the boundaries of the manipulated variable. In fact, the range defined in "**Vary**" tab window will tell the optimizer where to look at the critical (optimal) diameter such that "**TOTCOST**" will be a local minimum.



☑ Optimization is active

○ Maximize

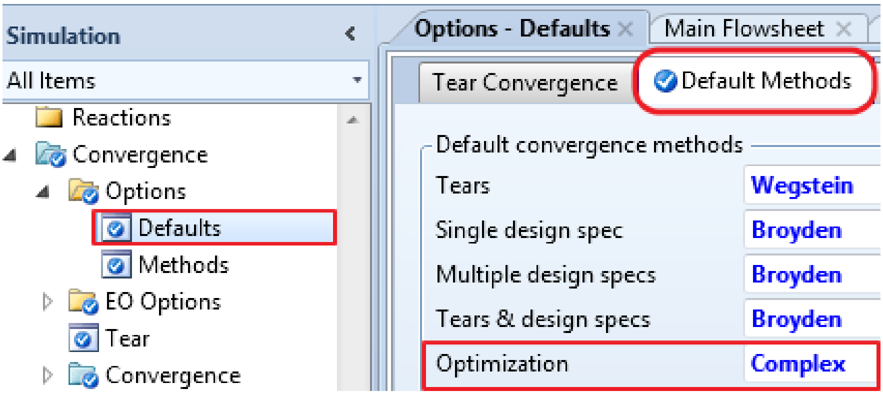
● Minimize

TOTCOST

Figure 9.13 In "**Objective & Constraints**" tab window, the user names the objective function to be either minimized or maximized.

> **NOTE #3:** *One more important thing, that is, the default convergence method assigned to optimization algorithm. By default, Aspen Plus assigns* ***S****uccessive* ***Q****uadratic* ***P****rogramming ("****SQP****") algorithm to solve small or large-scale optimization problems. Replace the default method by "****Complex****" method. The reason for this replacement is discussed at the end of this chapter. The "****Complex****" method is useful in optimization problems with bounds on the manipulated variables and, optionally, inequality constraints. "****Complex****" method is a direct search method; it does not require numerical derivatives. "****Complex****" method may be useful for simple problems without recycle loops or equality constraints (design specifications).*

To replace the default ("*SQP*") method by "*Complex*" method go to "**Convergence**" | "**Options**" | "**Defaults**" | "**Default Methods**" tab window, as shown in Figure 9.14.



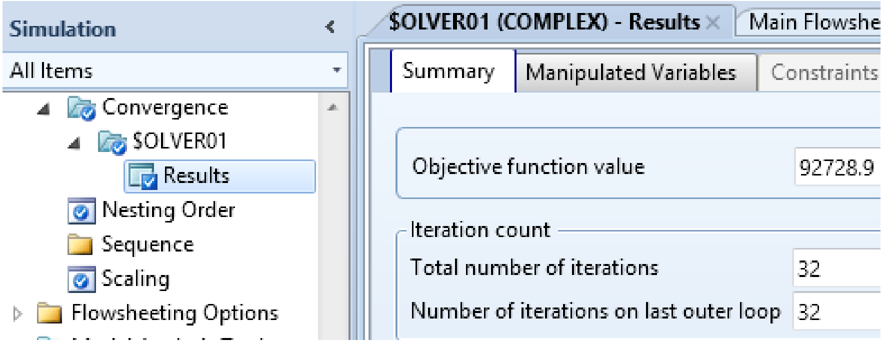
Default convergence methods

Tears	Wegstein
Single design spec	Broyden
Multiple design specs	Broyden
Tears & design specs	Broyden
Optimization	Complex

Figure 9.14 Replacement of the default ("*SQP*") convergence method by the "*Complex*" method.

Reinitialize and run the show. Watch out for any error or serious warning in "**Control Panel**".

The results of optimization are shown in Figures 9.15 and 9.16. Figure 9.15 shows the minimum total annual cost of $92,729/year, evaluated at the optimum diameter.



Objective function value 92728.9

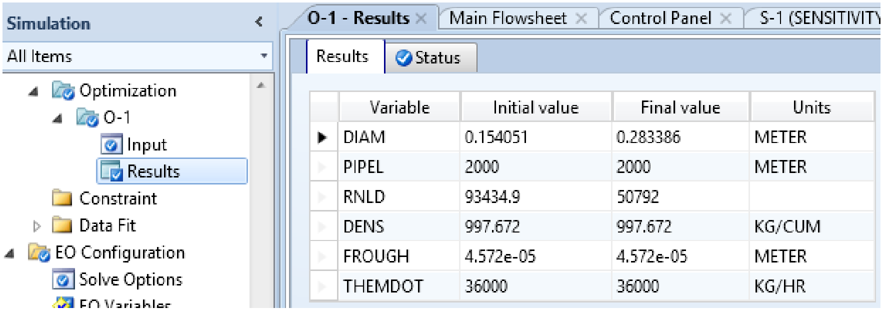
Iteration count

Total number of iterations 32

Number of iterations on last outer loop 32

Figure 9.15 The minimum total annual cost of $92,729/year, evaluated at the optimum diameter.

Figure 9.16 shows the initial and final values for each variable defined in the optimization list "**O-1**". Notice that the optimum diameter is reported as 283.4 mm, which amounts to 11.16 inches (nominal 12″).

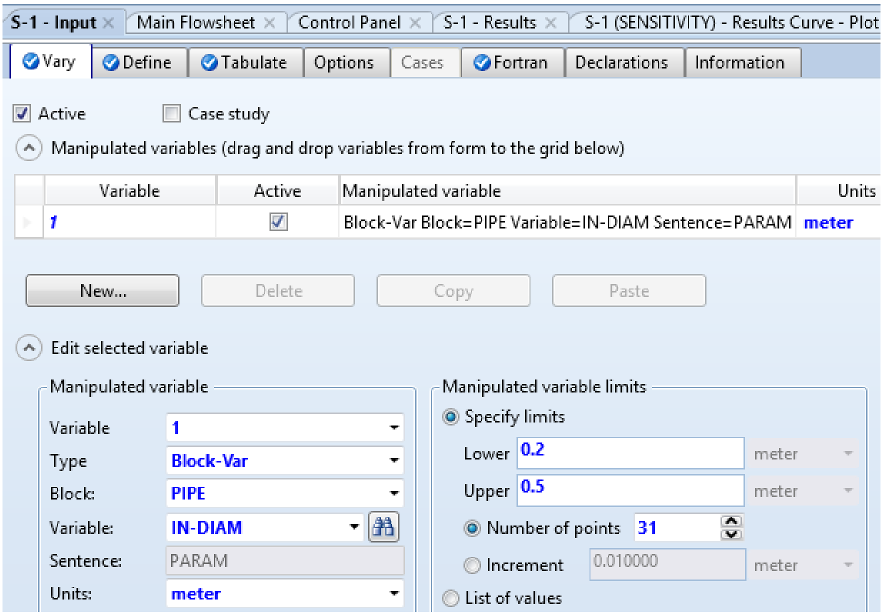


Variable	Initial value	Final value	Units
DIAM	0.154051	0.283386	METER
PIPEL	2000	2000	METER
RNLD	93434.9	50792	
DENS	997.672	997.672	KG/CUM
FROUGH	4.572e-05	4.572e-05	METER
THEMDOT	36000	36000	KG/HR

Figure 9.16 The optimum inside pipe diameter, reported by Aspen Plus, is 283.4 mm or 11.16 inches.

9.6 MODEL ANALYSIS TOOLS: THE SENSITIVITY TOOL

In addition to the optimization case study, a sensitivity analysis can be carried out using the same notion of optimization. Create "**S-1**" as a new sensitivity set under "**Model Analysis Tools**" | "**Sensitivity**" subfolder. The same list that was defined earlier in Figure 9.8 can be now copied by highlighting one line at a time or all lines together, then use "**Copy**" button at the bottom of the same window (i.e., "**Define**" tab window of "**O-1**" set). Go to "**Define**" tab window of "**S-1**" set, and use "**Paste**" button found at the bottom of the active window, saving the user the time and effort needed to redefine them. The manipulated variable under “**Vary**” tab window of “**O-1**” set can be also copied to that of “**S-1**” set; nevertheless, the lower and upper limits are modified to avoid simulation errors and make the cost plot a more plausible, without really affecting the heart of sensitivity analysis, as shown in Figure 9.17.



☑ Active ☐ Case study

Variable	Active	Manipulated variable	Units
1	☑	Block-Var Block=PIPE Variable=IN-DIAM Sentence=PARAM	meter

Variable: 1
Type: Block-Var
Block: PIPE
Variable: IN-DIAM
Sentence: PARAM
Units: meter

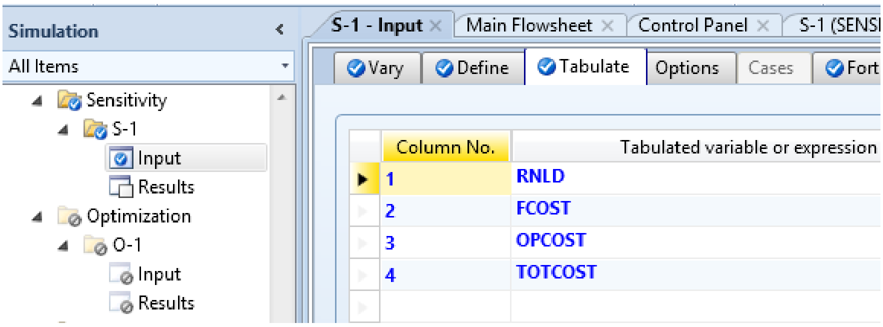
● Specify limits
Lower: 0.2 meter
Upper: 0.5 meter
● Number of points: 31
○ Increment: 0.010000 meter
○ List of values

Figure 9.17 The manipulated variable of “**S-1**” set is essentially the same as that of “**O-1**”, except for the modification of both lower and upper limit.

In “**Fortran**” tab window, the same set of FORTRAN code will be borrowed from that of “**O-1**” set (see Figure 9.12).

NOTE #4: *Always watch out how Aspen Plus defines a property. For example, “**THEMDOT**” is defined as the water mass flow rate in stream “**3**”, expressed in kg/h in both “**O-1** and “**S-1**” set. This explains why we divided by the conversion factor to convert **THEMDOT** into kg/s. Alternatively, you may select to express “**THEMDOT**” in kg/s, instead of kg/h.*

The “**Tabulate**” tab window of “**S-1**” set is shown in Figure 9.18. The total, operational, and fixed annual cost will be shown as a function of pipe diameter. The Reynolds number is used as indicator for the user that whether or not the prevailing flow regime is turbulent.

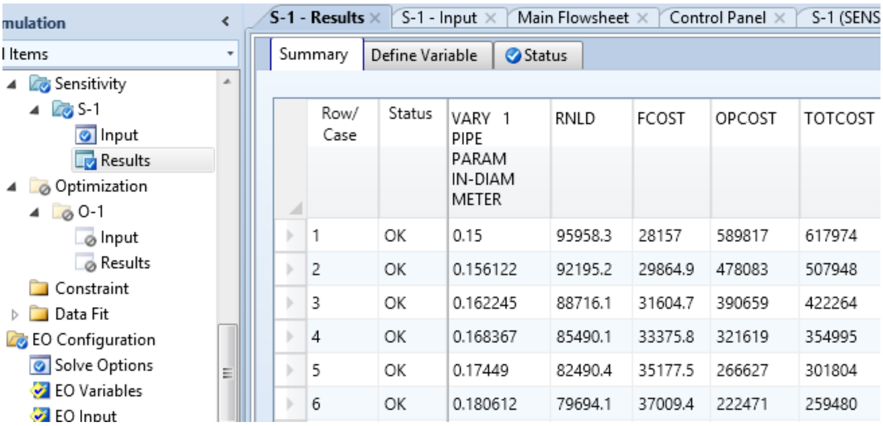


Column No.	Tabulated variable or expression
1	RNLD
2	FCOST
3	OPCOST
4	TOTCOST

Figure 9.18 Tabulation of “**RNLD**”, “**FCOST**”, “**OPCOST**”, and “**TOTCOST**” as a function of pipe diameter “**DIAM**”. “**RNLD**” is used to tell the flow regime.

> <u>**NOTE #5:**</u> *If an attempt is made to simultaneously run both model analysis tools: the optimization and sensitivity, then annoying simulation warnings (or even errors) may develop and show up in “**Control Panel**”. To avoid this situation, deactivate the optimization case study via right clicking on “**O-1**” set and selecting “**Deactivate**” command from the shortcut context menu. Doing this will make your life easier.*

Figure 9.19 shows a portion of sensitivity results where the cost data are shown for each examined diameter. To gain a better insight and while the “**S-1**” | “**Results**” | “**Summary**” tab window <u>is still active</u>, go to “**Plot**” tab found in “**Home**” ribbon and click on “**Results Curve**” button to activate the plot features of Aspen Plus. Follow the instructions on how to generate a plot for the cost data as a function of pipe diameter.



Row/ Case	Status	VARY 1 PIPE PARAM IN-DIAM METER	RNLD	FCOST	OPCOST	TOTCOST
1	OK	0.15	95958.3	28157	589817	617974
2	OK	0.156122	92195.2	29864.9	478083	507948
3	OK	0.162245	88716.1	31604.7	390659	422264
4	OK	0.168367	85490.1	33375.8	321619	354995
5	OK	0.17449	82490.4	35177.5	266627	301804
6	OK	0.180612	79694.1	37009.4	222471	259480

Figure 9.19 A portion of the results for the sensitivity analysis “**S-1**”. Notice that “**O-1**” optimization case study is deactivated.

Figure 9.20 shows the plot for the three annual cost indices as a function of inside pipe diameter.

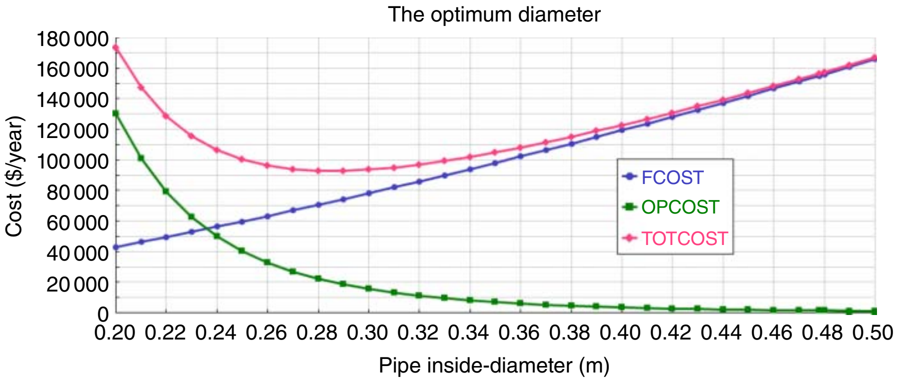


Figure 9.20 The plot of three annual cost indices as a function of the inside pipe diameter (m). The minimum lies at $D = 283.4$ mm (11.16″) with a total annual cost of \$92,729/year, as was found in optimization "**O-1**" case study.

9.7 LAST COMMENTS

1. If we look at Equation 9.5, we will realize that it is highly non-linear in *D*, and this may result, in general, in more than one local minimum. In other words, from convergence criterion point of view, if the function topology exhibits a valley more than once over a wide range of *D*, then the optimization method may report more than a local minimum, depending on the starting diameter range that is assigned by the user to search for the minimum diameter. In fact, I have used Aspen Plus to run the optimization problem but with the default (**SQP**) method and the simulator converged to different local minima. "**SQP**"-based optimization algorithm may converge to a local minimum and it gets stuck over there. On the other hand, "**Complex**"-based optimization algorithm shows a global minimum over different starting diameter ranges.
2. The optimum diameter value itself may vary from one model to another, depending on the set of factors to be accounted for in the fixed or operational cost, in addition to quantifying the role each factor contributes to the overall picture. The reported value here (283.4 mm, or 11.16″) is larger than that given by Peters *et al.* [3]. For our case (i.e., $Q = 0.01\ \mathrm{m^3/s}$ that is equivalent to 10 kg/s or 36,000 kg/h), the value of the optimum diameter will be

$$D_{\mathrm{i,opt}} = 0.363 \times Q^{0.45} \times \rho^{0.13} = 0.363 \times 0.01^{0.45} \times 997.7^{0.13} = 0.112\,\mathrm{m}$$
$$= 112\,\mathrm{mm} = 4.41\,\mathrm{in.}$$

3. I referred back to Genić *et al.*'s [2] article and found that they gave a straight equation (eq. 23 in their article) for calculating the optimum *D* for a rough pipe as

$$D_{\mathrm{rpf}} = 0.665\left[\frac{(1+J)YC_{\mathrm{en}}}{XxE(1+F)(a+b)} \times \frac{G^3}{\rho^2}\right]^{1/6.722}$$
$$= 0.665\left[\frac{(1+0.5)8760 \times 0.072}{153.2 \times 1.472 \times 0.5(1+6.5)(0.1+0.1)} \times \frac{10^3}{997.7^2}\right]^{1/6.722}$$

$$D_{\text{rpf}} = 0.665\left[\frac{946.08}{169.13} \times \frac{10^3}{997.7^2}\right]^{1/6.722}$$

$$= 0.665 \times [0.0056196]^{0.148765} = 0.3076\,\text{m} = 12.1''$$

The last answer is even slightly larger than the value of 0.2834 m, reported by Aspen Plus.

REFERENCES

[1] Peters, M.S. and Timmerhaus, K.D. (1991) *Plant Design and Economics for Chemical Engineers*, 4th edn, McGraw-Hill, New York, p. 496.

[2] Genić, S.B., Jaćimović, B.M., and Genić, V.B. (2012) Economic optimization of pipe diameter for complete turbulence. *Energy and Buildings*, **45**, 335–338.

[3] Peters, M.S., Timmerhaus, K.D., and West, R.E. (2003) *Plant Design and Economics for Chemical Engineers*, 5th edn, McGraw-Hill, New York, p. 501.

HOMEWORK/CLASSWORK 9.1 (SWAMEE–JAIN EQUATION)

The Swamee–Jain equation, which is used to directly solve for the Darcy–Weisbach friction factor f for a fully developed flow in a circular pipe and is thus an approximation of the implicit Colebrook–White equation, gives the friction faction f as

$$f = \frac{0.25}{\left[\log_{10}\left(\frac{\varepsilon}{3.7D} + \frac{5.74}{N_{\text{Re}}^{0.9}}\right)\right]^2} \tag{9.6}$$

f, Darcy's friction factor, is exactly equal to ξ in Equation 9.4. Rerun both optimization and sensitivity studies while replacing the dimensionless friction factor ξ in Equation 9.4, using that given by Equation 9.6. Rewrite the code in "**Fortran**" tab window in line with the new definition of friction factor as shown earlier. Report the value of optimum D. Is it equal to or different from $D_{\text{Optimum}} = 0.2834$ m?

HOMEWORK/CLASSWORK 9.2 (A SIMPLIFIED PIPE DIAMETER OPTIMIZATION)

Given that the objective function:

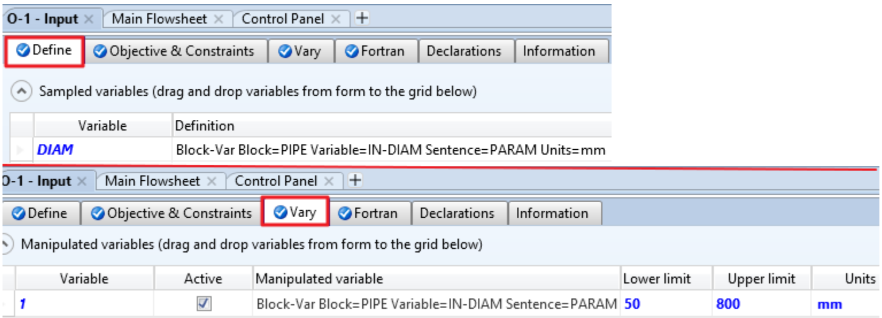
$$f(D) = 1000.0 \times D + \frac{10^{17}}{D^5} \qquad D\ [\text{mm}]$$

a) Solve analytically and find the optimum diameter that will minimize *f(D)*. Check that it is minimum not maximum via the sign of the second derivative of *f(D)*.

b) Using the same flowsheet shown in Figure 9.1, use Aspen Plus optimization tool to find the optimum D that will minimize the total cost as in the following FORTRAN code:

```
FCOST=1000.0*DIAM
OPCOST=(10.0**17)/(DIAM**5)
TOTCOST=FCOST+OPCOST
```

where the pipe diameter will be the defined (i.e., “**DIAM**”) and also the manipulated (i.e., “**Variable**” *1*) variable, as shown in Figure 9.21. Verify that the answer here and that in “Part a” are the same.



Sampled variables (drag and drop variables from form to the grid below)

Variable	Definition
DIAM	Block-Var Block=PIPE Variable=IN-DIAM Sentence=PARAM Units=mm

Manipulated variables (drag and drop variables from form to the grid below)

Variable	Active	Manipulated variable	Lower limit	Upper limit	Units
1	☑	Block-Var Block=PIPE Variable=IN-DIAM Sentence=PARAM	50	800	mm

Figure 9.21 The inside pipe diameter is defined as “**DIAM**” variable in “**Define**” tab window (*top*) and as the manipulated variable in “**Vary**” tab window (*bottom*) for a typical optimization case study.

HOMEWORK/CLASSWORK 9.3 (THE OPTIMUM DIAMETER FOR A VISCOUS FLOW)

Replace water by glycerol as the process fluid. Glycerol is a highly viscous material compared with water. It has a viscosity of 866 cP at room temperature, which is about three orders of magnitude larger than that of water.

Since the prevailing flow regime will be laminar, here is the FORTRAN code to use in defining the friction factor under laminar and turbulent region.

```
IF (RNLD .LE. 2100) THEN
 FRIC =64/RNLD
 ELSE IF (RNLD .GT. 2100) THEN
 ARGTRM=FROUGH/(3.7*DIAM)+5.74/(RNLD**0.9)
 FRIC=0.25/(DLOG10(ARGTRM))**2
 END IF
 FCOST=216.6*(DIAM**1.472)*PIPEL
 TERM=PIPEL*((THEMDOT)**3)/((DENS)**2)
 OPCOST=1533.7*(FRIC/(DIAM**5))*TERM
 TOTCOST=FCOST+OPCOST
```

See Figure 9.9 for deciphering the legend of such terms. You may have to multiply/divide "**THEMDOT**" term by a conversion factor, depending on how Aspen Plus defines it for you. With a pump discharge pressure of 16 atm and a flow rate of 36,000 kg/h (10 kg/s) of glycerol, carry out both sensitivity and optimization analyses and find the optimum diameter that will minimize the total annual cost for the process. Adjust the pipe diameter and the pipe diameter range in "**Vary**" tab window under both analyses such that you avoid any simulation errors (i.e., a negative absolute pressure). Show a plot for the annual cost indices as a function of pipe diameter.

HOMEWORK/CLASSWORK 9.4 (THE SELECTIVITY OF PARALLEL REACTIONS)

Consider the following process flowsheet (Figure 9.22) that represents "**RGibbs**"-type reactor, where two simultaneous gas-phase reactions take place. The two reactions exist under equilibrium condition (i.e., no need for kinetic data).

$$\text{Toluene} + H_2 \leftrightarrow \text{Benzene} + CH_4 \qquad \text{(Desired)} \tag{9.7}$$

$$2\ \text{Benzene} \leftrightarrow \text{Diphenyl} + H_2 \qquad \text{(Undesired)} \tag{9.8}$$

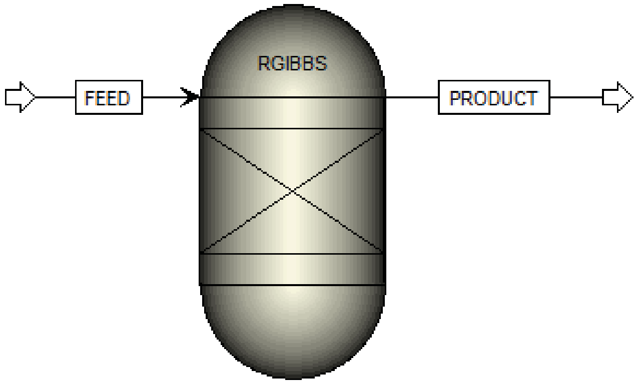
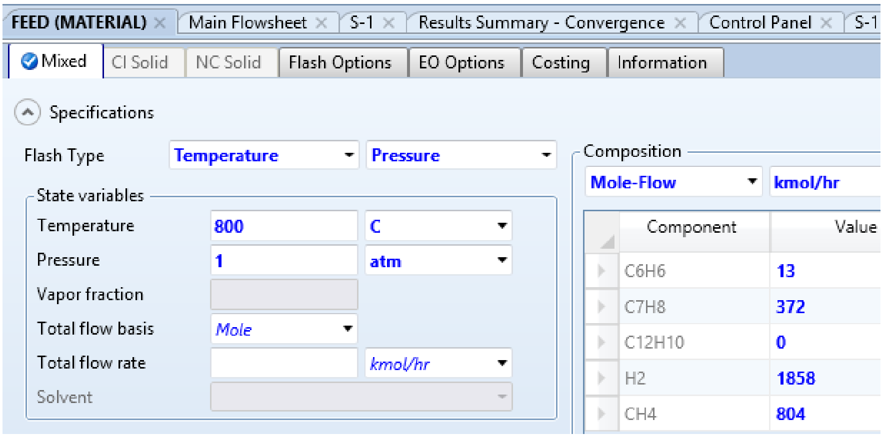


Figure 9.22 The "**RGibbs**"-type reactor where two simultaneous gas-phase equilibrium reactions occur.

Our mission is to maximize the production of benzene and minimize the formation of diphenyl for the following feed composition, as shown in Figure 9.23:



Flash Type: Temperature, Pressure

Temperature: 800 C

Pressure: 1 atm

Vapor fraction:

Total flow basis: Mole

Total flow rate: kmol/hr

Solvent:

Composition: Mole-Flow, kmol/hr

Component	Value
C6H6	13
C7H8	372
C12H10	0
H2	1858
CH4	804

Figure 9.23 The feed compositional flow rate, pressure, and temperature.

Create both sensitivity and optimization analysis to find the optimum pressure and temperature, which will maximize the selectivity defined as BOVERDP = (YBENZ/YDP), where "**YBENZ**" and "**YDP**", respectively, represent the benzene and diphenyl mole fraction in the product stream. Notice that "**BOVERDP**" should be defined in "**Fortran**" tab window and both "**YBENZ**" and "**YDP**" in "**Define**" tab window of both analyses. In sensitivity analysis, allow both pressure and temperature of "**RGibbs**" block to vary between 1 and 20 bar for pressure and 800 and 1000°C for temperature. Choose the proper increment for both. After finding the best value of pressure, allow only the temperature to change in optimization analysis. For the given feed composition, report the best values of *P* and *T*, which will maximize benzene over diphenyl production.

10

HEAT EXCHANGER (H.E.) DESIGN

10.1 PROBLEM DESCRIPTION

Freon-12 (R-12), at a flow rate of 12,000 kg/h, is to be heated from 250 to 300 K. Ethylene glycol (EG) is available at 370 K. A typical shell and tube heat exchanger will be used. The plant engineer recommends that the minimum temperature approach should be at least 15 K. She/he also recommends using 20 BWG carbon-steel tubing with a pressure drop not exceeding 5 psi (0.34 atm) for either the shell or tube side (see Figure 10.1).

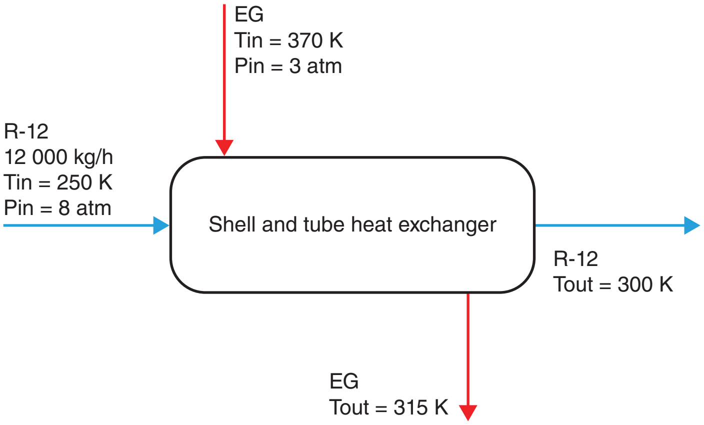


Figure 10.1 A schematic for shell and tube heat exchanger to cool ethylene glycol (**EG**) using Freon-12 (**R-12**).

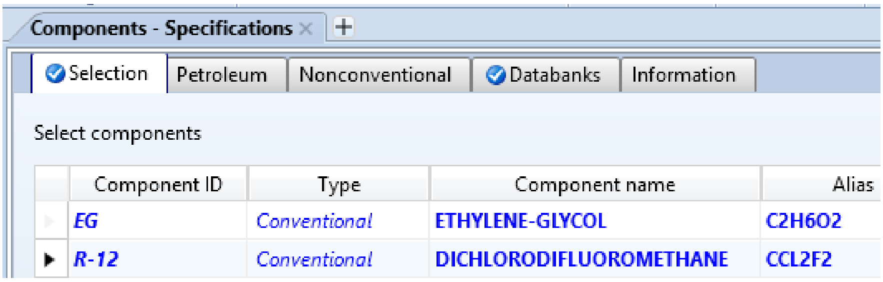
This chapter guides you through the procedure necessary to design a shell and tube heat exchanger unit using Aspen Plus®. It also includes recommendations for the design process.

Aspen Plus®: Chemical Engineering Applications, First Edition. Kamal I.M. Al-Malah.

Companion Website: www.wiley.com/go/Al-Malah/AspenPlusApplications

10.2 TYPES OF HEAT EXCHANGER MODELS IN ASPEN PLUS

Using Aspen Plus, choose “**Specialty Chemicals with Metric Units**” template to create the process flow sheet. The default property model will be “**NRTL**”. Add the two components, ethylene glycol (EG) and dichlorodifluoromethane (R-12), as shown in Figure 10.2.



Select components

Component ID	Type	Component name	Alias
EG	Conventional	ETHYLENE-GLYCOL	C2H6O2
R-12	Conventional	DICHLORODIFLUOROMETHANE	CCL2F2

Figure 10.2 Adding **EG** ($C_2H_6O_2$) and **R-12** (CCl_2F_2) to “**Components**” list.

To avoid annoying warnings, you may go to “**Methods**” | “**Parameters**” | “**Binary Interaction**” | “**NRTL-1**” sheet and ensure that the “*Estimate missing parameters by UNIFAC*” option is selected. Click “**Reset**” followed by “**Next**” button to run the simulation and assure that properties analysis completed successfully. Switch to “**Simulation**” environment.

Figure 10.3 shows the “**Exchangers**” tab in “**Model Palette**”. It shows the four options of a heat exchanger type. These represent four different calculation models, not physically different heat exchangers.

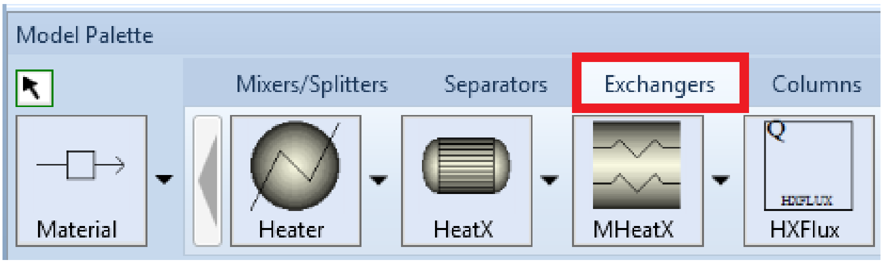


Figure 10.3 Different options (i.e., models) for a heat exchanger type.

The description of each item is quoted from Aspen Plus built-in help.

1. “**Heater**”: The basic heat exchanger model that performs simple energy balance calculations; it requires only one process stream. You can use “**Heater**” to represent heaters, coolers, valves, pumps (whenever work-related results are not needed), and compressors (whenever work-related results are not needed). You can also use “**Heater**” to set the thermodynamic condition of a stream. When the user specifies the outlet conditions, “**Heater**” will determine the

thermal and phase conditions of a mixture with one or more inlet streams. *This block will be initially used in this running tutorial for calculating the heat duty, which will then be used to calculate heat-transfer area requirement*.

2. "**HeatX**": The fundamental heat exchanger model that is used in a rigorous design; it will calculate energy balance, pressure drop, exchanger area, velocities, and so on and requires two process streams: hot and cold. "**HeatX**" can model a wide variety of shell and tube heat exchanger types and perform heat transfer related tasks, including
   a) countercurrent and co-current exchangers
   b) TEMA E, F, G, H, I/J, K, X shells (see Figure 10.19), and double pipe and multi-tube exchangers
   c) bare, low-finned, and longitudinal-finned tubes exchangers
   d) single and double segmental baffles, rod baffles, and unbaffled exchangers
   e) "**HeatX**" will perform the required calculations (all combinations of a single-phase boiling or condensing heat transfer, with associated pressure drop calculations), returning key calculation results to be viewed within Aspen Plus.
   f) perform mechanical vibration and Rhov2 (ρv^2) analysis
   g) estimate maximum fouling
   h) display setting plan and tube-sheet layout drawing.

   "**HeatX**" can perform a full zone analysis with heat transfer coefficient and pressure drop estimation for single- and two-phase streams. For rigorous heat transfer and pressure drop calculations, you must supply the exchanger geometry. If exchanger geometry is unknown or unimportant, "**HeatX**" can perform simplified shortcut rating calculations. For example, you may want to perform only heat and material balance calculations. "**HeatX**" has correlations to estimate sensible heat, nucleate boiling, and condensation film coefficients. "**HeatX**" uses a rigorous heat exchanger program to perform these calculations. Available programs include "*Shell&Tube*", "*AirCooled*", and "*Plate*". Collectively, these programs are referred to as Aspen Exchanger Design and Rating (EDR). *This block will be used in this running tutorial for design calculations*.

NOTE #1: *The version V7.1 was the last version of Aspen Plus to support the legacy heat exchanger programs: Aspen TASC, Aspen Hetran, and Aspen Aerotran. You should upgrade old simulations to "Shell&Tube" and "AirCooled".*

3. "**MHeatX**": As its name tells, a multi-heat-exchanger model can be used to represent heat transfer between multiple hot and cold streams, as in an LNG exchanger, for example. "**MHeatX**" can perform a detailed and rigorous internal zone analysis to determine the internal pinch points and heating and cooling curves for all streams in the heat exchanger. "**MHeatX**" can also calculate, UA, the multiplication of the overall heat transfer coefficient by the area, for the exchanger and model heat leak to or from an exchanger. "**MHeatX**" uses multiple heater blocks and heat streams to enhance flowsheet convergence. Aspen Plus automatically sequences block and stream convergence unless you specify a sequence or tear stream.
4. "**HXFlux**": A heat exchanger model that is used to perform heat transfer calculations between a heat sink and a heat source, using convective heat transfer and does not

> require any input or output material stream; nevertheless, you may add heat streams to substitute the heat exchange duty. The driving force for the convective heat transfer is calculated as a function of log-mean temperature difference (LMTD). The user has to specify all variables, except one, among inlet and outlet stream temperatures, duty, heat transfer coefficient, and heat transfer area. "**HXFlux**" calculates the unknown variable and determines the LMTD, using either the rigorous or the approximate method.

For the sake of calculating the heat duty that will be used to calculate the area requirement, let us use the first type, that is, "**Heater**".

10.3 THE SIMPLE HEAT EXCHANGER MODEL ("HEATER")

As a preliminary step, we will add the first type of heat exchangers (i.e., "**Heater**") to the flowsheet just to calculate the amount of heat (heat duty), which will then enable us to calculate the area available for heat transfer using the "**HeatX**" model, where the latter is more fundamental than the former primitive type.

Figure 10.4 shows the insertion of "**Heater**" type heat exchanger to simply calculate the heat duty, Q. Freon-12 stream is simply chosen because it is well defined in terms of the flow rate and operating conditions.

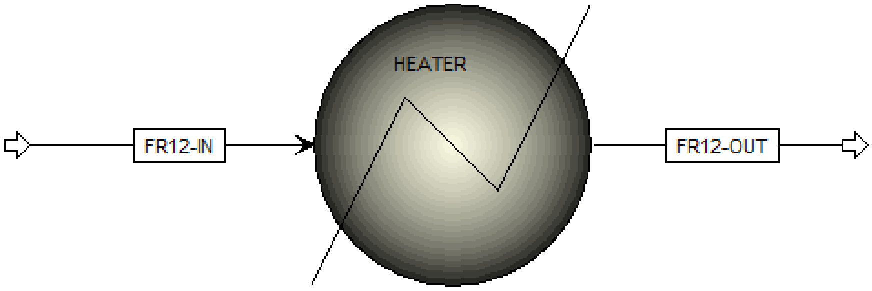
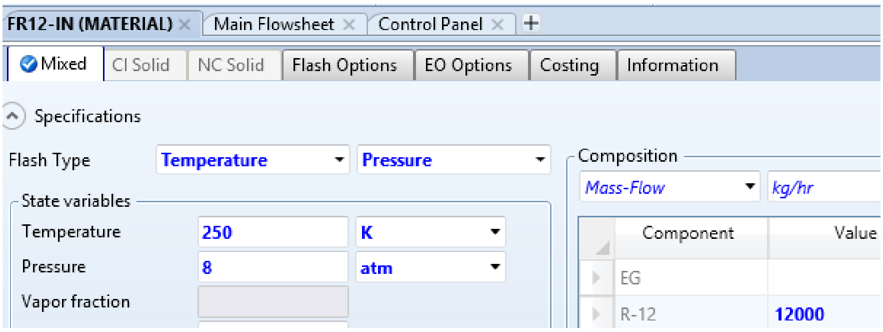


Figure 10.4 Addition of "**Heater**" type heat exchanger for the sake of calculating the heat duty, Q.

Figure 10.5 shows the specifications of Freon-12 inlet stream.



Flash Type: Temperature | Pressure

State variables

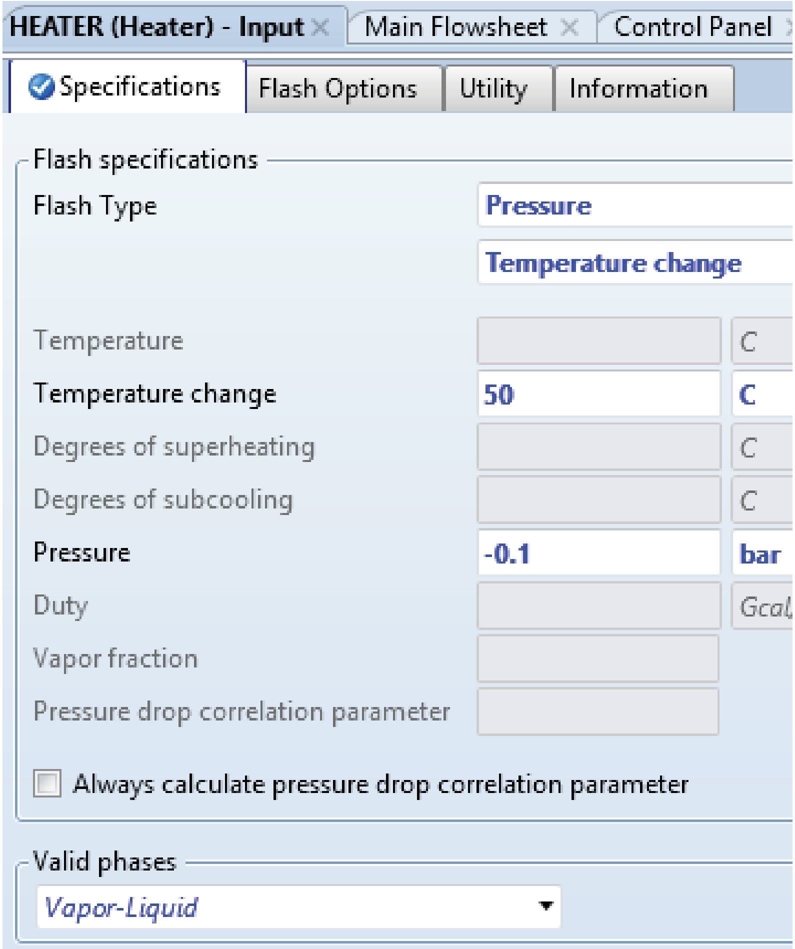
Temperature	250	K
Pressure	8	atm
Vapor fraction		

Composition: Mass-Flow | kg/hr

Component	Value
EG	
R-12	12000

Figure 10.5 Entering the specifications of “**FR12-IN**” stream.

Figure 10.6 shows that we have entered the pressure drop (−0.1 bar) and temperature change (300 K − 250 K = 50 K = 50°C). For pressure, you have two options. You can key



Flash specifications

Flash Type: Pressure | Temperature change

Temperature		C
Temperature change	50	C
Degrees of superheating		C
Degrees of subcooling		C
Pressure	-0.1	bar
Duty		Gcal
Vapor fraction		
Pressure drop correlation parameter		

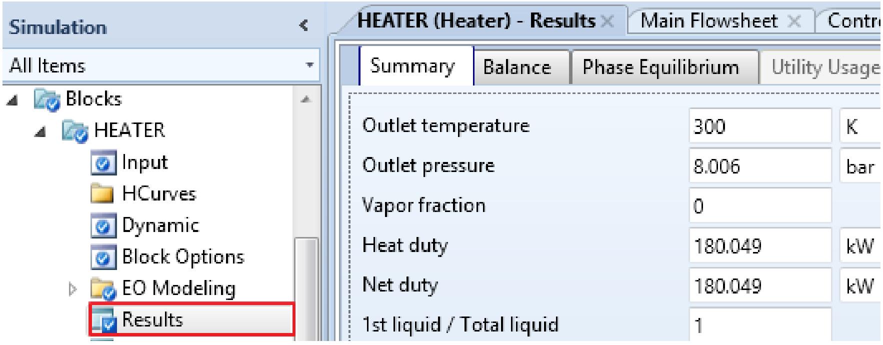
☐ Always calculate pressure drop correlation parameter

Valid phases: Vapor-Liquid

Figure 10.6 Entering the pressure drop (a negative value) and temperature change for the “**Heater**”.

in the outlet pressure or key in the pressure drop for the unit. Here, the pressure drop was entered. This value is just an initial estimate of the pressure drop. Notice that the value is negative and Aspen Plus assumes that the negative number means a pressure drop. On the other hand, a positive number would mean a value for the actual outlet pressure. Keep the "**Valid phases**" option set to "*Vapor–liquid*".

Reset and run the simulation to see the results. Figure 10.7 shows that the heat duty, *Q*, is 180.049 kW and the outlet temperature is 300 K. Notice that the vapor fraction is 0, which means that both streams exist as liquid Freon under the given pressure and temperature.



Outlet temperature	300	K
Outlet pressure	8.006	bar
Vapor fraction	0	
Heat duty	180.049	kW
Net duty	180.049	kW
1st liquid / Total liquid	1	

Figure 10.7 Calculation of the heat duty, *Q*, based on the given inlet and outlet Freon flow rate and the temperature change.

10.4 THE RIGOROUS HEAT EXCHANGER MODEL ("HEATX")

Replace the "**Heater**" block by "**HeatX**" type block from "**Model Palette**". For "**HeatX**" block, the ethylene glycol stream will need to be added. Make sure that the proper stream is connected to the correct port of the block. The Freon-12 stream will be on the cold side and the glycol stream will be on the hot side of the heat exchanger. Figure 10.8 shows the addition of a "**HeatX**" type block to the flowsheet.

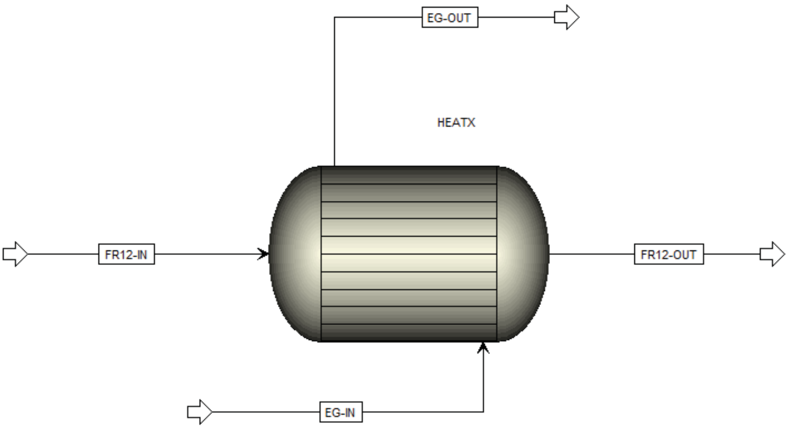
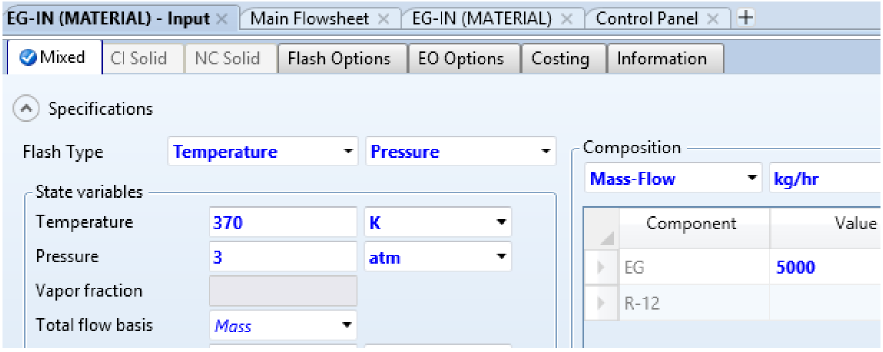


Figure 10.8 Insertion of a "**HeatX**" type heat exchanger to the process flowsheet. FR-12 is connected as both the inlet and outlet cold stream, whereas EG as the inlet and outlet hot stream.

Since the mass flow rate of EG is unknown, we will utilize the calculated heat duty, Q, and find the mass flow rate of EG such that it gives the right outlet temperature of “**EG-OUT**” stream, which is 315 K. If you create a new simulation file, then enter the properties of “**FR12-IN**” stream as was done in the simplified “**HEATER**” case. For “**EG-IN**” stream flow rate, it will be a matter of a “trial-and-error” attempt until the correct value of “**EG-OUT**” stream temperature is obtained. Figure 10.9 shows the input properties of “**EG-IN**” stream where the mass flow rate is assumed to be 5000 kg/h of EG.



Flash Type: Temperature, Pressure

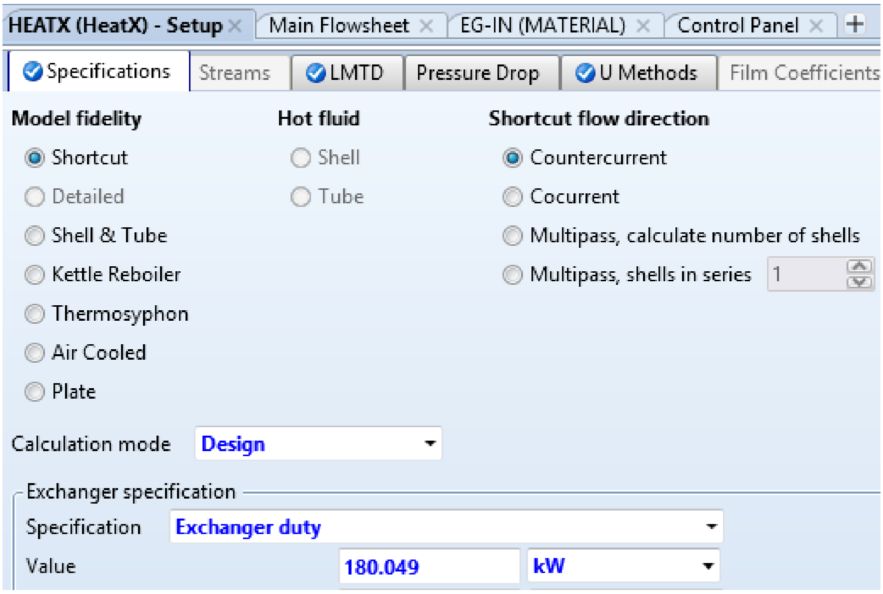
State variables
Temperature: 370 K
Pressure: 3 atm
Vapor fraction:
Total flow basis: Mass

Composition: Mass-Flow, kg/hr

Component	Value
EG	5000
R-12	

Figure 10.9 The inlet flow rate is tentatively assumed to be 5000 kg/h of EG.

Go to “**Blocks**” | “**HEATX**” | “**Setup**” | “**Specifications**” tab window, where the window shows up as in Figure 10.10. At this stage, choose the simplest method of calculation,



Model fidelity
● Shortcut
○ Detailed
○ Shell & Tube
○ Kettle Reboiler
○ Thermosyphon
○ Air Cooled
○ Plate

Hot fluid
○ Shell
○ Tube

Shortcut flow direction
● Countercurrent
○ Cocurrent
○ Multipass, calculate number of shells
○ Multipass, shells in series 1

Calculation mode: Design

Exchanger specification
Specification: Exchanger duty
Value: 180.049 kW

Figure 10.10 Selection of “**Model fidelity**” option as “*Shortcut*”, of “**Calculation mode**” option as “*Design*”, and of “**Exchanger specification**” option as “*Exchanger duty*” will allow the calculation of “**EG-OUT**” temperature, for a given EG flow rate.

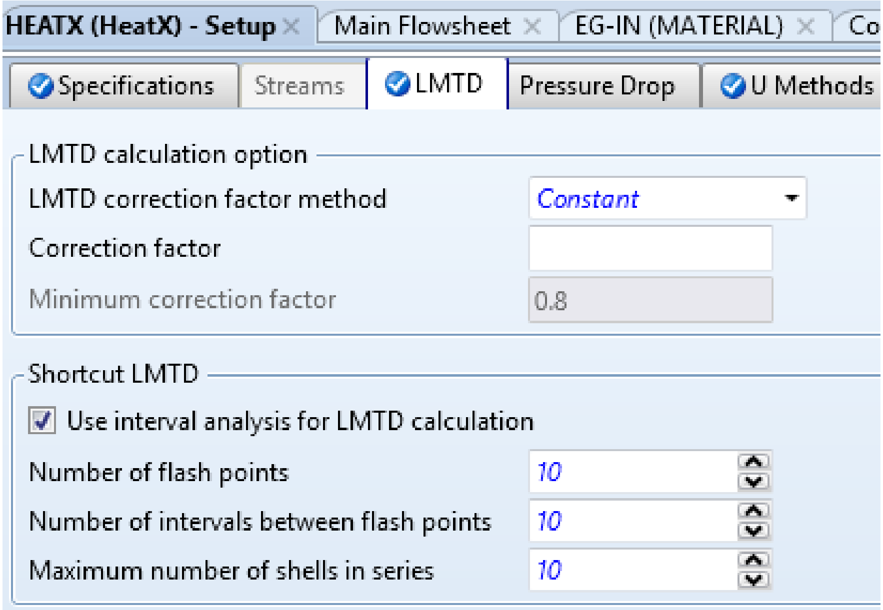
that is, "*Shortcut*" with "**Calculation mode**" as "*Design*". For "**Exchanger specification**" option, there are different options to choose from. Remember that each specification gives a different calculation scenario for Aspen Plus to execute. They are as follows:

1. **Hot stream outlet temperature**: Specifies the outlet temperature of the hot stream, *used for situations where there is no phase change on the hot stream side.*
2. **Hot stream outlet temperature decrease**: Specifies the temperature decrease for the hot stream.
3. **Hot outlet–cold inlet temperature difference**: Specifies the temperature difference between the hot stream outlet temperature and the cold stream inlet temperature, *used with the countercurrent flow.*
4. **Hot stream outlet degrees subcooling**: Specifies the outlet temperature below the dew point for the hot stream, *used for boiling and condensation*.
5. **Hot stream outlet vapor fraction**: Specifies the outlet vapor fraction for the hot stream (1.0 = sat. vapor and 0.0 = sat. liquid), *used for boiling and condensation.*
6. **Hot inlet–cold outlet temperature difference**: Specifies the temperature difference between the hot stream inlet temperature and the cold stream outlet temperature, *used with the countercurrent flow.*
7. **Cold stream outlet temperature**: Specifies the outlet temperature of the cold stream, *used for situations where there is no phase change on the cold stream side.*
8. **Cold stream outlet temperature increase**: Specifies the temperature increase for the cold stream.
9. **Cold stream outlet degrees superheat**: Specifies the outlet temperature above the bubble point for the cold stream, *used for boiling and condensation***.**
10. **Cold stream outlet vapor fraction**: Specifies the outlet vapor fraction for the cold stream (1.0 = sat. vapor and 0.0 = sat. liquid), *used for boiling and condensation.*
11. **Exchanger duty**: Specifies the amount of energy transferred from one stream to another.
12. **Hot/cold outlet temperature approach**: Specifies the temperature difference between the hot/cold stream outlet temperature and the cold/hot stream inlet temperature, *used with the countercurrent flow.*

We will choose "*Exchanger duty*" for "**Exchanger specification**" and assign a value of 180.049 kW as was calculated earlier in the simplified "**HEATER**" case.

For the "**Model fidelity**" option set to "*Shortcut*" and the "**Calculation mode**" set to "*Design*" do not require the user to enter the heat transfer area requirement at this stage. The "**Shortcut flow direction**" option will be set to "*Countercurrent*".

Go to "**LMTD**" tab window and enable "*Use interval analysis for LMTD calculation*" option, as shown in Figure 10.11.



LMTD calculation option

LMTD correction factor method: Constant

Correction factor

Minimum correction factor: 0.8

Shortcut LMTD

☑ Use interval analysis for LMTD calculation

Number of flash points: 10

Number of intervals between flash points: 10

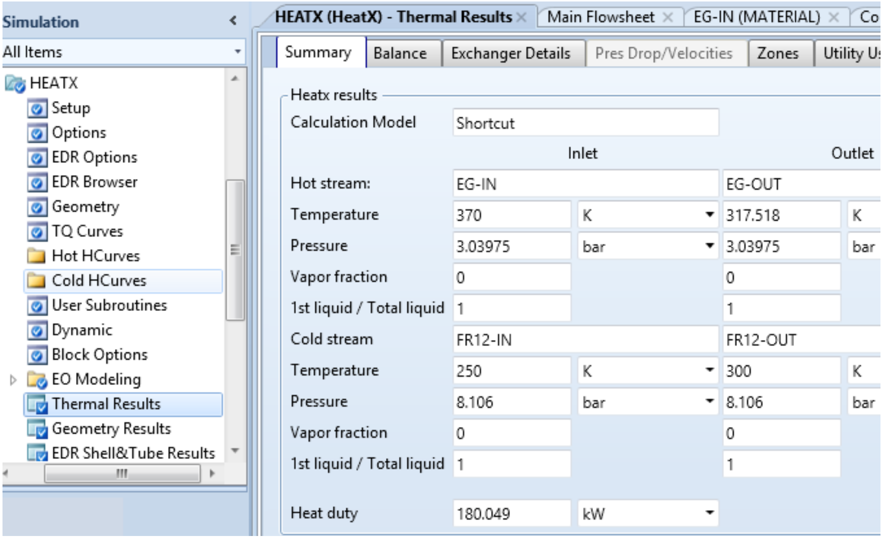
Maximum number of shells in series: 10

Figure 10.11 Specifications of "**Shortcut LMTD**" method of calculation.

In "**Pressure Drop**" tab window, assign "*0*" value for "**Outlet Pressure**" to tell Aspen Plus that the pressure drop is zero and enable "*Always calculate pressure drop correlation parameter*" option for both streams of the exchanger. Anyhow, this is a shortcut method and the results will be modified or further refined using one of the applicable rigorous Aspen Plus Exchanger Design and Rating (EDR) options.

In "**U Methods**" tab window, select "*Phase specific values*" option for "**Selected calculation method**" of the overall heat transfer coefficient, *U*.

Reset, run the simulation, and check the results to see what the output temperature is. Figure 10.12 shows a small portion of the block results, where "**EG-OUT**" temperature is about 317.52 K, which is slightly higher than the required temperature of 315 K. Notice that there are more sheets than one results sheet dedicated for "**HeatX**" type block.



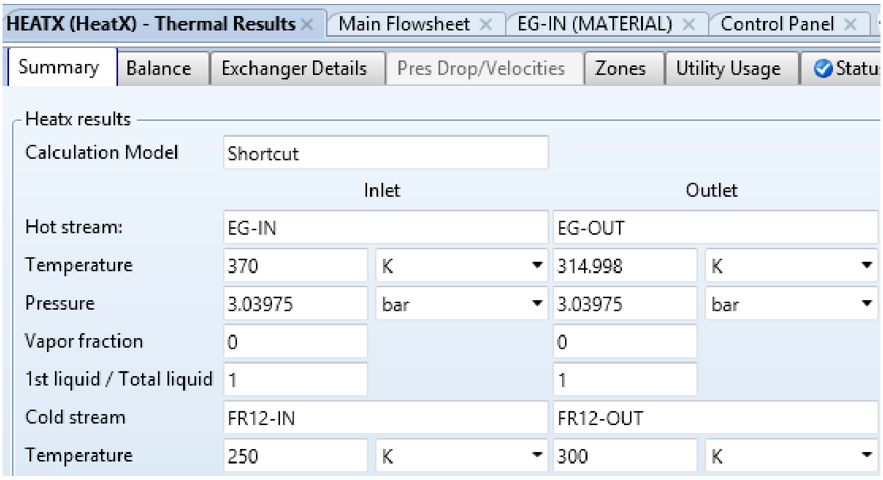
Heatx results

Calculation Model: Shortcut

	Inlet		Outlet	
Hot stream:	EG-IN		EG-OUT	
Temperature	370	K	317.518	K
Pressure	3.03975	bar	3.03975	bar
Vapor fraction	0		0	
1st liquid / Total liquid	1		1	
Cold stream	FR12-IN		FR12-OUT	
Temperature	250	K	300	K
Pressure	8.106	bar	8.106	bar
Vapor fraction	0		0	
1st liquid / Total liquid	1		1	
Heat duty	180.049	kW		

Figure 10.12 A portion of the block results (here "**Thermal Results**" | "**Summary**" sheet) where "**EG-OUT**" temperature is about 317.52 K, which is slightly higher than the correct value of 315 K.

Since it is slightly higher than 315 K, we have to decrease the flow rate a little bit until we hit the value of 315 K. By the trial-and-error game, a value of 4780 kg/h for mass flow rate of EG is found to give the correct value of "**EG-OUT**" temperature, as shown in Figure 10.13.



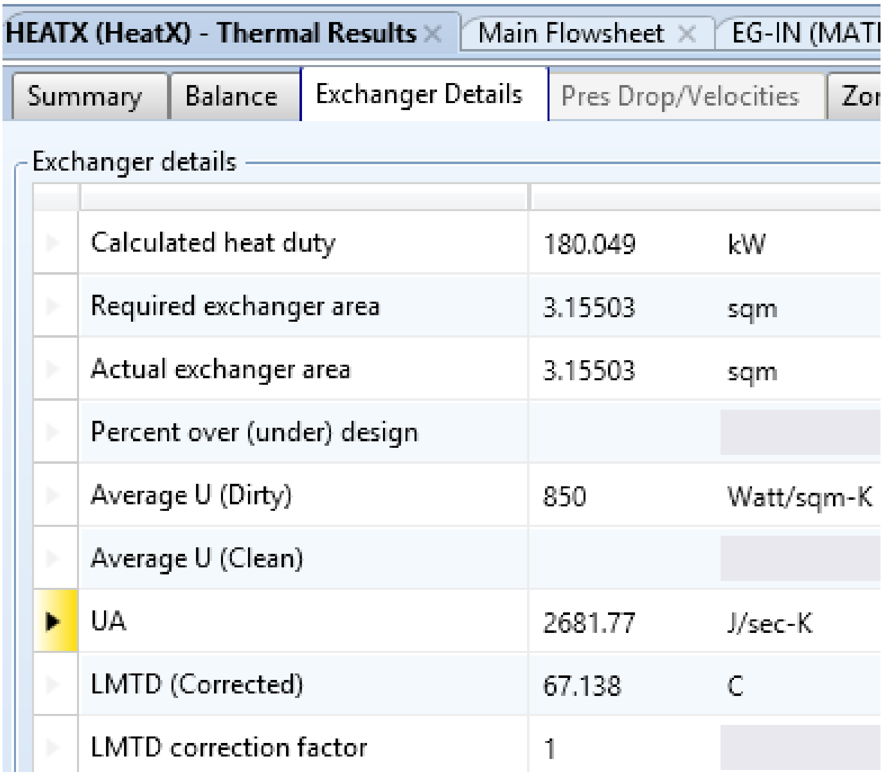
Heatx results

Calculation Model: Shortcut

	Inlet		Outlet	
Hot stream:	EG-IN		EG-OUT	
Temperature	370	K	314.998	K
Pressure	3.03975	bar	3.03975	bar
Vapor fraction	0		0	
1st liquid / Total liquid	1		1	
Cold stream	FR12-IN		FR12-OUT	
Temperature	250	K	300	K

Figure 10.13 A mass flow rate 4780 kg/h of EG will result in the correct value of **EG-OUT** temperature.

Figure 10.14 shows the "**Exchanger Details**" tab window after entering the right mass flow rate of EG while still selecting the "*Shortcut*" method (see Figure 10.10).



Exchanger details

Calculated heat duty	180.049	kW
Required exchanger area	3.15503	sqm
Actual exchanger area	3.15503	sqm
Percent over (under) design		
Average U (Dirty)	850	Watt/sqm-K
Average U (Clean)		
UA	2681.77	J/sec-K
LMTD (Corrected)	67.138	C
LMTD correction factor	1	

Figure 10.14 The "**Exchanger Details**" tab window after selecting the right flow rate of EG while still selecting the shortcut method.

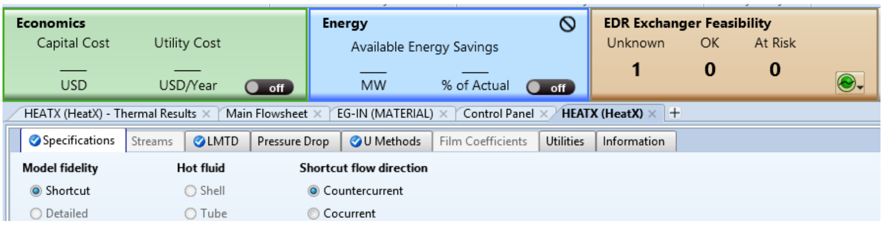
10.5 THE RIGOROUS EXCHANGER DESIGN AND RATING (EDR) PROCEDURE

Since we have found the right mass flow rate of EG, which gives the correct "**EG-OUT**" stream temperature, we can go and make further calculations regarding both the heat transfer and pressure drop aspects. We will approach the rigorous Aspen Exchanger Design and Rating (EDR) to perform a detailed modeling of "**HeatX**" blocks via two routes:

1. The EDR Exchanger Feasibility panel on the Activation dashboard to view a summary of results and risks for rigorous heat exchangers modeled with EDR.
2. The rigorous mode within the "**HeatX**" block.

10.5.1 The EDR Exchanger Feasibility Panel

If the activation dashboard is not active, then from "**File**" menu, click on "**Options**" submenu and the "**Simulation Run Options**" window will pop up. Go to "**Advanced**" tab and deselect "**Disable activation dashboard**" followed by clicking on "**Apply**" and "**OK**" button. As a result, the activation dashboard will appear now as part of Aspen Plus main window as in Figure 10.15. Notice that we ended up with the "*Shortcut*" option for "**Model fidelity**" as was shown in Figure 10.10.



Model fidelity
● Shortcut
○ Detailed

Hot fluid
○ Shell
○ Tube

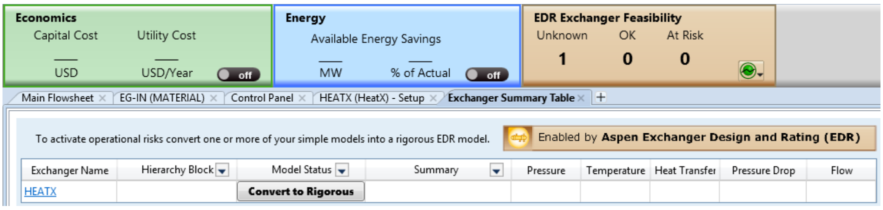
Shortcut flow direction
● Countercurrent
○ Cocurrent

Figure 10.15 Activation of "**EDR Exchanger Feasibility**" dashboard.

In addition, for "**Model fidelity**" option we have to choose either "*Shortcut*" option or one of the available rigorous exchanger types found in Aspen Plus EDR. Keep in mind that the "*Detailed*" method is only available for compatibility purpose with older versions of Aspen Plus. For example, selecting the rigorous "*Shell & Tube*" option, "**HeatX**" model can perform detailed design, rating, or simulation calculations using an Aspen "*Shell&Tube*" model, which has a large variety of shell and tube heat exchanger types available for users.

When a heat exchanger model in the simulation uses a simple (*Shortcut*) model, it is not possible to determine the operational performance or risk. The dashboard reports these exchangers as "*Unknown*" as shown in Figure 10.15. EDR determines the risks for each rigorous exchanger. The dashboard reports rigorous exchangers with no operational or performance issues as "*OK*", and ones with operational or performance risks as "*At Risk*". A single exchanger may have multiple risk conditions; it is only counted once in the "*At Risk*" scenario regardless of the number of critical issues. Risks are problems such as vibration, erosion, and excessive operating temperature and pressure, which could occur while an exchanger is in use. Also, warnings are also included in "*At Risk*" case.

From the dashboard, click on "**EDR Exchanger Feasibility**" button and the "**Exchanger Summary Table**" window will show up as in Figure 10.16.

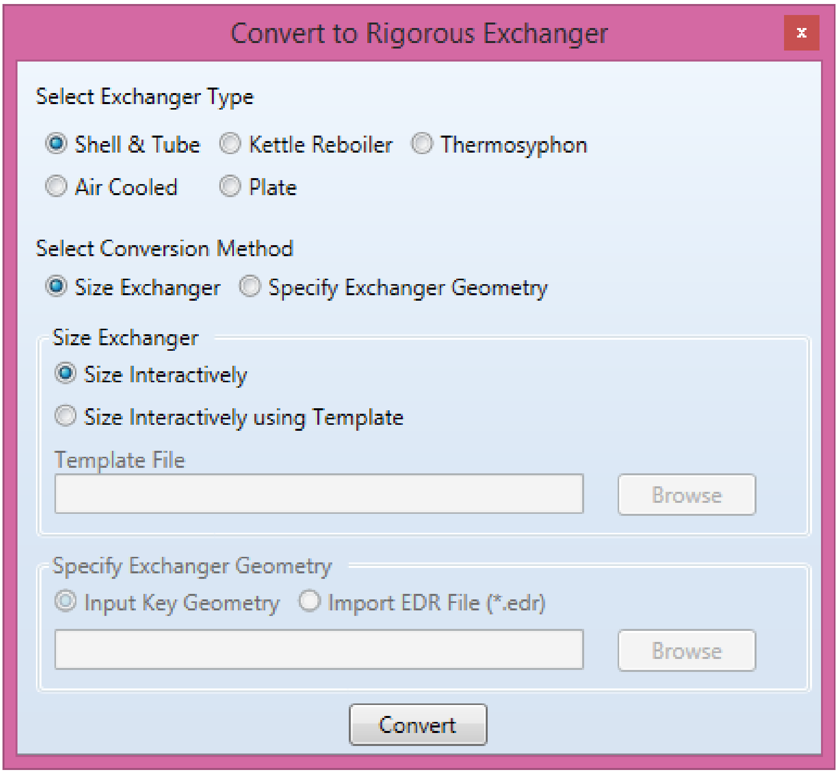


To activate operational risks convert one or more of your simple models into a rigorous EDR model.

Exchanger Name	Hierarchy Block	Model Status	Summary	Pressure	Temperature	Heat Transfer	Pressure Drop	Flow
HEATX		Convert to Rigorous						

Figure 10.16 The "**Exchanger Summary Table**" window that allows conversion of a simple to rigorous exchanger.

Click on "**Covert to Rigorous**" button to start the process of conversion into a rigorous model. The "**Convert to Rigorous Exchanger**" window will pop up as shown in Figure 10.17.



Convert to Rigorous Exchanger

Select Exchanger Type

● Shell & Tube ○ Kettle Reboiler ○ Thermosyphon
○ Air Cooled ○ Plate

Select Conversion Method

● Size Exchanger ○ Specify Exchanger Geometry

Size Exchanger

● Size Interactively
○ Size Interactively using Template

Template File

Specify Exchanger Geometry

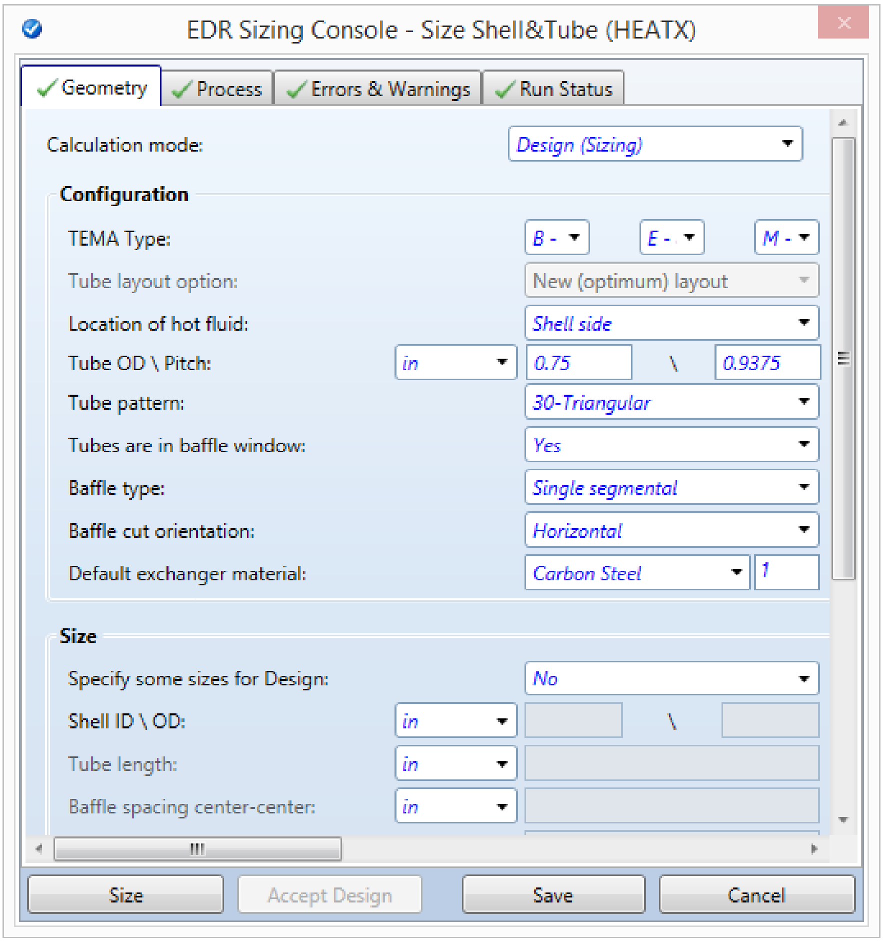
○ Input Key Geometry ○ Import EDR File (*.edr)

Figure 10.17 The "**Convert to Rigorous Exchanger**" window for selecting the exchanger type and conversion method using either built-in templates or user-specified parameter values.

You can choose whether to use an EDR template, and if so, select an EDR/EDTemplate (*.edr/*.edt) file to use for certain geometric details of the exchanger; otherwise, Aspen Plus EDR defaults are used. Alternatively, you can click on "**Specify Exchanger Geometry**" radio button to convert to a rigorous exchanger type and enter your own geometry later in the EDR Browser or import EDR (*.edr) file. Typically, the built-in templates are installed in "**C:\Program Files (x86)\AspenTech\Aspen Exchanger Design and Rating V8.8\Examples**" folder.

Let us go with "Shell & Tube", "*Size Exchanger*", and "*Size Interactively*" option.

Clicking on "**Convert**" button will bring "**EDR Sizing Console – Size Shell&Tube HEATX**" window where we need to either retain Aspen Plus initially assigned parameters related to the exchanger geometry and process conditions, or modify them, as shown in Figure 10.18.



Calculation mode: Design (Sizing)

Configuration

TEMA Type: B - E - M -

Tube layout option: New (optimum) layout

Location of hot fluid: Shell side

Tube OD \ Pitch: in 0.75 \ 0.9375

Tube pattern: 30-Triangular

Tubes are in baffle window: Yes

Baffle type: Single segmental

Baffle cut orientation: Horizontal

Default exchanger material: Carbon Steel 1

Size

Specify some sizes for Design: No

Shell ID \ OD: in \

Tube length: in

Baffle spacing center-center: in

Figure 10.18 The "**EDR Sizing Console – Size Shell&Tube HEATX**" window where the user has the choice to either retain or modify Aspen Plus initially assigned parameters related to exchanger geometry and process conditions.

Consequently, in light of items appearing in Figure 9.18, elaboration will be made on each item from top to bottom, under each tab.

In "**Geometry**" tab window, let us start with the "**Calculation mode**", which can take on: "*Design (Sizing)*", "*Rating*", "*Simulation*", or "*Find Fouling*" option. See also Figure 10.10.

Design mode is available for "*Shortcut*", "*Shell&Tube*", "*Kettle Reboiler*", "*Thermosyphon*", and "*AirCooled*" option for "**Model fidelity**". Given a specified load, "**HeatX**" model will determine the area required and the number of shells in series that are required. In addition, the rigorous methods will also define the optimum geometry for the exchanger.

Rating mode is available for all options of "**Model fidelity**". Given a specified load and exchanger geometry, "**HeatX**" model will predict the percent over or under surface for the unit. In addition, the rigorous methods will also estimate the level of fouling that may exist in the unit if the unit is over-surfaced for those specified operating conditions.

Simulation mode is available for all options of "**Model fidelity**". Given an area or geometry for an exchanger, the methods will determine the outlet conditions for the hot and cold side streams.

Maximum Fouling mode is only available for the "*Shell&Tube*", "*Kettle Reboiler*", and "*Thermosyphon*" option of "**Model fidelity**". This method determines the amount of fouling resistance based on the given process condition and geometry.

> **NOTE #2:** *With all rigorous options of "**Model fidelity**", you can use a "**Utility**" on one side of the exchanger only in "Design" and "Rating" mode. A utility can be Aspen Plus- or user-defined, which can be in the form of steam, cooling water, or heating/cooling fluid, in general. The block utility is part of cost estimate as is discussed in Chapter 17.*

We will go with the "*Design*" option for "**Calculation mode**". With such an option, the geometry of the exchanger need not be initially provided by the user. Sizing of exchanger geometry will be done shortly in the second case (i.e., under "*Rating*" mode).

"B" stands for TEMA type B (bonnet bolted or integral with tubesheet), which is one selection for front head (A, B, C, N, and H) to be used. Program will default to TEMA type B.

The TEMA shell type can be one-pass, two-pass, split-flow, and so on. Examples of each shell type can be seen on pages 11–34 of Perry and Green [1] as also shown in Figure 10.19. Type "*E*" will be our choice.

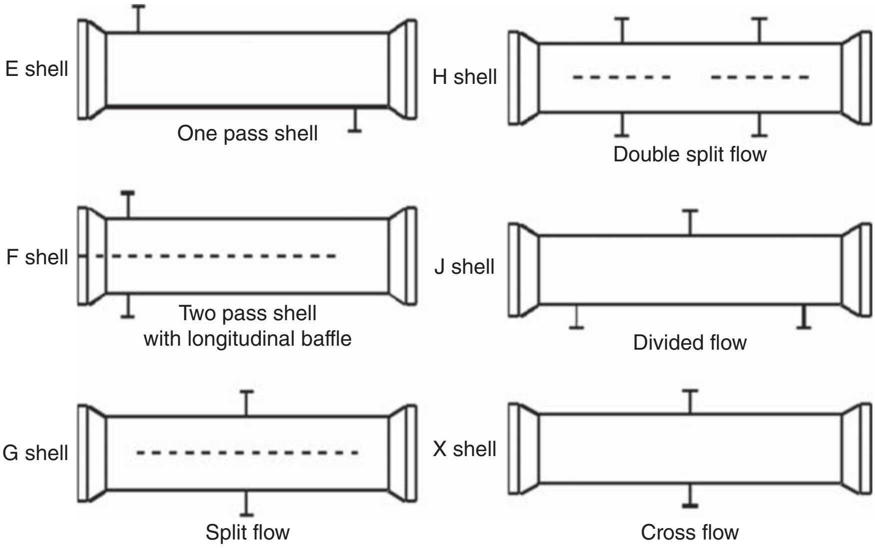


Figure 10.19 Different configurations of TEMA shell type.

"M" stands for TEMA type M (bonnet), which represents one selection for the rear head (L, M, N, P, S, T, U, and V) arrangement. Program will default to TEMA type M.

Location of hot fluid: What is where?

NOTE #3: *The decision on which fluid to be located on what side of the exchanger will have a direct impact on the performance, economics, and durability aspects of an exchanger. The following issues can be used as rules of thumb in decision making* [2]*:*

- *Fouling:* *Allocating the most fouling fluid to the tube side will be more favorable as mechanical cleaning of the inside of the tubes will be much easier. Moreover, the allowable velocity in the tubes is usually higher than that at the shell side and a high fluid velocity causes less deposit formation.*
- *Working Pressure:* *It will be more economical to assign the medium with the highest maximum allowable working pressure to the tube side. If the shell side needs to be designed for a high pressure, the wall thickness will increase; hence, making the heat exchanger more expensive.*
- *Corrosion:* *If an expensive corrosion-resistant material is needed, it will be more economical to place the corrosive fluid on the tube side, as this will reduce the cost of the shell material, or protective shield.*
- *High Viscosity or Low Flow Rate:* *To obtain an economic design, high heat transfer coefficients are required. Heat transfer coefficients are much higher for turbulent flow than laminar, and this represents the most important aspect to take care of. For a highly viscous medium, or a low flow rate, turbulent flow can be easily created at the shell side. However, if Reynolds number at the shell side falls below 200, it will probably be cheaper to allocate this fluid to the tube side and use a high number of tube passes.*

In light of the previous arguments, both fluids are neither corrosive nor causing fouling; hence, we are left by the high-pressure and flow rate issue. The high-pressure and high flow rate FR-12 (cold fluid) stream will be on the tube-side and the low-pressure and low flow rate EG (hot fluid) stream will be on the shell-side.

Tube OD: The outside diameter of a single tube within the tube bundle.

NOTE #4: *Set the dimensions of one tube by specifying the tube diameter and length. As a rule of thumb, start with 1-inch pipe diameter if the fluid is liquid and 1.5 inches if the fluid is vapor. However, this is a start and the user may attempt to go higher or lower than recommended, depending on other factors, such as pressure drop restriction, heat transfer requirement, and degree of fluid cleanliness. Preferred tube lengths are 1.83 m (6 ft), 2.44 m (8 ft), 3.88 m (12 ft), and 4.88 m (16 ft).*

Tube pitch: The distance between tube centers within the tube bundle. In general, the pitch is 1.25 times the outside diameter of one tube, to ensure adequate strength for tube rolling. We will stick to the initially assigned tube diameter. Then, the tube pitch is $1.25 \times 0.75'' = 0.9375''$.

Tube pattern: Specify the tube layout, either a triangular or square pitch; triangular pitch is used here. In general, the triangular 30° layout is used for clean fluids, both laminar and turbulent flow, and a 45° or 90° layout is used whenever mechanical cleaning is required for fouling fluids. In addition, the 45°-rotated square tube layout can be selected to create more turbulence on the shell-side whenever the shell-side Reynolds' number is low [3]. See Figure 10.20.

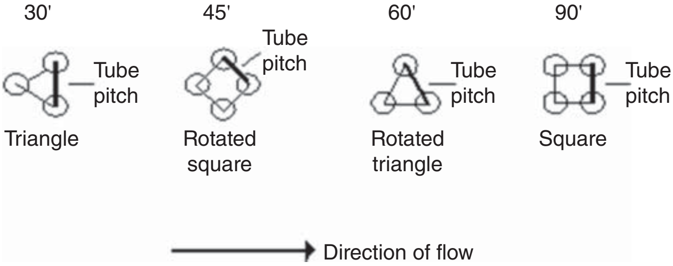


Figure 10.20 Different tube bank layout patterns.

Baffle type: Baffles are either segmental or rod, as shown in Figure 10.21. Segmental baffles are perforated metal sheets that partially block the shell-side flow while rod types are simply rods that cause more turbulent flow in the shell-side via partial obstruction of fluid flow. The baffle cut specifies the fraction of a baffle cut, that is, the height of the segment that is cut in each baffle to permit the shell-side fluid to flow across the baffle. This is expressed as a percentage of the shell's inner diameter. The baffle cut is also an important factor for S&T H.E. design; however, its effect is less pronounced than that of the baffle spacing. Baffle cut can vary between 15 and 45% of the shell's inner diameter.

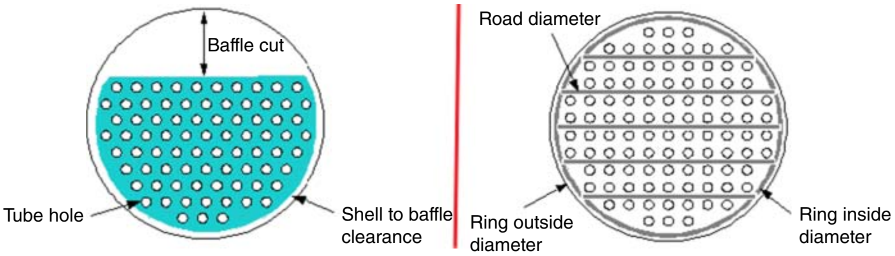
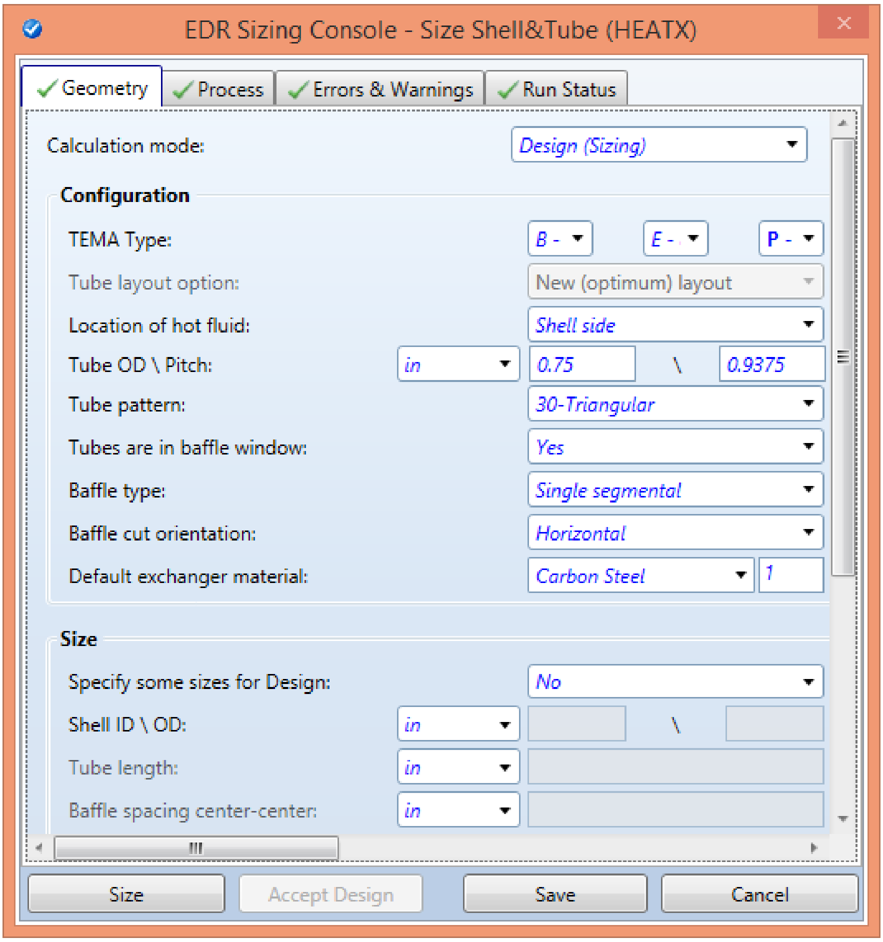


Figure 10.21 Segmental baffle (*left*) and rod baffle (*right*).

Default exchanger material: Select from the drop-down list the material of construction of the tubes. "*Carbon Steel*" option will be assigned here.

Based on the previous recommendations and calculations, the final geometrical parameters are shown in Figure 10.22 in "**Geometry**" tab window. Notice that the type of TEMA rear head pattern is selected as "*P*", outside packed floating head simply because the temperature difference (i.e., LMTD) between hot and cold fluid is larger than 50°C (see Figure 10.14) to allow for thermal expansion effects, as recommended by Aspen Plus.



Calculation mode: Design (Sizing)

Configuration

TEMA Type: B - E - P -

Tube layout option: New (optimum) layout

Location of hot fluid: Shell side

Tube OD \ Pitch: in 0.75 \ 0.9375

Tube pattern: 30-Triangular

Tubes are in baffle window: Yes

Baffle type: Single segmental

Baffle cut orientation: Horizontal

Default exchanger material: Carbon Steel 1

Size

Specify some sizes for Design: No

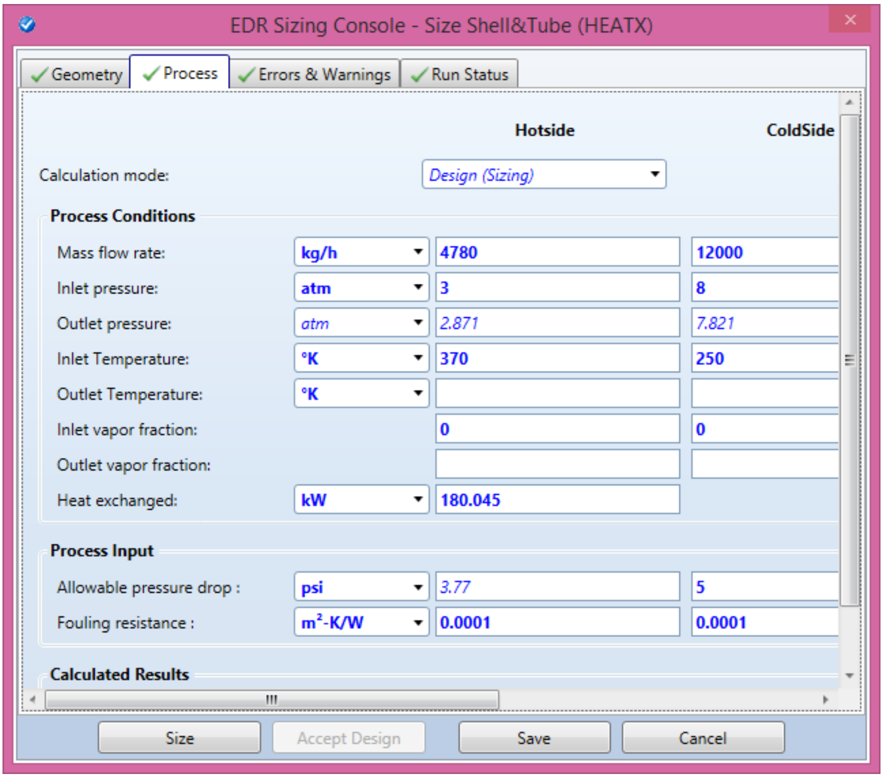
Shell ID \ OD: in \

Tube length: in

Baffle spacing center-center: in

Figure 10.22 The final recommended geometrical parameters in "**Geometry**" tab window.

On the other hand, the process variables have only a restriction on the pressure drop not to exceed 5 psi on either side of the heat exchanger. In addition, a fouling resistance value of 0.0001 $m^2 \cdot K/W$ is entered for either fluid. The final process parameters are shown in Figure 10.23 in "**Process**" tab window. Notice that other values are already borrowed from the "***Shortcut***" method.



	Unit	Hotside	ColdSide
Calculation mode:		Design (Sizing)	
Process Conditions			
Mass flow rate:	kg/h	4780	12000
Inlet pressure:	atm	3	8
Outlet pressure:	atm	2.871	7.821
Inlet Temperature:	°K	370	250
Outlet Temperature:	°K		
Inlet vapor fraction:		0	0
Outlet vapor fraction:			
Heat exchanged:	kW	180.045	
Process Input			
Allowable pressure drop :	psi	3.77	5
Fouling resistance :	m^2-K/W	0.0001	0.0001
Calculated Results			

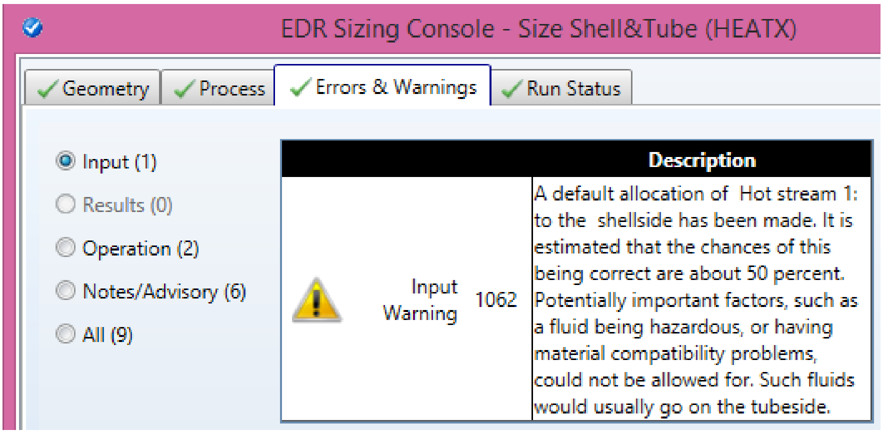
Figure 10.23 The final recommended process parameters in “**Process**” tab window.

Notice if there are errors or warnings, then they can be seen in “**Errors and Warnings**” tab window.

At this stage, you may save the user-entered specifications in the form of an Aspen Exchanger Design Document (*.edr) file so that you can import later in another design scenario.

Click on “**Size**” button to initiate the sizing process by Aspen Plus. After the completion of sizing, watch out for any warning under “**Errors and Warnings**” tab. If there exists any serious warning that requires the user to make correction(s), then he/she has to make the proper changes and resize via clicking on “**Size**” button until all serious warnings are taken care of.

Figure 10.24 shows a warning regarding the location of hot stream whether it be on the tube or on shell side. We have already elaborated on that (see **NOTE #3**).

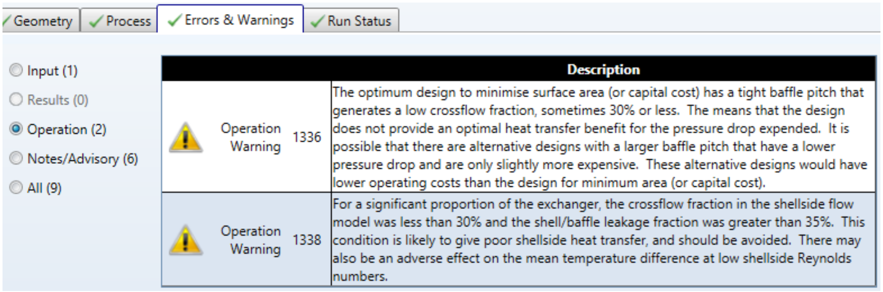


● Input (1)
○ Results (0)
○ Operation (2)
○ Notes/Advisory (6)
○ All (9)

			Description
⚠	Input Warning	1062	A default allocation of Hot stream 1: to the shellside has been made. It is estimated that the chances of this being correct are about 50 percent. Potentially important factors, such as a fluid being hazardous, or having material compatibility problems, could not be allowed for. Such fluids would usually go on the tubeside.

Figure 10.24 In "**Errors & Warnings**" tab window, the user has to look for critical issues raised by Aspen Plus EDR simulator.

On the other hand, Figure 10.25 shows some critical issues in the form of recommendation to take care regarding the shell-side flow pattern and geometrical constraints imposed on the shell-side fluid. The first precaution is not really a serious issue but the second issue has to be taken care of by not letting shell-side Reynolds number drop below 200 (see **NOTE #3**).

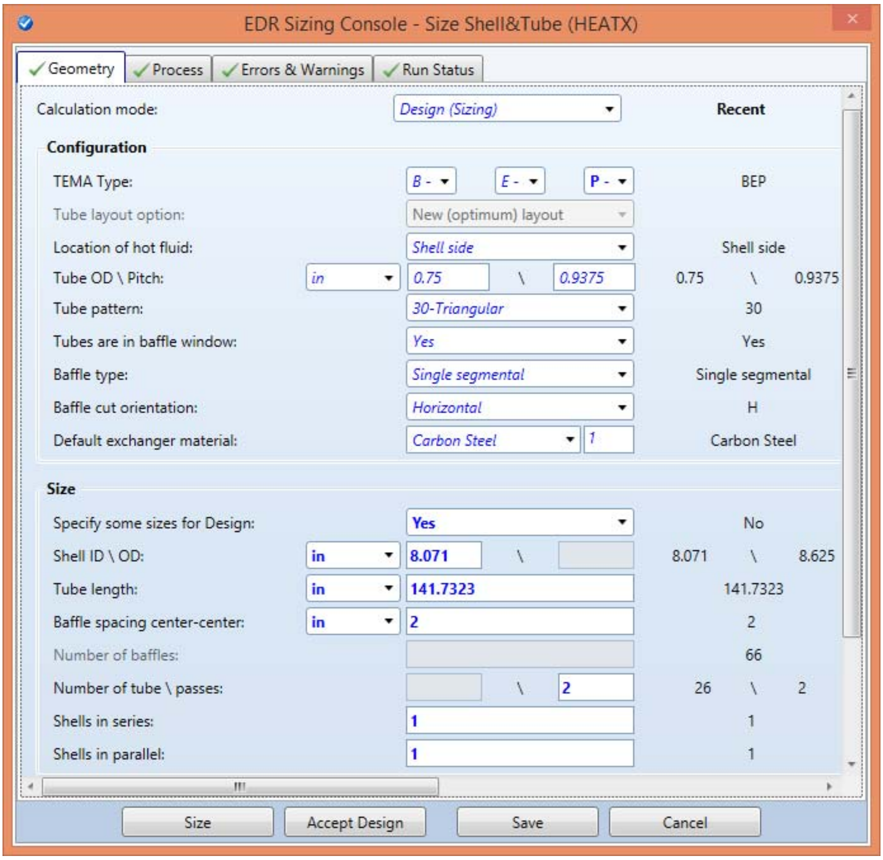


○ Input (1)
○ Results (0)
● Operation (2)
○ Notes/Advisory (6)
○ All (9)

			Description
⚠	Operation Warning	1336	The optimum design to minimise surface area (or capital cost) has a tight baffle pitch that generates a low crossflow fraction, sometimes 30% or less. The means that the design does not provide an optimal heat transfer benefit for the pressure drop expended. It is possible that there are alternative designs with a larger baffle pitch that have a lower pressure drop and are only slightly more expensive. These alternative designs would have lower operating costs than the design for minimum area (or capital cost).
⚠	Operation Warning	1338	For a significant proportion of the exchanger, the crossflow fraction in the shellside flow model was less than 30% and the shell/baffle leakage fraction was greater than 35%. This condition is likely to give poor shellside heat transfer, and should be avoided. There may also be an adverse effect on the mean temperature difference at low shellside Reynolds numbers.

Figure 10.25 Other precautions are brought to the user's attention, such as "**Operation**"-related issues.

To speed up the process of heat exchanger design via the rigorous approach, we will move one step further. Let us make use of the already calculated geometrical or size parameters given by Aspen Plus EDR simulator. Figure 10.26 shows that we have switched from "*No*" to "*Yes*" option for "**Specify some sizes for design**" scenario in "**Geometry**" tab window and entered some geometrical parameters as shown on the right side of each entry. Notice that number of tubes and number of baffles are disabled under "*Design*" mode.



Calculation mode: Design (Sizing) — Recent

Configuration

				Recent		
TEMA Type:		B -	E - / P -	BEP		
Tube layout option:		New (optimum) layout				
Location of hot fluid:		Shell side		Shell side		
Tube OD \ Pitch:	in	0.75	0.9375	0.75	\	0.9375
Tube pattern:		30-Triangular		30		
Tubes are in baffle window:		Yes		Yes		
Baffle type:		Single segmental		Single segmental		
Baffle cut orientation:		Horizontal		H		
Default exchanger material:		Carbon Steel	1	Carbon Steel		

Size

				Recent		
Specify some sizes for Design:		Yes		No		
Shell ID \ OD:	in	8.071		8.071	\	8.625
Tube length:	in	141.7323		141.7323		
Baffle spacing center-center:	in	2		2		
Number of baffles:				66		
Number of tube \ passes:			2	26	\	2
Shells in series:		1		1		
Shells in parallel:		1		1		

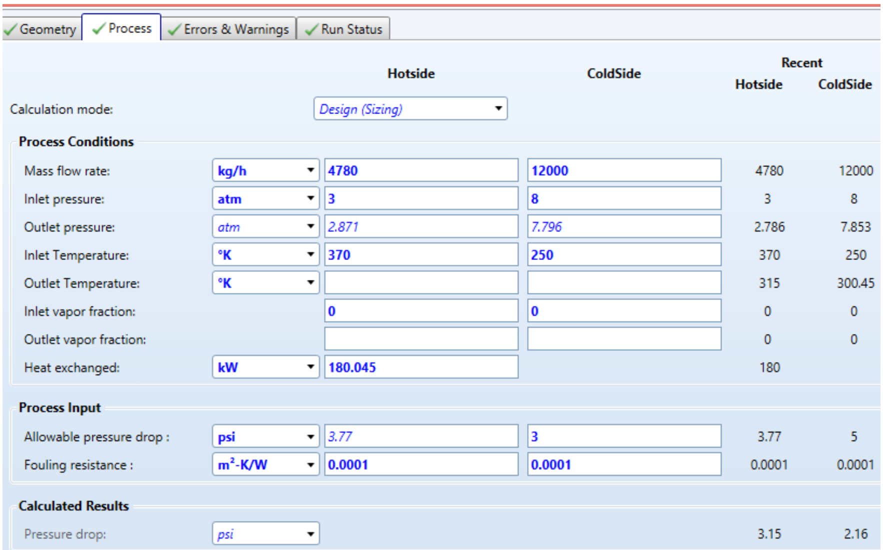
Figure 10.26 Specifying some geometrical parameters for the heat exchanger while utilizing the values as given by Aspen Plus EDR simulator. Number of tubes and baffles are disabled under "*Design*" mode.

Figure 10.27 shows further tune-up in "**Process**" tab window. The pressure drop on the tube (i.e., cold) side is reduced from 5 to 3 psi.

Click on "**Size**" button to see the exchanger performance with the newly entered settings. This will reveal the fact things turn out to be the same in terms of types of warnings and precautions as was shown earlier in Figures 10.24 and 10.25.

Nevertheless, in Figure 10.26, if we change the value of "**Baffle spacing center–center**" from "*2 inches*" to "*4 inches*" or "*6 inches*", we will get rid of the second "**Operation**" precaution, shown earlier in Figure 10.25 as "*Operation Warning 1338*". The baffle spacing is approximately equal to tube length divided by the (number of baffles + 1). More baffles can be added to increase the heat transfer coefficient, but at the expense of increasing pressure drop; hence, make sure that the pressure drop is below the maximum allowable pressure drop.

Let us switch from “*Design*” to “*Rating*” option for “**Calculation mode**”. Upon switching, a pop-up window will ask whether to use current or have a new rating. We will go with the current configuration; click on “**Use Current**” button to close the pop-up window.



Calculation mode: Design (Sizing)

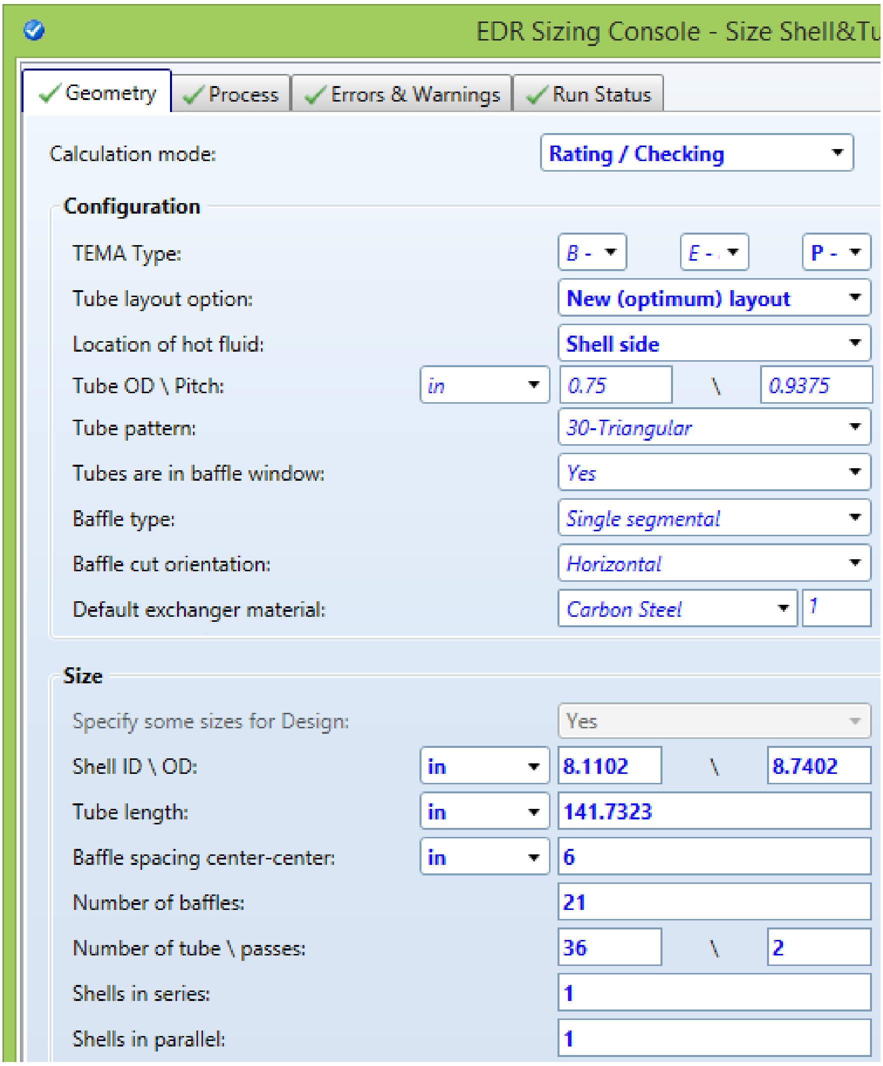
		Hotside	ColdSide	Recent Hotside	Recent ColdSide
Process Conditions					
Mass flow rate:	kg/h	4780	12000	4780	12000
Inlet pressure:	atm	3	8	3	8
Outlet pressure:	atm	2.871	7.796	2.786	7.853
Inlet Temperature:	°K	370	250	370	250
Outlet Temperature:	°K			315	300.45
Inlet vapor fraction:		0	0	0	0
Outlet vapor fraction:				0	0
Heat exchanged:	kW	180.045		180	
Process Input					
Allowable pressure drop :	psi	3.77	3	3.77	5
Fouling resistance :	m^2-K/W	0.0001	0.0001	0.0001	0.0001
Calculated Results					
Pressure drop:	psi			3.15	2.16

Figure 10.27 Further tune-up in “**Process**” tab window, where the pressure drop on the tube (i.e., cold) side is reduced from 5 to 3 psi.

With “*Rating*” mode on, Aspen Plus EDR simulator allows us to manipulate two extra features, which are, the number of tubes and baffles, in addition to other features or entries found in “*Design*” mode. We can stick to the estimated number of tubes, which is “*26*” (see Figure 10.26), or increase it to avoid shortage in available area for heat transfer.

The new settings are shown in Figure 10.28.

Moreover, in “**Process**” tab window, the “**Allowable pressure drop**” values were further reduced to “*1 psi*” and “*1.5 psi*” for “**Hotside**” and “**Coldside**” stream, respectively.



Calculation mode: Rating / Checking

Configuration

TEMA Type: B - E - P -

Tube layout option: New (optimum) layout

Location of hot fluid: Shell side

Tube OD \ Pitch: in 0.75 \ 0.9375

Tube pattern: 30-Triangular

Tubes are in baffle window: Yes

Baffle type: Single segmental

Baffle cut orientation: Horizontal

Default exchanger material: Carbon Steel 1

Size

Specify some sizes for Design: Yes

Shell ID \ OD: in 8.1102 \ 8.7402

Tube length: in 141.7323

Baffle spacing center-center: in 6

Number of baffles: 21

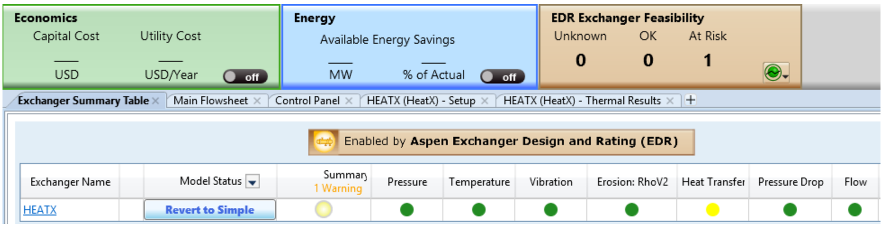
Number of tube \ passes: 36 \ 2

Shells in series: 1

Shells in parallel: 1

Figure 10.28 The updated geometrical settings of EDR exchanger, under "**Rating/Checking**" mode.

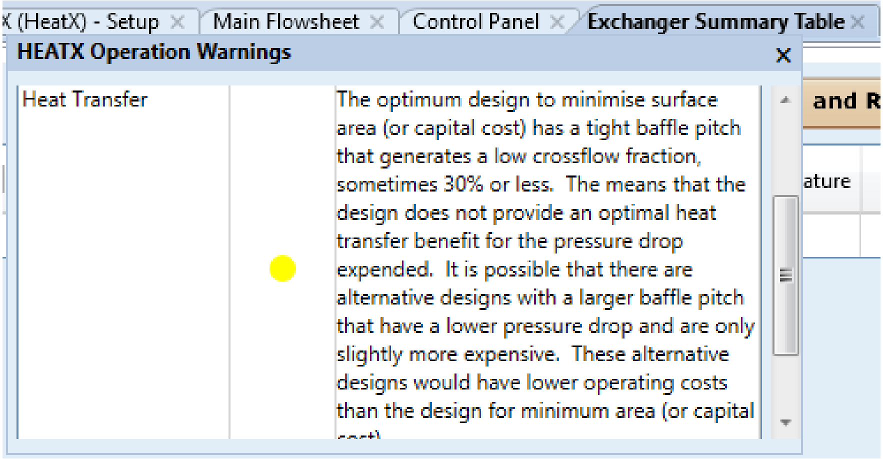
Click on "**Accept Design**" button to proceed to the final specifications. Figure 10.29 shows the decision/judgment by Aspen Plus EDR exchanger. All issues are okayed (green) except for one issue labeled as yellow (i.e., warning level).



Exchanger Name	Model Status	Summary 1 Warning	Pressure	Temperature	Vibration	Erosion: RhoV2	Heat Transfer	Pressure Drop	Flow
HEATX	Revert to Simple	○	●	●	●	●	●	●	●

Figure 10.29 The technical judgment by Aspen Plus EDR exchanger on the entered geometrical specifications. All issues are labeled as green except one issue (yellow) with warning. *See Plate section for color representation of this figure.*

Click on the circle shown below "**Summary 1 Warning**" tab to see further details. Figure 10.30 shows the details that Aspen Plus EDR worries about the heat transfer aspect, which is labeled as yellow, indicating a non-serious warning but definitely not a risk (error).

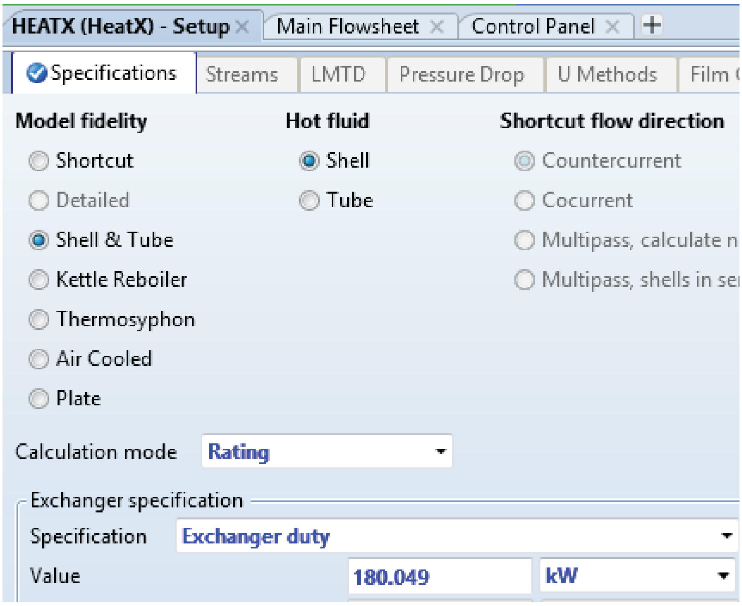


HEATX Operation Warnings

Heat Transfer	●	The optimum design to minimise surface area (or capital cost) has a tight baffle pitch that generates a low crossflow fraction, sometimes 30% or less. The means that the design does not provide an optimal heat transfer benefit for the pressure drop expended. It is possible that there are alternative designs with a larger baffle pitch that have a lower pressure drop and are only slightly more expensive. These alternative designs would have lower operating costs than the design for minimum area (or capital cost)

Figure 10.30 Aspen Plus EDR suggests other alternatives, geometrical configurations that may result in further lowering of pressure drop and are potentially slightly more expensive. *See Plate section for color representation of this figure.*

You may close the "**Exchanger Summary Table**" window shown in Figure 10.30. Let us go back to "**Blocks**" | "**HEATX**" | "**Setup**" | "**Specifications**" tab window and select the "**Calculation method**" option to be "*Rating*". Moreover, select the "**Hot fluid**" option to be "*Shell*", the "**Exchanger specification**" option to be "*Exchanger duty*" and assign its value in power unit, as shown in Figure 10.31.



Model fidelity
○ Shortcut
○ Detailed
● Shell & Tube
○ Kettle Reboiler
○ Thermosyphon
○ Air Cooled
○ Plate

Hot fluid
● Shell
○ Tube

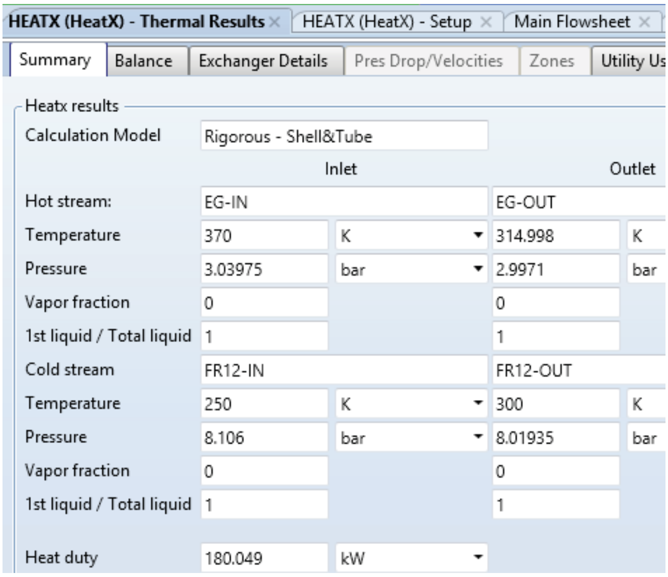
Shortcut flow direction
○ Countercurrent
○ Cocurrent
○ Multipass, calculate n
○ Multipass, shells in se

Calculation mode: Rating

Exchanger specification
Specification: Exchanger duty
Value: 180.049 kW

Figure 10.31 The Aspen Plus simulator will be ready to run under rigorous "**Model fidelity**" option being "*Shell&Tube*" while the "**Calculation mode**" is set to "*Rating*".

Click on "**Reset**" followed by "**Next**" button to run the simulator with the new settings. Notice that with this yellow-colored non-serious warning, Aspen Plus simulator via its "**Control Panel**" indicated that no warnings were issued during input translation and also no errors or warnings were issued during simulation. Figure 10.32 shows a summary of results including inlet and outlet temperatures and pressures.



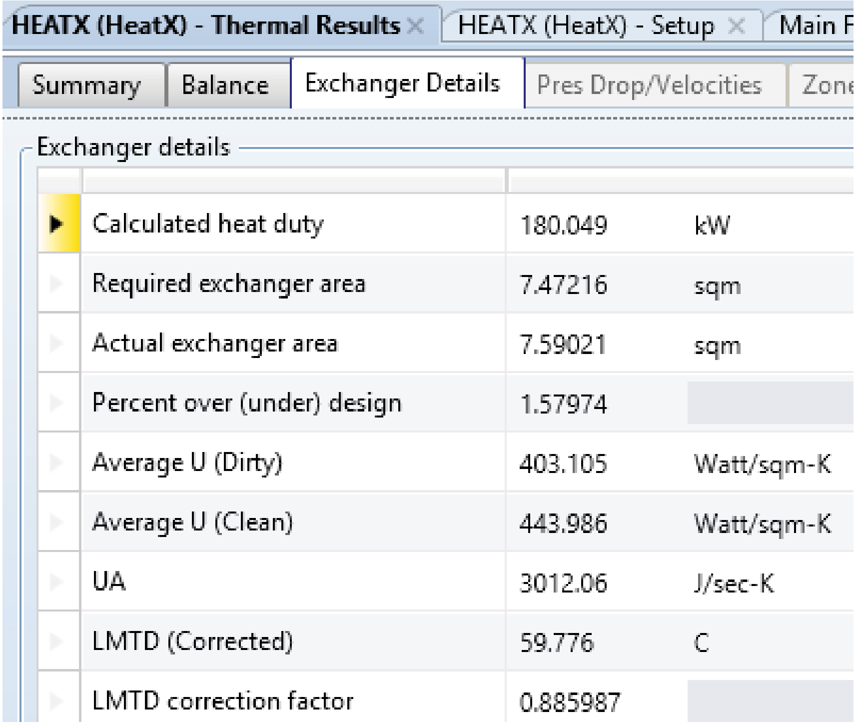
Heatx results

Calculation Model: Rigorous - Shell&Tube

	Inlet		Outlet	
Hot stream:	EG-IN		EG-OUT	
Temperature	370	K	314.998	K
Pressure	3.03975	bar	2.9971	bar
Vapor fraction	0		0	
1st liquid / Total liquid	1		1	
Cold stream	FR12-IN		FR12-OUT	
Temperature	250	K	300	K
Pressure	8.106	bar	8.01935	bar
Vapor fraction	0		0	
1st liquid / Total liquid	1		1	
Heat duty	180.049	kW		

Figure 10.32 A summary of results for inlet and outlet temperatures and pressures.

Figure 10.33 shows the exchanger details where the percent over design is about 1.6%. In general, the percent over design value has to be greater than zero and less than 10%, given the fact that the fouling vulnerability, on both sides of the exchanger, is taken care of via assigning a fouling resistance factor for both sides (see Figure 10.23).



Calculated heat duty	180.049	kW
Required exchanger area	7.47216	sqm
Actual exchanger area	7.59021	sqm
Percent over (under) design	1.57974	
Average U (Dirty)	403.105	Watt/sqm-K
Average U (Clean)	443.986	Watt/sqm-K
UA	3012.06	J/sec-K
LMTD (Corrected)	59.776	C
LMTD correction factor	0.885987	

Figure 10.33 The required, actual, percent over/under design, and other heat transfer-related parameters.

10.5.2 The Rigorous Mode Within the "HeatX" Block

We mention here how to initiate this procedure, and all other subsequent steps are exactly the same as those of the first procedure. Starting from Figure 10.10, where we ended up with the "*Shortcut*" option for "**Model fidelity**", once you click on "*Shell&Tube*" option, the "**Convert to Rigorous Exchanger**" window will show up as exactly as shown in Figure 10.17. Continue your journey of exchanger design as explained earlier in the first procedure.

10.6 GENERAL FOOTNOTES ON EDR EXCHANGER

a) To edit and modify a rigorous EDR exchanger, you may click on the hyperlink "**HeatX**" in "**Exchanger Summary Table**" tab window (see Figure 10.29). This window is accessed via clicking on "**EDR Exchanger Feasibility**" panel on the Activation dashboard. Alternatively, go to "**Blocks**" | "**HEATX**" | "**EDR Browser**" window, as shown in Figure 10.34.

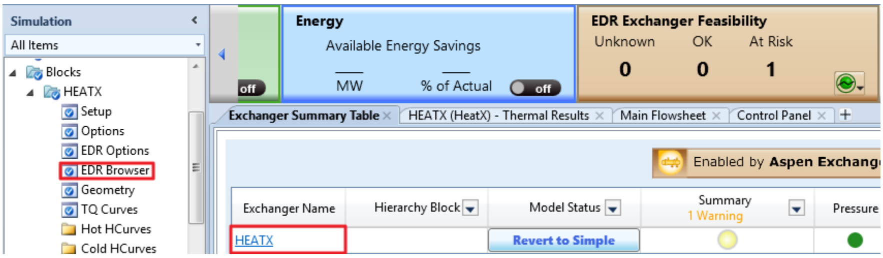
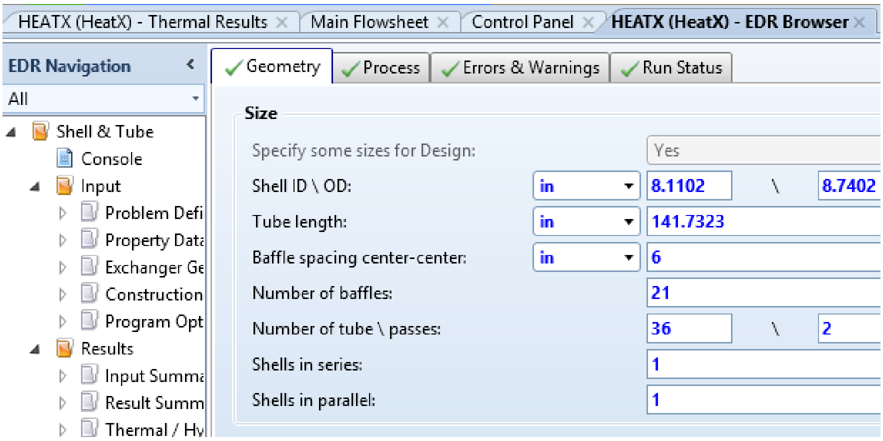


Figure 10.34 Editing a rigorous EDR exchanger.

b) Figure 10.35 shows the EDR navigation pane and the corresponding tab sheets.



Specify some sizes for Design: Yes
Shell ID \ OD: in 8.1102 \ 8.7402
Tube length: in 141.7323
Baffle spacing center-center: in 6
Number of baffles: 21
Number of tube \ passes: 36 \ 2
Shells in series: 1
Shells in parallel: 1

Figure 10.35 The EDR navigation pane where the user may modify any entry.

c) In Figure 10.35, if the user may attempt to modify any of the geometrical entries, he/she has to rerun the show via clicking on "**Next**" button while the EDR exchanger design is in "**Connected**" mode as shown in Figure 10.36 (*top*). For example, we may change the number of tubes from "*36*" to a higher number, say, "*40*", to increase the surface area available for the exchanger. The effect of changing any of the input parameters on exchanger performance can be seen via browsing through different "**Results**" sheets in EDR navigation pane. Always check for the adverse effects on exchanger performance via monitoring the "**Errors & Warnings**" tab form.

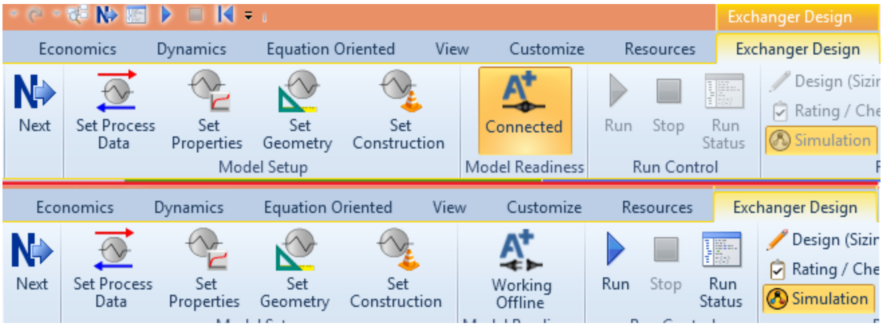
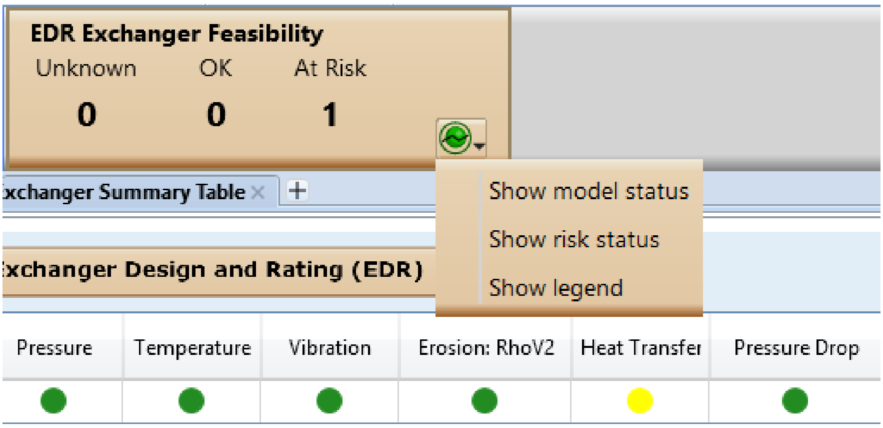


Figure 10.36 The EDR exchanger design is either in "**Connected**" (*top*) or "**Working Offline**" mode (*bottom*).

d) You can click on the small button at the lower right of the dashboard panel to highlight exchangers on the flowsheet by clicking on "**Show model status**" (which marks whether exchangers are simple or rigorous) or on "**Show risk status**". Click the active status choice again to turn off the flowsheet highlight feature. Click on "**Show legend**" to display the meanings of the colors. See Figure 10.37. When "**Show risk status**" is active, if you move the mouse over one of the flowsheet highlights, information appears about the risks in a small window. Operational or performance warnings are shown with a yellow status icon. Operational or performance risks are shown with a red icon. The most severe risk type is indicated at the top of this window as the overall exchanger status. Click this overall exchanger status icon to display more details about the risks.



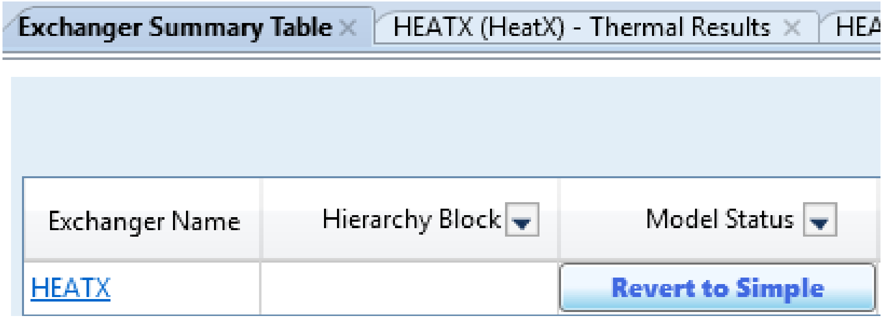
EDR Exchanger Feasibility

Unknown	OK	At Risk
0	0	1

Pressure	Temperature	Vibration	Erosion: RhoV2	Heat Transfer	Pressure Drop
●	●	●	●	●	●

Figure 10.37 Showing the model and risk status, in addition to the legend.

e) You can revert to the simple (i.e., **Shortcut**) method by clicking on "**Revert to Simple**" button as shown in Figure 10.38. Alternatively, in "**Blocks**" | "**HEATX**" | "**Setup**" | "**Specifications**" tab window when results are available for a rigorous exchanger type, you can click on "**Reconcile**" button next to **Constant UA** to switch this block back to a **Shortcut** model using the UA calculated by EDR as a specification.



Exchanger Name	Hierarchy Block	Model Status
HEATX		Revert to Simple

Figure 10.38 Reverting to the simple (**Shortcut**) calculation method.

f) Reynolds number for both sides of exchanger can be seen in EDR navigation panel in "**Thermal/Hydraulic Summary**" | "**Heat Transfer**" | "**Heat Transfer Coefficients**" tab sheet.

> **NOTE #5:** *In general, there is a trade-off between having a higher heat transfer coefficient and a lower pressure drop. This simply means that tightening on the fluid will result in a higher heat transfer coefficient but with a higher pressure drop at the same time. So, the heat transfer can be further improved until we hit the upper limit of pressure drop for both exchanger sides.*

REFERENCES

[1] Perry, P.H. and Green, D., "*Perry's Chemical Engineering Handbook*", 7th ed., 1987, McGraw-Hill Co., New York, USA.

[2] J.M. Coulson and J.F. Richardson with J.R. Backhurst and J. H. Marker, "*Chemical Engineering Fluid Flow, Heat Transfer and Mass Transfer*", Volume 1, 6th ed., 1999, Butterworth and Heinemann, Oxford, UK.

[3] Rajiv Mukherjee, "Effectively Design Shell-and-Tube Heat Exchangers", CHEMICAL ENGINEERING PROGRESS, FEBRUARY 1998. American Institute of Chemical Engineers.

HOMEWORK/CLASSWORK 10.1 (HEAT EXCHANGER WITH PHASE CHANGE)

The process data details used for this homework/classwork are shown in Table 10.1:

TABLE 10.1 Hot and Cold Stream Properties for Methanol and Water Stream, Respectively.

Fluid	Hot Side—Steam 55% and Methanol 45%	Cooling Water	Units
Total flow rate	10.0	80	kg/s
Temperature (in/out)	120/?	35/80	°C
Inlet pressure	1.5	6.5	atm (abs)
Maximum pressure drop[a]	0.5	8.1	psi
Fouling resistance	0.00018	0.00018	$(m^2 \cdot K)/W$

[a] Depending on the selected geometrical configuration, the pressure drop may exceed or go below the indicated maximum values.

Your task is

Design a shell and tube heat exchanger, with the shell side as a condenser containing a mixture of steam and methanol, using water as a coolant. The design calculations will determine the inner diameter of the shell, tube length and diameter, the nozzle sizes, the number of tubes and passes, and the number of baffles and baffle cut. The design logic will optimize the heat transfer against the allowable pressure drop on both the shell and tube sides.

To achieve the proper design, create an Aspen Plus steady-state flowsheet simulation using the Using Aspen Plus, choose "**Specialty Chemicals with Metric Units**" template to create the process flowsheet. The default property model will be "**NRTL**". Add the two components: methanol (CH_3OH) and water (H_2O). Go to "**Methods**" | "**Parameters**" | "**Binary Interaction**" | "**NRTL-1**" sheet and be sure that the "*Estimate missing parameters by UNIFAC*" option is affirmed. Click "**Reset**" followed by "**Next**" button to run the simulation and assure that properties analysis completed successfully. Switch to "**Simulation**" environment.

The flowsheet should contain the heat exchanger unit. Follow the design procedure outlined in the running tutorial of this chapter. You should realize that you have a mixture of steam and methanol where there is a phase change (i.e., partial condensation) for such a binary mixture. Moreover, keep in mind that the heat duty is about 85 times (85×) larger than the heat duty given in the solved example. Hence, consider the multipass option both for shell and tube sides. Run the simulator and be sure that the solver converges to reasonable results with a positive percent over design area factor while satisfying the pressure-drop requirement on both sides of the exchanger. Be sure that the shell-side Reynolds number does not drop below 200.

HOMEWORK/CLASSWORK 10.2 (HIGH HEAT DUTY HEAT EXCHANGER)

The process data details used for this homework/classwork are shown in Table 10.2:

TABLE 10.2 Hot and Cold Stream Properties for Thermalane-600 and Water, Respectively.

Fluid	Hot Side—Thermalane-600	Cooling Water	Units
Total flow rate	300.0	12.0	kg/s
Temperature (in/out)	185/?	25/60	°C
Inlet pressure	4.0	5.0	bar (abs)
Maximum pressure drop[a]	1.5	1.5	psi
Fouling resistance	0.00053	0.00018	$(m^2 \cdot K)/W$

[a] Depending on the selected geometrical configuration, the pressure drop may exceed or go below the indicated maximum values.

<u>Your task is</u>

Design a shell and tube heat exchanger, with the shell side having thermalane-600 and tube side having cooling water. Thermalane-600 is heat transfer oil, used in industrial process heating applications. The design calculations will determine the inner diameter of the shell, tube length and diameter, the nozzle sizes, the number of tubes and passes, and the number of baffles and baffle cut. The design logic will optimize the heat transfer against the allowable pressure drop on both the shell and tube sides.

To achieve the proper design, create an Aspen Plus steady-state flowsheet simulation using the Using Aspen Plus, choose "**Specialty Chemicals with Metric Units**" template to create the process flow sheet. Add the two components: Thermalane-600 (THERMOIL) and water (H_2O). Choose "**NRTL**" as the property method. The flowsheet should contain the heat exchanger unit. Follow the design procedure outlined in the running tutorial of this chapter. However, keep in mind that the heat duty is about 10 times (10×) larger than the heat duty given in the solved example. Hence, consider the multipass option both for shell and tube sides. Run the simulator and be sure that the solver converges to reasonable results with a positive percent over-design area factor while satisfying the pressure-drop requirement on both sides of the exchanger. Be sure that the shell-side Reynolds number does not drop below 200.

HOMEWORK/CLASSWORK 10.3 (DESIGN SPEC HEAT EXCHANGER)

The process data details used for this homework/classwork are shown in Table 10.3:

TABLE 10.3 Hot and Cold Water Stream Properties.

Fluid	Hot Side—Water	Cooling Water	Units
Total flow rate	7000	13 500	kg/h
Temperature (in/out)	95/?	35/55	°C
Inlet pressure	2.0	2.0	bar (abs)
Maximum pressure drop[a]	0.5	0.5	psi
Fouling resistance	0.001	0.001	(hr-ft^2-°F/Btu)

[a] Depending on the selected geometrical configuration, the pressure drop may exceed or go below the indicated maximum values.

Water with a mass flow rate of 13 500 kg/h is heated from 35 to 55°C in a tube and shell heat exchanger. A single pass of water at 7000 kg/h and 95°C is used on the shell side as the heating fluid. Because of space limitations, the heat exchanger must be no longer than 8 ft.

Your task is

Consistent with the aforementioned restriction, design a shell and tube heat exchanger, with the shell side having hot water and tube side cooling water. The design calculations will determine the inner diameter of the shell, tube length and diameter, the nozzle sizes, the number of tubes and passes, and the number of baffles and baffle cut. The design logic will optimize the heat transfer against the allowable pressure drop on both the shell and tube sides.

To achieve the proper design, create an Aspen Plus steady-state flowsheet simulation using the Using Aspen Plus, choose "**Specialty Chemicals with Metric Units**" template to create the process flow sheet. Add the only component: water (H_2O). Choose "**STEAMNBS**" as the property method. The flowsheet should contain the heat exchanger unit. Follow the design procedure outlined in the running tutorial of this chapter. Run the simulator and be sure that the solver converges to reasonable results with a positive percent over-design area factor while satisfying the pressure-drop requirement on both sides of the exchanger. Be sure that the shell-side Reynolds number does not drop below 200.

11

ELECTROLYTES

11.1 PROBLEM DESCRIPTION: WATER DE-SOURING

A sour water stream, which contains 0.20 wt% CO_2, 0.15 wt% H_2S, and 0.1 wt% NH_3 at a temperature of 85°C and pressure of 1 atm with a mass flow rate of 5000 kg/h, is to be treated by a dry steam at 1.1 atm and a mass flow rate of 1500 kg/h. The water polluting compounds will be stripped off the sour water and vented, with some amount of water vapor, off the top of the stripping tower. The sweet water will be withdrawn from the bottom of the stripper with almost nil carbon, nitrogen, and sulfur content. The dry stream, entering from the bottom, will act as the vapor stream within the column; hence, there is no need for a reboiler. On the other end, the rising vapor stream will be substantially condensed and recycled to the top of the column as a liquid reflux, whereas the rest of it will be vented off the top of the tower.

11.2 WHAT IS AN ELECTROLYTE?

In general, an electrolyte system is made of chemical species that can dissociate partially or totally into ions in a polar liquid medium (i.e., solvent). The liquid phase reaction always exists at its chemical equilibrium condition between the associate (i.e., condensed state) and dissociate (i.e., loose or ionic) form. The presence of ions in the liquid phase requires non-ideal solution thermodynamics, where the activity coefficient, in general, is not unity. Some examples of electrolytes are solutions of acids, bases, or salts, sour water solutions, aqueous amines, and hot carbonates. An electrolytic component can be classified under one of the following categories:

- Solvent: the polar medium. Examples are water, methanol, ethanol, and acetic acid.

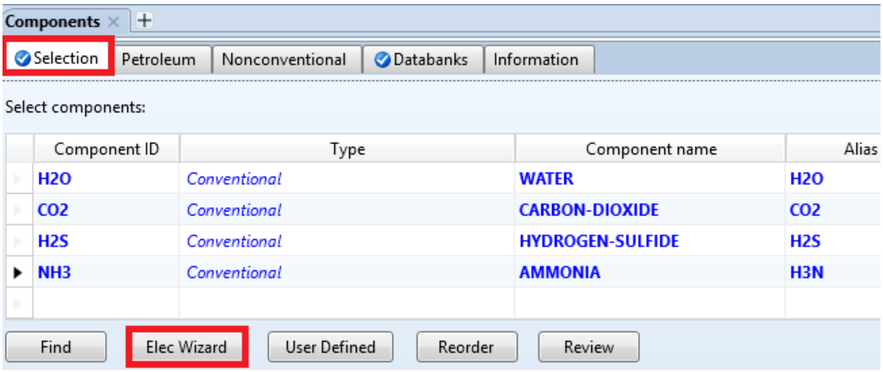
Aspen Plus®: Chemical Engineering Applications, First Edition. Kamal I.M. Al-Malah.

Companion Website: www.wiley.com/go/Al-Malah/AspenPlusApplications

- Soluble Gas: a non-condensable gas where its gas liquid equilibrium (alternatively, its solubility in the given solvent) is described by Henry's law. Examples are N_2, O_2, Cl_2, NH_3, and CO_2.
- Ion: an ionic (cationic or anionic) moiety with a formal charge. Examples are H_3O^+, OH^-, Cl^-, Na^+, $HCO_3{}^-$, $CO_3{}^{-2}$, Ca^{+2}, Fe^{+2}, and Fe^{+3}.
- The condensed (aggregate) matter: this form represents the associate (lattice) form of an ionic substance, which can exist in either solid (e.g., salt) or liquid form. Examples are $NaCl_{(s)}$, $NaOH_{(s)}$, $H_2SO_{4(l)}$, $HCOOH_{(l)}$, $CH_3CH_2COOH_{(l)}$, $CaCO_{3(s)}$, $CaSO_4\bullet 2H_2O_{(s)}$, $K_2SO_{4(s)}$, $Na_2HPO_{4(s)}$, and $NaHCO_3\bullet 2H_2O_{(s)}$.

11.3 THE PROPERTY METHOD FOR ELECTROLYTES

Using Aspen Plus®, choose "**Electrolytes with Metric Units**" template to create the process flowsheet. The default property model is "**ELECNRTL**". By default, water is added to the "**Components**" list. Add the three components: CO_2, H_2S, and NH_3, as shown in Figure 11.1.



Select components:

Component ID	Type	Component name	Alias
H2O	Conventional	WATER	H2O
CO2	Conventional	CARBON-DIOXIDE	CO2
H2S	Conventional	HYDROGEN-SULFIDE	H2S
NH3	Conventional	AMMONIA	H3N

Figure 11.1 Entering the three components: CO_2, H_2S, and NH_3, in addition to H_2O.

However, we will show here how to properly define each component as part of the electrolyte system.

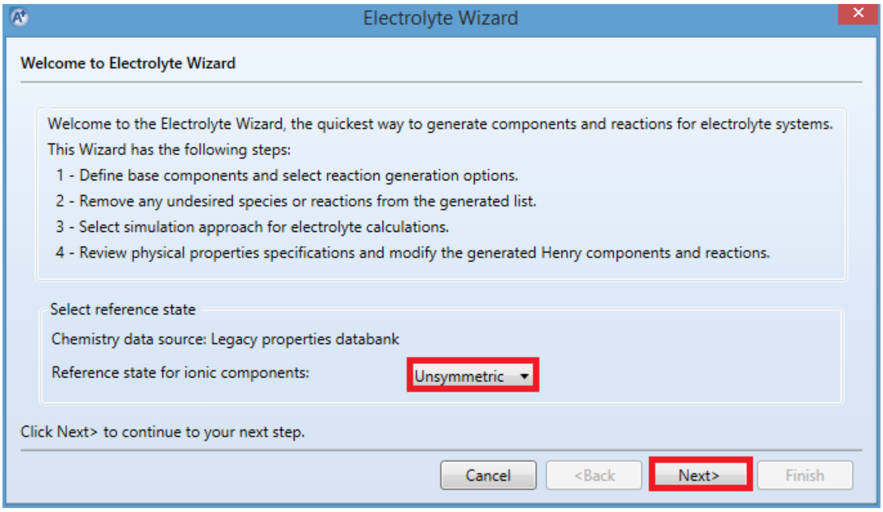
11.4 THE ELECTROLYTE WIZARD

In "**Components**" | "**Specifications**" | "**Selection**" tab window, click on "**Elec Wizard**" button (shown in Figure 11.1). This will bring the first "**Electrolyte Wizard**" window where the user can choose between symmetric and unsymmetric reference state for ionic components.

- For the unsymmetric reference state of ions, the equilibrium constants are calculated from the reference state Gibbs free energies of the participating components. Activity coefficients of ions are based on infinite dilution in pure water. We must have already defined water as a component to use electrolyte wizard for this case.

- For the symmetric reference state of ions, the equilibrium constants are not automatically calculated, and must either be entered here or regressed from data. Activity coefficients of ions are based on pure fused salts. Water is not necessary (though it may be included as a solvent).

We will choose the unsymmetric reference state for ionic components, as it does not require any further input about the equilibrium constants as functions of temperature for the dissociation reactions, as shown in Figure 11.2. See the appendix at the end of this chapter for more information on the development of electrolyte NRTL ("**ELECNRTL**") property model.



Welcome to the Electrolyte Wizard, the quickest way to generate components and reactions for electrolyte systems.
This Wizard has the following steps:
1 - Define base components and select reaction generation options.
2 - Remove any undesired species or reactions from the generated list.
3 - Select simulation approach for electrolyte calculations.
4 - Review physical properties specifications and modify the generated Henry components and reactions.

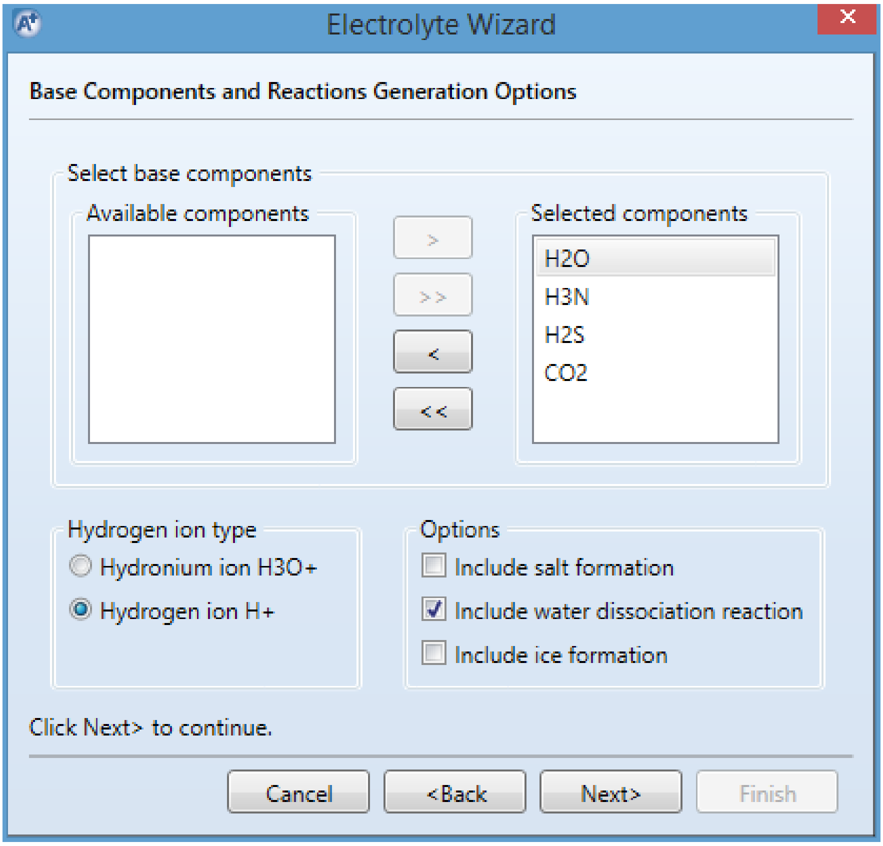
Select reference state
Chemistry data source: Legacy properties databank
Reference state for ionic components: Unsymmetric

Click Next> to continue to your next step.

Figure 11.2 The selection between "*Symmetric*" and "*Unsymmetric*" reference state for ionic components. The "*Unsymmetric*" option does not require further input for equilibrium constants.

Click on "**Next**" button to proceed to the next step.

Figure 11.3 shows the second "**Electrolyte Wizard**" window where the user selects what components to include in the electrolyte system. All components are selected to participate in the electrolytic scene. Moreover, the user may select/deselect the appropriate option and how hydrogen ion should be expressed.



Electrolyte Wizard

Base Components and Reactions Generation Options

Select base components

Available components

Selected components

H2O

H3N

H2S

CO2

Hydrogen ion type

○ Hydronium ion H3O+

● Hydrogen ion H+

Options

☐ Include salt formation

☑ Include water dissociation reaction

☐ Include ice formation

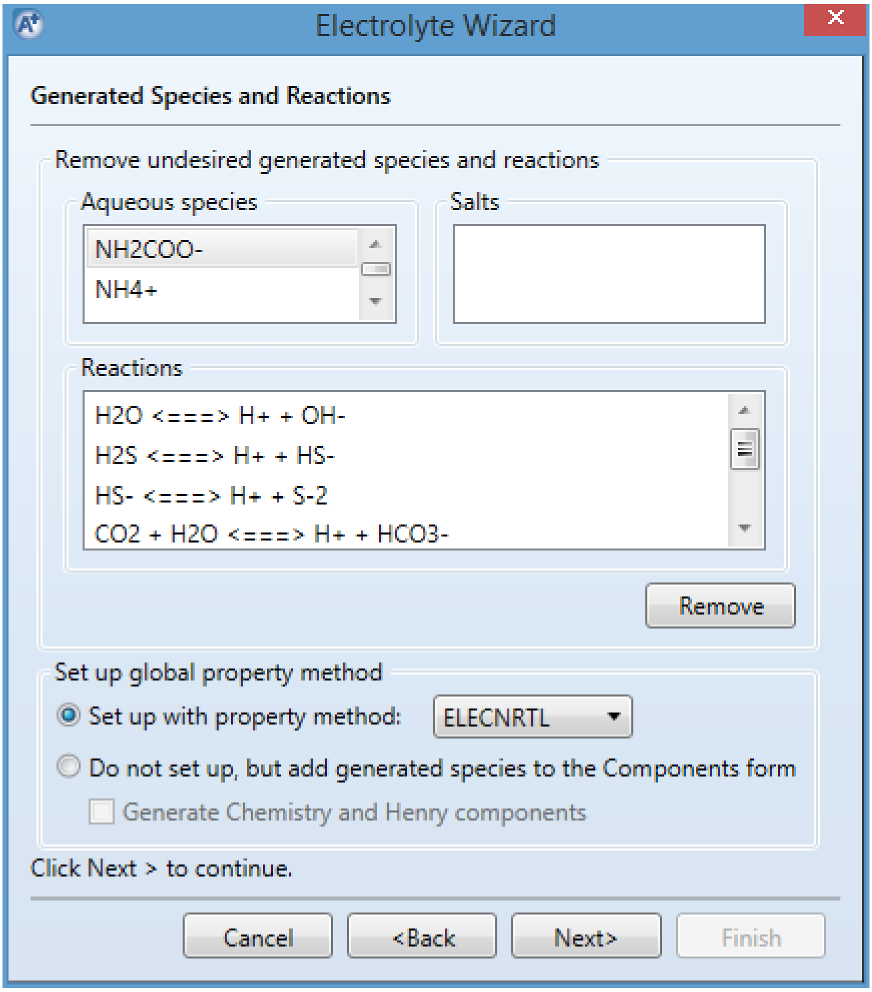
Click Next> to continue.

Figure 11.3 Selection of chemical species that are thought to participate in the electrolytic arena.

NOTE #1: *It is a multifaceted decision, made by the user, to decide what to include in the list of participating players in the electrolytic portray and the extent of participation each player will do, in addition to the interplay between one player and another. Precisely speaking, let us take* CO_2 *species as an example. We have to decide first whether or not to include* CO_2 *in the first place. If the decision is yes for considering* CO_2 *as an important electrolytic player, then we will have to decide on the assigned task for this player, that is, telling Aspen Plus what reactions are associated with this chemical species. Shall we consider its dissociation into water in the form of* HCO_3^- *only? Or, shall we consider further dissociation of* HCO_3^- *into* CO_3^{-2}*? Finally, what about the interplay between* HCO_3^- *and* NH_3*? Keep in mind that the more reactions you add to the electrolytic portray, the more complex the picture will be (or, longer CPU time), which may end up under some circumstances in a non-converging solution, (i.e., errors reported by Aspen Plus simulator), because of missing some pairwise interactions, which need to be plugged in by the user. If it happens that Aspen Plus fails to converge, then you may attempt to remove what you think is the least important electrolytic player (i.e., chemical reaction/species).*

Click on “**Next**” button to proceed to the next step.

Figure 11.4 shows the third "**Electrolyte Wizard**" window where Aspen Plus provides a list of potential reactions based on the stand-alone or interplay role of each of the chemical players nominated in the previous step.



Generated Species and Reactions

Remove undesired generated species and reactions

Aqueous species:
NH2COO-
NH4+

Reactions:
$H_2O \Longleftrightarrow H^+ + OH^-$
$H_2S \Longleftrightarrow H^+ + HS^-$
$HS^- \Longleftrightarrow H^+ + S^{-2}$
$CO_2 + H_2O \Longleftrightarrow H^+ + HCO_3^-$

Set up global property method

● Set up with property method: ELECNRTL

○ Do not set up, but add generated species to the Components form

☐ Generate Chemistry and Henry components

Click Next > to continue.

Figure 11.4 The "**Generated Species and Reaction**" list that provides the user with the possible reactions, based on the participation of a single- or team-player of each of the chemical players nominated in the previous step.

Notice that the user may select to remove one or more of ionic species that are listed and Aspen Plus will remove the corresponding reaction(s). Of course, the decision will be based on experimental observations that a particular ionic species is absent or its presence in the aqueous medium can be neglected.

Alternatively, the user may directly remove a specific reaction out of those suggested by Aspen Plus, with the understanding that this reaction contributes little or nothing to the electrolytic portray and thus can be neglected. In other words, at a given pH, the pK_a/pK_b will tell the user if the dissociation extent for an acid/base is significant or can be ignored. We will proceed without removing any chemical species or chemical reaction.

Moreover, the third “**Electrolyte Wizard**” window (Figure 11.4) allows the user to stick to the default (“**ELECNRTL**”) method or change to “**ENRTL-RK**” method. The “**ELECNRTL**” property method will be selected as it is the most versatile electrolyte property method. Both methods, however, can be used in our case.

NOTE #2: *Electrolyte solutions are extremely non-ideal because of the presence of charged species. The electrolyte-NRTL-based property methods: “**ELECNRTL**”, “**ENRTL-RK**”, and “**ENRTL-SR**” can all handle mixed-solvent systems at any concentration. The “**ELECNRTL**” property method is the most versatile electrolyte property method. It can handle very low and very high concentrations. It can handle aqueous and mixed-solvent systems as well. The “**ELECNRTL**” is fully consistent with the “**NRTL-RK**” property method (i.e., the molecular interactions are calculated exactly the same way; therefore, “**ELECNRTL**” can inherit from the databank for binary molecular interaction parameters of the “**NRTL-RK**” property method).*

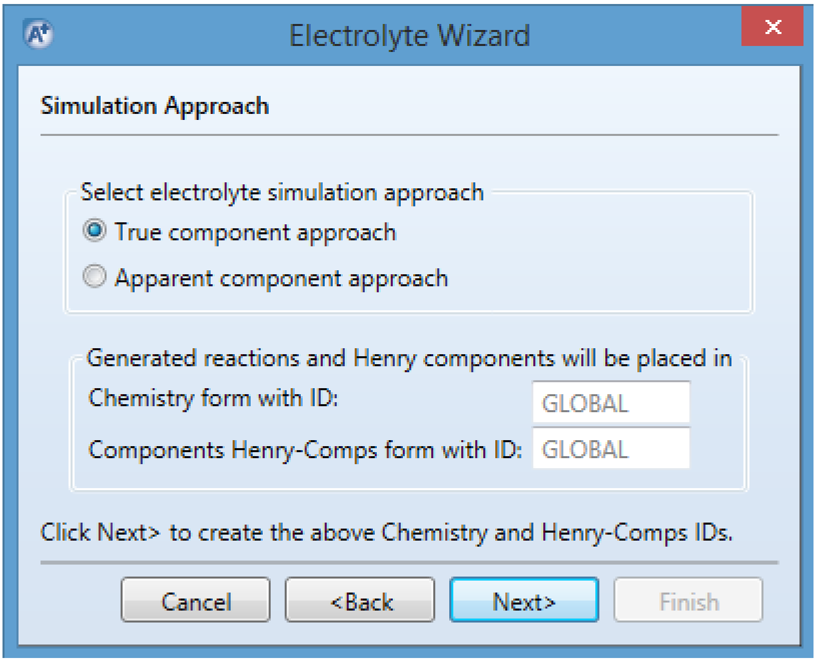
On the other hand, the solubility of supercritical gases can be modeled using Henry’s law. Henry coefficients are available from the databank. Heats of mixing are calculated using “**ELECNRTL**” *model.*

Moreover, the “**ENRTL-RK**” *method is identical to* “**ELECNRTL**” *for systems containing a single electrolyte. However, for mixed-electrolyte systems, the* “**ENRTL-RK**” *method uses the mixing rules only to calculate pairwise interaction parameters, instead of calculating both pairwise interaction parameters and Gibbs free energy from mixing rules. Furthermore, the* “**ENRTL-RK**” *uses a single thermodynamics framework to calculate the activity coefficients, Gibbs free energy, and enthalpy, instead of using separate models as in* “**ELECNRTL**”.

Finally, “**ENRTL-RK**” *uses the Redlich–Kwong equation of state for all vapor-phase properties, except for association behavior in the vapor phase; the unsymmetric reference state (infinite dilution in aqueous solution) for ionic species; Henry’s law for solubility of supercritical gases; and unsymmetric Electrolyte NRTL method of handling zwitterions.*

Click on “**Next**” button to proceed to the next step.

The fourth “**Electrolyte Wizard**” window will show up as shown in Figure 11.5, where the user is given the choice to select between *true*- and *apparent*-component approaches. The difference in the approaches lies in the level of technical details on how Aspen Plus shall present the results of calculation of electrolyte solution properties. The “**True component approach**”, I call it the chemist’s approach, reports results in terms of the ions, salts, and molecular species present (i.e., showing the details of solution chemistry). On the other hand, the “**Apparent component approach**”, I call it the chemical engineer’s approach, reports results in terms of base components present without showing the details of solution chemistry. In the latter approach, ions and precipitated salts cannot be apparent components; specifications must be expressed in terms of apparent components and not in terms of ions or solid salts. Of course, results of both approaches are equivalent. Let us take a simple example, that is, *NaCl* in water.



Simulation Approach

Select electrolyte simulation approach

● True component approach

○ Apparent component approach

Generated reactions and Henry components will be placed in

Chemistry form with ID: GLOBAL

Components Henry-Comps form with ID: GLOBAL

Click Next> to create the above Chemistry and Henry-Comps IDs.

Figure 11.5 The selection is made between the true- and apparent-component approaches.

a) For the "**True component approach**" (i.e., showing solution chemistry):

$$NaCl_{(s)} \overset{H_2O}{\Longleftrightarrow} Na^+ + Cl^-$$

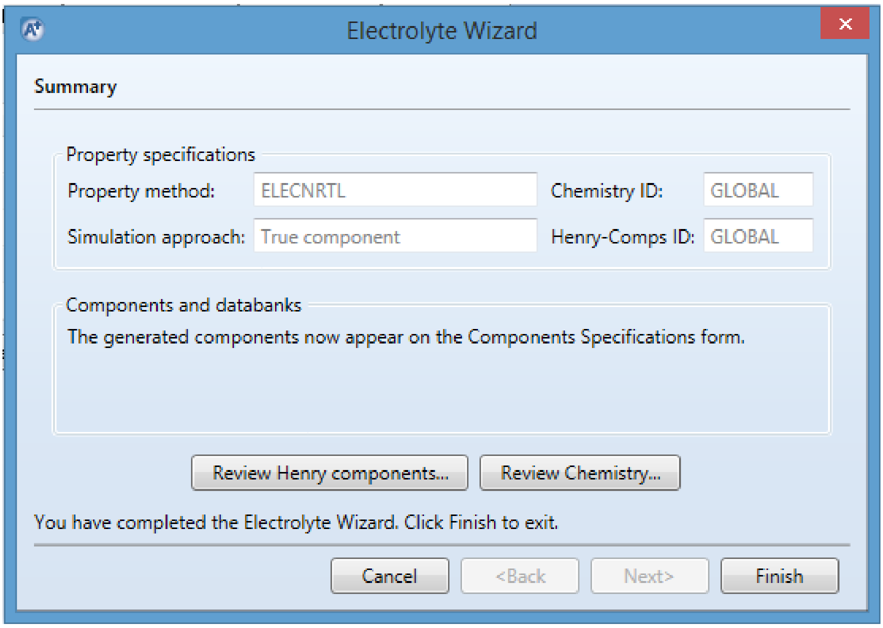
$$Na^+ + Cl^- \leftrightarrow NaCl_{(s)}$$

Results are thus reported in terms of Na^+, Cl^-, $NaCl_{(s)}$, and H_2O.

b) For the "**Apparent component approach**" (i.e., hiding the solution chemistry), the results are reported in terms of *NaCl (Conventional) and* H_2O *only*.

Click on "**Next**" button to proceed to the next step. The "**Update Parameters**" window will pop up requesting to update the form parameters (i.e., list of components). Click on "**Yes**" button to proceed. You may have to click more than once.

Figure 11.6 shows the fifth "**Electrolyte Wizard**" window summarizing what the user has already selected in previous steps and giving the chance to review and modify the chemistry of the electrolyte system under study.



Summary

Property specifications

Property method: ELECNRTL

Chemistry ID: GLOBAL

Simulation approach: True component

Henry-Comps ID: GLOBAL

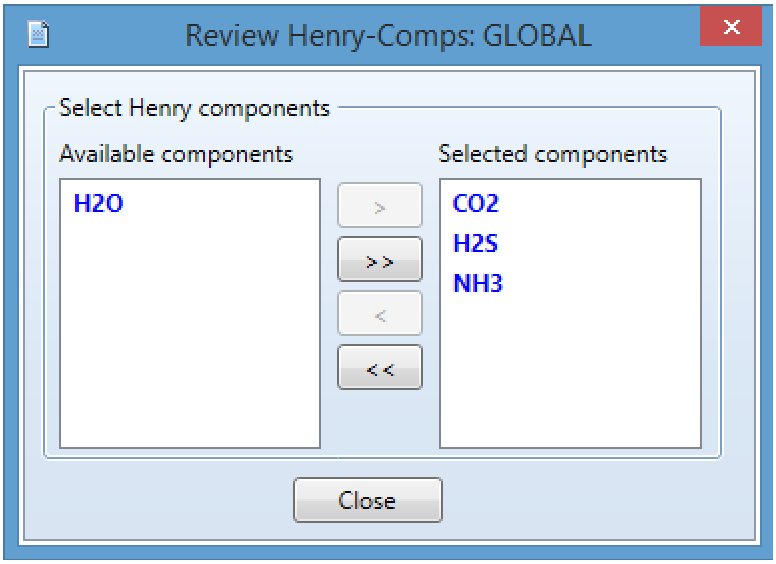
Components and databanks

The generated components now appear on the Components Specifications form.

You have completed the Electrolyte Wizard. Click Finish to exit.

Figure 11.6 The fifth "**Electrolyte Wizard**" window, where the user may review/modify the components that will obey Henry's law in determining its solubility in the given medium and also modify the list of electrolytic equilibrium reactions.

The user ought to click on "**Review Henry components** … " button to review the list of components that should be dealt with as Henry's case (Figure 11.7). Alternatively, Henry's



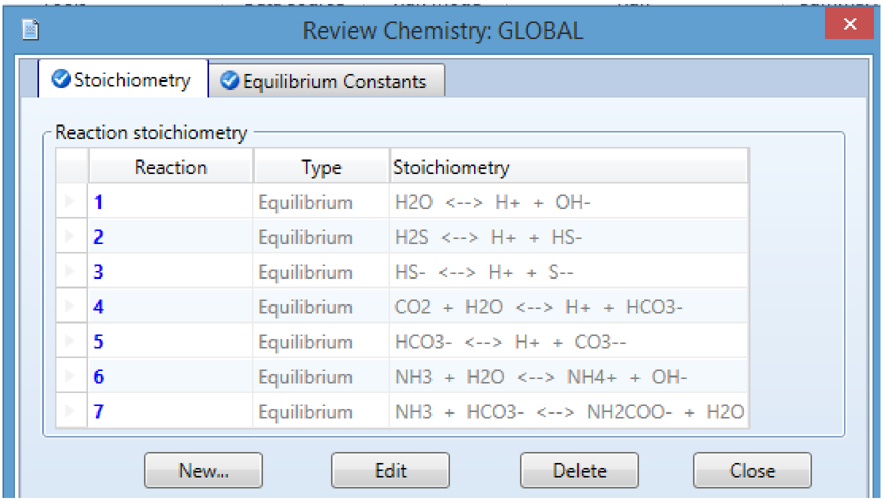
Available components: H2O

Selected components: CO2, H2S, NH3

Figure 11.7 The list of the three solutes to obey Henry's law, which are considered non-condensable gases at the given pressure and temperature.

set can been seen via visiting “**Components**” | “**Henry Comps**” | “**Global**” | “**Selection**” tab form.

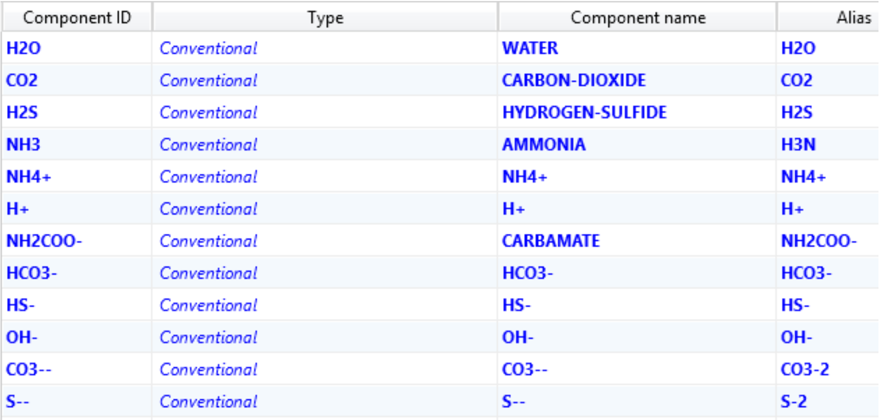
On the other hand, the user may click on “**Review Chemistry** … ” button to see the list of electrolytic equilibrium reactions, which are considered important players in the arena of the given electrolytic system (Figure 11.8). The user may edit, modify, or delete a given reaction and/or add a new one. Alternatively, the user may later go to “**Chemistry**” | “**GLOBAL**” | “**Input**” | “**Chemistry**” tab window and modify them from there. Moreover, if you click on “**Equilibrium Constants**” tab (the second tab in Figure 11.8), you will notice that Aspen Plus has already taken care of calculating the equilibrium constant, K_{eq}, for each electrolytic equilibrium reaction.



Reaction	Type	Stoichiometry
1	Equilibrium	H2O <--> H+ + OH-
2	Equilibrium	H2S <--> H+ + HS-
3	Equilibrium	HS- <--> H+ + S--
4	Equilibrium	CO2 + H2O <--> H+ + HCO3-
5	Equilibrium	HCO3- <--> H+ + CO3--
6	Equilibrium	NH3 + H2O <--> NH4+ + OH-
7	Equilibrium	NH3 + HCO3- <--> NH2COO- + H2O

Figure 11.8 The list of equilibrium-type reactions, which are considered important in making up the electrolytic picture.

Click on “**Finish**” button (Figure 11.6) to close the wizard. Figure 11.9 shows that, under “**Components**” list, more chemical species are added, reflecting the types of ionic species that are considered important in portraying the electrolytic picture, as agreed upon earlier in Figure 11.4.



Component ID	Type	Component name	Alias
H2O	Conventional	WATER	H2O
CO2	Conventional	CARBON-DIOXIDE	CO2
H2S	Conventional	HYDROGEN-SULFIDE	H2S
NH3	Conventional	AMMONIA	H3N
NH4+	Conventional	NH4+	NH4+
H+	Conventional	H+	H+
NH2COO-	Conventional	CARBAMATE	NH2COO-
HCO3-	Conventional	HCO3-	HCO3-
HS-	Conventional	HS-	HS-
OH-	Conventional	OH-	OH-
CO3--	Conventional	CO3--	CO3-2
S--	Conventional	S--	S-2

Figure 11.9 Ionic species are added to the list of components, based on the types of chemical reactions depicting the electrolytic picture.

From "**Navigation**" pane, you will notice that there are half-filled red circles, which means that they require either more input data or parameter estimation. Click on "**Next**" button more than once until you get rid of all red signs and the Aspen Plus sky becomes clear blue. Assure that the missing pairwise interaction parameters can be calculated by "**UNIFAC**" method. Once the properties analysis completed successfully, switch to "**Simulation**" environment.

NOTE #3: *You may end up having a warning such as in the following "**Control Panel**" message:*

```
WARNING IN PHYSICAL PROPERTY SYSTEM
      PROP-NAME RENON FOR COMPONENT PAIR H2O AND NH4+
      CANNOT BE ESTIMATED USING THE UNIFAC METHOD AS SPECIFIED
      BECAUSE OF MISSING INPUT PARAMETERS:
         STRUCTUR, GMUFR   , GMUFQ
```

*This should not be a serious warning and it can be ignored. In fact, after you get such a type of warning, if you click on "**Next**" button while in "**Properties**" environment, you will be prompted by the "**Properties Analysis/Setup Complete**" dialog window telling you that properties analysis and setup completed successfully.*

11.5 WATER DE-SOURING PROCESS FLOWSHEET

From "**Model Palette**" select "**Columns**" tab. Go to "**RadFrac**" subcategory and select the icon that shows a column with a condenser but without a reboiler, as shown in Figure 11.10. If the mouse hovers over the column icon, the tooltip will tell that it is "**RECT**" type column. Add the proper input and output streams. Notice that the distillate will be the top vented off sour vapor stream and the bottom will be the sweet liquid water stream. Two feeds are used: one for the sour water stream that enters into the top and another enters into the bottom as a saturated dry steam.

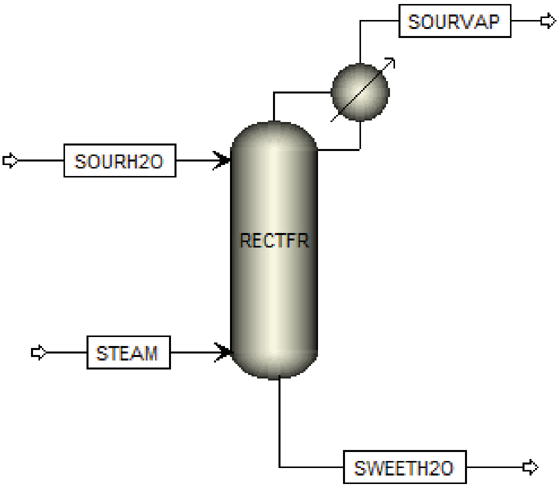
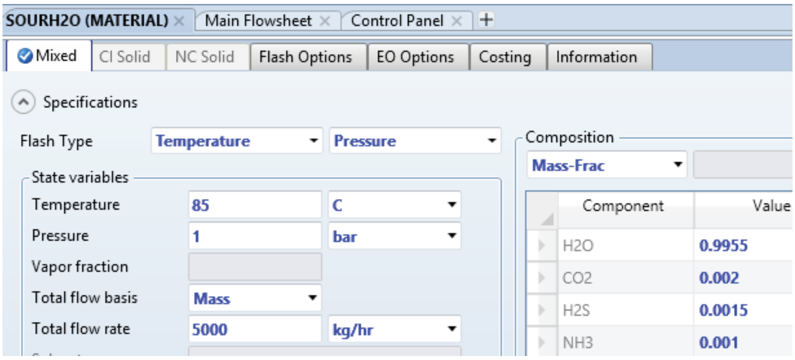


Figure 11.10 De-souring of sour water stream using the dry steam as the stripping agent.

It is worth mentioning here that there might be more than one school in describing what a stripper means as opposed to a scrubber. I refer to Wang *et al*. [1] in defining the stripping condition: "It is a stripping process if (1) the gas stream is the scrubbing agent (such as air with or without gaseous chemicals depending on the waterborne pollutants to be removed) and (2) the liquid stream contains the targeted pollutant (such as ammonia, chlorine, and VOCs) that will be removed by the reactor". Notice that how they describe the gas stream as the scrubbing agent, not the stripping, although the phrase is inserted within the definition of a stripping process. We will go with describing the removal of pollutants from a liquid by a dry steam as stripping process.

11.6 ENTERING THE SPECIFICATIONS OF FEED STREAMS AND THE STRIPPER

Figure 11.11 shows the input properties of "**SOURH2O**" feed stream.



Flash Type: Temperature, Pressure

State variables

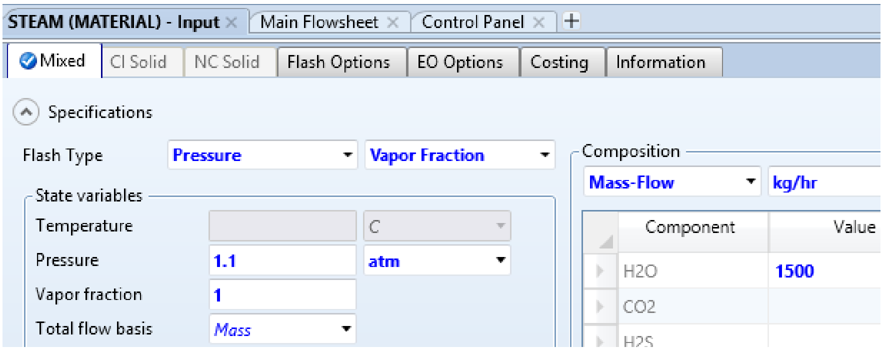
Temperature	85	C
Pressure	1	bar
Vapor fraction		
Total flow basis	Mass	
Total flow rate	5000	kg/hr

Composition: Mass-Frac

Component	Value
H2O	0.9955
CO2	0.002
H2S	0.0015
NH3	0.001

Figure 11.11 Properties of "**SOURH2O**" feed stream in terms of T, P, and composition.

Figure 11.12 shows the input properties of “**STEAM**” feed stream.



Flash Type: Pressure, Vapor Fraction

State variables

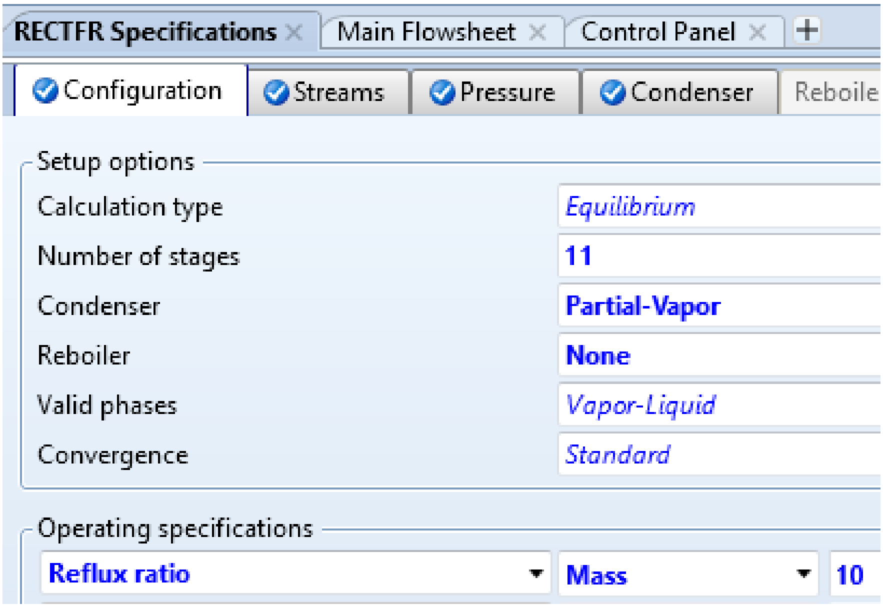
Temperature		C
Pressure	1.1	atm
Vapor fraction	1	
Total flow basis	Mass	

Composition: Mass-Flow, kg/hr

Component	Value
H2O	1500
CO2	
H2S	

Figure 11.12 Properties of “**STEAM**” feed stream in terms of *P*, vapor fraction, and flow rate.

Figure 11.13 shows the Stripper’s specification starting with the “**Configuration**” tab window. A partial vapor condenser is used and there is no need for a reboiler, because we have the steam acting as the vapor phase within the column. We have chosen 11 trays and a reflux mass ratio of 10.



Setup options

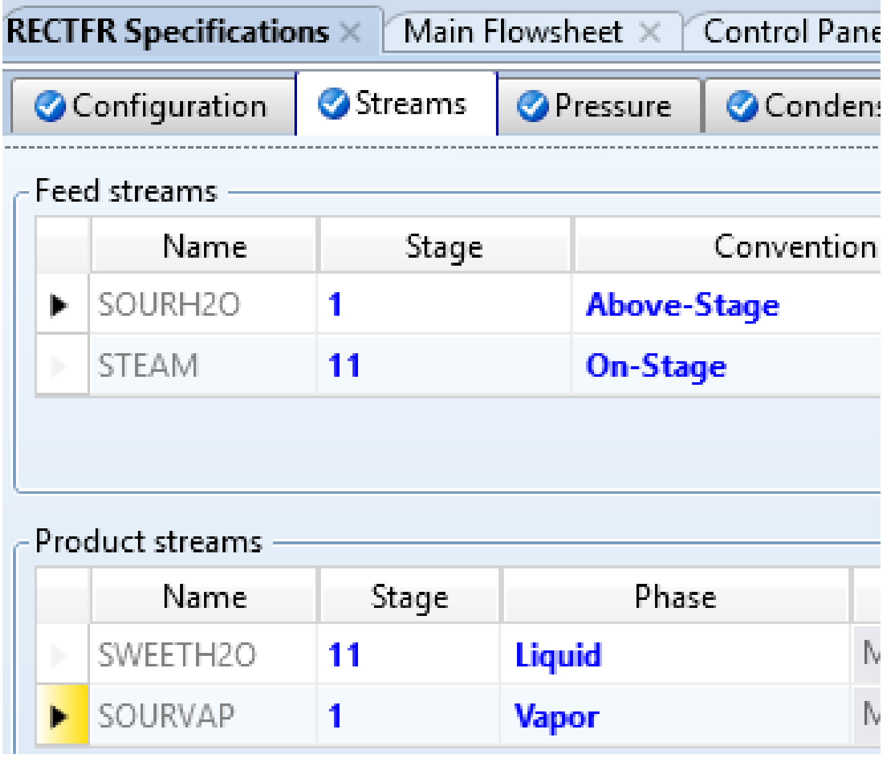
Calculation type	Equilibrium
Number of stages	11
Condenser	Partial-Vapor
Reboiler	None
Valid phases	Vapor-Liquid
Convergence	Standard

Operating specifications

Reflux ratio, Mass, 10

Figure 11.13 The number of trays, type of condenser, and the mass reflux ratio are assigned for the rectifying column (i.e., stripper).

Figure 11.14 shows the feed and product stream locations. The sour water stream enters into the top above stage #1 and the dry steam enters into the bottom as vapor.



Feed streams

Name	Stage	Convention
SOURH2O	1	Above-Stage
STEAM	11	On-Stage

Product streams

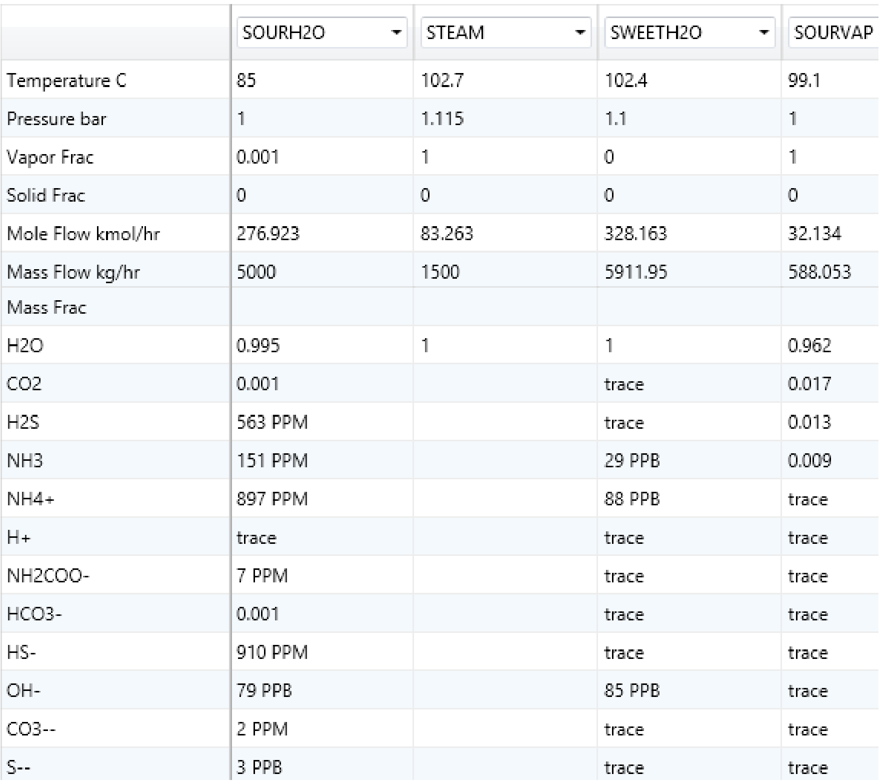
Name	Stage	Phase
SWEETH2O	11	Liquid
SOURVAP	1	Vapor

Figure 11.14 The location of feed and product streams with sour water at the top and dry steam at the bottom of the stripper.

For the “**Pressure**” tab window, the pressure at the condenser is set to 1 bar with a column pressure drop set to *0.1 bar*. For the “**Condenser**” tab window, both reflux and distillate are set at *0* degrees subcooled temperature, which means that both reflux and distillate exist at the equilibrium saturation temperature and pressure; however, the reflux will be saturated liquid mixture and “**SOURVAP**” will be withdrawn as saturated vapor mixture.

Reinitialize, run the show, and watch if there is any error or serious warning.

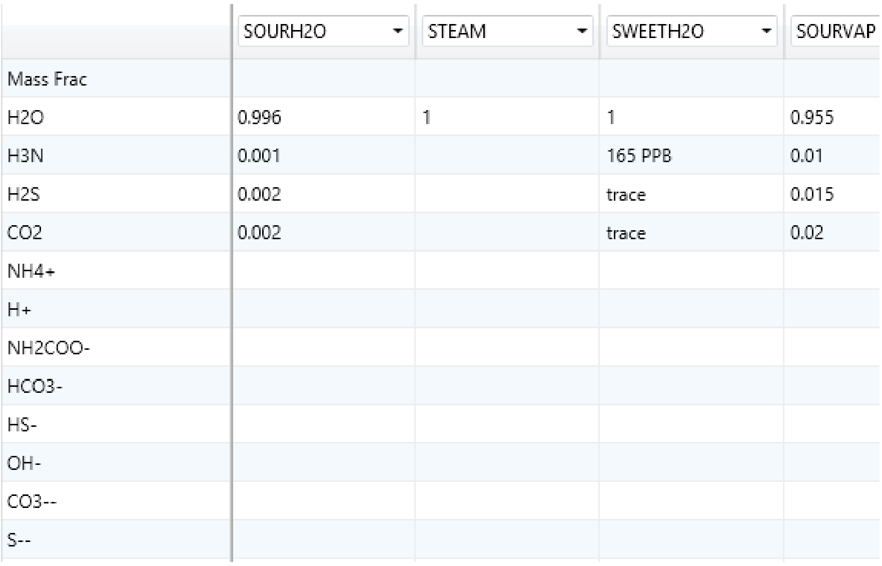
Figure 11.15 shows the composition of product streams where the contaminants were completely removed off the sour water stream and knocked out into the vapor stream. One more important thing, which is, with the “**True component approach**” option being selected (see Figure 11.5), the concentration for each ionic species is also shown here.



	SOURH2O	STEAM	SWEETH2O	SOURVAP
Temperature C	85	102.7	102.4	99.1
Pressure bar	1	1.115	1.1	1
Vapor Frac	0.001	1	0	1
Solid Frac	0	0	0	0
Mole Flow kmol/hr	276.923	83.263	328.163	32.134
Mass Flow kg/hr	5000	1500	5911.95	588.053
Mass Frac				
H2O	0.995	1	1	0.962
CO2	0.001		trace	0.017
H2S	563 PPM		trace	0.013
NH3	151 PPM		29 PPB	0.009
NH4+	897 PPM		88 PPB	trace
H+	trace		trace	trace
NH2COO-	7 PPM		trace	trace
HCO3-	0.001		trace	trace
HS-	910 PPM		trace	trace
OH-	79 PPB		85 PPB	trace
CO3--	2 PPM		trace	trace
S--	3 PPB		trace	trace

Figure 11.15 The composition of the product streams showing that the contaminants were completely removed off the sour-water stream. The concentration for each ionic species is also shown using the "**True component approach**" option.

On the other hand, all previous steps can be repeated except for one thing, which is, selecting "**Apparent component approach**" instead of "**True component approach**" option shown in Figure 11.5. Doing so will end up with results similar to Figure 11.15 but this time only the non-ionic species concentrations are shown, as can be seen in Figure 11.16. Notice that the stream flow rates and operating conditions are the same as those of "**True component approach**" option.



	SOURH2O	STEAM	SWEETH2O	SOURVAP
Mass Frac				
H2O	0.996	1	1	0.955
H3N	0.001		165 PPB	0.01
H2S	0.002		trace	0.015
CO2	0.002		trace	0.02
NH4+				
H+				
NH2COO-				
HCO3-				
HS-				
OH-				
CO3--				
S--				

Figure 11.16 The composition of the product streams showing that the contaminants were completely removed off the sour water stream. The concentration of any ionic species is not shown using the "**Apparent component approach**" option. The stream flow rates and operating conditions are the same as those shown in Figure 11.15.

REFERENCES

[1] Wang, Lawrence K., Pereira, Norman C., Hung, Yung-Tse, "*Air Pollution Control Engineering*", Springer Science & Business Media, LLC, New York, (2004), 276.

[2] Chen, C.-C., Britt, H.I., Boston, J.F., and Evans, L.B. (1982) Local compositions model for excess Gibbs energy of electrolyte systems: part I: single solvent, single completely dissociated electrolyte systems. *AIChE Journal*, **28** (4), 588–596.

[3] Chen, C.-C. and Evans, L.B. (1986) A local composition model for the excess Gibbs energy of aqueous electrolyte systems. *AIChE Journal*, **32** (3), 444–459.

[4] Mock, B., Evans, L.B. and Chen, C.-C. Phase equilibria in multiple-solvent electrolyte systems: a new thermodynamic model. Proceedings of the 1984 Summer Computer Simulation Conference, p. 558–562 (1984), held in Boston, Massachusetts, USA.

[5] Mock, B., Evans, L.B., and Chen, C.-C. (1986) Thermodynamic representation of phase equilibria of mixed-solvent electrolyte systems. *AIChE Journal*, **32** (10), 1655–1664.

[6] Eisa, O. and Shuhaimi, M. (2010) Thermodynamic study of hot potassium carbonate solution using Aspen Plus. *World Academy of Science, Engineering and Technology*, **4** (2), 221–225.

HOMEWORK/CLASSWORK 11.1 (AN ACIDIC SLUDGE NEUTRALIZATION)

Consider the treatment of H_2SO_4-containing wastewater by lime solution, as shown in Figure 11.17.

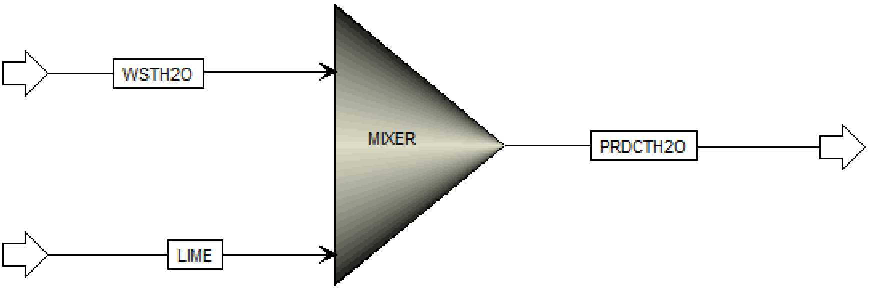


Figure 11.17 Treatment of H_2SO_4-containing wastewater by lime solution.

Using Aspen Plus, choose “**Electrolytes with Metric Units**” template to create the process flow sheet. The default property model is “**ELECNRTL**”. By default, water is added to the “**Components**” list. Enter the additional two components: $Ca(OH)_2$ and H_2SO_4 to the list of components. With the support of the Electrolyte Wizard, use the unsymmetric reference of state for ionic components to analyze such an electrolytic system. Include salt formation and water dissociation reaction (see Figure 11.3) in your analysis. Remove the solid salt $Ca(OH)_{2(s)}$ from the “**Salts**” column (see Figure 11.4) and keep other generated salts. Use the “**True component approach**” option (see Figure 11.5). There will be no component obeying Henry’s law. Finish dealing with the Electrolyte Wizard. You will have all possible ionic species appear in “**Components**” list.

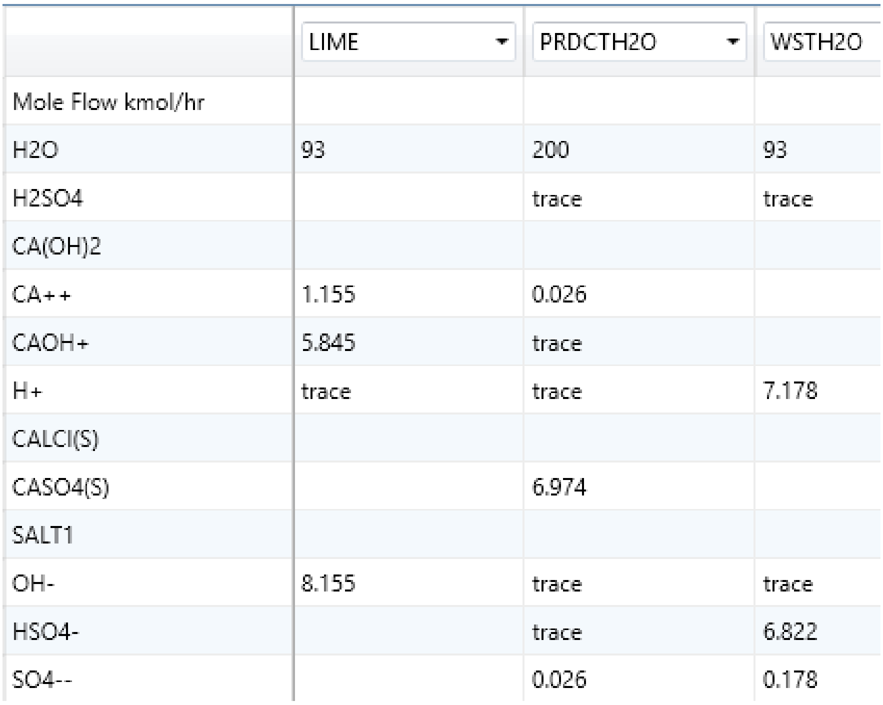
From “**Navigation**” pane, you will notice that there are half-filled red circles, which means that they require more parameter estimation. Click on “**Next**” button more than once until you get rid of all red signs and the Aspen Plus sky becomes clear blue. Once the properties analysis completed successfully, switch to “**Simulation**” environment.

The molar flow rate of wastewater stream is 100 (kmol/h) with 7 mol% H_2SO_4. It enters the mixer at room temperature and pressure. So is the case with lime solution that has the same molar flow rate, pressure, and temperature, but with 7 mol% $Ca(OH)_2$.

After entering all the required input data (i.e., all half-filled red circles disappear from “**Navigation**” pane), reinitialize, run the show, and watch out any simulation serious warning or error (if any).

Report the output product (“**PRDCTH2O**”) stream both on a molar and mass basis.

Figure 11.18 shows typical results for the treatment process.



	LIME	PRDCTH2O	WSTH2O
Mole Flow kmol/hr			
H2O	93	200	93
H2SO4		trace	trace
CA(OH)2			
CA++	1.155	0.026	
CAOH+	5.845	trace	
H+	trace	trace	7.178
CALCI(S)			
CASO4(S)		6.974	
SALT1			
OH-	8.155	trace	trace
HSO4-		trace	6.822
SO4--		0.026	0.178

Figure 11.18 The molar flow rate and composition of the feed and product streams.

Answer the following questions:

a) The water flow rate in the product stream is 200 (kmol/h), whereas the sum of inlet water is 186 (kmol/h); where did this excess amount of water come from?

b) What is the main solid precipitate in the product stream?

c) What is the name of the dissolved salt in the product stream?

d) Is the principle of electrical neutrality (the summation of formal charges should add up to zero) violated in any stream?

e) Given that the molar flow rate of both feed streams is entered as 100 (kmol/h); nevertheless, Figure 11.18 shows that the molar flow rate for either stream is different from 100 (kmol/h), is there anything wrong with Aspen Plus calculations?

f) Under **Properties | Prop-Sets**, define a new property set that enables the user to see the pH of a given stream both at 25°C and stream temperature. What will be the pH for each stream? Which of the streams does have a negative pH? Is it possible to have a negative pH? Does pH increase or decrease with temperature?

HOMEWORK/CLASSWORK 11.2 (CO_2 REMOVAL FROM NATURAL GAS)

Hot potassium carbonate process is an important technology that is used for CO_2 removal from natural gas streams using the chemical absorption method. The chemical solvent normally contains (20–40) wt% potassium carbonate, (1–3) wt% DEA activator, and (0.4–0.7) wt% V_2O_5 corrosion inhibitor. The normal operation conditions of CO_2 absorption process is pressure range (1–2 atm) and temperature range (70–140°C) as reported by

Eisa and Shuhaimi [6]. Consider the flowsheet shown in Figure 11.19, where a “**RadFrac**” type absorption column is used with no condenser and no reboiler. The hot potassium carbonate (“**HPC**”) stream enters at the top with a mass flow rate of 300 kg/h, a mass composition of 70% H_2O and 30% K_2CO_3, $P = 8$ bar, and $T = 100°C$. The natural gas (“**FEED**”) stream enters the column from the bottom with a mass flow rate of 500 kg/h, a mass composition of 96% CH_4 and 4% CO_2, $P = 9$ bar, and $T = 100°C$.

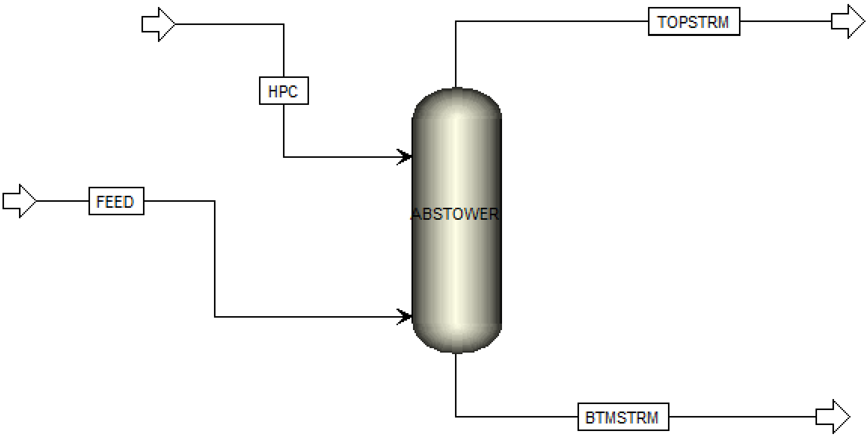
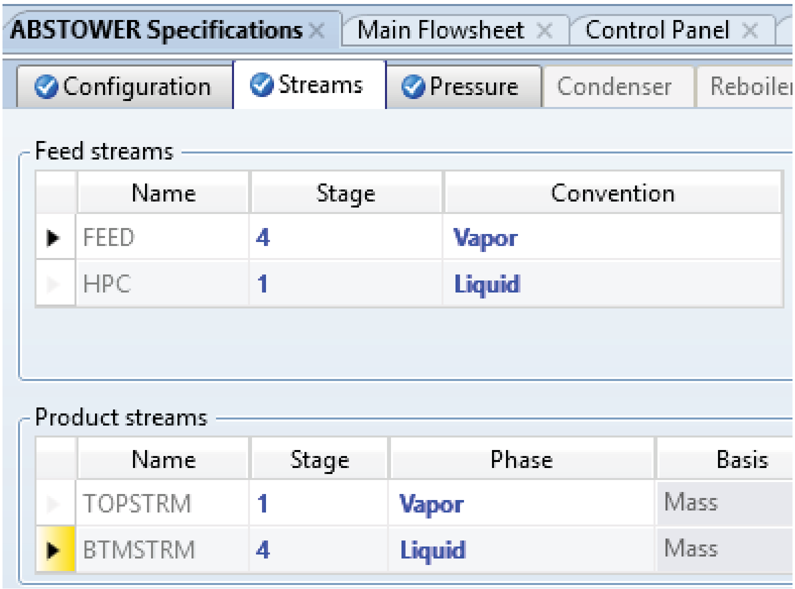


Figure 11.19 Removal of CO_2 from natural gas using potassium carbonate solution as the liquid scrubber.

Using Aspen Plus, choose “**Electrolytes with Metric Units**” template to create the process flowsheet. The default property model is “**ELECNRTL**”. By default, water is added to the “**Components**” list. Enter the additional three components: K_2CO_3, CH_4, and CO_2 to the list of components. With the support of the Electrolyte Wizard, use the unsymmetric reference of state for ionic components to analyze such an electrolytic system. Include only the three components: H_2O, K_2CO_3, and CO_2 in the electrolytic system. Include salt formation and deselect water dissociation reaction (see Figure 11.3) in your analysis. Retain the solid salts $K_2CO_{3(s)}$ and $KHCO_{3(s)}$ in the “**Salts**” column and the global property is set to “**ELECNRTL**” (see Figure 11.4). Use the “**True component approach**” option (see Figure 11.5). There will be CO_2 and CH_4 that obey Henry’s law. Finish dealing with the Electrolyte Wizard. All possible ionic species will appear in “**Components**” list. From “**Navigation**” pane, you will notice that there are half-filled red circles, which means that they require more parameter estimation. Click on “**Next**” button more than once until you get rid of all red signs and the Aspen Plus sky becomes clear blue. Once the properties analysis completed successfully, switch to “**Simulation**” environment.

The absorption tower (or scrubber) will be made of four equilibrium stages. There is no need for condenser or reboiler. “**FEED**” stream will act as the rising vapor phase and “**HPC**” stream as the falling liquid phase as shown in Figure 11.20.



Feed streams

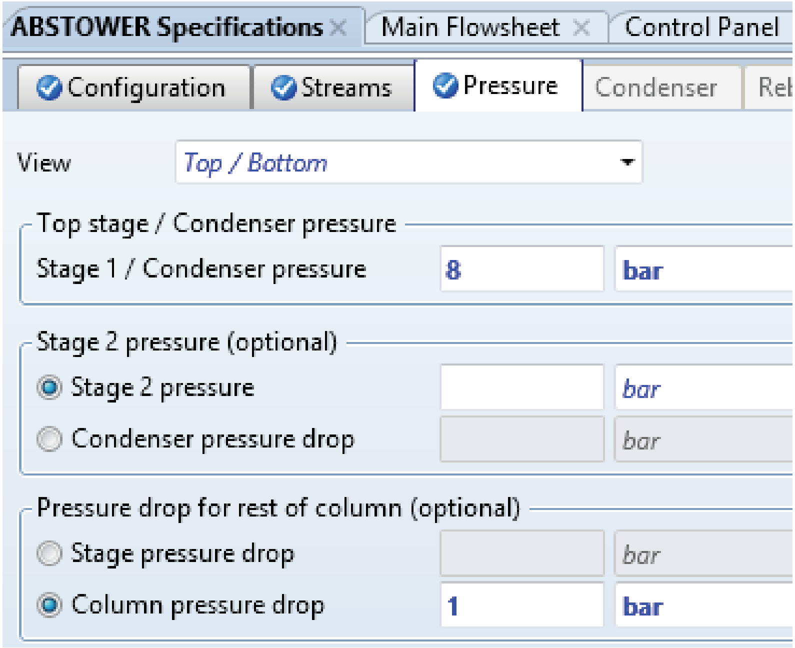
Name	Stage	Convention
FEED	4	Vapor
HPC	1	Liquid

Product streams

Name	Stage	Phase	Basis
TOPSTRM	1	Vapor	Mass
BTMSTRM	4	Liquid	Mass

Figure 11.20 The scrubber is made of four stages and "**HPC**" stream acts as the falling liquid phase while "**FEED**" stream as the rising vapor phase; hence, there is no need for a reboiler or condenser.

Figure 11.21 shows the "**Pressure**" tab form for the adsorption tower.



View: Top / Bottom

Top stage / Condenser pressure
Stage 1 / Condenser pressure: 8 bar

Stage 2 pressure (optional)
● Stage 2 pressure: bar
○ Condenser pressure drop: bar

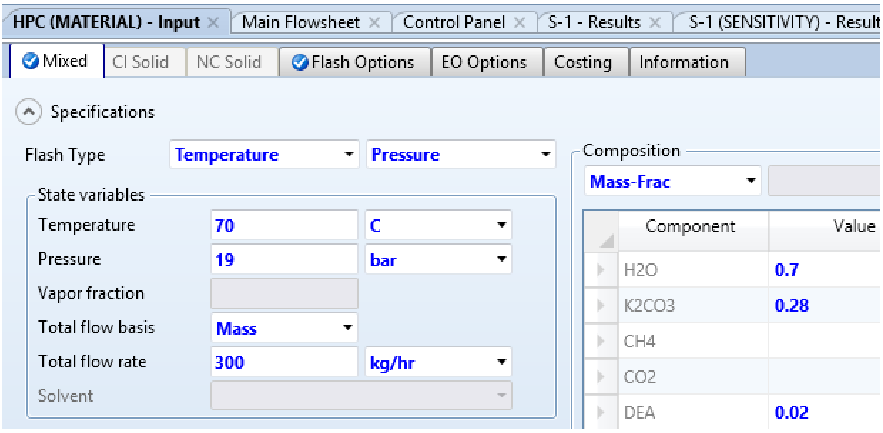
Pressure drop for rest of column (optional)
○ Stage pressure drop: bar
● Column pressure drop: 1 bar

Figure 11.21 The "**Pressure**" tab form for the adsorption tower, where the top pressure is set to 8 bar with a column pressure drop equal to 1 bar.

c) Reinitialize, run the show, and watch out any simulation error or serious warning. Report the flow rate and composition of top and bottom stream. Write down the dissolved salts found in the bottom stream. Do we have any precipitating salt?

d) Repeat the procedure but this time use the "**Apparent component approach**" option (see Figure 11.5). Remember to include only the three components: H_2O, K_2CO_3, and CO_2 in the electrolytic system. Include salt formation and water dissociation reaction (see Figure 11.3) in your analysis. Retain all possible solid salts in the "**Salts**" column and the global property is set to "**ENRTL-RK**" (see Figure 11.4) because the operating pressure can go higher than 10 bar. Again, both CO_2 and CH_4 obey Henry's law. The absorption tower (or scrubber) can be made of four equilibrium stages. Report the flow rate and composition of top and bottom stream. Notice the difference between the true- and apparent-component approaches in terms of reporting the salt in the bottom stream. Using the "**Apparent component approach**" case, carry out a sensitivity analysis where you vary, first, the block variable of the absorption tower ("**ABSTOWER**") called "**STAGE-PRES**" between 1 and 19 bar and, second, the top feed ("**HPC**") stream temperature between 70 and 140°C so as to minimize the sum of mole fraction of both water and CO_2 over methane in the top stream (i.e., $YRATIO = (YCO_2 + YH_2O)/YCH_4$). This is to minimize the vaporization of water and presence of CO_2 in the top stream. Do not forget to set the top feed stream pressure to 19 bar and the bottom feed to 20 bar with a column pressure drop equal to 1 bar. Make a parametric plot showing the effect of feed temperature and top stage pressure on the *YRATIO*. Report the optimum pressure and temperature that will end up with a minimum value of *YRATIO*.

e) Repeat step (d) but with the following top ("**HPC**") stream composition as shown in Figure 11.22:



Flash Type: Temperature, Pressure

State variables

Temperature: 70 C

Pressure: 19 bar

Vapor fraction:

Total flow basis: Mass

Total flow rate: 300 kg/hr

Solvent:

Composition: Mass-Frac

Component	Value
H2O	0.7
K2CO3	0.28
CH4	
CO2	
DEA	0.02

Figure 11.22 The "**HPC**" stream contains 2 wt% diethanolamine (DEA).

HOMEWORK/CLASSWORK 11.3 (PH OF AQUEOUS SOLUTIONS OF SALTS)

Salts, when dissolved in water, will often react with water to produce H_3O^+ (H^+) or OH^-. This is known as hydrolysis reaction. Based on how strong the ion acts as an acid or base, it will produce a solution with a different pH level. When water and salts react, there are many possibilities due to the varying structures of salts. A salt can be made of a strong acid and strong base, a weak acid and strong base, strong acid and weak base, or a weak acid and weak base.

a) A salt that is formed from a strong base and strong acid will, respectively, yield a weak conjugate acid and weak conjugate base. This will have no effect on $H^+ \rightarrow OH^-$ balance. The pH will remain practically neutral, at about 7. An example is NaCl. On one hand, Na^+ (a weak conjugate acid) will weakly attract OH^- and, on the other hand, Cl^- (a weak conjugate base) will weakly attract H+; hence, both dipoles are weak but equal. In general, salts containing halides (except F^-) and an alkaline metal (except Be^{2+}) will dissociate and form a neutral medium.

b) A salt that is born from a strong base and weak acid will, respectively, yield a weak conjugate acid and strong conjugate base. This will disrupt $H^+ \rightarrow OH^-$ balance resulting in the pH greater than 7. An example is sodium acetate (CH_3COONa) salt. On one hand, the cation (Na^+), being derived from a strong base (NaOH), will be a weak conjugate acid that will weakly bind to OH^-. On the other hand, the anion (CH_3COO^-) in the salt, being derived from a weak acid (CH_3COOH), will be a strong conjugate base that will strongly bind to the proton H^+. So, in terms of gain and loss balance, the aqueous medium will lose more H^+ than losing OH^-, resulting in “excess” of OH^- and “shortage” in H^+ (i.e., more basic or alkaline medium).

c) A salt that is formed from a weak base and strong acid will, respectively, yield a strong conjugate acid and weak conjugate base. This will disrupt $H^+ \rightarrow OH^-$ balance resulting in the pH lower than 7. An example is ammonium chloride (NH_4Cl) salt. On one hand, the cation (NH_4^+), being derived from a weak base (NH_3), will be a strong conjugate acid that will strongly bind to OH^-. On the other hand, the anion (Cl^-) in the salt, being derived from a strong acid (HCl), will be a weak conjugate base that will weakly bind to the proton H^+. So, in terms of gain and loss balance, the aqueous medium will lose more OH^- than losing H^+, resulting in “excess” of H^+ and “shortage” in OH^- (i.e., more acidic medium).

d) A salt that is formed from a weak base and weak acid. In general, this will disrupt $H^+ \rightarrow OH^-$ balance; however, the resulting pH may be equal to, lower than, or greater than 7, depending on the relative strengths of the acid and base. If $K_a > K_b$, the solution of the salt will be acidic and vice versa. Obviously, if both are equal then, we will end up with the first case (i.e., $pH \approx 7.0$). An example for $K_a > K_b$ is ammonium oxalate, where $K_a(\text{oxalic acid}) = 5.6 \times 10^{-2} > K_b(NH_3) = 1.8 \times 10^{-5}$. An example for $K_a < K_b$ is ammonium cyanide, where $K_a(\text{hydrogen cyanide}) = 6.2 \times 10^{-10} < K_b(NH_3) = 1.8 \times 10^{-5}$. An example for $K_a = K_b$ is ammonium acetate, where $K_a(\text{acetic acid}) = 1.85 \times 10^{-5} \approx K_b(NH_3) = 1.8 \times 10^{-5}$.

Let us demonstrate one case using the powerful features of Aspen Plus electrolyte model. Using Aspen Plus, choose “**Electrolytes with Metric Units**” template to create the process flow sheet. The default property model is “**ELECNRTL**”. By default, water is added to the “**Components**” list. Enter NaCl to the list of components. With the support of the Electrolyte Wizard, use the unsymmetric reference of state for ionic components to analyze such an electrolytic system. Include the two components: H_2O and NaCl in the electrolytic system. Do not include salt formation (as we run the system below the saturation limit of solubility) and select water dissociation reaction (see Figure 11.3) in your analysis. The global property is set to "**ELECNRTL**" (see Figure 11.4). Use the "**True component approach**" option (see Figure 11.5). There will be HCl that obeys Henry's law. Finish dealing with the Electrolyte Wizard. All possible ionic species will appear in "**Components**" list. From "**Navigation**" pane, you will notice that there are half-filled red circles, which means that they require more parameter estimation. Click on "**Next**" button more than once until you get rid of all red signs and the Aspen Plus sky becomes clear blue. Once the properties analysis completed successfully, switch to "**Simulation**" environment. Figure 11.23 shows a simple flowsheet made of a mixer with one input and output stream.

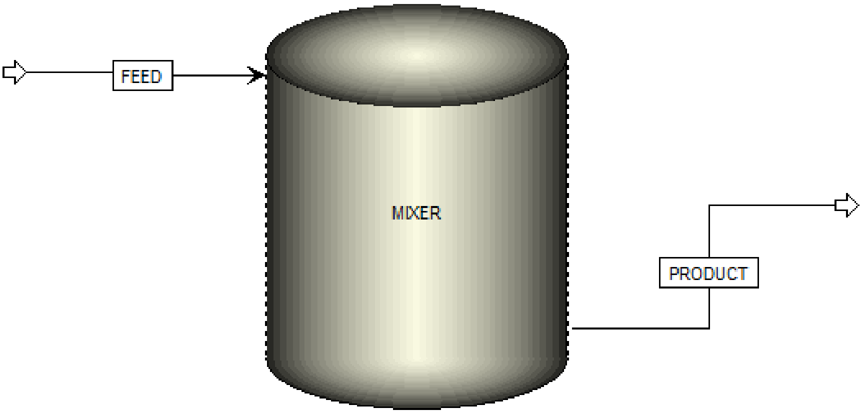
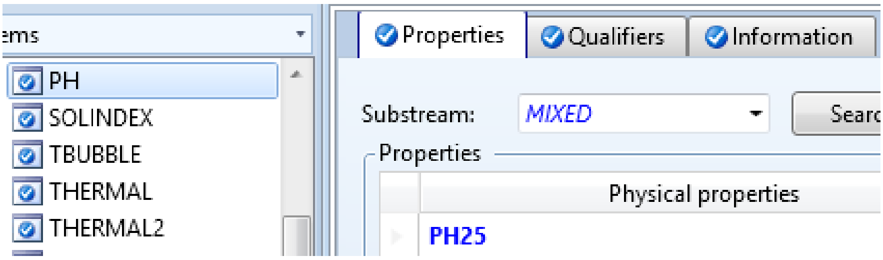


Figure 11.23 A simple flowsheet to demonstrate the pH of the product stream as a function of solute type.

The flow rate of feed stream is 100 kg/h, which enters at room temperature and pressure, and is made of H_2O and NaCl with NaCl mass fraction of 0.25. Notice that the maximum solubility of NaCl at 25°C is 0.36 kg/kg of water (i.e., $X_{NaCl} = 0.36/(1 + 0.36) = 0.265$).

By default, there exists a property set named "**PH**" for "**Electrolytes with Metric Units**" template; modify it to be PH25 instead of PH, as shown in Figure 11.24. pH is a function of temperature and the product stream may slightly shift from the feed temperature; hence, we will standardize the pH measurement.



Substream: MIXED

PH25

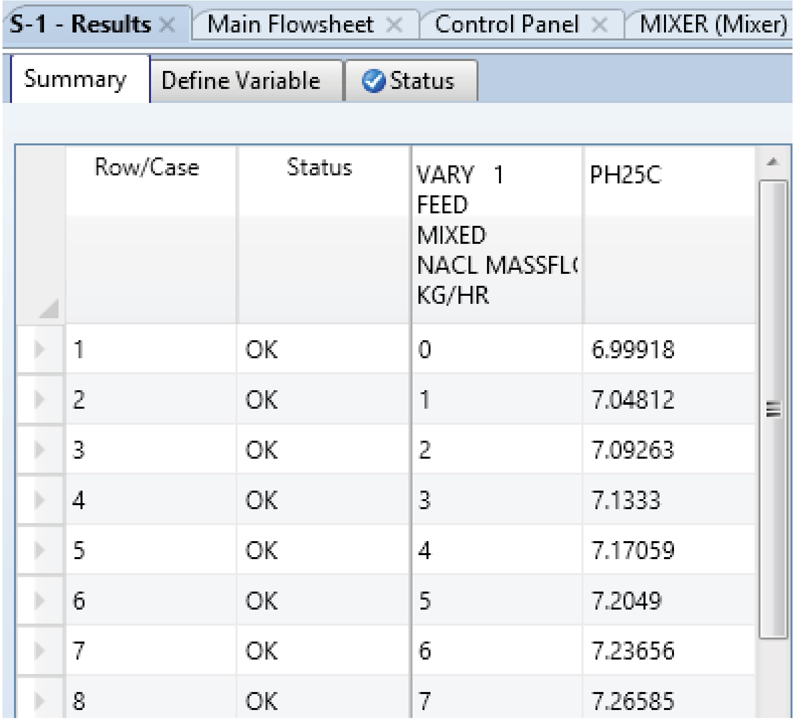
Figure 11.24 Setting the property set "**PH**" to estimate pH of the stream at 25°C.

Under “**Model Analysis Tools**” | “**Sensitivity**” | create a new sensitivity analysis called “**S-1**”. Under “**Vary**” tab, create a new variable named, by default, “**1**”, to represent the mass flow rate of *NaCl* in “**FEED**” stream, and it will vary between *0* and *25* kg/h with an increment of *1*. The upper limit is selected such that it will not exceed the maximum solubility, thus, avoiding formation of solid crystals in the product stream. Under “**Define**” tab, define a new variable named “**PH25C**”, which will account for pH of the product stream evaluated at 25°C. So, “**PH25C**” will be classified as:

“**Category**”: “*Streams*”, “**Type**”: “*Stream-Prop*”, “**Stream**”: “*PRODUCT*”, and “**Prop Set**”: “*PH*”.

Under “**Tabulate**” tab, there will be column #1 with variable “**PH25C**”.

“**Reset**”, run the show, and watch out for any serious warning or error that may appear in “**Control Panel**”. Figure 11.25 shows a portion of the sensitivity analysis where pH slightly increases with the addition of NaCl up to pH value of 7.57, at the saturation limit.



Row/Case	Status	VARY 1 FEED MIXED NACL MASSFL(KG/HR	PH25C
1	OK	0	6.99918
2	OK	1	7.04812
3	OK	2	7.09263
4	OK	3	7.1333
5	OK	4	7.17059
6	OK	5	7.2049
7	OK	6	7.23656
8	OK	7	7.26585

Figure 11.25 The continuous addition of NaCl to water will cause a slight increase in pH from 7.0 up to 7.57, at the saturation limit.

Your task is to replace NaCl each time by one of the following salty solutes and carry out all the steps needed to see how pH changes as a function of mass flow rate of solute up to the maximum solubility limit at 25°C.

a) Sodium hypochlorite (NaClO): the maximum solubility 29.3/100 g water (0°C) ↔ ($X_{NaClO} = 0.227$).
b) Ammonium cyanide (NH_4CN): very soluble (Take $X_{NH_4CN} = 0.5$).

c) Barium nitrate ($Ba(NO_3)_2$): the maximum solubility 10.0/100 g water (25°C) ↔ $X_{Ba(NO_3)_2} = 0.09$).

APPENDIX 11.A DEVELOPMENT OF “ELECNRTL” MODEL

The Electrolyte NRTL model was originally proposed by Chen *et al.* [2, 3], for aqueous electrolyte systems. It was later extended to mixed-solvent electrolyte systems by Mock *et al.* [4, 5]. The model is based on two fundamental assumptions:

1. The like-ion repulsion assumption, which states that the local composition of cations around cations is zero (and likewise for anions around anions). This is based on the assumption that the repulsive forces between ions of like charge are extremely large. This assumption may be justified on the basis that repulsive forces between ions of the same sign are very strong for neighboring species. For example, in salt crystal lattices the immediate neighbors of any central ion are always ions of opposite charge.
2. The local electroneutrality assumption, which states that the distribution of cations and anions around a central molecular species is such that the net local ionic charge is zero. Local electroneutrality has been observed for interstitial molecules in salt crystals.

Chen proposed an excess Gibbs energy expression, which contains two contributions: one contribution for the long-range ion–ion interactions that exist beyond the immediate neighborhood of a central ionic species and the other related to the local interactions that exist at the immediate neighborhood of any central species.

On the one hand, the unsymmetric Pitzer–Debye–Hückel (PDH) model and the Born model are used to represent the contribution of the long-range ion–ion interactions. On the other hand, the non-random two liquid (NRTL) theory is used to represent the local interactions. The model for local interaction contribution is developed as symmetric, based on reference states of a pure solvent and a pure, completely dissociated liquid electrolyte. The model is then normalized by infinite dilution activity coefficients in order to obtain an unsymmetric model. This NRTL expression for the local interactions, the Pitzer–Debye–Hückel expression, and the Born expression are all added to give Equation 11.A.1 for the excess Gibbs energy:

$$\frac{G_m^{*E}}{RT} = \frac{G_m^{*E,\mathrm{PDH}}}{RT} + \frac{G_m^{*E,\,\mathrm{Born}}}{RT} + \frac{G_m^{*E,\mathrm{loc}}}{RT} \tag{11.A.1}$$

This leads to:

$$\ln(\gamma_i^*) = \ln(\gamma_i^{*,\mathrm{PDH}}) + \ln(\gamma_i^{*,\mathrm{Born}}) + \ln(\gamma_i^{*,\mathrm{loc}}) \tag{11.A.2}$$

NOTE: *The notation using * to denote an unsymmetric reference state is well accepted in electrolyte thermodynamics. Beware of the meaning of * in classical thermodynamics according to IUPAC/ISO, referring to a pure component property. In fact, in the context of G or γ, the asterisk as superscript is never used to denote pure component property, so the risk of confusion is minimal.*

12

POLYMERIZATION PROCESSES

12.1 THE THEORETICAL BACKGROUND

The fact that you have reached here and you are still alive and interested to know about polymerization reactions using Aspen Plus® Polymers is just by itself thrilling. Good news; just relax and keep in mind that polymer reaction engineering, unlike classical chemical reaction engineering, requires the user to keep track on many granular details. So, be patient and do not go away as we will be back soon with another poly-cartoon.

12.1.1 Polymerization Reactions

Polymerization is a reaction where monomers are converted into a polymer. There are two types of polymerization reactions:

1. Step-Growth Polymerization (decrepit name: Condensation Polymerization). It applies to monomers with functional groups such as –COOH, –COOR, –COOOC–, –COCl, –OH, $–NH_2$, –CHO, and –NCO.
2. Chain Polymerization (decrepit name: Addition Polymerization). It applies to monomers having double bonds or ring structure. The polymerization of a given monomer may proceed by the free radical, anionic, or cationic mechanism, depending on the chemical structure of the monomer (steric and electronic effect).

Both classes of reaction can lead to the formation of either linear polymers or branched polymers (i.e., polymer networks). Whether the polymer is of linear or branched chains only depends on the number of reactive entities per monomer. The degree or extent of polymerization can be expressed in terms of number average molecular weight (MWN)

Aspen Plus®: Chemical Engineering Applications, First Edition. Kamal I.M. Al-Malah.

Companion Website: www.wiley.com/go/Al-Malah/AspenPlusApplications

and weight average molecular weight (MWW). For example, step-growth polymerization usually has MWN < 30,000 and MWW/MWN ≈ 2. On the other hand, chain polymerization usually has MWN > 50,000 and MWW/MWN = [1.01–50]. For definition of MWW and MWN, refer to APPENDIX 12.B.

The Ziegler–Natta polymerization is of the second type. The term Ziegler–Natta polymerization is used here to describe a variety of stereospecific multisite and single-site catalyzed addition polymerization systems, including the traditional Ziegler–Natta catalyzed systems, chromium-based catalyzed systems (Phillips type), and the more recent metallocene-based catalyzed systems. Several examples for applications based on the Ziegler–Natta polymerization model are given in the *Aspen Polymers Examples & Applications Case Book*. In addition, the *Examples & Applications Case Book* provides process details and the kinetics of polymerization for specific monomer–polymer systems. In addition, some polymer-based processes are also shown in "**C:\Program Files (x86)\AspenTech\Aspen Plus V8.8\GUI\Examples\Polymers**" folder.

The Ziegler–Natta polymerization model is applicable to processes that utilize coordination catalysts for the production of stereospecific polymers. Some examples are as follows:

- Linear low-density polyethylene (LLDPE): Ethylene is copolymerized with an α-olefin, such as 1-butene, 1-hexene, or 1-octene. Commercial processes include low pressure, slurry phase, solution phase, and gas phase.
- High-density polyethylene (HDPE): Ethylene homopolymers or copolymers with high α-olefins with a density of 0.940 g/cm^3 and higher. Commercial processes include solution, slurry or suspension, and gas-phase polymerization.
- Ethylene–propylene elastomers: Polymerization proceeds by solution or slurry processes. Both are operated continuously in liquid-phase back-mixed reactors.
- Polypropylene: Commercial processes include liquid pool, diluent slurry, and gas-phase polymerization.

Ziegler–Natta polymerization accounts for a significant chunk of the polyethylene polymers and all the polypropylene homopolymers and copolymers commercially produced. The commercial production of such polyolefins is exclusively carried out by continuous processes using several different processes and reactor types operating over a wide range of conditions. A high-density polyethylene (HDPE) and linear low-density polyethylene (LLDPE) are produced via catalyzed polymerization processes. The operating conditions for the catalyzed processes are relatively less severe compared with the high pressure LDPE (HP-LDPE) process. The pressure generally varies between 10 and 80 atm while the temperature between 80 and 110°C. The pressure and temperature may jump to 200 atm and 250°C, respectively, for the solution polymerization processes.

12.1.2 Catalyst Types

There are several catalysts used for ethylene polymerization, including both *supported* and *unsupported* heterogeneous and homogeneous catalyst systems. The Ziegler–Natta transition metal titanium-based catalysts are often used. Some vanadium-based catalysts are also used. Recently, several commercial processes have been developed using metallocene-based catalysts, including zirconium- and titanium-based types. These catalysts are thought to be single-site catalysts that are capable of producing high yields, combined with narrow molecular weight and copolymer composition distributions. All commercial brands of isotactic polypropylene homopolymer are manufactured using heterogeneous Ziegler–Natta catalyst systems. The catalyst consists of a solid transition metal halide, usually $TiCl_3$, with an organoaluminum compound cocatalyst, such as diethylaluminum chloride or an $MgCl_2$-supported triethylaluminum chloride catalyst.

12.1.3 Ethylene Process Types

There are three types of catalyzed ethylene polymerization processes in commercial use today:

1. Liquid slurry
2. Solution
3. Gas phase.

For the liquid slurry process, a hydrocarbon diluent is used, typically a $C4$–$C7$ paraffin, isoparaffin, or cycloparaffin. Under the process conditions, polyethylene is essentially insoluble in the diluent; hence, a slurry is formed.

For the solution process, the conditions are such that the polyethylene is completely dissolved in the solvent.

For the gas-phase process, gaseous ethylene and co-monomers are contacted with a polymer–catalyst powder. Polymerization occurs in the monomer-swollen polymer particles, which contain embedded catalyst fragments with active sites.

Ethylene polymerization processes have been extensively reviewed; more details of such processes are available in the open literature [1, 3, 6, 7].

12.1.4 Reaction Kinetic Scheme

The Aspen Plus Polymers built-in catalyst/polymerization kinetic scheme represents the typical scheme described in the open literature [9]. Although a number of reaction mechanisms have been proposed to describe stereospecific Ziegler–Natta polymerization, there is still no perfect reaction mechanism to completely describe the kinetic behavior of these complex catalyst/polymerization systems.

Most of the proposed mechanisms include a detailed set of reactions. However, not all of these reactions are applicable to every catalyst system nor can they be verified. The kinetic scheme for chromium- and metallocene-catalyzed systems can be considered to be a subset of a comprehensive Ziegler–Natta kinetic scheme.

12.1.5 Reaction Steps

There are a few key elementary reactions that apply to almost all catalyzed chain polymerization systems. These include the three basic reaction steps:

1. Chain initiation
2. Propagation
3. Chain transfer (spontaneous from and to small molecules such as monomer, solvent, and chain transfer agents).

For chromium and metallocene catalyst systems, additional reactions for long-chain branching via terminal double-bond (TDB) polymerization must also be included. In addition to the polymerization reactions, there are reactions affecting the catalyst active sites on which the polymerization reactions take place. These include catalyst site activation, inhibition, and deactivation. These catalyst reactions and the polymerization reactions occur simultaneously during the polymerization. A comprehensive kinetic scheme for the catalyzed multisite homo- and copolymerization of any number of monomers has been built into Aspen Plus Polymers.

12.1.6 Catalyst States

The multisite catalyst and the accompanying reactions are shown in Figure 12.1.

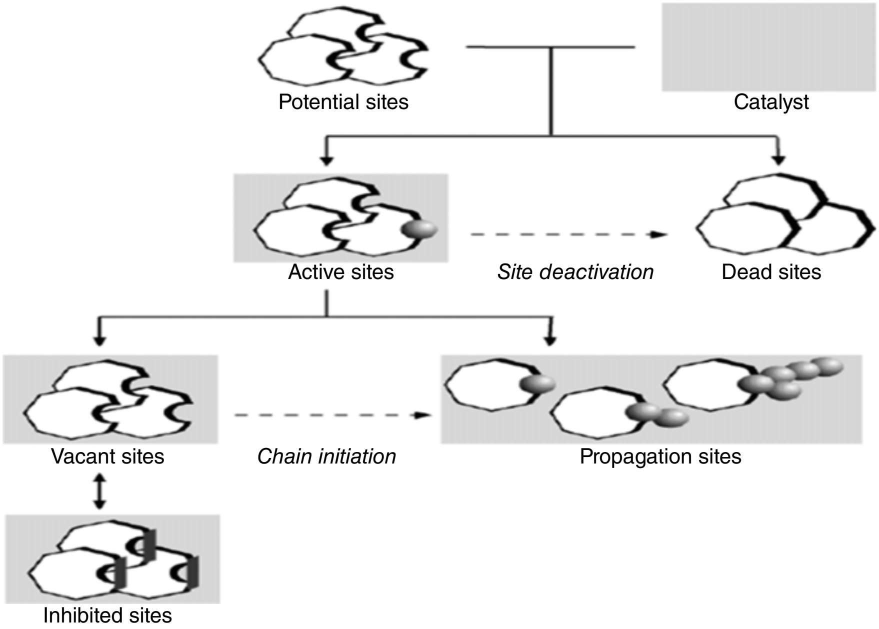


Figure 12.1 The multisite catalyst and the types of reactions involved.

In setting up a simulation, the user specifies the catalyst flow rate for the feed stream, and a catalyst parameter, that is, the moles of sites per unit mass of catalyst. This parameter together with the catalysts flow rate is used to compute the total moles of sites. The total moles of sites are made up of potential sites, active sites of different reactivities, and dead sites. Site activation reactions convert potential sites to active sites, while site deactivation reactions convert active to dead sites. There are several different site activation/deactivation reactions found in the built-in "Ziegler–Natta Catalysts and Polymerization Kinetic Scheme".

In Figure 12.1, potential and dead sites are considered to be independent of one another. The following analogy is drawn. In this regard, a dead site (a dead woman) is either a deactivated (rendered dead) state of an active site or is originally born dead (i.e., defected catalyst site). Under both circumstances, such as death, the dead state is irreversible.

The user specifies the number of site types to be included for a particular simulation.

- A vacant site (an uncoupled single woman) is an active (vivid) site that does not have a polymer or other molecule attached to it.
- A propagation site (a woman with a series of kids) has a *growing polymer molecule* attached to it. Here, a woman can have one, two, three, or more kids at a time.
- An inhibited site (a divorced woman from a bad ex-husband; hence, temporarily unwilling to socialize) is attached to *small molecules (toys)*, such as hydrogen or poisons, temporarily blocking them from becoming propagation sites. The small molecule may dissociate from an inhibited site, which then becomes a vacant site once again. Therefore, the site inhibition reaction is considered reversible; similar to saying a divorced woman is cured from the past history and now she is ready for a new relationship with a new guest (or ghost).

NOTE #1: *When a vacant site is involved in a chain initiation reaction (marriage relationship), it is converted to a propagation site. When a propagation site is involved in a chain transfer reaction (expiry of marriage contract), a vacant site (an uncoupled woman) and a dead polymer molecule (a series of kids alone with no parents) are formed.*

For more information on mechanism of polymerization, copolymerization, and different catalyst site reactions, refer to APPENDIX 12.A at the end of this chapter. Moreover, the Aspen Plus Polymers built-in model features and assumptions are also explained in APPENDIX 12.A.

12.2 HIGH-DENSITY POLYETHYLENE (HDPE) HIGH-TEMPERATURE SOLUTION PROCESS

The following example is borrowed from: “Aspen Polymers: Examples & Applications, Version 7.0, July, 2008”. However, changes were made with respect to feed flow rates, their compositions, and most important the property method.

The HDPE high-temperature solution process model illustrates the use of Aspen Plus Polymers to model a Ziegler–Natta solution polymerization of ethylene. The model is used to study the effect of feed flow rate on conversion and polymer properties, and to study the effect of hydrogen concentration on melt index and polydispersity index. Ziegler–Natta catalysts are multisite catalysts containing different site types, with each type having different reactivities. For this reason, each site type produces a polymer with a distinct molecular weight. As a result, the composite polymer has a broad molecular weight distribution.

The Ziegler–Natta model in Aspen Plus Polymers takes into account the important reactions found in this chemistry, including site activation, chain initiation, chain propagation, chain transfer, site deactivation, site inhibition, branching reactions, and so on. So, unlike previous chapters, dealing with polymers requires the user to input so many kinetic parameters that describe the complex interplay among all different reaction steps. The model is quite flexible and can be configured for homo- or copolymerization with any number of monomers. The user can also specify any number of site types for the catalyst. The model predicts the various polymer properties, such as molecular weight, polydispersity index, melt index, and copolymer composition, and returns this information for the polymer produced at each catalyst site.

12.2.1 Problem Definition

In this example, the solution polymerization of ethylene is carried out at 160°C using *n*-hexane as a solvent. Hydrogen is used as a chain transfer agent to control the molecular weight. The flowsheet consists of two reactors and a flash unit as shown in Figure 12.2.

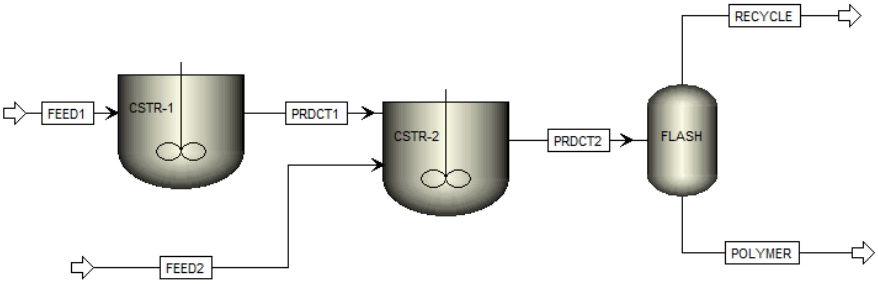


Figure 12.2 High-density polyethylene (HDPE) high-temperature solution process with two reactors and a flash unit.

The first reactor produces a high-molecular-weight polymer while the second produces a low-molecular-weight polymer. Solvent, unreacted monomer, and hydrogen are removed from the product in a flash tank. An intermediate feed stream going to the second reactor is used to set the concentration of hydrogen in that reactor to be several times higher than in the first reactor.

12.2.2 Process Conditions

The process conditions are shown in Table 12.1:

I discuss in the next section polymer-related input data that are specific to polymer industries and are quite uncommon in the previous chapters.

TABLE 12.1 Process Conditions for High-Density Polyethylene High-Temperature Solution Process with Two Reactors and a Flash Unit.

Components	Name	Description
Ethylene	C_2H_4	Monomer
Hydrogen	H_2	Chain transfer agent
n-Hexane	HEXANE	Solvent
Catalyst	$TiCl_4$	Catalyst (titanium-tetrachloride)
Cocatalyst	TEA	Cocatalyst (triethylaluminum)
HDPE	HDPE	Polymer
C2H4-R	C2H4-R	Ethylene segment
Physical properties	POLYNRTL property method	

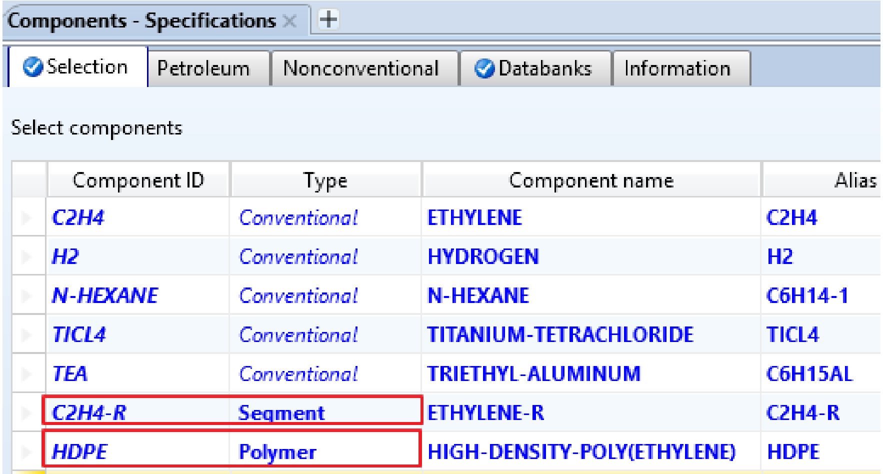
Feeds	Feed Specs.	FEED1	FEED2
Composition (mass fraction)	Ethylene (E2)	0.200	0.200
	Hydrogen (H_2)	0.001	0.010
	Hexane	0.789	0.780
	Catalyst ($TiCl_4$)[a]	0.005	0.005
	Cocatalyst (TEA)	0.005	0.005
Feed condition	Temperature	60°C	60°C
	Pressure	200 bar	200 bar
	Phase	Liquid	Liquid
Mass flow		90,000 kg/h	15,000 kg/h

Operating Conditions for Blocks	Temp (°C)	Pressure (bar)	Size (m^3)
CSTR-1	160	200	80
CSTR-2	160	200	80
FLASH	160	20	—

[a] Mole fraction of potential site fraction is one.

12.3 CREATING ASPEN PLUS FLOWSHEET FOR HDPE

Using Aspen Plus, start a new simulation by choosing the "**Polymers**" category and selecting "**Polymers with Met-C_bar_hr Units**" template to create a steady-state flowsheet. Notice that the property method originally used in: "Aspen Polymers: Examples & Applications" was set to **POLYPCSF**; nevertheless, it requires more input parameters, such as "**PCSFTM**", "**PCSFTU**", and "**PCSFTV**" both for the catalyst and cocatalyst. "**PCSFTM**" was supplied by Aspen Plus Polymers manual; unfortunately, the other two parameters are missing and must be supplied by the user as input parameters, or else there will be no solution and no chance to negotiate with Aspen Plus in this regard. Consequently, I tried all other property methods as recommended by the "**Property Method Selection Assistant**" and found that "**POLYNRTL**" gives reasonable results and requires the least input data. Moreover, there is no need to externally link with USERFORT.DLL file. However, if more data are available regarding properties of the monomer, solvent, polymer, catalyst, and cocatalyst, then it will be more accurate to switch to such property methods that can exploit the additional input data. Using "**POLYNRTL**" method will be good enough to touch the premises of polymerization reaction technology. Moreover, the free water method was set to “**SYSOP0**” instead of “**STEAM-TA**” in “**Methods**” | “**Global**” sheet. Give a title for the project and add the components as shown in Figure 12.3. Do not forget to change component “**Type**” of both “**C2H4-R**” and “**HDPE**” from *Conventional* to *Segment* and *Polymer*, respectively.

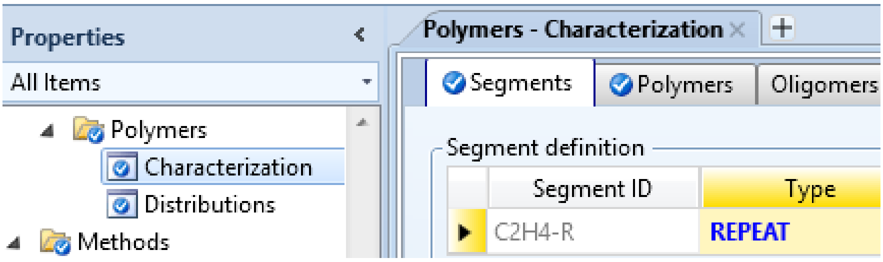


Select components

Component ID	Type	Component name	Alias
C2H4	Conventional	ETHYLENE	C2H4
H2	Conventional	HYDROGEN	H2
N-HEXANE	Conventional	N-HEXANE	C6H14-1
TICL4	Conventional	TITANIUM-TETRACHLORIDE	TICL4
TEA	Conventional	TRIETHYL-ALUMINUM	C6H15AL
C2H4-R	Segment	ETHYLENE-R	C2H4-R
HDPE	Polymer	HIGH-DENSITY-POLY(ETHYLENE)	HDPE

Figure 12.3 List of components to be entered. The component “**Type**” of both “**C2H4-R**” and “**HDPE**” are manually entered as “*Segment*” and “*Polymer*”, respectively.

Figure 12.4 shows “**Components**” | “**Polymers**” | “**Characterization**” | “**Segments**” tab window, where “**C2H4-R**” is defined as the repeat segment or building block for the polymer.

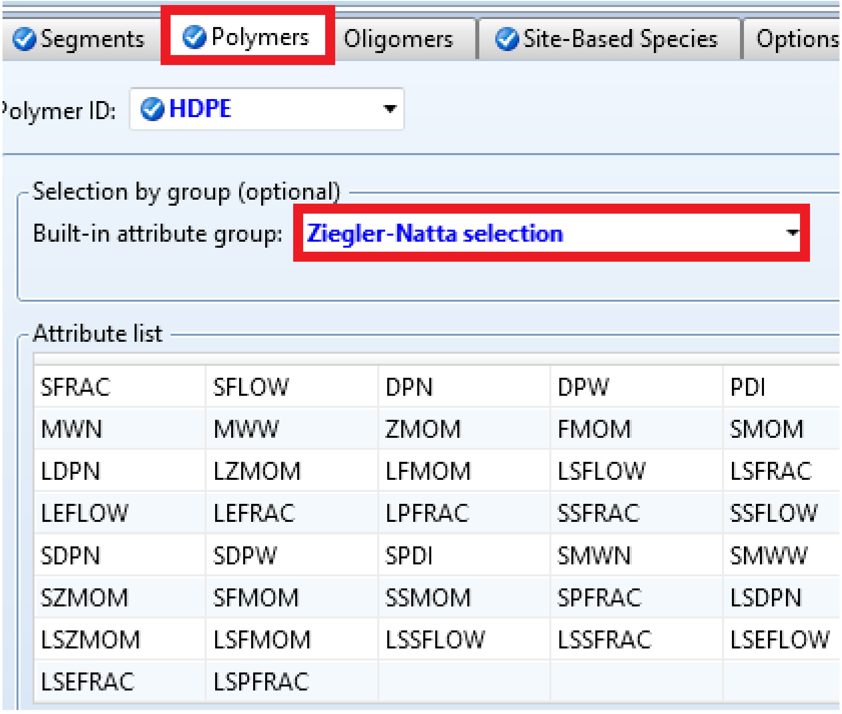


Segment definition

Segment ID	Type
C2H4-R	REPEAT

Figure 12.4 In “**Components**” | “**Polymers**” | “**Characterization**” | “**Segments**” tab window, “**C2H4-R**” is defined as “*REPEAT*” type (i.e., the monomeric building block of HDPE polymer).

Figure 12.5 shows the “**Polymers**” tab window where the user identifies the polymer, which is HDPE in this case, and selects the “**Built-in attribute group**” as “*Ziegler–Natta selection*” from the drop-down list. For more information on what these symbols stand for, refer to “**APPENDIX 12.A**” | “**Calculated Polymer Properties**” section and also refer to Aspen Plus built-in help for further information. Notice that only streams containing HDPE will be augmented by such attributes.



olymer ID: HDPE

Selection by group (optional)

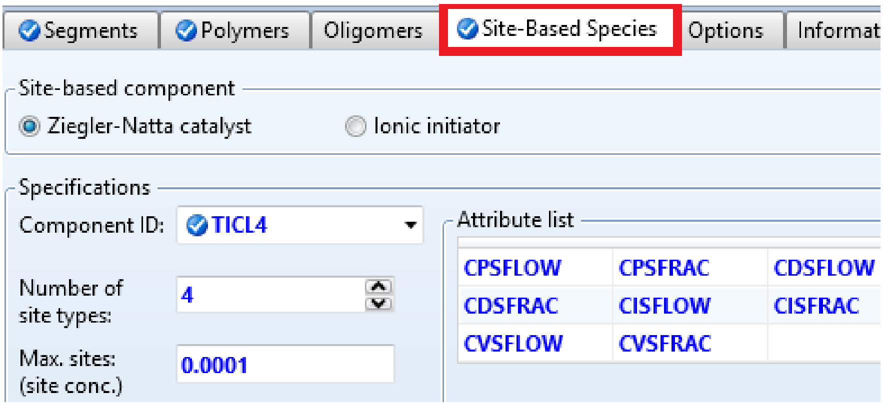
Built-in attribute group: Ziegler-Natta selection

Attribute list

SFRAC	SFLOW	DPN	DPW	PDI
MWN	MWW	ZMOM	FMOM	SMOM
LDPN	LZMOM	LFMOM	LSFLOW	LSFRAC
LEFLOW	LEFRAC	LPFRAC	SSFRAC	SSFLOW
SDPN	SDPW	SPDI	SMWN	SMWW
SZMOM	SFMOM	SSMOM	SPFRAC	LSDPN
LSZMOM	LSFMOM	LSSFLOW	LSSFRAC	LSEFLOW
LSEFRAC	LSPFRAC			

Figure 12.5 The built-in attribute group is selected in "**Polymers**" tab window. Aspen Plus will report such attributes only for streams containing HDPE polymer constituent.

Figure 12.6 shows that a total of four site types are used for the catalyst (TiCl$_4$). Two sites will be considered active in the first reactor and all four sites in the second reactor. Moreover, the molar concentration of catalytic sites is assumed as 0.0001 (kmol/kg catalyst).



Site-based component

● Ziegler-Natta catalyst ○ Ionic initiator

Specifications

Component ID: TICL4

Number of site types: 4

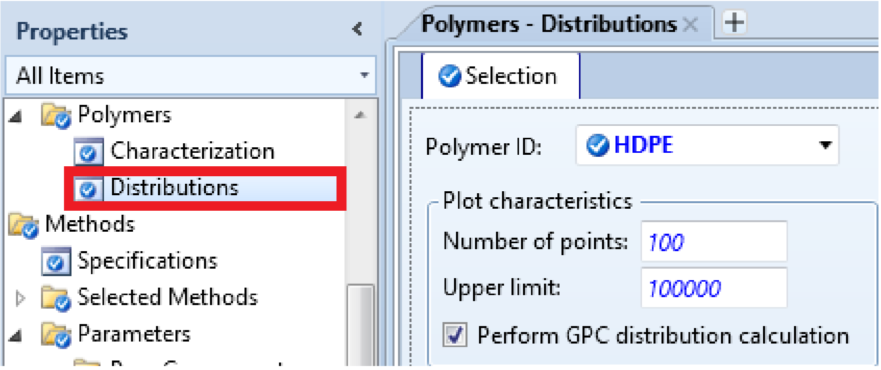
Max. sites: (site conc.) 0.0001

Attribute list

CPSFLOW	CPSFRAC	CDSFLOW
CDSFRAC	CISFLOW	CISFRAC
CVSFLOW	CVSFRAC	

Figure 12.6 Number of types of a catalyst site and their molar concentration are entered in "**Site-Based Species**" tab window.

Figure 12.7 shows the selection to perform **G**el **P**ermeation **C**hromatography (**GPC**) to request tracking of distributions. You need to specify the type of distribution, the polymer, and the display characteristics for the generated distribution data. In order to track distributions in your simulation, you must select the distribution characteristics. After the simulation is complete, you must retrieve the distribution data for plotting purpose. *You can display/plot the distribution data for the polymerization reactor, for a stream, or for the entire flowsheet*. In "**Plot characteristics**" box, select "**Perform GPC distribution calculation**" option. The distribution is calculated as $rW(r)$ versus r, where r is the number-average degree of polymerization. The common polymer structural properties for which distributions (i.e., $W(r)$) are typically considered include the chain length distribution (CLD) and molecular weight distribution (MWD). In order to accurately characterize a polymer component, and maintain a control of polymer product properties, engineers must be acquainted by these distributions. For further information, refer to Aspen Plus built-in help under "**Verifying the Accuracy of Distribution Calculations**" and "**Calculating Distribution Increments**".



Polymer ID: HDPE

Plot characteristics

Number of points: 100

Upper limit: 100000

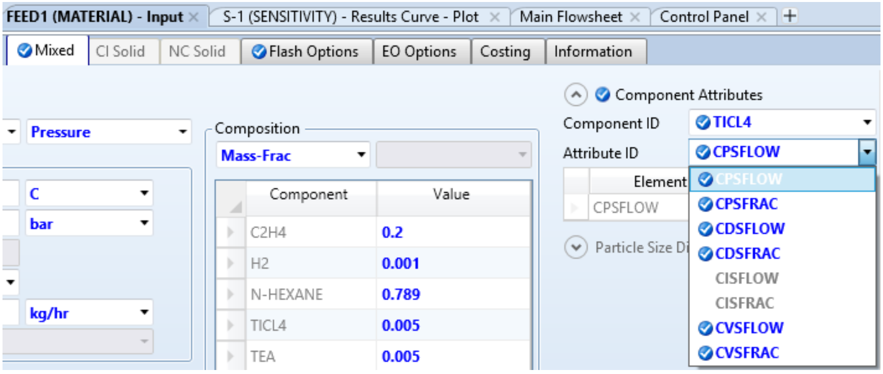
☑ Perform GPC distribution calculation

Figure 12.7 In "**Selection**" tab window, selecting "**Perform GPC distribution calculation**" option enables the user to see distribution plots for product quality control purposes. The distribution is calculated as $rW(r)$ versus r, where r is the number-average degree of polymerization.

Under "**Properties**" environment, go to "**Methods" | "Parameters" | "Binary Interaction" | "NRTL-1**" sheet and be sure that the "**Estimate missing parameters by UNIFAC**" option is enabled. Click on "**Reset**" followed by "**Next**" button to run the simulation and assure that properties analysis completed successfully. Switch to "**Simulation**" environment.

From "**Model Palette**", select "**Reactors**" tab, click on "**RCSTR**" icon, and add it twice to the flowsheet area. In addition, add one "**Flash2**" type separator. Add the proper input and output streams, as shown in Figure 12.2. The feed stream input properties and the operating conditions of each of three blocks are shown in Table 12.1.

Figure 12.8 shows "**Streams**" | "**FEED1**" | "**Input**" | "**Mixed**" tab window, where part of, or all catalyst attributes (Table 12.2) may be entered. Keep in mind that the catalyst is introduced to the reactor with the feed stream (i.e., not present in the reactor).



Pressure

C

bar

kg/hr

Composition: Mass-Frac

Component	Value
C2H4	0.2
H2	0.001
N-HEXANE	0.789
TICL4	0.005
TEA	0.005

Component ID: TICL4

Attribute ID: CPSFLOW

Figure 12.8 “**FEED1**” stream catalyst ($TiCl_4$) attributes need to be entered by the user.

TABLE 12.2 The Entered Catalyst ($TiCl_4$) Component Attributes and Their Description.

Attribute	Description for COMP-ATTR for $TiCl_4$	Value
CPSFLOW	Mole flow of potential sites	[0.0001]
CPSFRAC	Mole fraction of potential sites	[1.0]
CDSFLOW	Mole flow of dead sites	[0.0]
CDSFRAC	Mole fraction of dead sites	[0.0]
CVSFLOW	Mole flow of vacant sites of type *k*	[0.0, 0.0, 0.0, 0.0]
CVSFRAC	Mole fraction of vacant sites of type *k*	[0.0, 0.0, 0.0, 0.0]

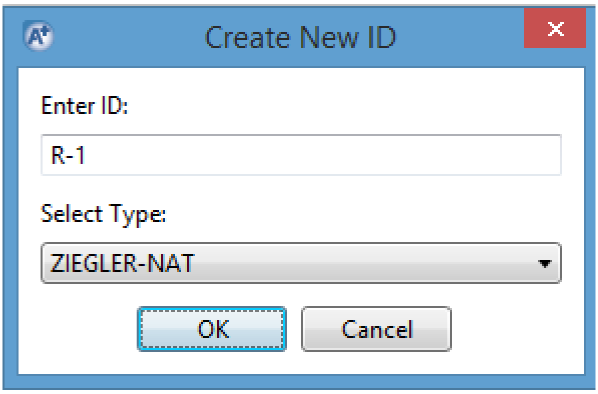
Component attributes are used to track the multisite Ziegler–Natta catalyst site activity, in terms of mole flow and fraction of potential, vacant, inhibited, dead, and occupied sites. The occupied sites are not tracked since that information may be obtained from the live polymer zeroth moment of chain length distribution (ZMOM). The site types are defined as follows:

- Potential sites: sites that are not yet activated.
- Vacant sites: activated sites without an attached growing polymer.
- Inhibited sites: activated sites that are temporarily in an inactive state.
- Dead sites: sites that have permanently lost their catalytic activity.
- Occupied sites: activated sites with an attached growing polymer.

Table 12.2 lists the entered catalyst component attributes and their description:

Notice that the values of catalyst ($TiCl_4$) attributes are exactly repeated for “**FEED2**” stream.

Let us show the critical part of polymerization reactions. Under “**Reactions**” folder, click on “**New …** ” button to create a reaction. Figure 12.9 shows the creation of “**R-1**” reaction set of *Ziegler–Natta* type.

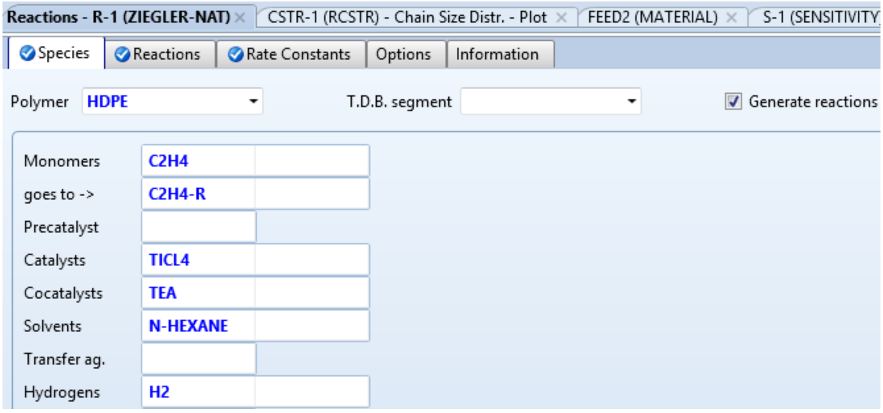


Enter ID: R-1

Select Type: ZIEGLER-NAT

Figure 12.9 The creation of Ziegler–Natta type reaction set.

Figure 12.10 shows the "**Species**" tab window where the user defines the polymer, the monomer, the repeat or building unit, the catalyst, the cocatalyst, the solvent, and the hydrogen (also acts as a transfer agent).



Polymer: HDPE

T.D.B. segment:

☑ Generate reactions

Monomers: C2H4

goes to ->: C2H4-R

Precatalyst:

Catalysts: TICL4

Cocatalysts: TEA

Solvents: N-HEXANE

Transfer ag.:

Hydrogens: H2

Figure 12.10 Defining the polymer, the monomer, the repeat unit, the catalyst, the cocatalyst, and the hydrogen agent, in "**Species**" tab window.

NOTE #2: *Do not select the terminal double-bond segment ("**T.D.B. segment**") as C2H4-R in both ("**R-1**") and ("**R-2**") sets (see Figure* 12.10*). The TDB segment should be of type end segment and should not be substituted by a repeat segment.*

Once you select "**Generate reactions**" option (deselect later), as shown in Figure 12.10, Aspen Plus will create many different reaction steps that all in all describe the overall mechanism of conversion of ethylene to HDPE using Ziegler–Natta approach. We will retain reaction substeps with known kinetics, as given in Figure 12.11 for "**R-1**" set and

#	Type	Site #	Comp1	Comp2	Pre-Exp (1/hr)
1.	ACT-SPON	1	TICL4		0.08
2.	ACT-SPON	2	TICL4		0.08
3.	ACT-SPON	3	TICL4		0.0
4.	ACT-SPON	4	TICL4		0.0
5.	ACT-COCAT	1	TICL4	TEA	0.15
6.	ACT-COCAT	2	TICL4	TEA	0.15
7.	ACT-COCAT	3	TICL4	TEA	0.0
8.	ACT-COCAT	4	TICL4	TEA	0.0
9.	CHAIN-INI	1	C2H4		255.0
10.	CHAIN-INI	2	C2H4		90.0
11.	CHAIN-INI	3	C2H4		0.0
12.	CHAIN-INI	4	C2H4		0.0
13.	PROPAGATION	1	C2H4-R	C2H4	255.0
14.	PROPAGATION	2	C2H4-R	C2H4	90.0
15.	PROPAGATION	3	C2H4-R	C2H4	0.0
16.	PROPAGATION	4	C2H4-R	C2H4	0.0
17.	CHAT-MON	1	C2H4-R	C2H4	0.09
18.	CHAT-MON	2	C2H4-R	C2H4	0.24
19.	CHAT-MON	3	C2H4-R	C2H4	0.0
20.	CHAT-MON	4	C2H4-R	C2H4	0.0
21.	CHAT-H2	1	C2H4-R	H2	5.55
22.	CHAT-H2	2	C2H4-R	H2	18.5
23.	CHAT-H2	3	C2H4-R	H2	0.0
24.	CHAT-H2	4	C2H4-R	H2	0.0
25.	CHAT-SPON	1	C2H4-R		0.004
26.	CHAT-SPON	2	C2H4-R		0.012
27.	CHAT-SPON	3	C2H4-R		0.0
28.	CHAT-SPON	4	C2H4-R		0.0
29.	DEACT-SPON	1			0.0001
30.	DEACT-SPON	2			0.0006
31.	DEACT-SPON	3			0.0
32.	DEACT-SPON	4			0.0

Figure 12.11 The Ziegler–Natta based kinetic parameters for 32 substeps that make up the overall "**R-1**" polymerization reaction. Two active sites are assumed.

in Figure 12.12 for "**R-2**" set. This means that you delete all other reaction substeps that are not listed here, using "**Delete**" button at the bottom of "**Reactions**" tab window. Notice that the pre-exponential factor is entered, under "**Rate Constants**" tab, for each considered substep.

#	Type	Site #	Comp1	Comp2	Pre-Exp (1/hr)
1.	ACT-SPON	1	TICL4		0.08
2.	ACT-SPON	2	TICL4		0.08
3.	ACT-SPON	3	TICL4		0.08
4.	ACT-SPON	4	TICL4		0.08
5.	ACT-COCAT	1	TICL4	TEA	0.15
6.	ACT-COCAT	2	TICL4	TEA	0.15
7.	ACT-COCAT	3	TICL4	TEA	0.15
8.	ACT-COCAT	4	TICL4	TEA	0.15
9.	CHAIN-INI	1	C2H4		255.0
10.	CHAIN-INI	2	C2H4		90.0
11.	CHAIN-INI	3	C2H4		255.0
12.	CHAIN-INI	4	C2H4		90.0
13.	PROPAGATION	1	C2H4-R	C2H4	255.0
14.	PROPAGATION	2	C2H4-R	C2H4	90.0
15.	PROPAGATION	3	C2H4-R	C2H4	255.0
16.	PROPAGATION	4	C2H4-R	C2H4	90.0
17.	CHAT-MON	1	C2H4-R	C2H4	0.09
18.	CHAT-MON	2	C2H4-R	C2H4	0.24
19.	CHAT-MON	3	C2H4-R	C2H4	0.09
20.	CHAT-MON	4	C2H4-R	C2H4	0.24
21.	CHAT-H2	1	C2H4-R	H2	5.55
22.	CHAT-H2	2	C2H4-R	H2	18.5
23.	CHAT-H2	3	C2H4-R	H2	5.55
24.	CHAT-H2	4	C2H4-R	H2	18.5
25.	CHAT-SPON	1	C2H4-R		0.004
26.	CHAT-SPON	2	C2H4-R		0.012
27.	CHAT-SPON	3	C2H4-R		0.004
28.	CHAT-SPON	4	C2H4-R		0.012
29.	DEACT-SPON	1			0.0001
30.	DEACT-SPON	2			0.0006
31.	DEACT-SPON	3			0.0001
32.	DEACT-SPON	4			0.0006

Figure 12.12 The Ziegler–Natta based kinetic parameters for 32 substeps that make up the overall "**R-2**" polymerization reaction. Four active sites are assumed.

12.4 IMPROVING CONVERGENCE

Polymer reaction kinetics present very difficult convergence problems, so the standard convergence options are frequently insufficient. To resolve this problem, perform the following steps:

a) Go to "**Blocks**" | "**CSTR-1**" | "**Convergence**" form.
b) Click on "**Parameters**" tab and change the "**Solver**" to "*Newton*".

c) Click on "**Newton Parameters**" button and change the "**Stabilization strategy**" to "*Line-Search*". Click on "**Close**" button.

NOTE #3: *Implementing these two steps (b and c) are recommended for all chain polymerization kinetics.*

d) In the "**Parameters**" tab sheet, click on "**Advanced Parameters**" button and change the "**Scaling method**" to "*Component-based*".

NOTE #4: *Component-based scaling is recommended for all Aspen Plus Polymers simulations.*

e) In the "**Parameters**" tab sheet, select "*Initialize using integration*" option under "**Initialization**" section. When this option is selected, CSTR uses an integrator to provide an initial guess to the simultaneous equation solver.

f) Repeat previous steps for "**CSTR-2**" block.

12.5 PRESENTING THE PROPERTY DISTRIBUTION OF POLYMER

After finishing the "one thousand and one night" novel about entering such an immense number of input parameters, reinitialize, run the show, and check for warnings and errors (if any).

To see some HDPE polymer characteristics for either a block or a stream object, in "**Navigation**" pane, select that object and then from the top toolbar go to "**Plot**" tab found in "**Home**" ribbon followed by clicking on "**Chain Size Distr**". button. Follow the steps instructed by the plot wizard to show some polymer characteristics.

Figure 12.13 shows the chain length distribution (CLD) for HDPE polymer inside "**CSTR-1**", based on two calculation methods for average molecular properties: Instantaneous distribution and Moments of distribution. The word "**Composite**" in Figure 12.13 refers to the sum of the four types of catalyst active sites (two sites are considered active in the first reactor). Notice that DPW = DPN × PDI.

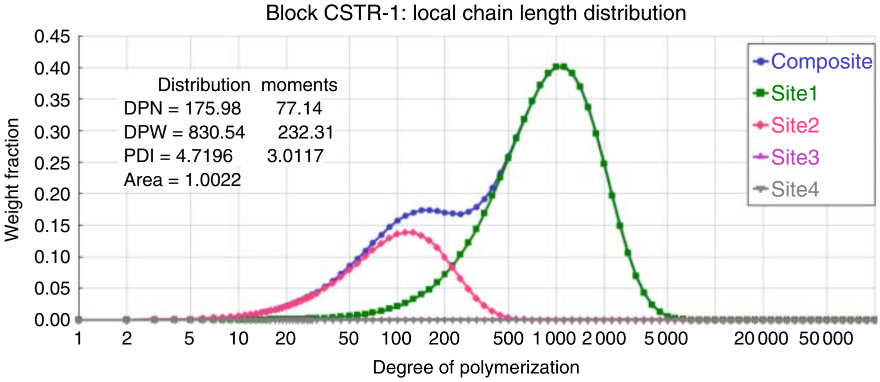
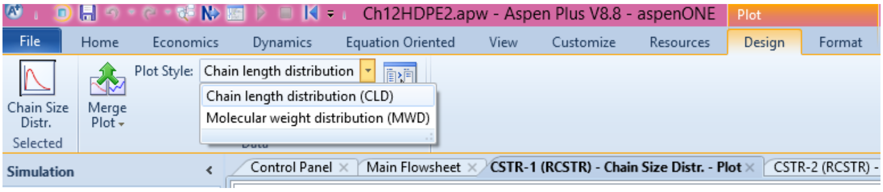


Figure 12.13 The chain length distribution (CLD) for HDPE polymer inside the first reactor, "**CSTR-1**". Two sites are considered active in the first reactor.

On the other hand, to get the molecular weight distribution, you have to select that from the drop-down list shown in “**Top Toolbar**” under “**Design**” tab as shown in Figure 12.14. Of course, the plot (“**CSTR-1 (RCSTR) – Chain Size Distr. – Plot**”) window has to be active.



Plot Style: Chain length distribution

Figure 12.14 The selection between CLD and MWD is made via the “**Design**” tab in “**Top Toolbar**”.

Figure 12.15 shows the molecular weight distribution (MWD) for HDPE polymer inside “**CSTR-1**”, based on two calculation methods for average molecular properties: Instantaneous distribution and Moments of distribution. Notice that MWW = MWN × PDI. For more information on molecular weight distribution properties, see APPENDIX 12.B.

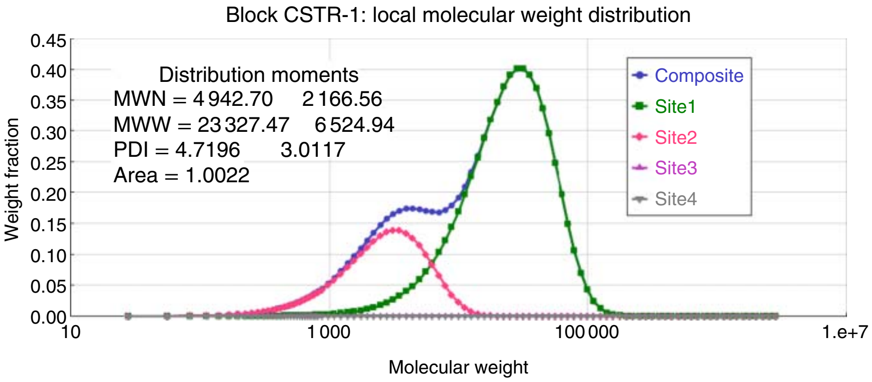


Figure 12.15 The molecular weight distribution (MWD) for HDPE polymer inside the first reactor, “**CSTR-1**”. Two sites are considered active in the first reactor.

Referring to Aspen Plus built-in help, here is a summary about the assessment methods of polymer properties or attributes.

Keep in mind that the polymer is a mixture of chains; hence, there is normally a distribution of these structural characteristics. It will be a more convenient way to examine polymer molecular properties in terms of averages instead of considering only the complete distribution. Average properties must be determined from the actual distributions either through distribution moments or through instantaneous properties.

Method of moments (called Moments in Figures 12.13 and 12.15), developed by Tompa [8], continues to be the preferred approach for calculating average properties whether the distribution is unimodal (e.g., binomial, Poisson, or Gaussian) or non-unimodal (such complex distributions having a shoulder, or are even bimodal in behavior as in a multireactor system).

Nevertheless, applying the method of moments for the calculation of property distributions has several drawbacks; in addition to CPU requirements and computational complexity, a larger number of moments than currently calculated would be required. A better approach is to use the instantaneous distribution (called Distribution in Figures 12.13 and 12.15) method for generating molecular weight distributions via storing reaction rate data throughout the kinetic calculations, and later using them to construct the full distribution of polymer accumulated in the reactor system. Such an approach was developed by Hamielec [5]. In the simplest case, a linear polymerization in a single CSTR reactor, the ratios of termination and chain transfer reaction rates to propagation reaction rates are stored. The instantaneous chain length distribution is expressed as a function of these ratios and chain length. For the case of two CSTRs in series, at steady-state, the outlet polymer distribution function is the weighted average of the distribution function in each CSTR taken separately. The case of a plug-flow reactor can be approximated using multiple CSTRs, and similarly for a batch reactor.

Finally, the method of instantaneous distribution assumes that the polymer molecules are conserved once they are formed; unfortunately, this assumption can be invalid in the presence of certain side reactions, such as

- random (thermal) scission, which destroys polymer molecules;
- chain transfer to polymer, which causes inactive polymer molecules to become active again, leading to long-chain branch formation and significantly increasing the weight-average molecular weight and PDI.

Keep in mind that the molecular weight distribution charts display the MWW and PDI calculated both by the method of moments and the method of instantaneous properties. If the predicted values for the PDI are not in reasonable agreement (but not necessarily equal) with each other, it will be most likely due to these types of side reactions.

Figure 12.16 shows the chain length distribution (CLD) for HDPE polymer inside "**CSTR-2**", based on the previously explained two calculation methods for average molecular properties. Again, the word "**Composite**" in Figure 12.16 refers to the sum of the four

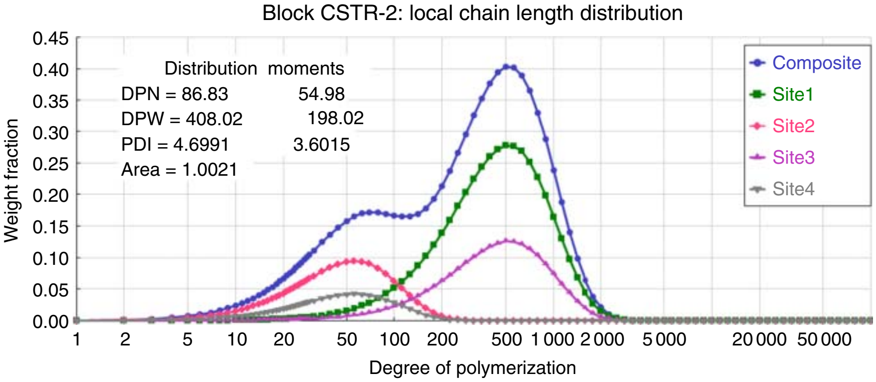
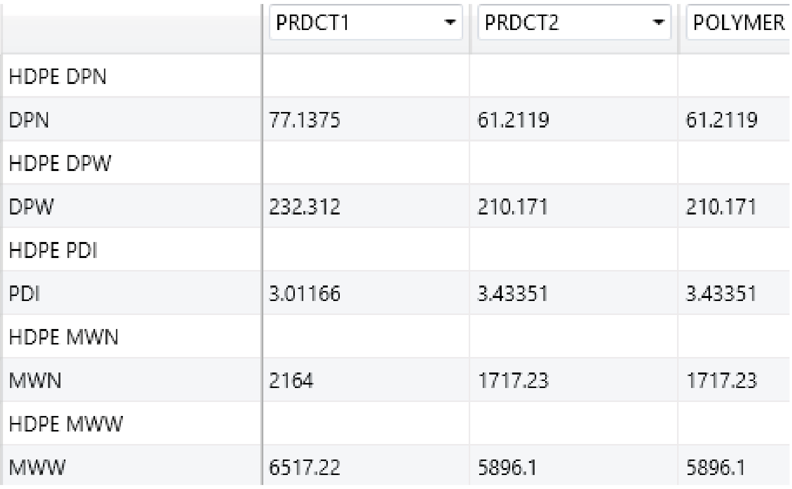


Figure 12.16 The chain length distribution (CLD) for HDPE polymer inside the second reactor. Four sites are considered active in the second reactor.

types of catalyst active sites. A similar figure can be obtained for the molecular weight distribution (MWD) for HDPE polymer inside the same reactor.

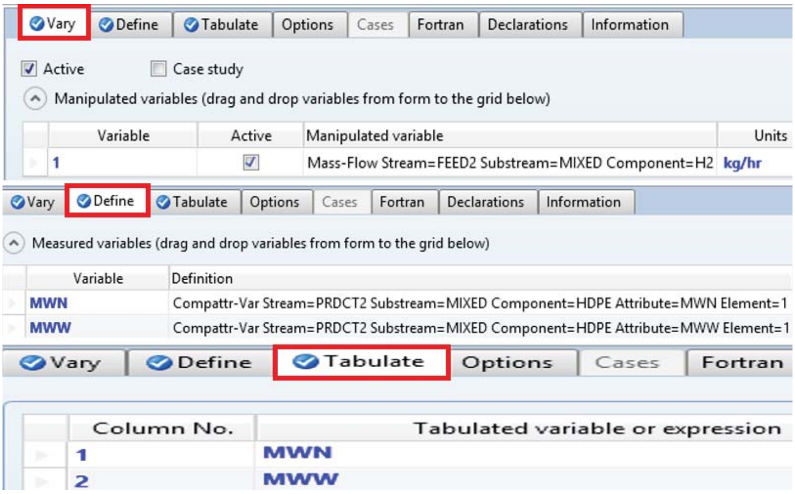
Figure 12.17 shows a portion of product streams properties where HDPE average molecular properties of "**PRDCT1**" stream are essentially the same as those for "**CSTR-1**". On the other hand, the "**PRDCT2**" stream average molecular weight properties fall somewhere between those of "**CSTR-1**" and "**CSTR-2**". For example, DPN for "**PRDCT2**" stream, which is 61.2119 (Figure 12.17), lies between DPN of 54.98 (Figure 12.16) for "**CSTR-2**" and 77.14 (Figure 12.13) for "**CSTR-1**".



	PRDCT1	PRDCT2	POLYMER
HDPE DPN			
DPN	77.1375	61.2119	61.2119
HDPE DPW			
DPW	232.312	210.171	210.171
HDPE PDI			
PDI	3.01166	3.43351	3.43351
HDPE MWN			
MWN	2164	1717.23	1717.23
HDPE MWW			
MWW	6517.22	5896.1	5896.1

Figure 12.17 Average molecular properties of HDPE polymer for product streams.

A sensitivity analysis was carried out to see the effect of H_2 flow rate in "**FEED2**" stream on HDPE polymer attributes MWN and MWW. Figure 12.18 shows "**Vary**" and



☑ Active ☐ Case study

Manipulated variables (drag and drop variables from form to the grid below)

Variable	Active	Manipulated variable	Units
1	☑	Mass-Flow Stream=FEED2 Substream=MIXED Component=H2	kg/hr

Measured variables (drag and drop variables from form to the grid below)

Variable	Definition
MWN	Compattr-Var Stream=PRDCT2 Substream=MIXED Component=HDPE Attribute=MWN Element=1
MWW	Compattr-Var Stream=PRDCT2 Substream=MIXED Component=HDPE Attribute=MWW Element=1

Column No.	Tabulated variable or expression
1	MWN
2	MWW

Figure 12.18 A sensitivity analysis was carried out to see the effect of H_2 flow rate on "**MWN**" and "**MWW**" of "**HDPE**" in "**PRDCT2**" stream.

"**Define**" tab window related to the sensitivity analysis tool. The mass flow rate of H_2 will be varied from 50 to 500 kg/h. "**MWW**" and "**MWN**" are defined as "**Compattr-Var**" type belonging to "**HDPE**" component in "**PRDCT2**" stream, which will be monitored as a function of varying the hydrogen flow rate in "**FEED2**" stream.

Figure 12.19 shows the plot of both "**MWN**" and "**MWW**" as a function of H_2 flow rate in "**FEED2**" stream. Notice that both decrease with increasing H_2 flow rate, indicating that H_2 competes with the repeat unit (C_2H_4) in prematurely terminating (or aborting) the polymerization process.

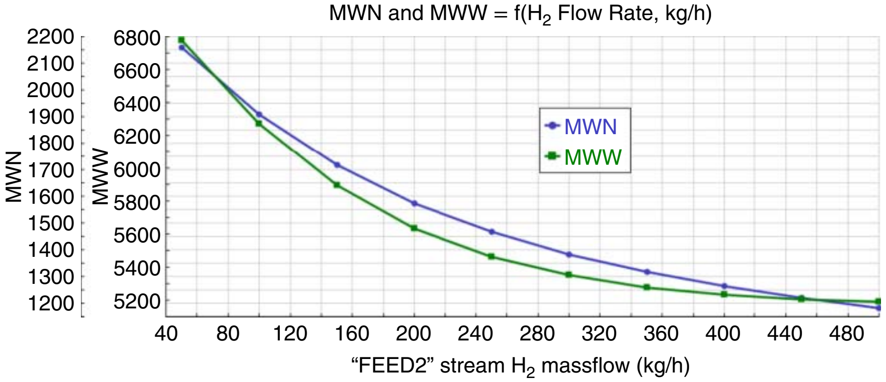


Figure 12.19 The effect of H_2 flow rate on MWN and MWW of HDPE in "**PRDCT2**" stream.

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HOMEWORK/CLASSWORK 12.1 (MAXIMIZING THE DEGREE OF HDPE POLYMERIZATION)

Consider again the HDPE polymerization as described by reaction set "**R-2**" in the running tutorial of this chapter.

a) Using Aspen Plus, start a new simulation by choosing the "**Polymers**" category and selecting "**Polymers with Met-C_bar_hr Units**" template to create a steady-state flowsheet.
b) Set the property method to "**POLYNRTL**" and the free water method to "**SYSOP0**", instead of "**STEAM-TA**" in "**Methods**" | "**Global**" sheet.
c) Give a title for the project and add the same components shown in Figure 12.3. Do not forget to change component "**Type**" of both "**C2H4-R**" and "**HDPE**" from "*Conventional*" to "*Segment*" and "*Polymer*", respectively.
d) Under "**Properties**" environment, go to "**Methods**" | "**Parameters**" | "**Binary Interaction**" | "**NRTL-1**" sheet and assure that the "**Estimate missing parameters by UNIFAC**" option is selected.
e) Redo the additional steps that have been carried out in light of Figures 12.4–12.6, and 12.7.
f) Click on "**Reset**" followed by "**Next**" button to run the simulation and assure that properties analysis completed successfully. Switch to "**Simulation**" environment.
g) From "**Model Palette**", select "**Reactors**" tab, click on "**RCSTR**" icon, and add it once to the flowsheet area. Add the proper input and output stream, as shown in Figure 12.20.

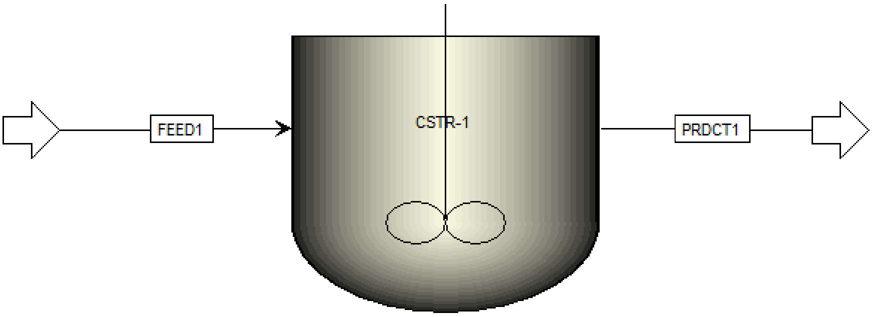


Figure 12.20 The process flowsheet for HDPE polymerization as described by reaction set "**R-2**" in the text.

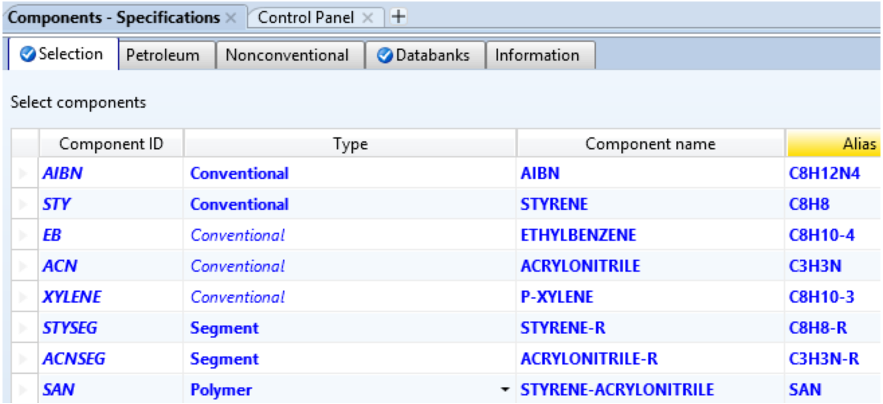
The feed stream input properties and the operating conditions of "**CSTR-1**" are shown in Table 12.1. To make simulation life easier for you, let the total feed flow rate be 100,000 instead of 90,000 kg/h.

h) Define the catalyst attributes present in "**FEED1**" stream as described in Figure 12.8 and Table 12.2.
i) Define the reaction set as exactly as "**R-2**" set in the text and associate it to "**CSTR-1**" block.
j) Do not forget to improve the convergence of the simulator. See Section 12.4.
k) Reset and run the show. Check for possible errors or serious warnings.
l) Suppose that we would like to end up with a high-molecular-weight HDPE. You will basically carry out a sensitivity analysis study, called "**S-1**", to see the optimum feed composition, which will maximize the degree of polymerization. To simplify the task, we consider only the effect of C_2H_4 and *n*-hexane flow rates on the degree of polymerization, which is manifested via MWN and MWW of HDPE in the product ("**PRDCT1**") stream. This means that the feed flow rates for other components will be held constant. Vary the flow rate of C_2H_4 between 10,000 and 30,000 with an increment of 1000 kg/h. On the other hand, vary *n*-hexane between 70,000 and 90,000 with an increment of 5000 kg/h. Define two variables MWN and MWW as shown in Figure 12.18.
m) Reset and run the show. Check for possible errors or serious warnings.
n) Go to "**Model Analysis Tools**" | "**Sensitivity**" | "**S-1**" | "**Results**" | "**Summary**" tab sheet and clicking on "**Results Curve**" button found in "**Home**" ribbon, make two parametric plots one for MWN and another for MWW as a function of C_2H_4 and *n*-hexane feed flow rates. Report the optimum value for both varied feed variables and recalculate the feed composition at the optimum condition.

HOMEWORK/CLASSWORK 12.2 (STYRENE ACRYLONITRILE (SAN) POLYMERIZATION)

Consider the free radical polymerization reaction between acrylonitrile ($N{\equiv}C{-}CH{=}CH_2$) and styrene ($C_6H_5{-}CH{=}CH_2$) to form the styrene acrylonitrile (SAN) polymer. The reaction is initiated by 2,2'-azobis-isobutyronitrile (AIBN, $C_8H_{12}N_4$) and will be carried out in liquid xylene. Ethylbenzene (EB) will be used as the chain transfer agent.

a) Using Aspen Plus, start a new simulation by choosing the "**Polymers**" category and selecting "**Polymers with Met-C_bar_hr Units**" template to create a steady-state flowsheet.
b) Set the property method to "**POLYNRTL**".
c) Give a title for the project and Figure 12.21 shows the list of components that are involved in this free radical polymerization process to produce SAN.



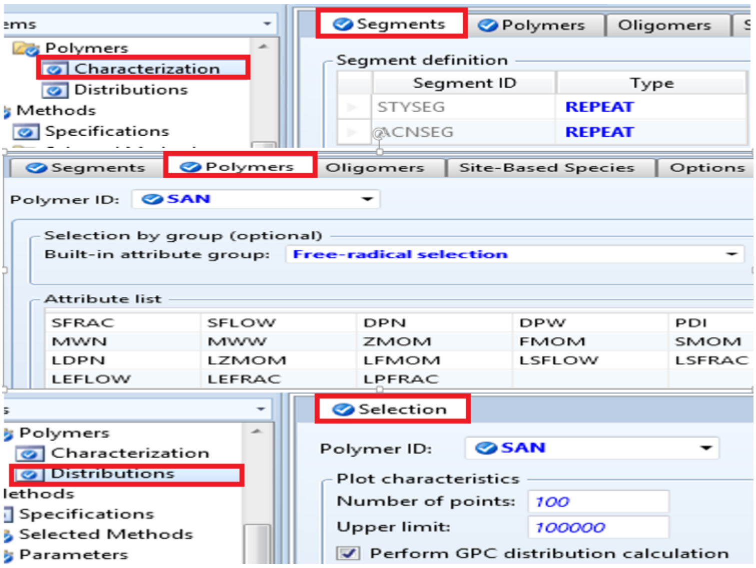
Select components

Component ID	Type	Component name	Alias
AIBN	Conventional	AIBN	C8H12N4
STY	Conventional	STYRENE	C8H8
EB	Conventional	ETHYLBENZENE	C8H10-4
ACN	Conventional	ACRYLONITRILE	C3H3N
XYLENE	Conventional	P-XYLENE	C8H10-3
STYSEG	Segment	STYRENE-R	C8H8-R
ACNSEG	Segment	ACRYLONITRILE-R	C3H3N-R
SAN	Polymer	STYRENE-ACRYLONITRILE	SAN

Figure 12.21 The list of components involved in a free radical polymerization for production of SAN.

d) Under “**Properties**” environment, go to “**Methods**” | “**Parameters**” | “**Binary Interaction**” | “**NRTL-1**” sheet and assure that the “**Estimate missing parameters by UNIFAC**” option is selected.

e) Figure 12.22 shows the “**Components**” | “**Polymers**” | “**Characterization**” and “**Distributions**” folder where we introduce the polymer species to ASPEN, select its attributes group and its repeating units, and ask to perform GPC distribution calculation. Beware that under “**Site-Based Species**” tab, stick to the default “*Ziegler–Natta catalyst*” option.



Segment definition

Segment ID	Type
STYSEG	REPEAT
ACNSEG	REPEAT

Polymer ID: SAN

Selection by group (optional)

Built-in attribute group: Free-radical selection

Attribute list

SFRAC	SFLOW	DPN	DPW	PDI
MWN	MWW	ZMOM	FMOM	SMOM
LDPN	LZMOM	LFMOM	LSFLOW	LSFRAC
LEFLOW	LEFRAC	LPFRAC		

Polymer ID: SAN

Plot characteristics

Number of points: 100

Upper limit: 100000

☑ Perform GPC distribution calculation

Figure 12.22 Define the polymer species for Aspen Plus, its building blocks, and its attributes.

f) Click on “**Reset**” followed by “**Next**” button to run the simulation and assure that properties analysis completed successfully. Switch to “**Simulation**” environment.

g) From “**Model Palette**”, select “**Reactors**” tab, and add twice “**RCSTR**” type block. Add also a mixer. Add the proper input and output streams, as shown in Figure 12.23. The products from both reactors will be combined and leave the mixer as one product.

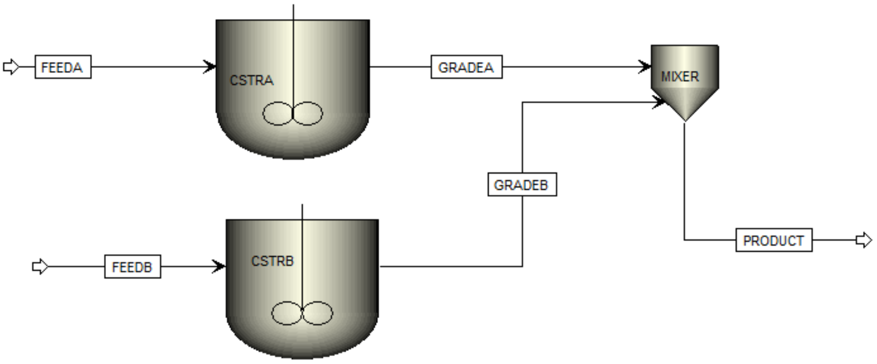


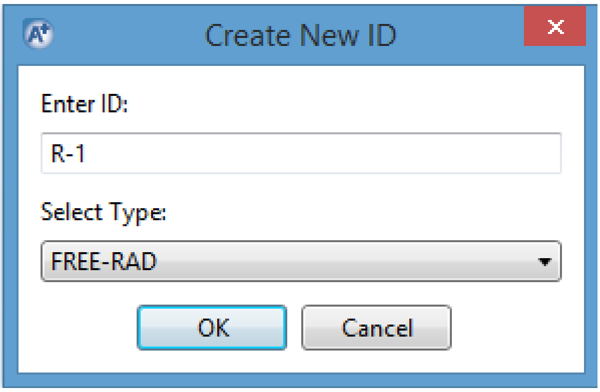
Figure 12.23 Production of SAN using two different feed conditions.

h) The feed and the block operating conditions are given in Figure 12.24. Do not forget to enter SAN attributes using “**Blocks**” | “**CSTRA**” or “**CSTRB**” | “**Setup**” | “**Component Attr.**” tab window for both reactors and later associate “**R-1**” reaction set with “**CSTRA**” and “**R-2**” set with “**CSTRB**”.

STREAM FEEDA
SUBSTREAM MIXED TEMP=70°C. PRES=2 atm. MASS-FLOW=24,000 kg/h.
MASS-FRAC AIBN 0.004 / STY 0.23 / EB 0.04 / ACN 0.23 / & XYLENE 0.496
STREAM FEEDB
SUBSTREAM MIXED TEMP=70°C. PRES=2 atm. MASS-FLOW=24,000 kg/h.
MASS-FRAC AIBN 0.004 / STY 0.25 / ACN 0.25 / & XYLENE 0.496
BLOCK MIXER
PARAM PRES=1 atm. NPHASE=1 PHASE=L MAXIT=60
BLOCK-OPTION FREE-WATER=NO
BLOCK CSTRA
FLASH-MAXIT=90 SCALING=COMPONENTS ALGORITHM=MIXED
PARAM VOL=10 m^3. TEMP=70°C. PRES=2 atm. NPHASE=1 PHASE=L &
FLASH-MAXIT=90 SCALING=COMPONENTS ALGORITHM=MIXED
COMP-ATTR MIXED SAN LPFRAC (1E-005)
COMP-ATTR MIXED SAN LEFRAC (0.5 0.5)
COMP-ATTR MIXED SAN LSFRAC (0.5 0.5)
COMP-ATTR MIXED SAN LDPN (500.0)
COMP-ATTR MIXED SAN SFRAC (0.5 0.5)
COMP-ATTR MIXED SAN PDI (1.5)
COMP-ATTR MIXED SAN DPN (1000.0)
CONVERGENCE SOLVER=NEWTON STAB-STRAT=LINE-SEARCH
BLOCK-OPTION TERM-LEVEL=4 FREE-WATER=NO
REACTIONS RXN-IDS=R-1
BLOCK CSTRB
All properties are the same as those of “**CSTRA**” except you associate “**R-2**” with “**CSTRB**”.

Figure 12.24 Operating conditions of feed streams and reactors, in addition to SAN component attributes within each reactor.

i) Go to “**Reactions**” folder and click on “**New** … ” button and the “**Create New ID**” form will appear, as shown in Figure 12.25, where you enter *R-1* for “**ID**” and “*FRRE-RAD*” for reaction type. Click on “**OK**” button to proceed.

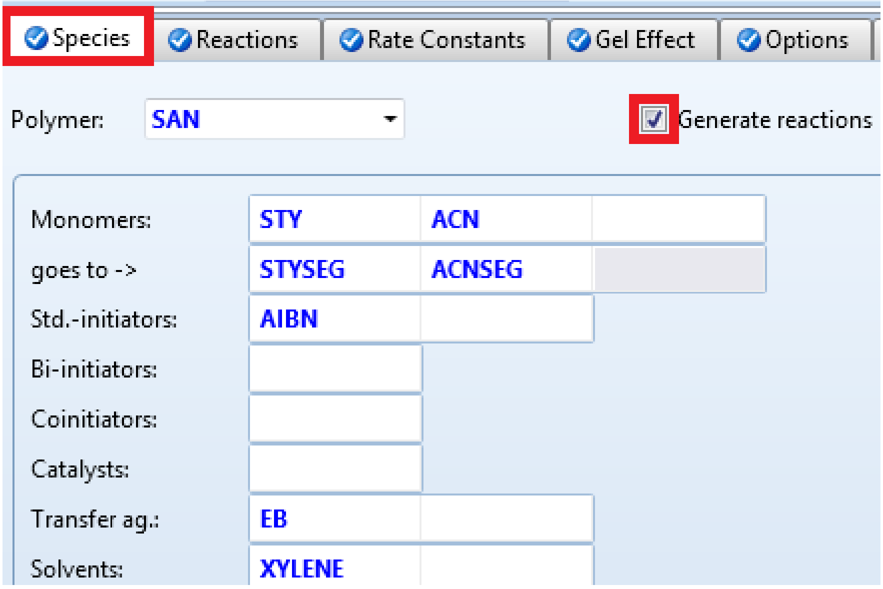


Enter ID: R-1

Select Type: FREE-RAD

Figure 12.25 Creation of a reaction of a free radical (*FREE-RAD*) type to describe polymer synthesis of SAN.

j) For “**Species**” tab window, define the records as shown in Figure 12.26, while select “**Generate reactions**” check button. Once Aspen Plus creates the detailed reaction steps turn it off.



Polymer: SAN

☑ Generate reactions

Monomers:	STY	ACN
goes to ->	STYSEG	ACNSEG
Std.-initiators:	AIBN	
Bi-initiators:		
Coinitiators:		
Catalysts:		
Transfer ag.:	EB	
Solvents:	XYLENE	

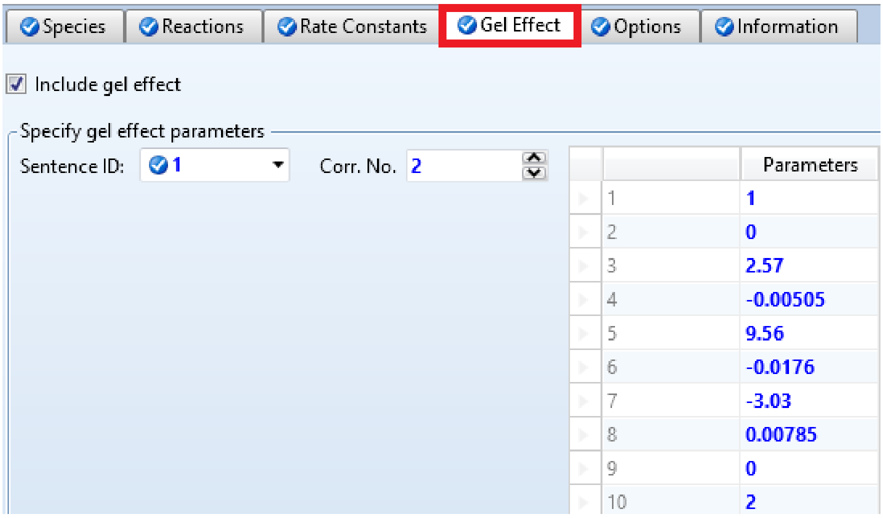
Figure 12.26 Defining the polymer, the two monomers, the two repeat units, the initiator, the chain transfer agent, and solvent for a free radical mechanism polymerization reaction.

k) Retain the reaction steps that are shown in Figure 12.27 and also enter their rate constants as given in the following text. Notice that the order of substeps may not be the same as shown in Figure 12.27; hence, pay attention for the corresponding pre-exponential value for each substep.

Type	Comp1	Comp2	Pre-Exp (1/s)
INIT-DEC	AIBN		3.71E-005
CHAIN-INI	STY		4820
CHAIN-INI	ACN		225
PROPAGATION	STY	STY	4820
PROPAGATION	STY	ACN	10277
PROPAGATION	ACN	STY	7165.6
PROPAGATION	ACN	ACN	225
CHAT-MON	STY	STY	0.289
CHAT-MON	STY	ACN	0.289
CHAT-MON	ACN	STY	0.006
CHAT-MON	ACN	ACN	0.006
TERM-COMB	STY	STY	1.39E7
TERM-COMB	STY	ACN	3.58E8
TERM-COMB	ACN	STY	3.58E8
TERM-COMB	ACN	ACN	1.02E7

Figure 12.27 The detailed reaction substeps that describe the overall free radical mechanism of monomeric conversion of styrene and acrylonitrile into SAN polymer.

l) In "**Gel-Effect**" tab window, enter the parameters as shown in Figure 12.28. Bimolecular termination reactions between chain radicals become diffusion controlled at high



☑ Include gel effect

Specify gel effect parameters

Sentence ID: 1

Corr. No. 2

	Parameters
1	1
2	0
3	2.57
4	-0.00505
5	9.56
6	-0.0176
7	-3.03
8	0.00785
9	0
10	2

Figure 12.28 Entering the gel effect parameters.

polymer concentrations or high conversion, leading to an initial increase in the polymerization rate and molecular weight. This condition is known as the *gel effect* or Trommsdorff effect. At high polymer concentrations, the increased viscosity of the reaction medium imposes a diffusional limitation on the polymer chains, which leads to lower effective termination rates. Typically, the termination rate coefficients are affected first by the gel effect because they involve diffusion of two bulky polymer radicals. Eventually at high enough conversions, efficiencies of initiation, chain transfer reactions, the initiator, and even the propagation are all lowered by the gel effect. Hence, in general, it may be necessary to allow gel/glass effects for all the polymerization reactions in the built-in kinetic scheme. The diffusional limitation is usually modeled by multiplying the low conversion reaction rate coefficients, k_o, by a gel effect factor, GF, that decreases with increasing conversion. Hence, the effective rate coefficient for a reaction is given by $k_{eff} = k_o \times \text{GF}$.

m) Repeat the previous (j → l) steps for “**R-2**” set.

n) Do not forget to improve the convergence of the simulator. See Section 12.4.

The Aspen Plus platform is now ready for analyzing the distribution of SAN polymer as a function of feed variables or if the user carries out a sensitivity analysis. You can always monitor the molecular weight or chain length distribution for a particular block or stream simply by clicking on that block (or stream), and clicking on “**Chain Size Distr**”. button under “**Plot**” tab found in “**Home**” ribbon. If interested in seeing all three streams together such as “**GRADEA**”, “**GRADEB**”, and “**PRODUCT**”, then go to “**Results Summary**” and select “**Streams**”. This will allow you to see the three of them together, as shown in Figure 12.29.

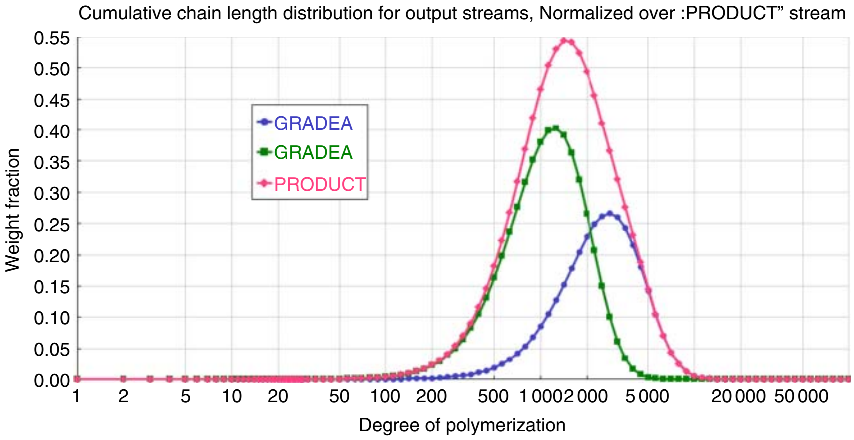


Figure 12.29 Showing the SAN polymer distribution curves for the three streams in one plot.

o) What do you conclude about the difference in MWW between “**GRADEA**” and “**GRADEB**” stream?

p) Increase the mass fraction of styrene at the expense of ACN in one feed and decrease it in favor of ACN in the second feed.

q) Repeat case two but switch the feeds in terms of increasing and decreasing styrene.

r) Change both reactor temperatures to $T = 90°C$ and see how an increase in T affects the degree of polymerization, manifested via MWW, MWN, and PDI. You may increase the pressure.

s) Change both reactor temperatures to $T = 50°C$ and see how a decrease in T affects the degree of polymerization, manifested via MWW, MWN, and PDI. Notice that, in current and previous steps, the effect of temperature will be picked up by the gel effect as the overall polymerization process will be mass transfer limited at a high conversion or yield.

t) Carry out a sensitivity analysis for "**CSTRA**", where you monitor MWW for SAN in "**GRADEA**" while manipulating the solvent mass flow rate in "**FEEDA**" stream.

u) Carry out a sensitivity analysis for "**CSTRB**", where you monitor MWW for SAN in "**GRADEB**" while manipulating the solvent mass flow rate in "**FEEDB**" stream.

APPENDIX 12.A THE MAIN FEATURES AND ASSUMPTIONS OF ASPEN PLUS CHAIN POLYMERIZATION MODEL

APPENDIX 12.A.1 Polymerization Mechanism

The catalyst active site is attached to one end of a live polymer chain via a metal–carbon bond. It is generally accepted that polymerization proceeds via a two-step mechanism. In the first step, monomer is complexed to the transition metal site. The second step is the coordinated insertion of the monomer into the metal–carbon bond. As a result, the polymer chain and the previously added segment grow away from the active site with every addition of a monomer molecule.

It is believed that the chain microstructure will not have a strong influence on the mode of monomer addition. For this reason, the built-in kinetic model assumes that the reactivity of a live polymer chain depends only on the active segment and the active site type, and is independent of the polymer chain length and other structural properties. That is, in the propagation reaction, *the rate of propagation* $R^k_{p,ij}$ *is independent of the polymer chain length*. It depends only on the concentration of monomer j, and the concentration of live polymer chains with an active segment of type i attached to an active site of type k. Models using this assumption are referred to as terminal models in the polymerization literature.

APPENDIX 12.A.2 Copolymerization Mechanism

For copolymerization, the built-in kinetic scheme allows the user to specify the number of monomer types used. Similarly, the user has the flexibility to specify the number of each type of reactive species present in the polymerization: catalysts, cocatalysts, chain transfer agents, solvents, and so on. The user is able to tailor the built-in kinetics to model a specific catalyzed polymerization system by selecting a subset of the reactions shown in the Built-In Ziegler–Natta Catalysts and Polymerization Kinetic Scheme.

However, it is important that the subset include a chain initiation, propagation, and at least one chain transfer or active site deactivation reaction to produce dead polymer.

APPENDIX 12.A.3 Rate Expressions

The rate expression for each reaction is generally written as a product of the rate constant and the concentrations of the reacting species. In many of the reactions, one of the reacting species is a polymer chain while the other is a small molecule such as monomer, chain transfer agent, and cocatalyst. A reaction order with respect to the small reacting molecule is included for some of the reactions. This reaction order has a default value of one. The rate constants for each reaction at sites of type k are calculated at the reaction temperature using the Arrhenius equation shown below. The user specified rate constant parameters are pre-exponential factor (k_{o}^{k}), activation energy (E_{a}^{k}) at sites of type k, and the reference temperature.

APPENDIX 12.A.4 Rate Constants

$$k^{k} = k_{\mathrm{o}}^{k} \exp\left[-\frac{E_{\mathrm{a}}^{k}}{R}\left(\frac{1}{T} - \frac{1}{T_{\mathrm{ref}}}\right)\right]$$

where

k_{o}^{k}	Pre-exponential factor in 1/s for first order reactions
E_{a}^{k}	Activation energy in mole enthalpy units
R	Universal gas constant
T_{ref}	Reference temperature in Kelvin

APPENDIX 12.A.5 Catalyst Preactivation

Some of the chromium catalysts used in these processes exhibit a slow activation with induction period. This slow activation can be modeled by catalyst preactivation reaction. The precatalyst goes to catalyst that further undergoes site activation, initiation, and propagation.

APPENDIX 12.A.6 Catalyst Site Activation

The catalyst site activation step involves the generation of reactive vacant active sites from potential sites. Depending on the catalysts system, the activation may be done before the catalyst is fed to the reactor or within the reactor.

There are several, different site activation reactions included in the built-in kinetic scheme. They include site activation by cocatalyst, by electron donors, by hydrogen, by monomer, and spontaneous site activation. Different catalyst systems tend to be activated by a different subset of the reactions in this scheme. For example, $TiCl_3$ catalyst systems are usually activated with an organoaluminum cocatalyst such as diethylaluminum chloride (DEAC), in the reactor. Chromic oxide catalysts are calcined by heating with air for several hours at temperatures of 400–975°C and cooled in dry air. Some of these catalysts may be activated with a reducing agent before introduction into the reactor, while others are activated within the reactor.

APPENDIX 12.A.7 Site Activation Reactions

Some of the site activation reactions (activation by monomer, electron donor, hydrogen) have been proposed to explain the observed rate enhancement behavior in different catalyst systems. For example, the activation of additional sites by co-monomer has been proposed to explain the rate enhancement observed with the addition of a co-monomer to ethylene and propylene homopolymerization reactors.

APPENDIX 12.A.8 Chain Initiation

Chain initiation involves the reaction of a monomer molecule at a vacant active site to form a live polymer molecule of unit length at that site. This reaction converts a vacant active site to a propagation site. The chain initiation reaction is shown here:

$$P_{\mathrm{o}}^k + M_i \rightarrow P_1^i \quad R_{\mathrm{ci}}^k = k_{\mathrm{ci}}^k P_{\mathrm{o}}^k (C_{Mi})^{O_{Mi}^k}$$

The rate of chain initiation at site type k, R_{ci}^k, is dependent on the concentration of vacant sites of type k and the concentration of monomer i. The user can also specify the reaction order with respect to the monomer concentration. The live polymer chains grow by successive addition of monomer molecules to form long polymer molecules.

APPENDIX 12.A.9 Propagation

The live polymer, at each active site type, grows or propagates through the addition of monomer molecules to form long polymer chains. The propagation reaction is represented by

$$P_{n,i}^k + M_j \rightarrow P_{n+1,j}^k \quad R_{p,ij}^k = k_{p,ij}^k C_{Mj} P_{n,i}^k \text{ (main propagation)}$$

where monomer j is being added to a polymer chain of length n, with an active segment of type i at an active site of type k. The resulting polymer chain will be of length $n + 1$ and the active segment will be of type j. The active segment type usually represents the last monomer type incorporated into the polymer chain.

For copolymerization, there will be $\boldsymbol{N_m \times N_m \times N_{site}}$ propagation reactions that may have different reactivities. For example, with two monomers and three site types, the monomer being added could be monomer 1 or monomer 2 while the active segment type could be segments from monomer 1 or monomer 2 at each site type.

As a result, there will be 12 *rate constants* ($k_{p,ij}^k$), where the subscript i refers to the active segment type while the second subscript j refers to the propagating monomer type. The superscript k refers to active site type. For the terminal model the rate of propagation is dependent only on the concentration of live polymer with active segment i at active site k and the concentration of the propagating monomer j. In Aspen Polymers Version 3.0 and higher, another propagation reaction has been added to account for formation of atactic polymer. This reaction has the same form as the main propagation reaction:

$$P_{n,i}^k + M_j \rightarrow P_{n+\delta i,i}^k \quad R_{paij}^k = k_{paij}^k \mu_{0,j}^k (C_{Mi})^{O_{paMi}^k} \text{ (atactic propagation)}$$

but uses a different rate constant k_{paij}^k. When the atactic propagation reaction is included in the simulation, the main propagation reaction should be considered to account for the formation of all polymer whether it is isotactic or atactic. Hence, the main propagation reaction is also termed the total propagation. The atactic propagation reaction only accounts for the formation of atactic polymer. The atactic content of the polymer is then calculated from the ratio of atactic to total polymer.

APPENDIX 12.A.10 Chain Transfer to Small Molecules

Chain transfer to small molecules such as monomer, solvent, or chain transfer agent usually involves the extraction of hydrogen from the small molecule by the active site and leads to the termination of the live chain. At the same time, a new vacant site is formed, which can undergo chain initiation to start polymerization. The effect of chain transfer on the polymerization kinetics depends on the reactivity of the transfer sites.

When the transfer site is very reactive, as is the case when the chain initiation rate constant is greater than the propagation rate constant, chain transfer will not lower the polymerization rate or conversion, but will reduce the molecular weight of the polymer. However, if the transfer site is less reactive, as in the case of low chain initiation rate constant, both the conversion and molecular weight of the polymer will be lowered. In the built-in kinetics, *chain transfer to hydrogen, cocatalysts, solvent, transfer agent, electron donor, monomer, and spontaneous chain transfer are included* in the Built-In Ziegler–Natta Catalysts and Polymerization Kinetic Scheme.

APPENDIX 12.A.11 Chain Transfer to Monomer

For chain transfer to monomer, a new polymer chain of unit length is generated while for the other transfer reactions a vacant site of that type is generated. The dead polymer chain formed by some of the chain transfer reactions will have an end-group with a TDB. In addition to the rate constant parameters and the reaction order, the user may also specify a parameter to track the fraction of dead polymer chains with TDBs that are generated from the chain transfer reactions. The default value for this parameter is zero.

APPENDIX 12.A.12 Site Deactivation

The catalyst site deactivation step involves the deactivation of active sites, vacant and propagation, to form dead sites. Depending on the catalyst system and operating conditions, the deactivation rate may be high or low. There are several different site deactivation reactions included in the built-in kinetic scheme. They include site deactivation by cocatalyst, by electron donors, by hydrogen, by monomer, by poisons, and spontaneous site deactivation. Different catalyst systems tend to be deactivated by a different subset of the reactions. The deactivation rate constants are assumed to be dependent only on the site type and not on the polymer segment attached to a site. Therefore, the same rate constant is applied to both vacant and propagation sites of the same type. Note that deactivation rates are per unit of active (vacant and propagation) site concentration.

APPENDIX 12.A.13 Site Inhibition

Inhibited sites have small molecules such as hydrogen or poisons attached. As a result, inhibited sites are temporarily blocked from becoming propagation sites. The site inhibition reaction is considered reversible. Therefore, the small molecule may dissociate from an inhibited site, which then becomes a vacant site once again. The user must specify rate constant parameters for both the forward (inhibition) and reverse (dissociation) reactions.

APPENDIX 12.A.14 Cocatalyst Poisoning

For some catalyst systems, additional amounts of cocatalysts are fed to the reactor to counteract the effect of any poisons present. This is modeled as a cocatalyst poisoning reaction in the built-in kinetics. The product of this reaction is designated as a by-product in the list of reactive species. The by-product is considered to be inert and does not participate in any reaction.

APPENDIX 12.A.15 Terminal Double Bond Polymerization

For some catalyst systems, primarily metallocene, polymer chains with long-chain branches are formed. However, the long-chain branching frequency is usually small. The long-chain branches are believed to be due to propagation reactions involving a live chain and a TDB on a dead polymer chain. Polymer chains with TDBs are formed by some of the chain transfer reactions. To form long-chain branches, the metal center must be open to provide a favorable reactivity ratio for the macro-monomer. The concentration of TDB end-groups on the dead polymer chains are tracked through an additional segment called the TDB-Segment. *TDB-Segments are generated through the chain transfer reactions and are consumed through the TDB polymerization reaction*. When the TDB reaction is used, one additional segment needs to be defined in the Components form for the TDB-Segment. Typically, for a copolymerization system with N monomers, N repeat segments would be defined in the Components form. However, with the TDB polymerization reaction, N repeat segments and one end segment should be defined in the Component form. The end segment must be specified as the TDB-Seg species in the Species folder of the Ziegler–Natta kinetics.

APPENDIX 12.A.16 Phase Equilibria

The polymerization model currently considers a single-phase system (vapor or liquid), two-phase system (vapor and liquid), or three-phase (VLL) system when calculating concentrations for the reaction kinetics. For single-phase systems, the reacting phase may be either vapor or liquid. In multiphase systems, reactions can occur in one or more phases simultaneously. Each reaction object is associated with a single reacting phase, identified on the options form.

By default, the reacting phase is assumed to be the liquid phase (for VLL systems, the reacting phase must be specified). Several reaction models can be referenced from a single reactor block to account for reactions in each phase.

APPENDIX 12.A.17 Rate Calculations

The Ziegler–Natta polymerization kinetic model supplies to the reactor models the reaction rates for the components and the rate of change of polymer attributes (e.g., the chain length distribution moments). The component reaction rates are computed from the kinetic scheme by summing over all reactions that involve the component. The site-based moment rates are derived from a population balance and method of moments approach.

APPENDIX 12.A.18 Calculated Polymer Properties

The following variables can be calculated by the built-in kinetics routine based on the polymer attributes selected, and the subset of the built-in kinetics used for a specific simulation:

- Zeroth, first, and second moments for the composite polymer (ZMOM, FMOM, and SMOM)
- Zeroth, first, and second moments for the live polymer (LZMOM, LFMOM, and LSMOM)
- Zeroth, first, and second moments for the site-based live polymer (SZMOM, SFMOM, and SSMOM)
- Number and weight degree of polymerization and polydispersity index for the composite and site-based bulk polymer (DPN, DPW, PDI and SDPN, SDPW, SPDI)
- Number and weight average molecular weight for the composite and site-based bulk polymer (MWN, MWW and SMWN, SMWW)
- Copolymer segment composition for composite and site-based bulk polymer (SFRAC and SSFRAC segment mole fractions)
- Total number long-chain branches (LCB)
- Long-chain branching frequencies (FLCB)
- Mole fraction of live bulk polymer chains (LPFRAC and LSPFRAC)
- Number average degree of polymerization for live polymer (LDPN and LSDPN)
- Copolymer segment composition for live polymer (LSFRAC and LSSFRAC)
- Live polymer active segment composition (LEFRAC and LSEFRAC).

These variables are stored as component attributes. It is assumed that attributes needed for the kinetic scheme are selected. In many cases, users may need to know polymer product properties related to the above-mentioned structural properties. For example, users may be interested in melt flow rate or melt index, viscosity, density, and so on. These properties can be calculated in user-supplied FORTRAN subroutines, which take the polymer moments and structural information and return the desired property.

APPENDIX 12.B THE NUMBER AVERAGE MOLECULAR WEIGHT (MWN) AND WEIGHT AVERAGE MOLECULAR WEIGHT (MWW)

The average properties can be calculated as ratios of the moments. The number average degree of polymerization (DPN) is the ratio of the first to the zeroth moment, λ_1/λ_0. On the other hand, the Weight or Volume average degree of polymerization (DPW) is the ratio of the second to the first moment, λ_2/λ_1.

In general, for a polymer with a chain length distribution, the moment frequency distribution is given by

$$\lambda_m = \sum_{n=1}^{N} n^m Q_n \tag{B.1}$$

where

λ	Moment
m	Moment order
n	Chain length or degree of polymerization
Q_n	Number of moles of polymer of length n

The polymer average chain length and weight properties are then calculated as follows:

$$\text{DPN} = \text{Number–average degree of polymerization} = \frac{\lambda_1}{\lambda_0} = \frac{\text{FMOM}}{\text{ZMOM}} \tag{B.2}$$

$$\text{DPW} = \text{Weight–average degree of polymerization} = \frac{\lambda_2}{\lambda_1} = \frac{\text{SMOM}}{\text{FMOM}} \tag{B.3}$$

$$\text{PDI} = \text{Poly dispersity index} = \frac{\text{DPW}}{\text{DPN}} = \frac{(\lambda_2/\lambda_1)}{(\lambda_1/\lambda_0)} = \frac{(\lambda_2 \times \lambda_0)}{(\lambda_1)^2} = \frac{(\text{SMOM} \times \text{ZMOM})}{(\text{FMOM})^2} \tag{B.4}$$

$$\text{MWN} = \text{Number–average molecular weight} = \text{DPN} \times \overline{\text{M}}_{\text{segment}} \tag{B.5}$$

$$\text{MWW} = \text{Weight–average molecular weight} = \text{DPW} \times \overline{\text{M}}_{\text{segment}} \tag{B.6}$$

I know ahead that the brain-average user will find it difficult to grasp or grab such terms. Therefore, I will explain the terminology based on a simple statistical approach.

Let us consider that we have <u>100 monomeric units of C_3H_6</u>. Let us say the homopolymerization reaction (i.e., formation of polypropylene polymer) is initiated via different catalyst sites. The 100 building blocks can be put in so many different ways (i.e., configurations), depending on the rate constant of each type of active site. For the sake of clarifying the aforementioned definitions, we consider the following cases:

<u>The First Case:</u> All 100 blocks (i.e., monomers) are put in one single polymer chain.

<u>The Second Case:</u> Two polymer chains each with 50 blocks.

<u>The Third Case:</u> Two polymer chains but one with 60 and another with 40 blocks.

<u>The Fourth Case:</u> Four polymer chains where the first has 10, the second 20, the third 30, and the fourth 40 blocks, adding up to 100 blocks.

Let us calculate the mean and variance for each case.

<u>The First Case:</u>

$$\text{MWN} = 100 \times M_o = 100M_o \tag{B.7}$$

$$\mu = \overline{X} = 100M_o \tag{B.8}$$

$$\text{Variance} = \sum_{i=1}^{N} \frac{(X_i - \overline{X})^2}{N} = \frac{(M_o 100 - M_o 100)^2}{1} = \frac{M_o^2(100 - 100)^2}{1} = 0 \tag{B.9}$$

$$\text{The standard deviation, } s = \sqrt{\text{Variance}} = 0 \tag{B.10}$$

Here, we have one polymer chain and the average of one chain will be the same as that of the chain itself. This also explains why the standard deviation is identically zero. M_o represents the molecular weight of one building block (i.e., $C_3H_6 = 42$ g/mol).

$$\mathrm{PDI} = \left(\frac{s}{\mu}\right)^2 + 1 = \frac{\mathrm{Variance}}{\mu^2} + 1 = \left(\frac{0}{100M_\mathrm{o}}\right)^2 + 1 = 1 \tag{B.11}$$

Equation B.11 simply says that if there is no deviation from the mean value, then all sampled polymer chains will lie on their mean value (i.e., a monodisperse solution with PDI = 1).

Thus,

$$\mathrm{MWW} = \mathrm{PDI} \times \mathrm{MWN} = 1 \times 100M_\mathrm{o} = 100M_\mathrm{o} \tag{B.12}$$

The Second Case:

$$\mathrm{MWN} = \frac{1 \times 50 \times M_\mathrm{o} + 1 \times 50 \times M_\mathrm{o}}{2} = 50M_\mathrm{o} \tag{B.13}$$

$$\mu = \overline{X} = 50M_\mathrm{o} \tag{B.14}$$

$$\mathrm{Variance} = \sum_{i=1}^{2} \frac{(X_i - \overline{X})^2}{N} = \frac{M_\mathrm{o}^2(50-50)^2 + M_\mathrm{o}^2(50-50)^2}{2} = 0 \tag{B.15}$$

$$s = \sqrt{\mathrm{Variance}} = 0 \tag{B.16}$$

$$\mathrm{PDI} = \left(\frac{s}{\mu}\right)^2 + 1 = \frac{\mathrm{Variance}}{\mu^2} + 1 = \frac{0}{\overline{X}^2} + 1 = 1 \tag{B.17}$$

Thus,

$$\mathrm{MWW} = \mathrm{PDI} \times \mathrm{MWN} = 1 \times 50M_\mathrm{o} = 50M_\mathrm{o} \tag{B.18}$$

Here, we have two polymer chains with identical number of blocks. Hence, the average will be equal to $50M_\mathrm{o}$, which is the same as that of either chain.

The Monodisperse Polymer: In general, if we have one single chain with 100 blocks, two chains each with 50 blocks, four chains each with 25 blocks, and so on, then PDI will be one and MWN = MWW. Any of the aforementioned cases, which has a uniform chain length, is called a monodisperse polymeric system.

The Third Case:

$$\mathrm{MWN} = \frac{1 \times 60 \times M_\mathrm{o} + 1 \times 40 \times M_\mathrm{o}}{2} = 50M_\mathrm{o} \tag{B.19}$$

$$\mu = \overline{X} = 50M_\mathrm{o} \tag{B.20}$$

$$\mathrm{Variance} = \sum_{i=1}^{2} \frac{(X_i - \overline{X})^2}{N} = \frac{M_\mathrm{o}^2(60-50)^2 + M_\mathrm{o}^2(40-50)^2}{2} = 100M_\mathrm{o}^2 \tag{B.21}$$

$$s = \sqrt{\text{Variance}} = 10M_o \tag{B.22}$$

$$\text{PDI} = \left(\frac{s}{\mu}\right)^2 + 1 = \left(\frac{10M_o}{50M_o}\right)^2 + 1 = 1.04 \tag{B.23}$$

Thus:

$$\text{MWW} = \text{PDI} \times \text{MWN} = 1.04 \times 50M_o = 52M_o \tag{B.24}$$

Here, we have two polymer chains with different number of blocks. Hence, the average will be equal to $50M_o$, which lies between $40M_o$ and $60M_o$. Since we have a mixture containing two polymer chains but with different chain lengths, then PDI will be greater than one, reflecting the degree of scatter around the mean value (i.e., $\mu = \text{MWN} = 50M_o$). Notice that for such a case, if we apply Equation B.1 thrice, we get

$$\lambda_0 = \sum_{n=1}^{2} n^0 Q_n = 60^0 \times 1 + 40^0 \times 1 = 2 \tag{B.25}$$

$$\lambda_1 = \sum_{n=1}^{2} n^1 Q_n = 60^1 \times 1 + 40^1 \times 1 = 100 \tag{B.26}$$

$$\lambda_2 = \sum_{n=1}^{2} n^2 Q_n = 60^2 \times 1 + 40^2 \times 1 = 5200 \tag{B.27}$$

Moreover, if we apply Equations B.2 through B.6, we get

$$\text{DPN} = \frac{\lambda_1}{\lambda_0} = \frac{100}{2} = 50 \tag{B.28}$$

$$\text{DPW} = \frac{\lambda_2}{\lambda_1} = \frac{5200}{100} = 52.0 \tag{B.29}$$

$$\text{PDI} = \frac{\text{DPW}}{\text{DPN}} = \frac{(\lambda_2 \times \lambda_0)}{(\lambda_1)^2} = \frac{(5200 \times 2)}{(100)^2} = \frac{104}{100} = 1.04 \tag{B.30}$$

$$\text{MWN} = \text{DPN} \times \overline{\text{M}}_{\text{segment}} = 50 \times M_o = \overline{X} \tag{B.31}$$

$$\text{MWW} = \text{DPW} \times \overline{\text{M}}_{\text{segment}} = 52 \times M_o \tag{B.32}$$

Notice that we have the same answer for PDI as given by both Equations B.23 and B.30; MWN is exactly $\overline{X}$; and MWW is the same as given by both Equations B.24 and B.32. We do not have to carry out the comparison between the methods anymore; this serves as an evidence that both methods quantitatively yield the same answer.

<u>The Fourth Case:</u>

$$\text{MWN} = \frac{(1 \times 10 \times M_o) + (1 \times 20 \times M_o) + (1 \times 30 \times M_o) + (1 \times 40 \times M_o)}{4} = 25M_o \tag{B.33}$$

$$\mu = \overline{X} = 25M_o \tag{B.34}$$

$$\text{Variance} = \sum_{i=1}^{2} \frac{(X_i - \overline{X})^2}{N} = \frac{M_o^2(40-25)^2 + M_o^2(30-25)^2 + M_o^2(20-25)^2 + M_o^2(10-25)^2}{4}$$

$$= 125M_o^2 \tag{B.35}$$

$$s = \sqrt{\text{Variance}} = 11.18M_o \tag{B.36}$$

$$\text{PDI} = \frac{\text{Variance}}{\mu^2} + 1 = \frac{125M_o^2}{(25M_o)^2} + 1 = 1.2 \tag{B.37}$$

Thus:

$$\text{MWW} = \text{PDI} \times \text{MWN} = 1.2 \times 25M_o = 30M_o \tag{B.38}$$

Here, we have four polymer chains with different number of blocks. Hence, the average will be equal to $25M_o$. Since we have a mixture containing four polymer chains but with different chain lengths, then PDI here will be greater than that of the third case, reflecting more degree of scatter around the mean value (i.e., $\mu = \text{MWN} = 25M_o$).

At the end, I hope that I managed to clarify for the reader the notion behind MWN, MWW, and PDI.

13

CHARACTERIZATION OF DRUG-LIKE MOLECULES USING ASPEN PROPERTIES

13.1 INTRODUCTION

Aspen Properties is a useful tool in characterization of drug-related compounds. In this content, the compound to be characterized can be the solvent itself and how it interacts with other solvents, such as examining the solubility of polar organic solvents in water or vice versa (i.e., mutual solubility). Alternatively, the compound can be the solute, or what is called the active ingredient, which is, in general, scarcely water soluble and requires a set of solvents, cosolvent, and/or emulsifying agent to make it soluble.

Organic solvents nowadays have many applications in almost all avenues of industrial life. They are used in emulsion and microemulsion formulations as a solvent, cosolvent, or cosurfactant as is the case in detergent, cosmetic, paint, and pharmaceutical industries. They are also used in liquid–liquid extraction and absorption processes. Moreover, solvents may be used as a reaction medium to bring reactants together, as a reactant to react with a solute when it cannot be dissolved, and as a carrier, to deliver chemical compounds in solutions to their point of use in the required amounts [1]. Organic solvents are constantly present in the pharmaceutical production processes. The pharmaceutical industry is one of the largest users of organic solvents per amount of the final product [2]. They are usually used at any step of the synthesis pathway of an active substance or excipients, and sometimes during the drug product formulation process.

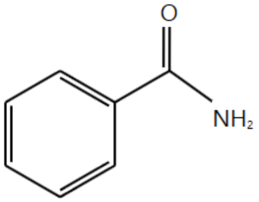
In pharmaceutical industries, crystallization from solution is widely used for the purification of pharmaceutical products during the final stages of manufacture. The type of solvent being used influences the morphology of obtained crystals. For example, the polarity of the solvent affects the crystal morphology of ibuprofen. The use of methanol results in symmetrical and smooth crystals while the use of a low polarity solvent (such as acetone) results in elongated crystals [3].

Aspen Plus®: Chemical Engineering Applications, First Edition. Kamal I.M. Al-Malah.

Companion Website: www.wiley.com/go/Al-Malah/AspenPlusApplications

With increasing pressure to identify high-quality drug candidates, it is critical to assess the absorption, distribution, metabolism, excretion (ADME) attributes of compounds early during the drug discovery phase. This may include properties such as aqueous solubility, permeability, metabolic stability, and *in vivo* pharmacokinetics. One of the properties crucial to candidate screening is the solubility of the compound. Aqueous solubility is an important property of drugs, which are administrated orally or by injection due to the fact that oral drugs must be absorbed through the gastrointestinal tract and should remain in solution to reach the intended therapeutic target. On the other hand, injectable drugs must be sufficiently water soluble to get a "free" ride in the blood and lymph system. *In silico* models that can predict the solubility without expending the compound are of great value to the pharmaceutical industry. Nevertheless, models can fail or result in little value if the data used to generate the model are of a poor quality or were obtained under varied experimental conditions.

13.2 PROBLEM DESCRIPTION

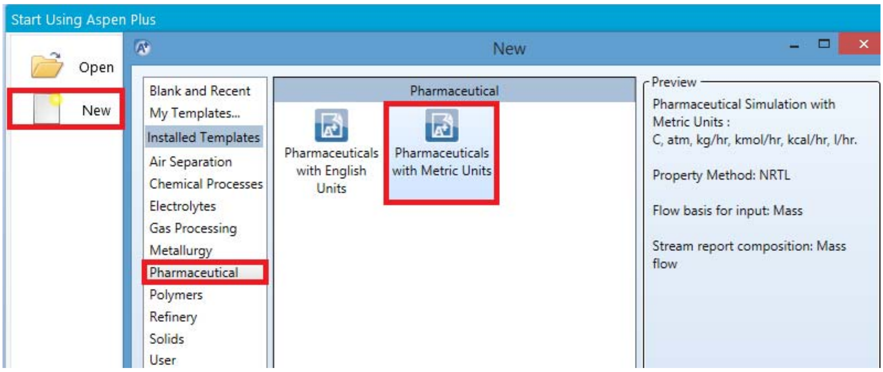


Benzamide (C_7H_7NO), with a molecular weight (MW) of 121.14, is an aromatic amide that consists of benzene bearing a single carboxamido substituent. Its **S**implified **M**olecular-**I**nput **L**ine-**E**ntry **S**ystem (SMILES) formula is NC(=O)C1=CC=CC=C1. It is a transparent crystalline substance, obtained by the action of ammonia upon chloride of benzoyl, as also by several other reactions with benzoyl compounds. It has a melting point of 130°C, a normal boiling point of 288°C, and a density of 1.341 g/cm^3. It is slightly soluble in water and more soluble in ethyl alcohol and carbon tetrachloride. It is used in chemical synthesis. Benzamide is the most potent poly(ADP-ribose) polymerase (PARP) inhibitor in the family of benzamides (PARP inhibitors can be used as anticancer agents, radiosensitizers, and antiviral agents). Benzamide is used as a potent antiemetic (against vomiting), antidepressant, and anticholinergic (a substance that opposes or blocks the action of acetylcholine, sleep aid, daytime sedative, when more potent agents are contraindicated).

In this chapter, I guide the reader through the procedure for estimating the physical properties for this component as if it were not present in the Aspen Plus databanks. Plugging the molecular structure and some known molecular properties of benzamide will be sufficient for Aspen Properties to estimate typical thermodynamic and transport properties. It should be noted that benzamide is already an Aspen Plus databank member (i.e., fully characterized). So, why do we need to use a known databank member? Well, it is simply for the sake of comparison; the estimated properties will be contrasted versus those of the built-in (Aspen Plus databank member) benzamide component. At the same time, it will be used as an example to demonstrate how to use Aspen Properties as a tool to almost fully characterize a material with a little information about it.

13.3 CREATING ASPEN PLUS PHARMACEUTICAL TEMPLATE

Using Aspen Plus, start a new simulation by choosing the “**Pharmaceutical**” category and selecting “**Pharmaceuticals with Metric Units**” template to create a steady-state flow sheet. Notice that the default property method is set to “**NRTL**” (Figure 13.1).



Pharmaceutical Simulation with Metric Units :
C, atm, kg/hr, kmol/hr, kcal/hr, l/hr.

Property Method: NRTL

Flow basis for input: Mass

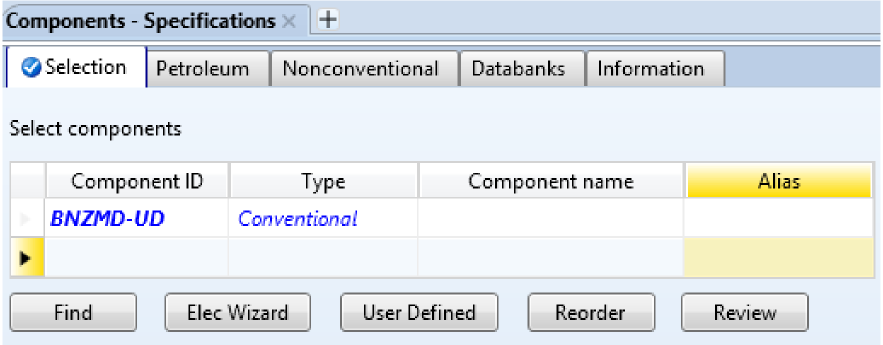
Stream report composition: Mass flow

Figure 13.1 Selection of “**Pharmaceuticals with Metric Units**” template from “**Pharmaceutical**” category.

Next, we will define a component called **BNZMD-UD**. The suffix “**UD**” means User-Defined.

13.3.1 Entering the User-Defined Benzamide (BNZMD-UD) as Conventional

1. In “**Navigation**” pane menu tree, go to “**Components**” | “**Specifications**” | “**Selection**” tab sheet.
2. In the first line of the “**Component ID**” column, enter “**BNZMD-UD**”. Diligently, hit “tab” or “enter” key and Aspen Plus will automatically assign the “*Conventional*” type for such an unrecognized name of a component. Notice that “**BNZMD-UD**” is not present in any of the Aspen Plus databanks; hence, “**Component name**” and “**Alias**” column remain empty, as shown in Figure 13.2.



Select components

Component ID	Type	Component name	Alias
BNZMD-UD	Conventional		

Figure 13.2 Entering the name for benzamide, “**BNZMD-UD**”, as “*Conventional*” and user-defined component.

Next, we will tell Aspen Plus to estimate missing parameters using “**UNIFAC**”.

13.3.2 Specifying Properties to Estimate

Under “**Properties**” environment, go to “**Methods**” | “**Parameters**” | “**Binary Interaction**” | “**NRTL-1**” sheet and be sure that the “**Estimate missing parameters by UNIFAC**” option is selected.

Next, enter the molecular structure of **BNZMD-UD**. Click on “Next (N→)” button and Aspen Plus will bring you to “**Components**” | “**Molecular Structure**” | “**BNZMD-UD**” | “**General**” tab sheet.

> **NOTE #1:** *You can define the molecular structure in different ways: Using the “**General**” sheet, which is based on individual atoms and bonds (i.e., molecular connectivity); using the “**Functional Group**” tab sheet in which you indicate the functional groups specific to a particular estimation method; or using “**Structure**” tab sheet. In old versions of Aspen, we used to define the molecular structure via the “**General**” tab sheet, or import *.mol file. In this chapter, we explain how to define the structure of a molecule using the “**Molecule Editor**” of Aspen Plus.*

13.4 DEFINING MOLECULAR STRUCTURE OF BNZMD-UD

Figure 13.3 shows the “**Structure**” tab sheet where it is still empty as we did not yet define the molecular structure of “**BNZMD-UD**”.

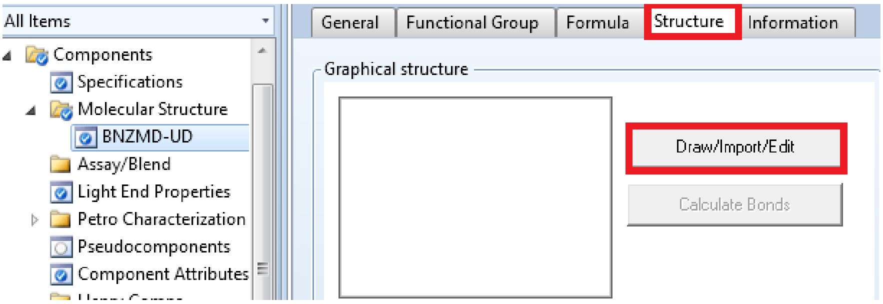


Figure 13.3 The “**Structure**” tab sheet where we define the molecular structure of “**BNZMD-UD**”.

Click on “**Draw/Import/Edit**” button, shown in Figure 13.3, to open the “**Molecule Editor**” window as shown in Figure 13.4. This window is made of the main window and three left panes. The first (i.e., top left) pane represents the types of bond (i.e., single, double, triple, neutral, or charged) to be used; the second (i.e., middle) pane allows the user to select the atom to be installed alone (for the first time), or attached to an existing structure with a type of bond already selected in the first pane; and the third (i.e., bottom left) pane gives the user the flexibility to choose a segment or fragment as part of a molecule, such as the phenyl aromatic ring, without having to build the segment itself from scratch.

Once you click on the phenyl ring from the “**Fragments**” panel, drag it to the working area, decide on the proper location of the phenyl ring, release the mouse, and hit one left-click. The phenyl group will then show up, as shown in Figure 13.5. Alternatively,

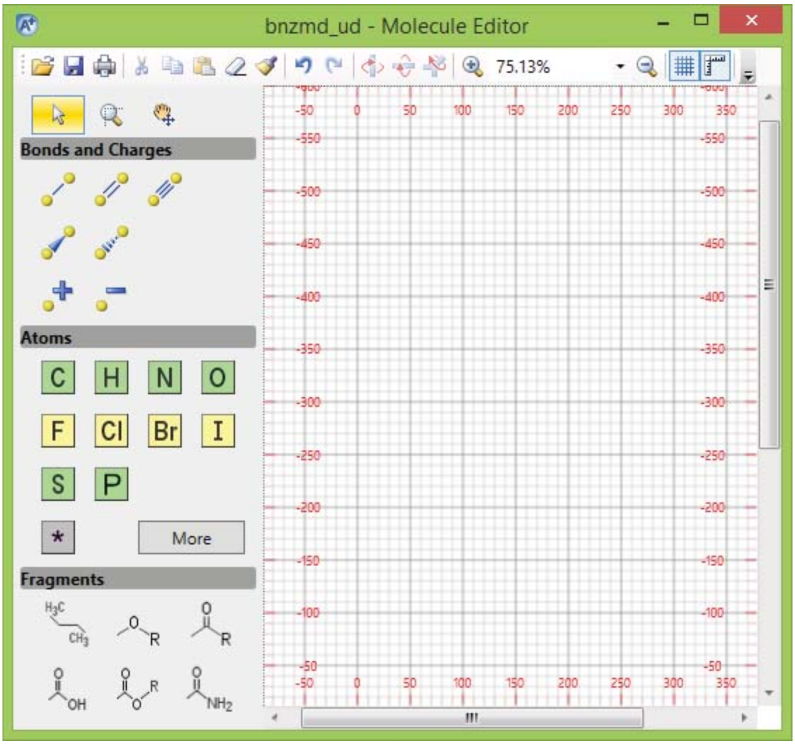


Figure 13.4 The "**Molecule Editor**" window of Aspen Plus where the user can construct the molecule, save it as *.mol file, and update the "**Structure**" tab sheet upon closing the editor.

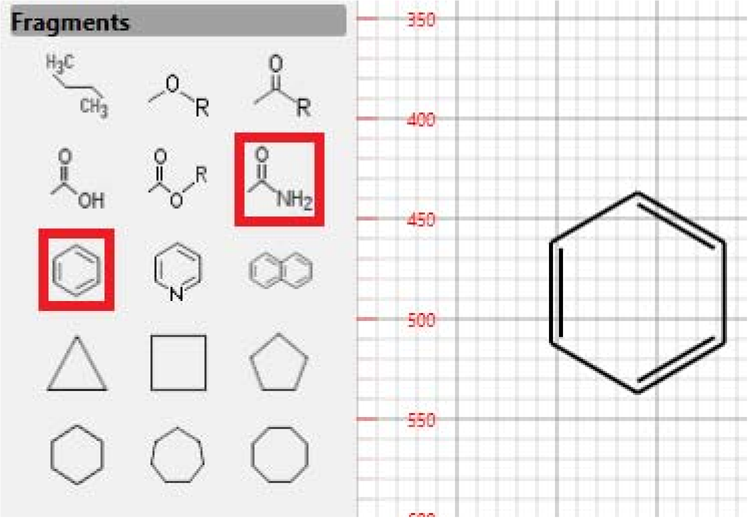


Figure 13.5 Selecting the phenyl ring from "**Fragments**" panel, moving the mouse toward the working area, and then releasing the mouse, followed by one left-click. To stop adding more of its kind, right-click the mouse or press "Escape" key.

click on the proper fragment and go to the proper location in the working area and hit one left-click. Either way, to stop adding more blocks of the same type, just right-click the mouse or press "Escape" key. Click on the arrow icon found in the top-left tool (second raw) and in drag (left mouse pressed) mode, you can draw a rectangle around any existing object, then you may delete that enclosed object.

NOTE #2: *Notice here that I can repeat the same procedure and attach the —(C═O)—NH_2 as one big fragment immediately to the phenyl ring; however, for the sake of learning I will incrementally attach one moiety at a time until I add all the required small fragments that make up the benzamide molecule.*

Figure 13.6 shows that once I highlight the "*C atom*" icon from "**Atoms**" pane and select the "*Single bond*" icon from "**Bonds and Charges**" pane; I move the mouse to one of the corners (i.e., ring carbon atoms) of phenyl ring, where "CH" group will appear exactly beneath the mouse at the selected corner; and then I left-click the mouse once. Right-click to stop adding more of the same type.

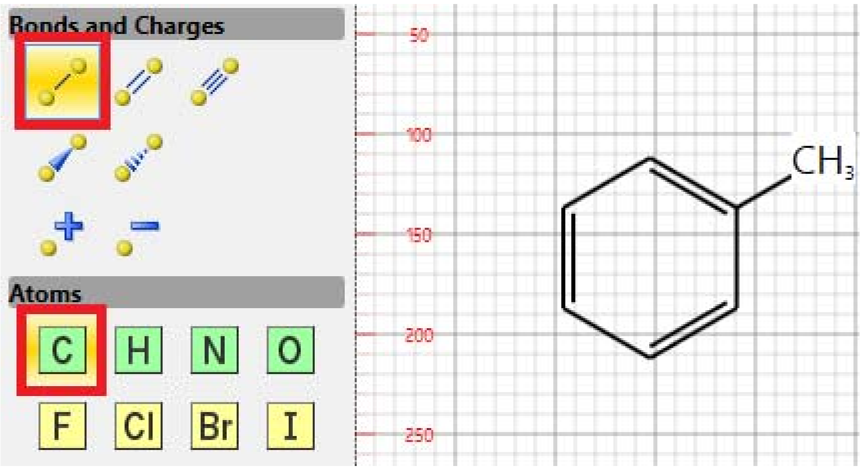


Figure 13.6 Attaching the methyl group to the existing phenyl ring while highlighting the "*C atom*" icon from "**Atoms**" pane, the "*Single bond*" icon from "**Bonds and Charges**" pane, hovering the mouse over one ring corner, left-clicking and dragging away the mouse; and finally releasing the left mouse.

As I did in the previous step, highlight the "*O atom*" icon from "**Atoms**" pane and select the "*Double bond*" icon from "**Bonds and Charges**" pane; move the mouse exactly onto the top of the methyl group; left-click and drag away the mouse; and then release the left mouse. Right-click the mouse to stop adding more of the same type. Figure 13.7 shows the new changes after the attachment of "*O*" atom to the methyl group via the double bond.

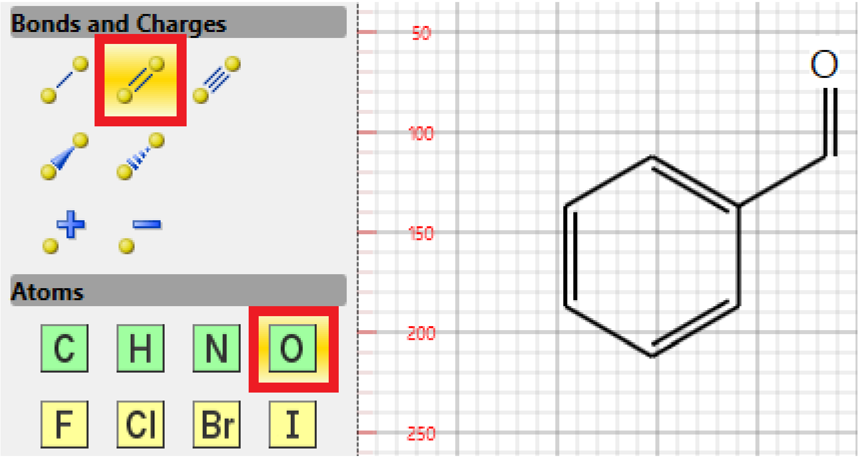


Figure 13.7 Attaching the "*O*" atom to the methyl group via the double bond by highlighting the "*O atom*" icon from "**Atoms**" pane and selecting the "*Double bond*" icon from "**Bonds and Charges**" pane; moving the mouse exactly onto the top of the methyl group; left-clicking and dragging away the mouse; and finally releasing the left mouse.

Finally, highlight the "*N atom*" icon from "**Atoms**" pane and select the "*Single bond*" icon from "**Bonds and Charges**" pane; move the mouse exactly onto the top of the carbon atom of the carbonyl group, where "CH" group will appear underneath the mouse; left-click and drag away the mouse; and then release the left mouse. Right-click the mouse to stop adding more of the same type. Figure 13.8 shows the latest changes after the attachment of "NH2" group to the carbonyl group via the single bond.

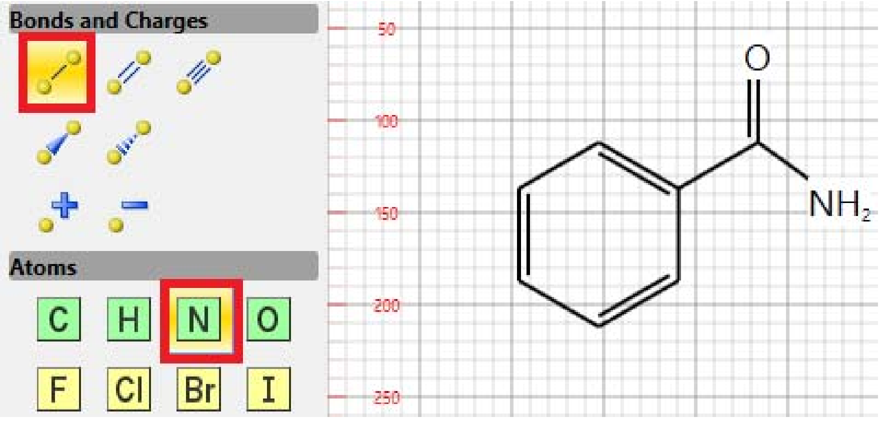
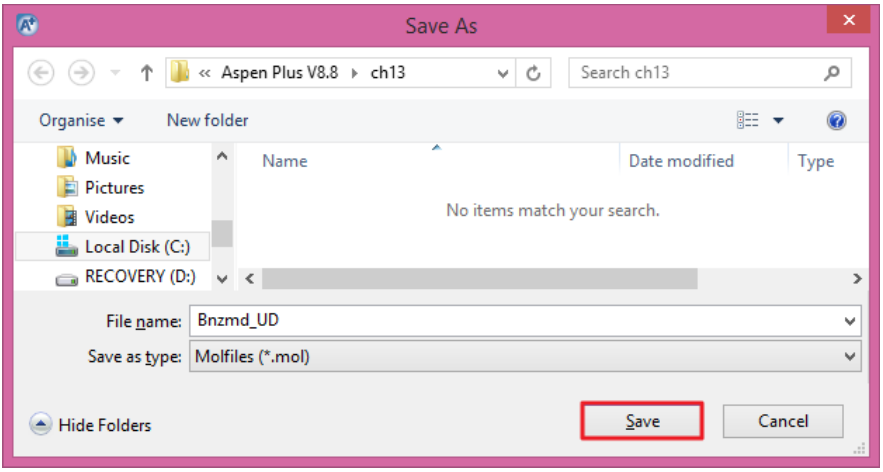


Figure 13.8 Attaching the "NH2" group to the carbonyl group via the single bond, while following the procedure outlined in Figure 13.7.

See; we are done with constructing the benzamide molecule. Save the file to "*Bnzmd_UD.mol*" file as shown in Figure 13.9.



File name: Bnzmd_UD

Save as type: Molfiles (*.mol)

Figure 13.9 Saving the artwork to *.mol type file.

After saving the file, close the molecule editor and be back to "**Structure**" tab window, as shown in Figure 13.10.

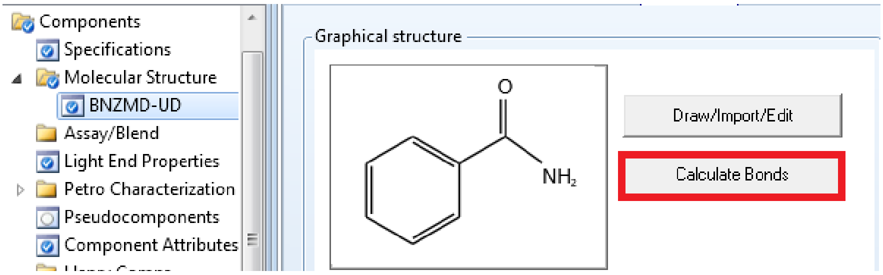
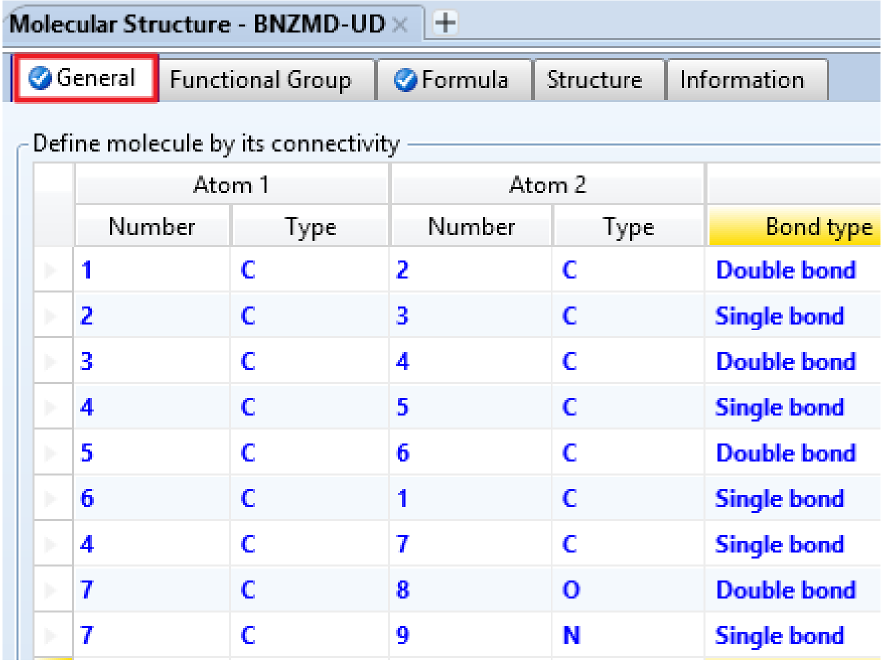


Figure 13.10 The molecular structure of benzamide ("**BNZMD-UD**") is uploaded to Aspen Plus environment.

NOTE #3: *If the image of the molecule does not immediately show up, you may click on the adjacent tab and then be back to "**Structure**" tab window. You have to be patient plus with Aspen Plus.*

Click on "**Calculate Bonds**" button so that Aspen Plus will transform the image into known bonds and atoms (i.e., their bond energies and lengths will be calculated).

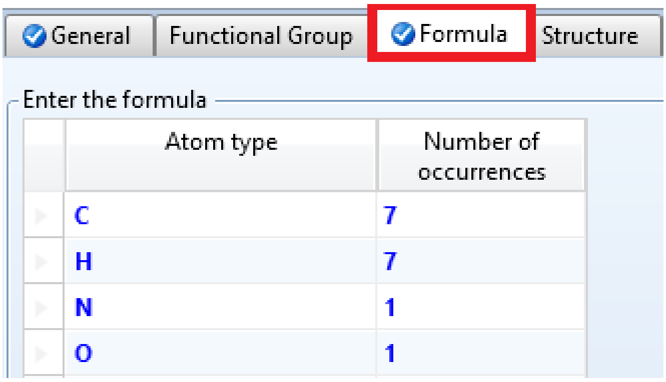
Figure 13.11 shows the "**General**" tab window where the atomic connectivity has been automatically calculated by Aspen Plus, based on the defined molecular structure under "**Structure**" tab.



Atom 1		Atom 2		
Number	Type	Number	Type	Bond type
1	C	2	C	Double bond
2	C	3	C	Single bond
3	C	4	C	Double bond
4	C	5	C	Single bond
5	C	6	C	Double bond
6	C	1	C	Single bond
4	C	7	C	Single bond
7	C	8	O	Double bond
7	C	9	N	Single bond

Figure 13.11 The atomic connectivity is automatically made by Aspen Plus once the user properly defines the molecular structure in "**Structure**" tab window.

Figure 13.12 shows the formula tab window where Aspen Plus tells us that our lovely benzamide molecule is made of seven carbon atoms, seven hydrogen atoms, one nitrogen atom, and finally one oxygen atom.



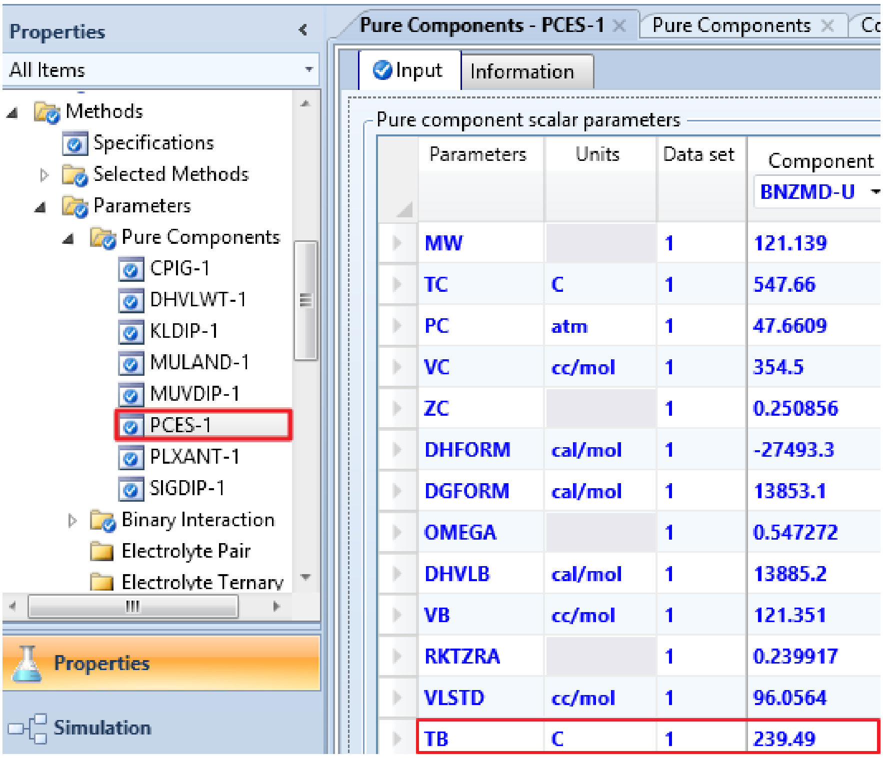
Atom type	Number of occurrences
C	7
H	7
N	1
O	1

Figure 13.12 The atomic content of benzamide molecule.

Next, we will enter the known property data for "**BNZMD-UD**".

13.5 ENTERING PROPERTY DATA

The molecular structure information is sufficient for Aspen Plus to estimate properties. However, entering all available data will further improve the accuracy of the Aspen Plus properties estimation. To demonstrate this point, if the user attempts to run the property estimator at this point, then Aspen Plus will do its best to carry out the property estimation process; nevertheless, the estimated properties will not be accurate enough. Figure 13.13 shows some of the estimated properties where the estimated boiling point ("**TB**") is given as 239.49°C. The experimental value is 288°C. This means that more experimental data are to be supplied by the user in order to have a better property estimate.



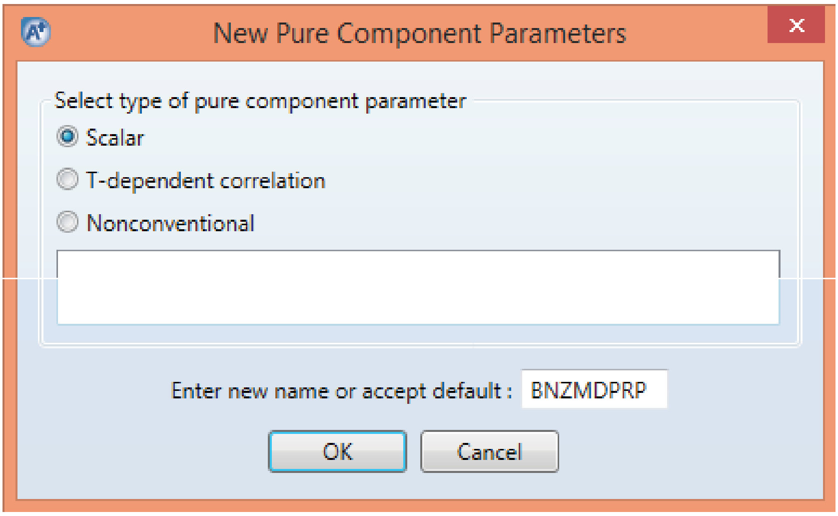
Pure component scalar parameters

Parameters	Units	Data set	Component BNZMD-U
MW		1	121.139
TC	C	1	547.66
PC	atm	1	47.6609
VC	cc/mol	1	354.5
ZC		1	0.250856
DHFORM	cal/mol	1	-27493.3
DGFORM	cal/mol	1	13853.1
OMEGA		1	0.547272
DHVLB	cal/mol	1	13885.2
VB	cc/mol	1	121.351
RKTZRA		1	0.239917
VLSTD	cc/mol	1	96.0564
TB	C	1	239.49

Figure 13.13 Estimation of boiling point of "**BNZMD-UD**" merely based on the molecular structure.

To enter the boiling and freezing point for "**BNZMD-UD**", execute the following steps:

1. In "**Navigation**" pane, go to "**Methods**" | "**Parameters**" | "**Pure Components**" and click on "**New** … " button.
2. In the "**New Pure Component Parameters**" dialog box, select "*Scalar*", as shown in Figure 13.14.
3. Enter the new name "**BNZMDPRP**" and click on "**OK**" button. The "**Methods**" | "**Parameters**" | "**Pure Components**" | "**BNZMDPRP**" | "**Input**" tab sheet appears.
4. In the first "**Component**"-labeled column, click the drop-down arrow and select "*BNZMD-UD*".


New Pure Component Parameters

Select type of pure component parameter

● Scalar

○ T-dependent correlation

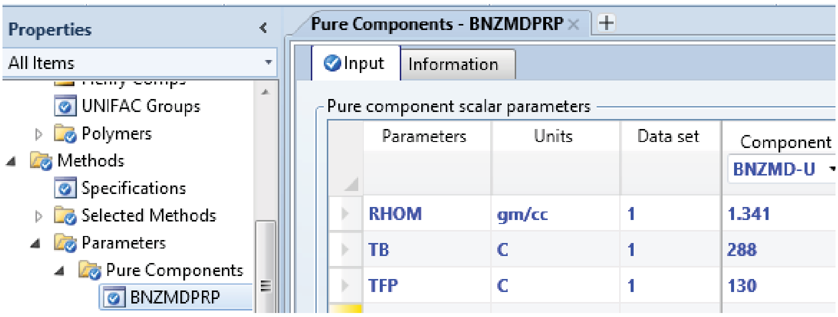
○ Nonconventional

Enter new name or accept default : BNZMDPRP

Figure 13.14 Selecting a new scalar property of pure component "**BNZMD-UD**".

5. Click beneath the "**Parameters**" column, and select "*RHOM*" (mass density).
6. Click the second horizontal cell under the "**Units**" column, and select *gm/cc* (g/cm^3) and in the corresponding cell, beneath the fourth column, enter *1.341* as the value of density.
7. Click below "*RHOM*" cell and select "*TB*" (normal boiling point).
8. Select °*C* for "*TB*" unit and in the corresponding cell, beneath the fourth column, enter *288* as the value of normal boiling point.
9. Click below "*TB*" cell and select "*TFP*" (freezing point).
10. Select °*C* for "*TFP*" unit and in the corresponding cell, beneath the fourth column, enter *130* as the value of freezing point.

Figure 13.15 shows that "**BNZMDPRP**" property is now defined and contains the mass density ("RHOM"), the normal boiling point temperature ("TB"), and the freezing point temperature ("TFP") for "**BNZMD-UD**" compound.



Pure component scalar parameters

Parameters	Units	Data set	Component BNZMD-U
RHOM	gm/cc	1	1.341
TB	C	1	288
TFP	C	1	130

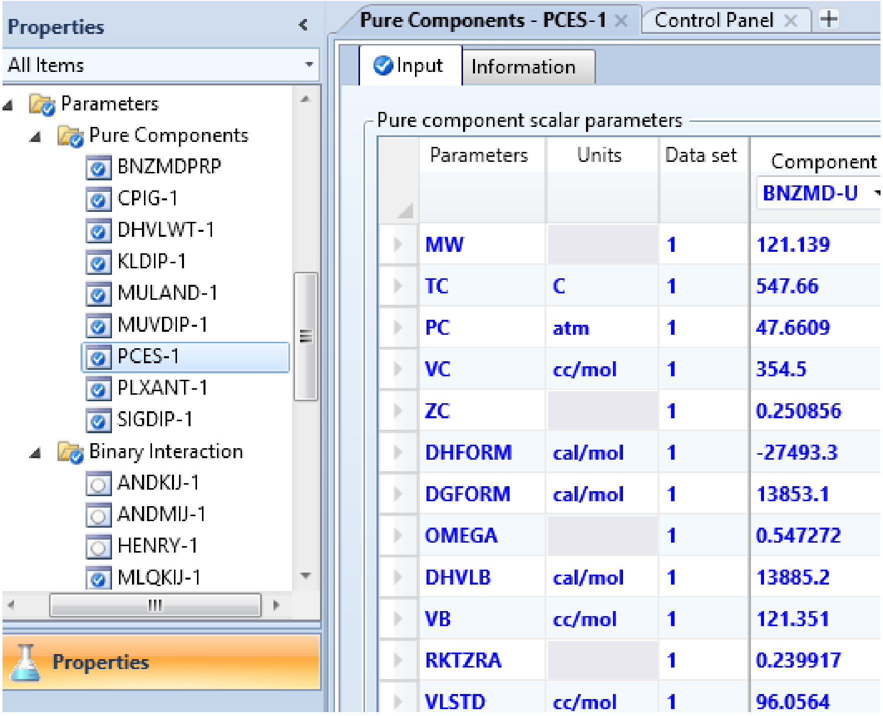
Figure 13.15 Assigning the mass density ("RHOM"), the normal boiling point temperature ("TB"), and the freezing point temperature ("TFP") for "**BNZMD-UD**" compound.

We have already entered the pure component property data for "**BNZMD-UD**" compound. Aspen Plus is now ready to compute the missing properties of "**BNZMD-UD**" compound. Run the simulator and monitor warning and errors (if any) via the "**Control Panel**". There might be some warnings as shown in Figure 13.16 but such a warning can be ignored.

```
*   WARNING IN PHYSICAL PROPERTY SYSTEM
   FUNCTIONAL GROUP GENERATION FOR THE UNIF-LBY METHOD CANNOT BE
COMPLETED
   FOR COMPONENT BNZMD-UD. THE FOLLOWING ATOMS WERE NOT MATCHED:

   C 7   O 8

            THE FUNCTIONAL GROUPS GENERATED

GROUP NUMBER    NO. OF OCCUR.   GROUP NUMBER    NO. OF OCCUR.

        1680     1               1105            5
        1100     1
```

Figure 13.16 A type of warnings during the property estimation step, which can be ignored.

Figure 13.17 shows a portion of estimated properties under "**PCES-1**" sheet for our lovely "**BNZMD-UD**" molecule. Typical physical (thermodynamic and transport) properties are also shown under the sheets starting from "**CPIG-1**" and ending up with "**SIGDIP-1**".

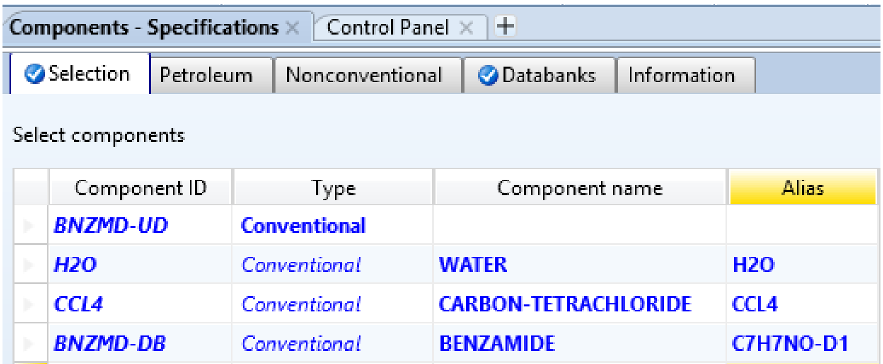


Pure component scalar parameters

Parameters	Units	Data set	Component BNZMD-U
MW		1	121.139
TC	C	1	547.66
PC	atm	1	47.6609
VC	cc/mol	1	354.5
ZC		1	0.250856
DHFORM	cal/mol	1	-27493.3
DGFORM	cal/mol	1	13853.1
OMEGA		1	0.547272
DHVLB	cal/mol	1	13885.2
VB	cc/mol	1	121.351
RKTZRA		1	0.239917
VLSTD	cc/mol	1	96.0564

Figure 13.17 A portion of estimated properties under "**PCES-1**" sheet for our lovely "**BNZMD-UD**" molecule. Other properties can be explored under other adjacent sheets, as well.

Next, add the following components: water ("**H2O**"), carbon tetrachloride ("**CCl4**"), and Aspen Plus databank benzamide ("**BNZMD-DB**") to the list of components. Figure 13.18 shows the new list of components.



Select components

Component ID	Type	Component name	Alias
BNZMD-UD	Conventional		
H2O	Conventional	WATER	H2O
CCL4	Conventional	CARBON-TETRACHLORIDE	CCL4
BNZMD-DB	Conventional	BENZAMIDE	C7H7NO-D1

Figure 13.18 Addition of ("**H2O**"), carbon tetrachloride ("**CCl4**"), and Aspen Plus databank benzamide ("**BNZMD-DB**").

In "**Setup**" | "**Specifications**" | "**Global**" tab sheet, change "**Free water**" option from "*No*" to "*Dirty water*". This is to account for any dispersed organic moiety in aqueous phase. Click on "**Next**" button, run the show, and watch any simulation error or serious warning.

At this stage, if the user wishes to remove the yellow-color exclamation mark that appears on both "**Estimation**" and "**Results**" folders found in "**Navigation**" pane, he/she may deselect "**Estimate missing parameters by UNIFAC**" option found in "**Methods**" | "**Parameters**" | "**Binary Interaction**" | "**NRTL-1**" sheet, rerun the show, and Aspen Plus sky becomes blue. This is simply because we have already calculated all possible permutations of pairwise interaction parameters using "**UNIFAC**" method.

Switch to "**Simulation**" environment.

13.6 CONTRASTING ASPEN PLUS DATABANK (BNZMD-DB) VERSUS BNZMD-UD

Add two mixing units and attach streams as shown in Figure 13.19. It shows a simplified flowsheet that mainly consists of the first mixer (**MIXER-1**) for handling the mixing process of the built-in databank benzamide (**BNZMD-DB**) and a second mixer (**MIXER-2**) for doing the same job as the first mixer but this time for the non-databank, user-defined benzamide (**BNZMD-UD**). Water and CCl_4 will be mixed with benzamide to create a mixture that will be separated into two streams one is mainly water phase and another is CCl_4 phase.

Notice that for both mixers, set the "**Valid phases**" option to "*Liquid-DirtyWater*" option, under "**Blocks**" | "**MIXER-1**" or "**MIXER-2**" | "**Input**" | "**Flash Options**" tab sheet. The word "dirty" here is coined for water systems whenever water is polluted by any organic substance. Yet, it will do the job here.

Next, we need to define the inlet streams for both mixers in terms of *T*, *P*, flow rate, and composition. All inlet liquid (both H_2O and CCl_4) streams are assumed at 50°C, 1 atm, and

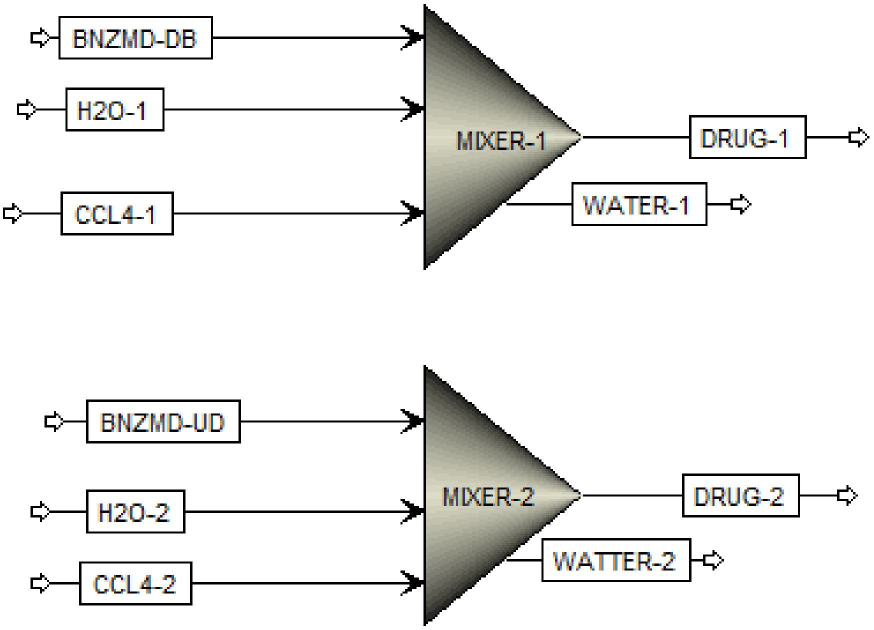
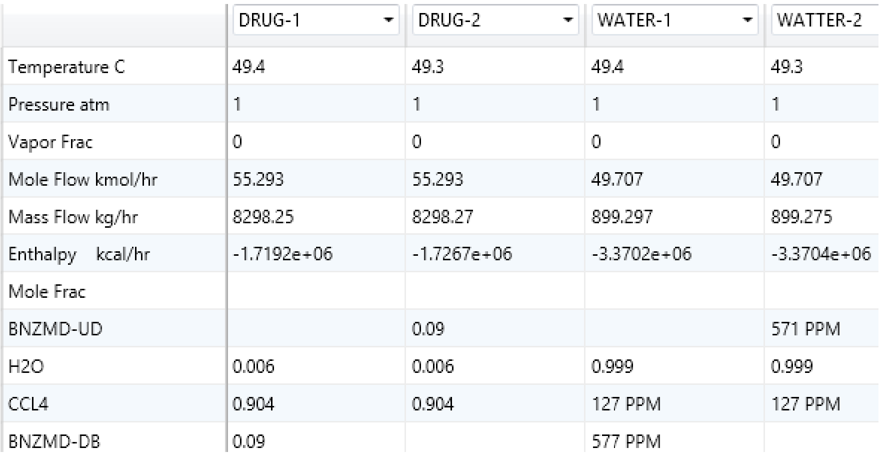


Figure 13.19 For the sake of comparison and testing the validity of the user-defined "**BNZMD_UD**" compound, two identical mixing units are used to see the flow rate and composition of the outlet streams from each unit, where the first unit contains the databank benzamide (**BNZMD-DB**) and the second the user-defined benzamide (**BNZMD-UD**) compound.

a flow rate of 50 kmol/h; on the other hand, "**BNZMD-DB**" and "**BNZMD-UD**" streams have the same flow rate of 5 kmol/h for each and are at the same *T* and *P* of other streams. Reinitialize, run the simulation, and watch out any serious warning or error. Figure 13.20 shows the results of the outlet stream for each mixer. One can see the outlet conditions



	DRUG-1	DRUG-2	WATER-1	WATTER-2
Temperature C	49.4	49.3	49.4	49.3
Pressure atm	1	1	1	1
Vapor Frac	0	0	0	0
Mole Flow kmol/hr	55.293	55.293	49.707	49.707
Mass Flow kg/hr	8298.25	8298.27	899.297	899.275
Enthalpy kcal/hr	-1.7192e+06	-1.7267e+06	-3.3702e+06	-3.3704e+06
Mole Frac				
BNZMD-UD		0.09		571 PPM
H2O	0.006	0.006	0.999	0.999
CCL4	0.904	0.904	127 PPM	127 PPM
BNZMD-DB	0.09		577 PPM	

Figure 13.20 The properties of product streams are accurately identical, indicating that properties of both "**BNZMD-DB**" and "**BNZMD-UD**" compound are essentially the same.

and properties in terms of pressure, temperature, molar flow rate, and mole fraction of each species are accurately identical for "**DRUG1**" and "**DRUG2**" streams.

This assures that the estimated properties of the user-defined "**BNZMD-UD**" are essentially the same as those of the built-in databank "**BNZMD-DB**" compound. Moreover, Aspen Plus predicts that benzamide substance whether it is a databank member or properly user-defined is much more soluble in CCl_4-phase than in water phase. In addition, trace amounts of benzamide are scarcely dispersed in the aqueous phase.

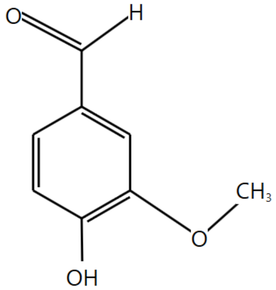
REFERENCES

[1] Al-Malah, K.I. (2012) Prediction of aqueous solubility of organic solvents as a function of selected molecular properties. *Journal of Pharmaceutics and Drug Delivery Research*, **1**, 2.

[2] Grodowska, K. and Parczewski, A. (2010) Organic solvents in the pharmaceutical industry. *Acta Poloniae Pharmaceutica: Drug Research*, **67** (1), 3–12.

[3] Karunanithi, A.T., Acquah, C., and Achenie, L.E.K. (2008) Tuning the morphology of pharmaceutical compounds via model based solvent selection. *Chinese Journal of Chemical Engineering*, **16**, 465–473.

HOMEWORK/CLASSWORK 13.1 (VANILLIN)



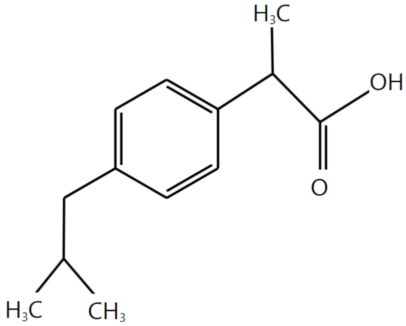
Vanillin, $C_8H_8O_3$, is a flavoring agent in foods, beverages, and pharmaceuticals. It is already defined as a databank member in Aspen Plus. It has a normal boiling point of 284.85°C, MW of 152.15, and a density of 1.056 g/cm^3.

Solubility of vanillin in 1,2-dichloroethane is 1.175 M, in THF is 3.594 M, in butanone is 2.138 M, and in water is 0.070 M. For vanillin, repeat the outlined procedure of this chapter.

1. Using Aspen Plus, start a new simulation by choosing the "**Pharmaceutical**" category and selecting "**Pharmaceuticals with Metric Units**" template to create a steady-state flowsheet.
2. Introduce vanillin as **user-defined structure** to Aspen Plus simulator. Call it "**VNLN-UD**".
3. Using the "**Molecule Editor**" of Aspen Plus, define its molecular structure.
4. Assign the normal boiling point ("**TB**") and mass density ("**RHOM**") to "**VNLN-UD**".
5. Run the simulator to estimate the missing properties of "**VNLN-UD**".

6. Add the following to the list of components, including the **Aspen Plus built-in vanillin** (**VANIL-DB**), water and 1,2-dichloroethane.
7. Go to "**Methods**" | "**Parameters**" | "**Binary Interaction**" | "**NRTL-1**" tab sheet and be sure that the "**Estimate missing parameters by UNIFAC**" option is selected.
8. Click on "**Next**" button, run the show, and check for potential errors or serious warnings. Ignore errors of the type shown in Figure 13.16.
9. Switch to "**Simulation**" environment.
10. Install two mixers as is explained in this chapter. Add **VNLN-DB** to **MIXER1** with water and 1,2-dichloroethane as solvents and **VANIL-UD** to **MIXER2**, again, with water and 1,2-dichloroethane as solvents. Use the same feed *P*, *T*, and molar flow rates.
11. Run the show and compare the simulation results of similar output streams.

HOMEWORK/CLASSWORK 13.2 (IBUPROFEN)



Ibuprofen ($C_{13}H_{18}O_2$) is a nonsteroidal anti-inflammatory drug (NSAID). It works by reducing hormones that cause inflammation and pain in the body. Ibuprofen is used to reduce fever and treat pain or inflammation caused by many conditions such as headache, toothache, back pain, arthritis, menstrual cramps, or minor injury. Ibuprofen is already defined as a databank member in Aspen Plus. It has a normal boiling point of 157°C and a density of 1.03 g/cm^3.

Ibuprofen is practically insoluble in water but very soluble in most organic solvents, such as ethanol, methanol, isopropyl alcohol, acetone, and dichloromethane. Repeat the outlined procedure of this chapter tutorial but for Ibuprofen.

1. Using Aspen Plus, start a new simulation by choosing the "**Pharmaceutical**" category and selecting "**Pharmaceuticals with Metric Units**" template to create a steady-state flowsheet.
2. Introduce vanillin as **user-defined structure** to Aspen Plus simulator. Call it "**BRFN-UD**".
3. Using the "**Molecule Editor**" of Aspen Plus, define its molecular structure.
4. Assign the normal boiling point ("**TB**") and mass density ("**RHOM**") to "**BRFN-UD**".
5. Run the simulator to estimate the missing properties of "**BRFN-UD**".

6. Add the following to the list of components, including the **Aspen built-in ibuprofen** (**BRFN-DB**), water, and isopropyl-alcohol.
7. Go to "**Methods**" | "**Parameters**" | "**Binary Interaction**" | "**NRTL-1**" sheet and be sure that the "**Estimate missing parameters by UNIFAC**" option is affirmed.
8. Click on "**Next**" button, run the show, and check for potential errors or serious warnings. Ignore errors of the type shown in Figure 13.16.
9. Switch to "**Simulation**" environment.
10. Install two mixers as is explained in this chapter tutorial. Add **BRFN-DB** to **MIXER1** with water and isopropyl-alcohol as solvents and **BRFN-UD** to **MIXER2**, again, with water and isopropyl-alcohol as solvents. Use the same feed P, T, and molar flow rates.
11. Run the show and compare the simulation results of similar output streams.

14

SOLIDS HANDLING

14.1 INTRODUCTION

Solids handling is important in some chemical industries, such as specialty chemicals (e.g., fertilizers and silicones), extractive processes (e.g., oil shale, copper, and alumina), and biofuel processes (e.g., corn stover and sugarcane).

Unlike liquids, solids handling requires the knowledge of additional characteristics, such as average particle size and density, moisture content, solubility, color, shape, porosity, and particle size distribution, which is usually expressed in terms of the mean particle size and a factor describing the degree of scatter around the mean (e.g., standard deviation). Moreover, it is not possible to infer bulk from microscopic (single particles) properties of solids, in general.

Aspen Plus has already many useful features that can deal with solids as it perfectly dealt with liquids and gases, as we have seen so far in the previous chapters. For more information about the different solids unit operations, refer to “APPENDIX 14.A”.

Since there are many applications that involve more or less solid materials, we pick up some of them to demonstrate the important features of Aspen Plus in dealing with solid materials.

14.2 PROBLEM DESCRIPTION #1: THE CRUSHER

To demonstrate the concept of particle size distribution (PSD), we consider a simple solid handling case. Figure 14.1 shows the flowsheet that is made of a crusher, one feed stream, and one output stream. The crusher, as its name suggests, will reduce the particle size of the feed stream.

Aspen Plus®: Chemical Engineering Applications, First Edition. Kamal I.M. Al-Malah.

Companion Website: www.wiley.com/go/Al-Malah/AspenPlusApplications

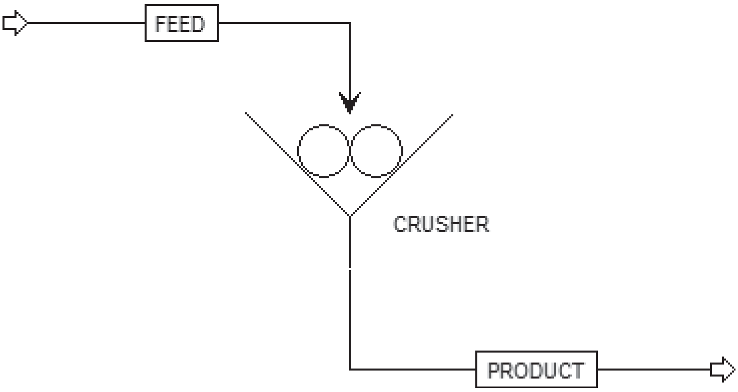


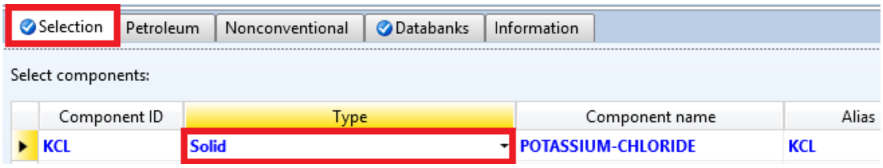
Figure 14.1 A simple solid handling process made of a crusher.

14.3 CREATING ASPEN PLUS FLOWSHEET

Using Aspen Plus, start a new simulation by choosing the “**Solids**” category and selecting “**Solids with Metric Units**” template to create a steady-state flowsheet. Notice that Aspen Plus does not assign a default property method. So, we will set it to “**SOLIDS**”.

14.3.1 Entering Components Information

In “**Navigation**” pane menu tree, go to “**Components**” | “**Specifications**” | “**Selection**” sheet. Click on “**Find**” button to search for “**KCL**”. Once you find “**KCL**”, add it to the list of components and change its “**Type**” from “*Conventional*” to “*Solid*”, as shown in Figure 14.2.



Select components:

Component ID	Type	Component name	Alias
KCL	Solid	POTASSIUM-CHLORIDE	KCL

Figure 14.2 Defining the “**Component ID**” as “*KCl*”, with “**Type**” as “*Solid*” in the list of components.

NOTE #1: “*KCL*” *being defined as solid type will be treated as an inert solid with known molecular structure and it will not be involved in aqueous phase equilibrium (i.e., no association/dissociation reactions). However, as we will see shortly that it requires knowledge of further attributes that have to deal with particle size distribution (PSD). Thus, the substream class type for the feed (or product) stream class will be Conventional Inert with* ***PSD*** (“***CIPSD***”).

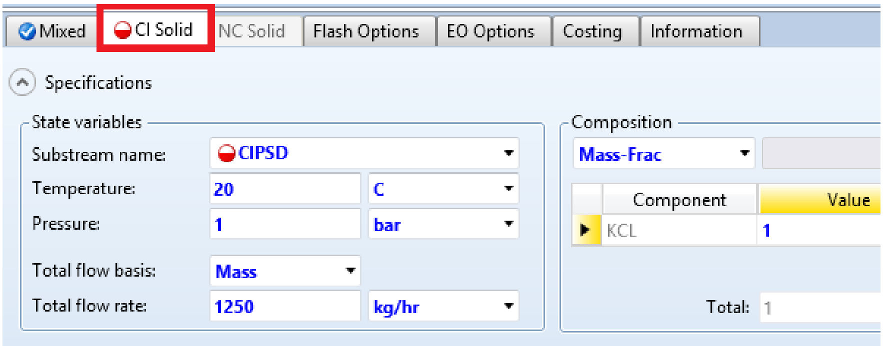
See “APPENDIX 14.B” for defining a solid material using different conventions. As explained in the appendix, one can define the same component in different ways; hence, a different “**Component ID**” will be created for each way. In other words, the same material can be defined in different ways, depending on whether or not the material is chemically active, and if it is inert whether or not it is of a known molecular structure.

Click on “**Next**” button, run the simulator, and monitor serious warning and errors (if any) via the “**Control Panel**”. Once you successfully manage to complete the property analysis step, switch to “**Simulation**” environment.

14.3.2 Adding the Flowsheet Objects

From “**Model Palette**”, select “**Solids**” tab, click on “**Crusher**” icon, and add the crusher icon to the flowsheet area. In addition, add the proper input and output stream, as shown in Figure 14.1. Click on “**Next**” button and Aspen Plus will bring you to “**FEED**” stream input form.

Notice here that entering solid-containing feed stream properties are different from those of a conventional feed stream, which has no “**Solid**” type component. Figure 14.3 shows the typical input data to be entered for a feed stream; however, we will use the second tab, that is, “**CI Solid**” tab for a conventional inert solid as in our case.



Substream name: CIPSD
Temperature: 20 C
Pressure: 1 bar
Total flow basis: Mass
Total flow rate: 1250 kg/hr

Composition: Mass-Frac

Component	Value
KCL	1

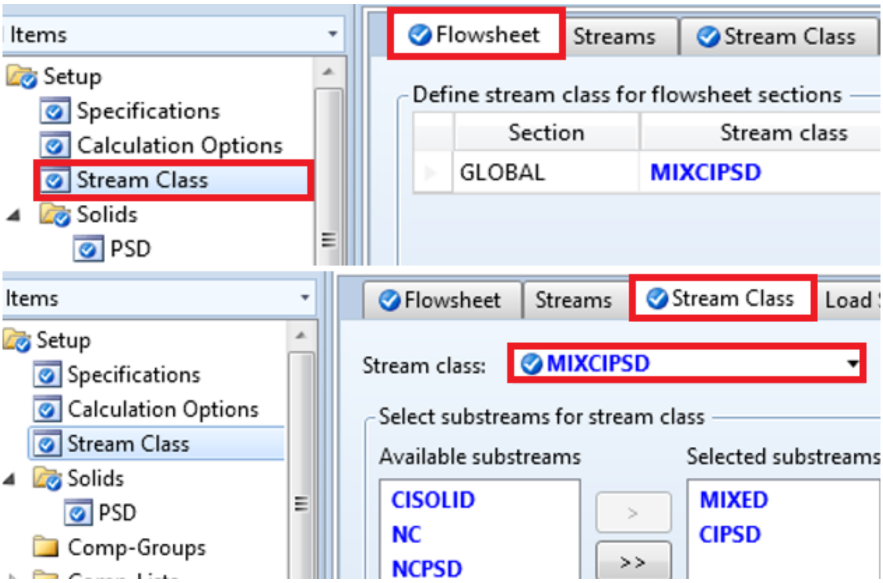
Total: 1

Figure 14.3 Entering *P*, *T*, flow rate, and composition of the feed stream, which is treated as **C**onventional **I**nert solid with **P**article **S**ize **D**istribution (“**CIPSD**”). *See Plate section for color representation of this figure.*

Notice that the half-filled red circle shown in Figure 14.3 indicates that input data pertaining to “**FEED**” stream is still incomplete, and the reason for this is simply because the stream class is of “**MIXCIPSD**” type with a substream of “**CIPSD**” type. Under such stream and substream definitions, we need to define or associate a PSD with the feed stream as well as define a simulation PSD for presentation of results.

Figure 14.4 (*top*) shows “**Setup**” | “**Stream Class**” | “**Flowsheet**” tab window where it shows that the stream class for the “**Global**” section (i.e., entire flowsheet) is of “**MIXCIPSD**” type. See “APPENDIX 14.C” for further information on stream classes. Stream classes ease the integration of solids and fluids in one simulation. The stream class can either be created or selected from a predefined type. Upon one’s need, a predefined class type can also be modified.

Moreover, the “**Stream Class**” tab window (Figure 14.4 *bottom*) shows the selected substream class types for the given stream class of type “**MIXCIPSD**”. One can select the stream class from the drop-down list and see what substreams are already associated with.



Define stream class for flowsheet sections

Section	Stream class
GLOBAL	MIXCIPSD

Stream class: MIXCIPSD

Select substreams for stream class

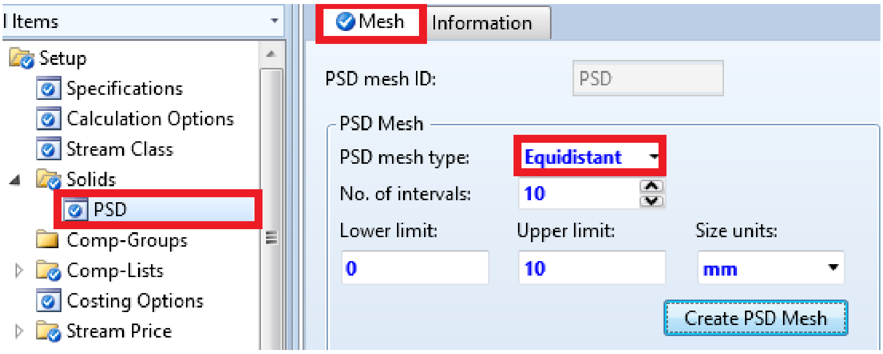
Available substreams	Selected substreams
CISOLID	MIXED
NC	CIPSD
NCPSD	

Figure 14.4 The flowsheet stream class type (*top*) and the substream class types (*bottom*).

See “APPENDIX 14.D” for further information on substream classes. Substream classes are the building blocks of stream classes. They can either be predefined or customized.

14.3.3 Defining the Particle Size Distribution (PSD)

Regarding the particle size distribution (PSD), we will define two PSD types one for the entire simulation and another for the feed stream. Refer to “APPENDIX 14.E” for further information on different particle size distributions (PSDs). Notice here that both PSD types have to be within the same range; that is, the PSD mesh of the simulation within which we monitor the product stream solid attributes should not be too fine or too coarse for the feed stream PSD mesh. So, let us define the simulation PSD first in terms of size unit, lower limit, and upper limit. Figure 14.5 shows that we have selected the “**PSD mesh type**” to be



PSD mesh ID: PSD

PSD Mesh

PSD mesh type: Equidistant

No. of intervals: 10

Lower limit: 0

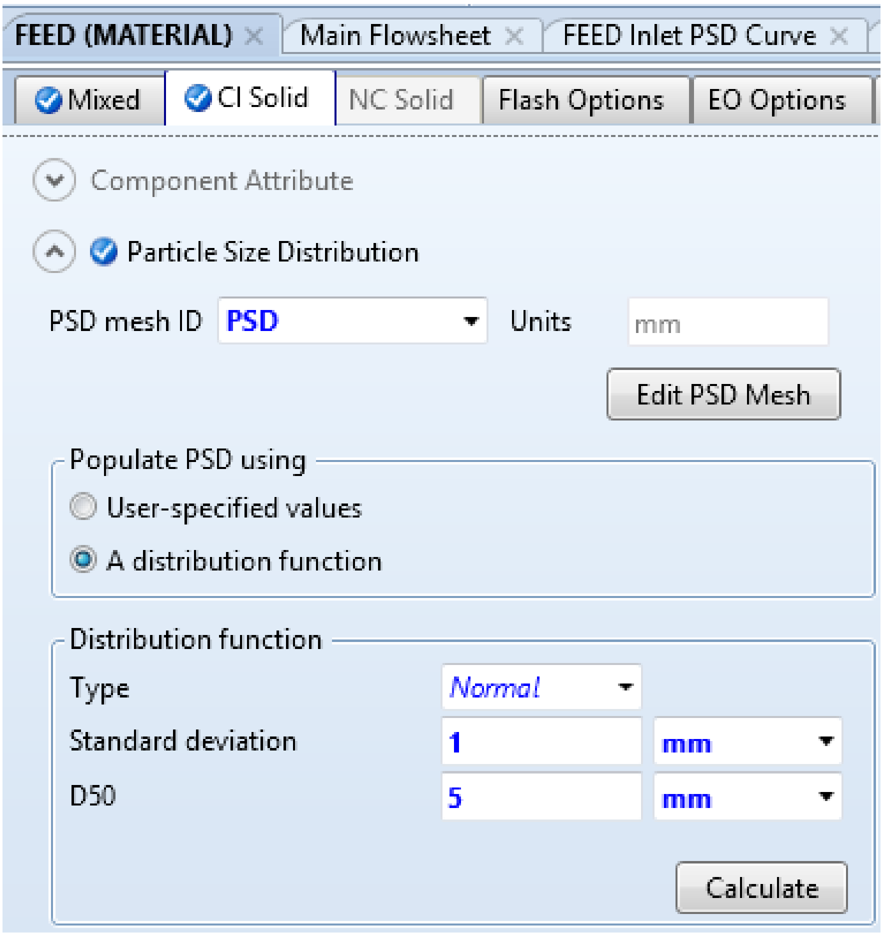
Upper limit: 10

Size units: mm

Figure 14.5 Selection of simulation PSD in terms of its type and accompanied parameters.

"*Equidistant*" with parameters as shown in the figure. For such types, refer to "APPENDIX 14.E" and to Aspen Plus built-in help: "**PSD Mesh Dialog Box**". Do not forget to click on "**Create PSD Mesh**" button to confirm the creation of the selected PSD.

Figure 14.6 shows the "**CI Solid**" tab window for "**FEED**" stream where we need to define a PSD for the solid of the feed stream. Notice here that you can edit (or modify) the simulation PSD via clicking on "**Edit PSD Mesh**" button, which will invoke the form shown earlier in Figure 14.5. Moreover, we define a PSD of "**FEED**" stream, here, as "*Normal*" with a standard deviation of 1 mm and median (D50) of 5 mm. For such types, refer to "APPENDIX 14.E" and to Aspen Plus built-in help: "**Distribution Functions**" and "**Distribution Functions and Comminution Laws for Crusher**".



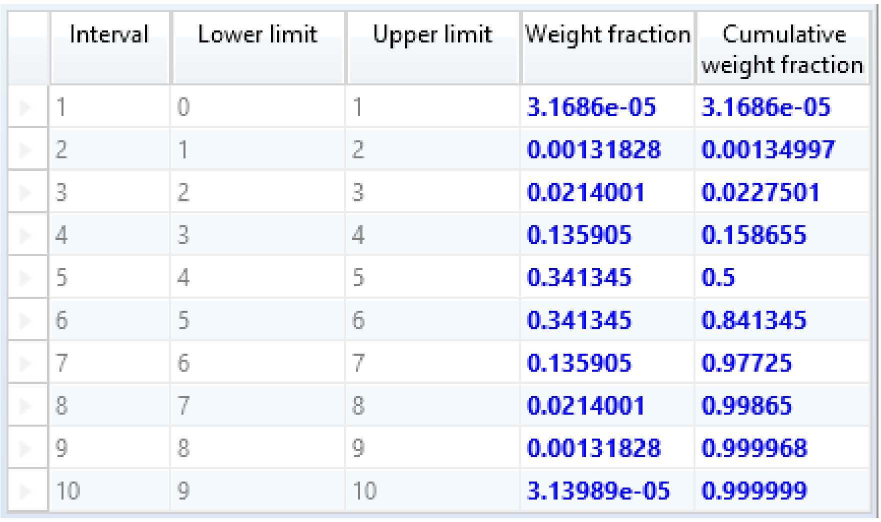
PSD mesh ID: PSD
Units: mm

Populate PSD using
○ User-specified values
● A distribution function

Distribution function
Type: Normal
Standard deviation: 1 mm
D50: 5 mm

Figure 14.6 Defining a PSD for "**FEED**" stream as "*Normal*" with a standard deviation of 1 mm and median (D50) of 5 mm.

Click on "**Calculate**" button to generate both the tabulated and graphic representation of PSD for "**FEED**" stream. Figure 14.7 shows the populated PSD values over the selected PSD mesh, which extends from 0 up to 10 mm with equal subintervals. Notice that we have



Interval	Lower limit	Upper limit	Weight fraction	Cumulative weight fraction
1	0	1	3.1686e-05	3.1686e-05
2	1	2	0.00131828	0.00134997
3	2	3	0.0214001	0.0227501
4	3	4	0.135905	0.158655
5	4	5	0.341345	0.5
6	5	6	0.341345	0.841345
7	6	7	0.135905	0.97725
8	7	8	0.0214001	0.99865
9	8	9	0.00131828	0.999968
10	9	10	3.13989e-05	0.999999

Figure 14.7 The generated data in the form of weight and cumulative weight fraction as a function of particle size (in mm) over the selected PSD mesh range.

the frequency (i.e., weight fraction) is normally (i.e., symmetrically) distributed around its mean value that lies at about 5 mm. The range of simulation PSD acts like a window through which we have the chance to look at the effect of solids crushing on the PSD of the feed stream.

Figure 14.8 shows the plot of cumulative mass fraction as a function of particle size (mm).

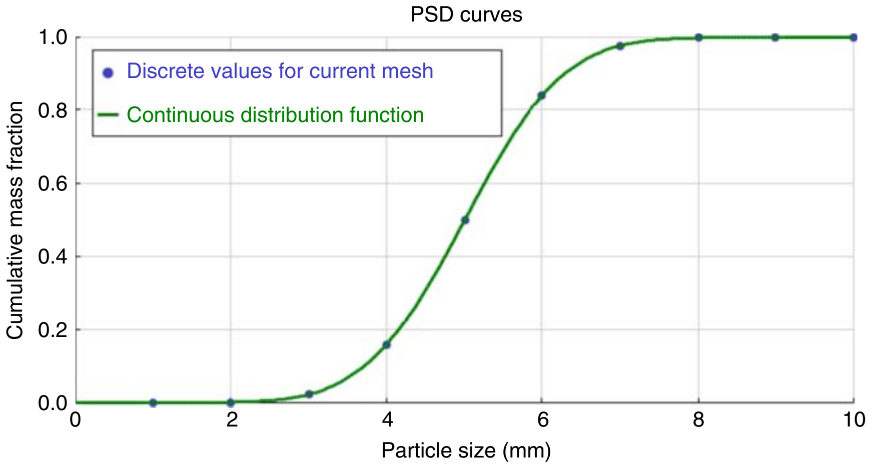
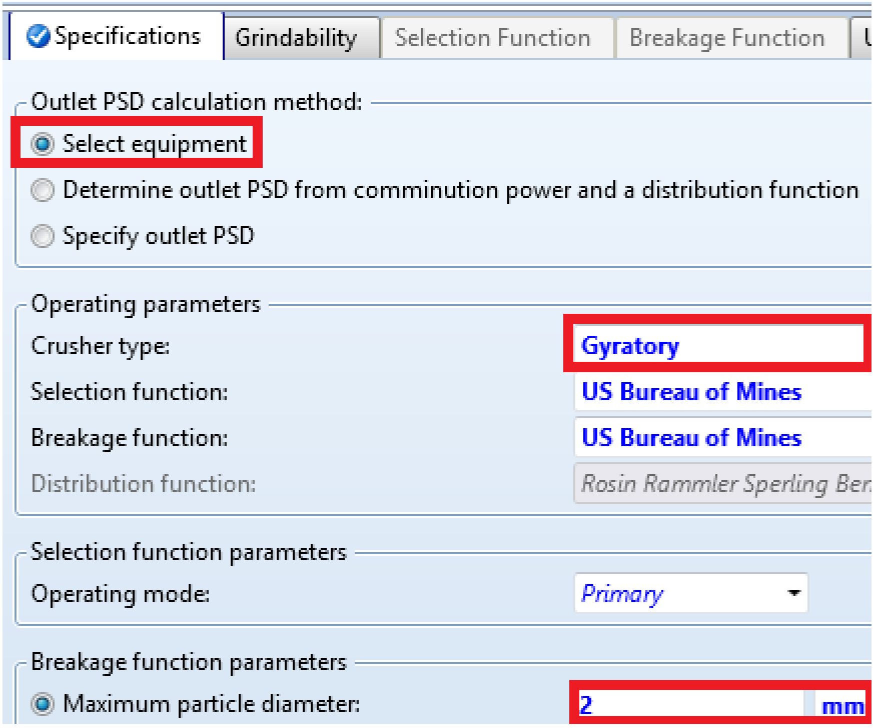


Figure 14.8 The cumulative PSD curve for “**FEED**” stream as a function of particle size (mm).

14.3.4 Calculation of the Outlet PSD

Click on "**Next**" button and the "**Blocks**" | "**CRUSHER**" | "**Input**" | "**Specifications**" tab sheet will show up, as shown in Figure 14.9. The outlet PSD will be calculated based on one of three methods: The first method is to spell out the crusher type, breakage function parameters, impact/rotor velocity, and/or some of its sizing parameters. For more information on different types of crushers, refer to Aspen Plus built-in help: "**About Crushers**". The second method is based on known comminution (disintegration) power and some specified distribution function parameters. Finally, the third method is based on known outlet PSD, which can be either user-specified or common built-in distribution function, such as GGS, RRSB, Normal, and Log normal (see "APPENDIX 14.E").



Outlet PSD calculation method:

● Select equipment

○ Determine outlet PSD from comminution power and a distribution function

○ Specify outlet PSD

Operating parameters

Crusher type: Gyratory

Selection function: US Bureau of Mines

Breakage function: US Bureau of Mines

Distribution function: Rosin Rammler Sperling Ber

Selection function parameters

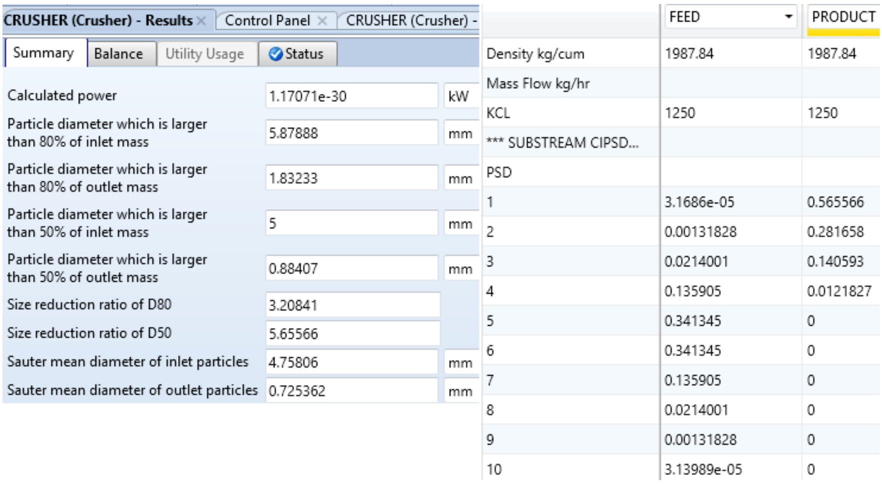
Operating mode: Primary

Breakage function parameters

● Maximum particle diameter: 2 mm

Figure 14.9 The calculation of outlet PSD using three different approaches.

Click on "**Next**" button, run the show, and watch out any serious warning or error in "**Control Panel**". Figure 14.10 (*left*) shows the "**Summary**" tab window for "**CRUSHER**" block under "**Results**" sheet. Obviously, there is a size reduction between the feed and the outlet stream. The size reduction ratio is 5.656 evaluated at the median. The Sauter mean diameter (see "APPENDIX 14.E") is also reduced from 4.76 to 0.725 mm. For example, Figure 14.10 (*right*) shows that 98.782% of total particles fall below 3 mm diameter size or 99.99997% of them lie below the 4 mm diameter dividing cut.



Calculated power	1.17071e-30	kW
Particle diameter which is larger than 80% of inlet mass	5.87888	mm
Particle diameter which is larger than 80% of outlet mass	1.83233	mm
Particle diameter which is larger than 50% of inlet mass	5	mm
Particle diameter which is larger than 50% of outlet mass	0.88407	mm
Size reduction ratio of D80	3.20841	
Size reduction ratio of D50	5.65566	
Sauter mean diameter of inlet particles	4.75806	mm
Sauter mean diameter of outlet particles	0.725362	mm

	FEED	PRODUCT
Density kg/cum	1987.84	1987.84
Mass Flow kg/hr		
KCL	1250	1250
*** SUBSTREAM CIPSD...		
PSD		
1	3.1686e-05	0.565566
2	0.00131828	0.281658
3	0.0214001	0.140593
4	0.135905	0.0121827
5	0.341345	0
6	0.341345	0
7	0.135905	0
8	0.0214001	0
9	0.00131828	0
10	3.13989e-05	0

Figure 14.10 Characterization of KCl solid particles both in the inlet and outlet stream in terms particle size cut, reduction, and mean (*left*) and PSD (*right*).

EXERCISE 14.1 (DETERMINE CRUSHER OUTLET PSD FROM COMMINUTION POWER)

Repeat the same task of reducing the particle size of "**FEED**" stream but this time using the second method, which is "*Determine outlet PSD from comminution power and a distribution function*" (see Figure 14.9). Under "**Specifications**" tab, use "*Rosin Rammler Sperling Bennet*" distribution function; power specification of 1 kW; and select "*D50*" parameter with "*1 mm*" from "**Distribution function parameters**" option. Under "**Grindability**" tab, use "*Bond's law*" as the "**Comminution law**" and for "**CIPSD**" substream use "*3 kW hr/ton*" under "**Bond work index**" column. See Aspen Plus built-in help: "**Bond's Law**" for further information on Bond work index. Bond considered that the work necessary for reduction is inversely proportional to the square root of the size produced. This applies for particles between 0.05 and 50 mm.

Report the outlet stream solid attributes in terms of particle size cut, reduction, mean, and distribution (i.e., PSD). Also, report the calculated power (kW) needed to carry out the crushing mission.

EXERCISE 14.2 (SPECIFYING CRUSHER OUTLET PSD)

Repeat the same task of reducing the particle size of "**FEED**" stream but this time using the third method, that is, "*Specify outlet PSD*" (see Figure 14.9).

Under "**Specifications**" tab, select "**Substream ID**" as *CIPSD*; select "*Use distribution function*"; the "*Bypass fraction*" is set to *0*; create a new distribution function ID and name it *1*; select the "*Distribution function*" as *Normal*; select D50 parameter with 1 mm and standard deviation of 1 mm.

Under "**Grindability**" tab, you may keep it blank (i.e., no entries at all); however, if you use Bond's law as the comminution law and for "**CIPSD**" substream use "*3 kW hr/ton*" under "**Bond work index**" column, then you will be able to calculate the power needed to achieve the mission, that is, size reduction of feed stream particles down to the specified outlet PSD.

Report the outlet stream solid attributes in terms of particle size cut, reduction, mean, and distribution (i.e., PSD). Also, report the calculated power (kW) needed to carry out the crushing mission. I hope toward the end of this exercise that you managed to crush the information needed to deal with crushers.

14.4 PROBLEM DESCRIPTION #2: THE FLUIDIZED BED FOR ALUMINA DEHYDRATION

In this problem, we will handle the fluidized bed with a chemical reaction. Fluidized beds are used in a variety of industrial processes, which include drying, cooling, heating, and as reactors. Have a look at "APPENDIX 14.F" for a general overview of the main features of Aspen Plus fluidized bed model. The feed stream is made of aluminum trihydroxide ($Al(OH)_3$), which will be dispensed in the form of solid particles to the entrance of the fluidized bed where it will be pneumatically lifted or fluidized by means of a hot air stream. This will cause the phenomenon known as fluidization visualizing solid particles behaving as fluid-like molecules (i.e., they gain the translational, vigorous vibrational, and rotational kinetic energy as well). This being the case, we will enhance the simultaneous mass and heat transfer rates from and to the solid particles. The dehydration reaction

$$2Al(OH)_3 \rightarrow Al_2O_3 + 3H_2O$$

can be put in another form:

$$Al_2O_3 \cdot 3H_2O \rightarrow Al_2O_3 + 3H_2O$$

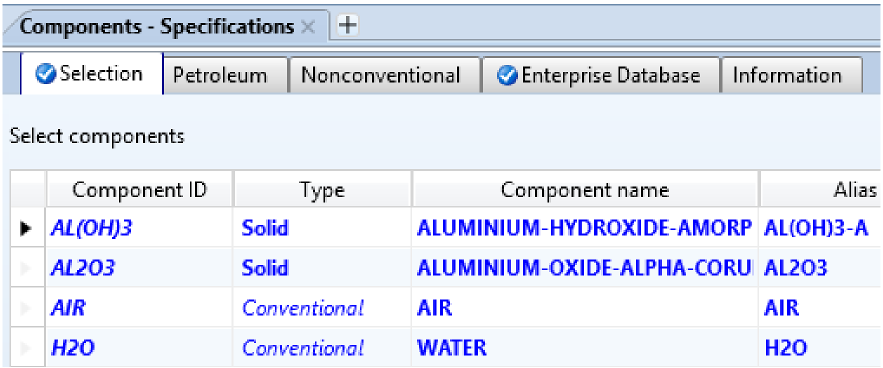
So, the reaction is basically a solid transformation from the hydrated into the anhydrous unit crystal. Thus, heating by convection (by the air) and conduction (through the solid particle) will liberate the combined water molecules from the crystal. Keep in mind that this process is a sort of "roasting" process rather than drying. For a typical wet-hydrated alumina or inorganic solids, in general, water molecules are trapped within the solid matrix itself (i.e., within the macropores of a solid pellet, compared with the tiny small size of the unit crystal).

14.5 CREATING ASPEN PLUS FLOWSHEET

Using Aspen Plus, start a new simulation by choosing the "**Solids**" category and selecting "**Solids with Metric Units**" template to create a steady-state flowsheet. We will set the default property method to "**SOLIDS**".

14.5.1 Entering Components Information

In "**Navigation**" pane menu tree, go to "**Components**" | "**Specifications**" | "**Selection**" tab sheet. Add the following components and change the "**Type**" of both "*AL*(*OH*)*3*" and "*AL2O3*" from "*Conventional*" to "*Solid*", as shown in Figure 14.11.



Select components

	Component ID	Type	Component name	Alias
▶	AL(OH)3	Solid	ALUMINIUM-HYDROXIDE-AMORP	AL(OH)3-A
	AL2O3	Solid	ALUMINIUM-OXIDE-ALPHA-CORU	AL2O3
	AIR	Conventional	AIR	AIR
	H2O	Conventional	WATER	H2O

Figure 14.11 Adding components and changing the "**Type**" of both "*AL(OH)3*" and "*AL2O3*" from "*Conventional*" to "*Solid*".

Click on "**Next**" button, run the simulator, and monitor warnings and errors (if any) via the "**Control Panel**". Once you successfully manage to complete the property analysis step, switch to "**Simulation**" environment.

14.5.2 Adding the Flowsheet Objects

From "**Model Palette**", select "**Solids**" tab, click on "**Fluidbed**" icon, and add the fluidized bed icon to the flowsheet area. Add one compressor unit from "**Pressure Changers**" tab. In addition, add the proper input and output streams, as shown in Figure 14.12. Notice that "**SIN**" and "**SOUT**" stream stand for the inlet and outlet solid streams, respectively.

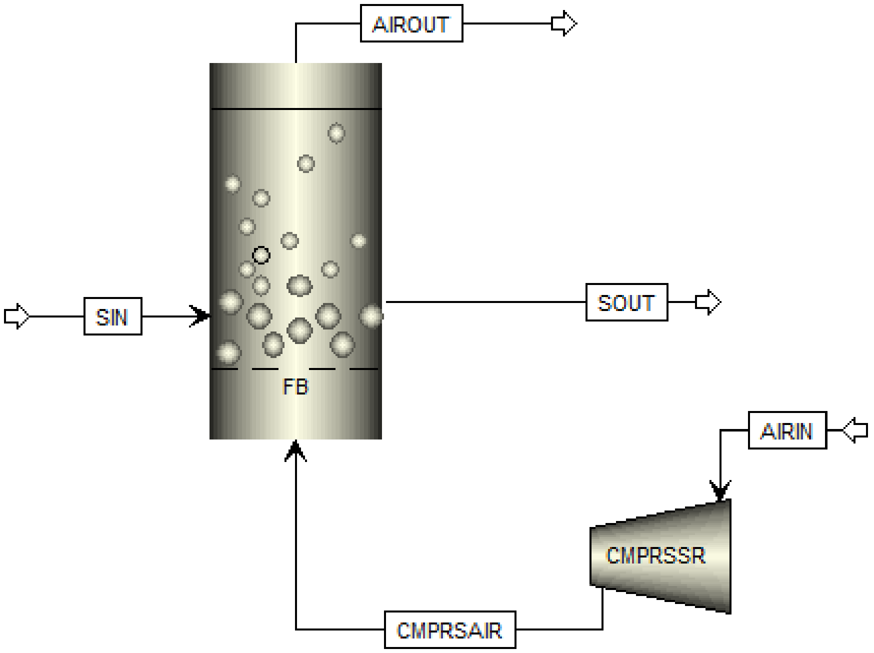
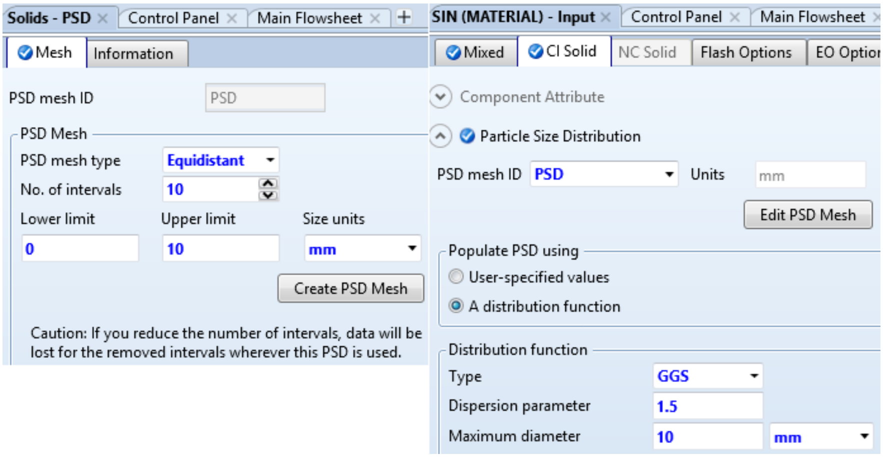


Figure 14.12 The process flowsheet for $Al(OH)_3$ "roasting".

14.5.3 Entering Input Data

Air stream (“**AIRIN**”) will be introduced to the compressor at a rate of 4500 kg/h at room temperature and pressure and the discharge pressure of the compressor will be set at 12 bar. Of course, the temperature of air will increase as a result of adiabatic compression. On the other hand, the solid feed stream (“**SIN**”) will enter at a rate of 300 kg/h at room temperature and a pressure of 12 bar as pure $Al(OH)_3$. Moreover, Figure 14.13 (*left*) shows the simulation PSD mesh and that of “**SIN**” stream (*right*).



PSD mesh ID PSD

PSD Mesh

PSD mesh type Equidistant

No. of intervals 10

Lower limit 0

Upper limit 10

Size units mm

Caution: If you reduce the number of intervals, data will be lost for the removed intervals wherever this PSD is used.

PSD mesh ID PSD

Units mm

Populate PSD using

○ User-specified values

● A distribution function

Distribution function

Type GGS

Dispersion parameter 1.5

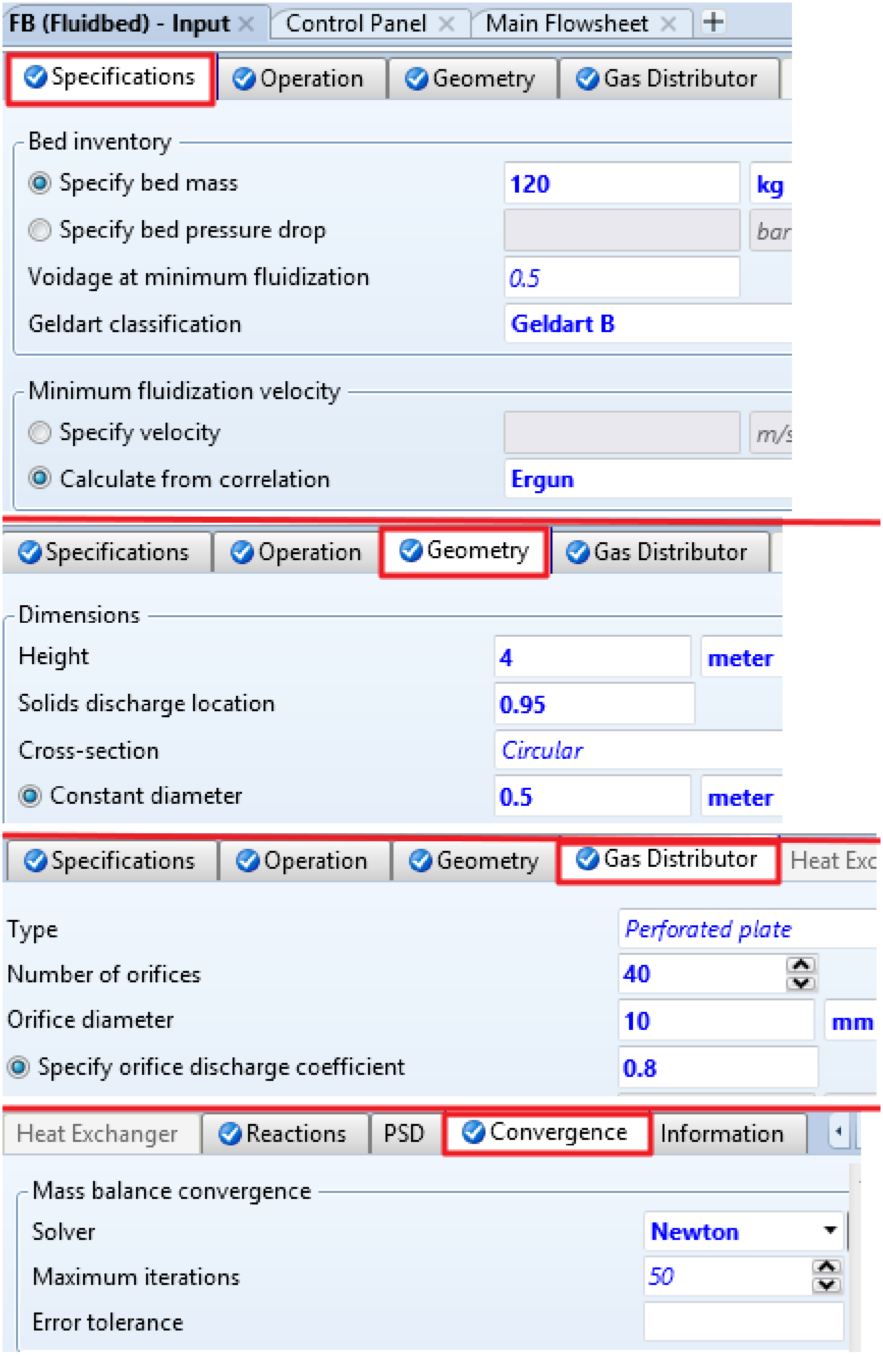
Maximum diameter 10 mm

Figure 14.13 The simulation PSD mesh (*left*) and that of solid feed “**SIN**” stream defined as Gates–Gaudin–Schuhmann (GSS) type (*right*).

For the fluidized bed block, the following design specifications are entered, as shown in Figure 14.14. **First**, under “**Specifications**” tab, the bed mass is set to *120 kg*; “*Geldart B*” classification; and “*Ergun*” model for finding the minimum fluidization velocity. **Second**, under “**Geometry**” tab, the bed height is set to *4 m*; the solid discharge location *0.95* (i.e., 0.95 × 4 = 3.8 m, measured from the bottom of the bed); and the cross-sectional area with a constant diameter equal to *0.5 m*. **Third**, under “**Gas Distributor**” tab, its type is set to “*Perforated plate*” with number of orifices equal to *40*, diameter equal to *10* mm each, and the default orifice discharge coefficient of *0.8*. **Fourth**, under “**Convergence**” tab, for mass balance convergence, the solver is set to “*Newton*” instead of “*Broyden*”, as the latter did not properly converge for a reasonable solution for the given fluidization case. Finally, under “**Reactions**” tab we will associate the reaction “**R-1**” set to the fluidized bed. The reaction “**R-1**” set will be created shortly.

NOTE #2: *For the fluidized bed, under “**PSD**” tab, the “**PSD calculation option**” has three choices; we have chosen the first choice, that is, “Keep PSD”. To know the difference between one choice and another, refer to Table 14.F.1.*

The reaction “**R-1**” set will be created under “**Reactions**” folder. Figure 14.15 shows the stoichiometry and kinetic data associated with alumina transformation from a hydrous to anhydrous state.



Bed inventory

● Specify bed mass 120 kg

○ Specify bed pressure drop bar

Voidage at minimum fluidization 0.5

Geldart classification Geldart B

Minimum fluidization velocity

○ Specify velocity m/s

● Calculate from correlation Ergun

Dimensions

Height 4 meter

Solids discharge location 0.95

Cross-section Circular

● Constant diameter 0.5 meter

Type Perforated plate

Number of orifices 40

Orifice diameter 10 mm

● Specify orifice discharge coefficient 0.8

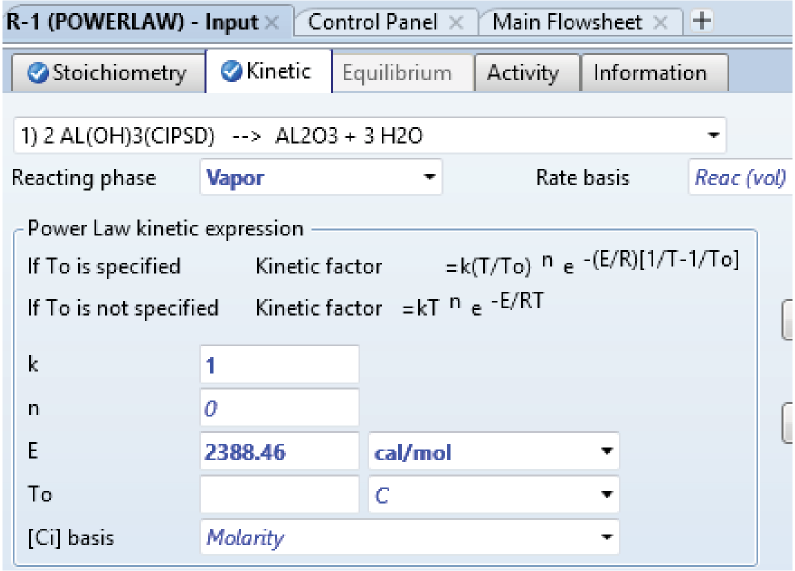
Mass balance convergence

Solver Newton

Maximum iterations 50

Error tolerance

Figure 14.14 Entering fluidized bed design (or geometric) specifications.



1) 2 AL(OH)3(CIPSD) --> AL2O3 + 3 H2O

Reacting phase: Vapor

Rate basis: Reac (vol)

Power Law kinetic expression

If To is specified: Kinetic factor $=k(T/To)^{n}\, e^{-(E/R)[1/T-1/To]}$

If To is not specified: Kinetic factor $=kT^{n}\, e^{-E/RT}$

k: 1

n: 0

E: 2388.46 cal/mol

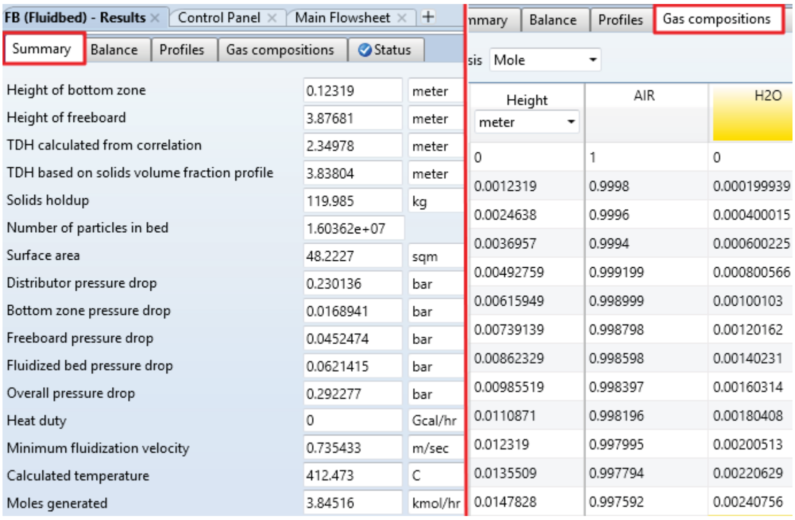
To: C

[Ci] basis: Molarity

Figure 14.15 The reaction stoichiometry and kinetic data for alumina transformation from a hydrous to anhydrous state.

14.5.4 Results

Figure 14.16 (*left*) shows the results summary of the calculated geometrical and operational variables of the fluidized bed and the moisture profile of air stream where dry air enters at the bottom and becomes moist as it moves upward (*right*).



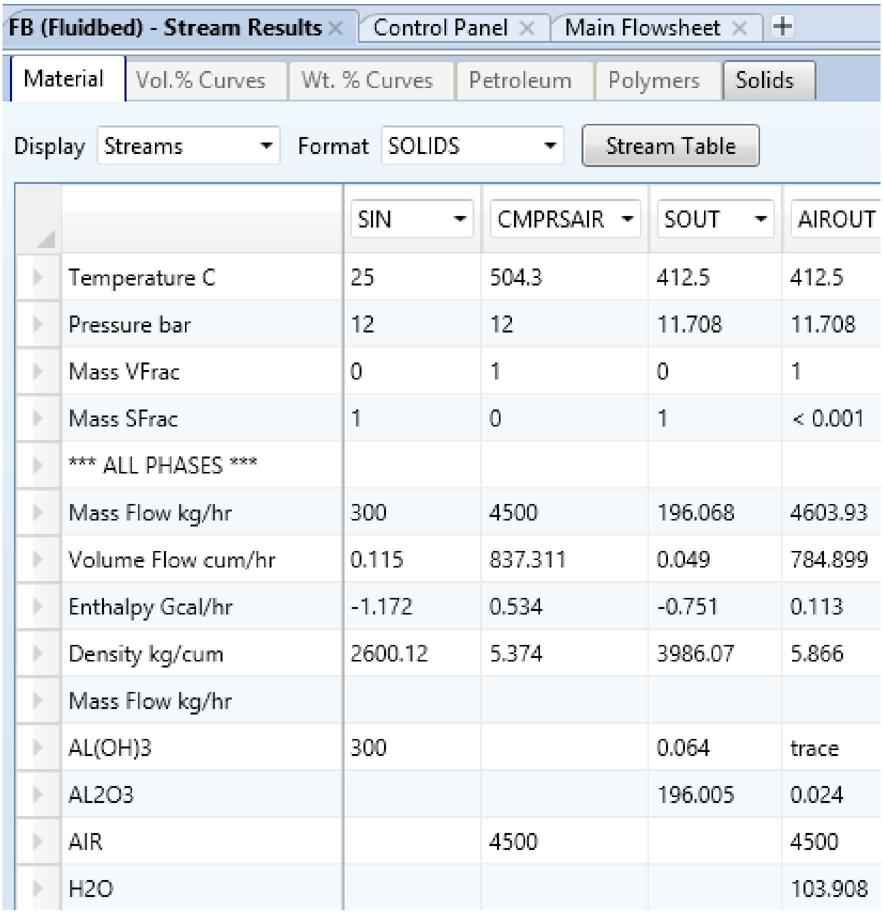
Height of bottom zone	0.12319	meter
Height of freeboard	3.87681	meter
TDH calculated from correlation	2.34978	meter
TDH based on solids volume fraction profile	3.83804	meter
Solids holdup	119.985	kg
Number of particles in bed	1.60362e+07	
Surface area	48.2227	sqm
Distributor pressure drop	0.230136	bar
Bottom zone pressure drop	0.0168941	bar
Freeboard pressure drop	0.0452474	bar
Fluidized bed pressure drop	0.0621415	bar
Overall pressure drop	0.292277	bar
Heat duty	0	Gcal/hr
Minimum fluidization velocity	0.735433	m/sec
Calculated temperature	412.473	C
Moles generated	3.84516	kmol/hr

sis: Mole

Height meter	AIR	H2O
0	1	0
0.0012319	0.9998	0.000199939
0.0024638	0.9996	0.000400015
0.0036957	0.9994	0.000600225
0.00492759	0.999199	0.000800566
0.00615949	0.998999	0.00100103
0.00739139	0.998798	0.00120162
0.00862329	0.998598	0.00140231
0.00985519	0.998397	0.00160314
0.0110871	0.998196	0.00180408
0.012319	0.997995	0.00200513
0.0135509	0.997794	0.00220629
0.0147828	0.997592	0.00240756

Figure 14.16 The summarized results of the calculated geometrical and operational variables of the fluidized bed (*left*) and the moisture profile of air stream where dry air enters at the bottom and becomes moist as it moves upward (*right*).

Figure 14.17 shows the stream results of the fluidized bed. The hydrated alumina was almost completely converted into anhydrous alumina with the liberation of water that went into air stream. The outlet PSD is the same as that of the inlet (see **NOTE**: #**2**). On the other hand, the outlet air ("**AIROUT**") stream contains extremely tiny amounts of dry alumina (i.e., dusty particles) the PSD of which tells that 99.92 % of total particles have a particle size less than 1 mm.



Display Streams Format SOLIDS

	SIN	CMPRSAIR	SOUT	AIROUT
Temperature C	25	504.3	412.5	412.5
Pressure bar	12	12	11.708	11.708
Mass VFrac	0	1	0	1
Mass SFrac	1	0	1	< 0.001
*** ALL PHASES ***				
Mass Flow kg/hr	300	4500	196.068	4603.93
Volume Flow cum/hr	0.115	837.311	0.049	784.899
Enthalpy Gcal/hr	-1.172	0.534	-0.751	0.113
Density kg/cum	2600.12	5.374	3986.07	5.866
Mass Flow kg/hr				
AL(OH)3	300		0.064	trace
AL2O3			196.005	0.024
AIR		4500		4500
H2O				103.908

Figure 14.17 Stream results for the fluidized bed showing the transformation of almost all hydrated into anhydrous alumina, while keeping the same PSD. Yet, extremely tiny amounts of anhydrous alumina (i.e., dusty particles) were found in the outlet air stream as losses.

EXERCISE 14.3 (RECONVERGING THE SOLUTION FOR AN INPUT CHANGE)

It is to be mentioned here that it is a matter of "trial-and-error" approach when the user reaches successful results regarding the geometrical specifications of the fluidized bed.

Thus, it will be the duty upon the shoulders of the user to tune up the process of reaching successful results. Change the bed inventory from 120 to 150 kg of bed mass (under "**Specifications**" tab, see Figure 14.14). Your task will be to reconverge the solution for this change.

REFERENCES

[1] Werther, J. and Wein, J. (1994) Expansion behavior of gas fluidized beds in the turbulent regime. *AIChE Symposium Series*, **90** (301), 31–44.

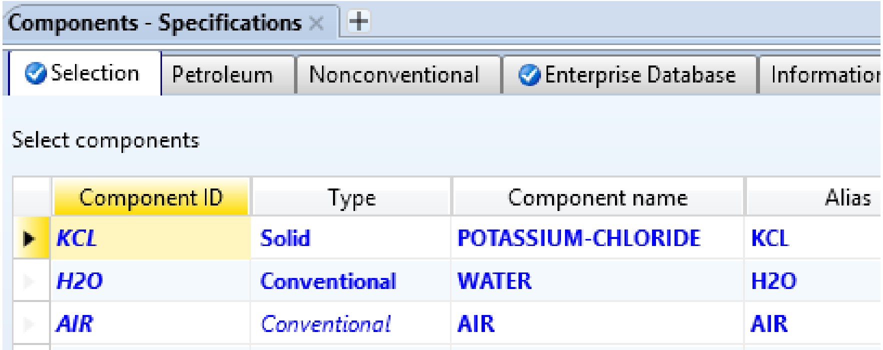
[2] Kunii, D. and Levenspiel, O. (1991) *Fluidization Engineering*, Butterworth-Heinemann, Boston.

HOMEWORK/CLASSWORK 14.1 (KCL DRYING)

Consider the process of KCl drying using hot air, where moisture will migrate from the wet solid to the dry air and the heat needed will be convectively supplied by the hot air.

Using Aspen Plus, start a new simulation by choosing the "**Solids**" category and selecting "**Solids with Metric Units**" template to create a steady-state flow sheet. Notice that Aspen Plus does not assign a default property method. So, we will set it to "**SOLIDS**".

In "**Navigation**" pane menu tree, go to "**Components**" | "**Specifications**" | "**Selection**" sheet. Click on "**Find**" button to search for "**KCL**". Once you find "**KCL**", add it to the list of components and change its "**Type**" from "*Conventional*" to "*Solid*". Add water and air as well, as shown in Figure 14.18.



Select components

Component ID	Type	Component name	Alias
KCL	Solid	POTASSIUM-CHLORIDE	KCL
H2O	Conventional	WATER	H2O
AIR	Conventional	AIR	AIR

Figure 14.18 Entering KCL, H2O, and AIR as components while changing the type from "*Conventional*" to "*Solid*" for KCL.

Click on "**Next**" button, run the simulator, and monitor warnings and errors (if any) via the "**Control Panel**". Once you successfully manage to complete the property analysis step, switch to "**Simulation**" environment. From "**Model Palette**", select "**Solids**" tab, click on "**Dryer**" icon, and add the dryer icon to the flowsheet area. Add one compressor unit from "**Pressure Changers**" tab. In addition, add the proper input and output streams, as shown in Figure 14.19.

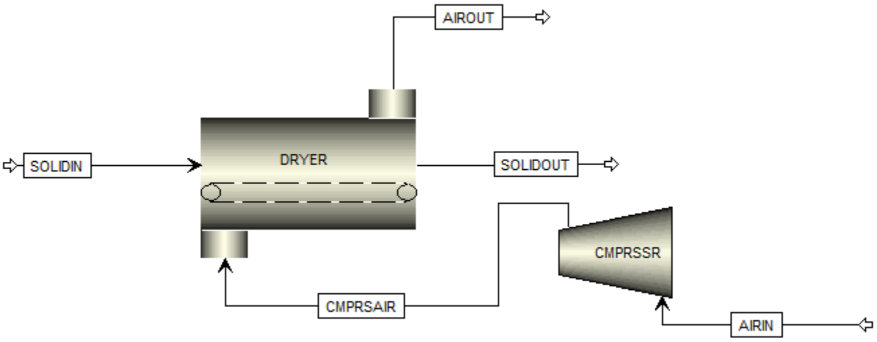
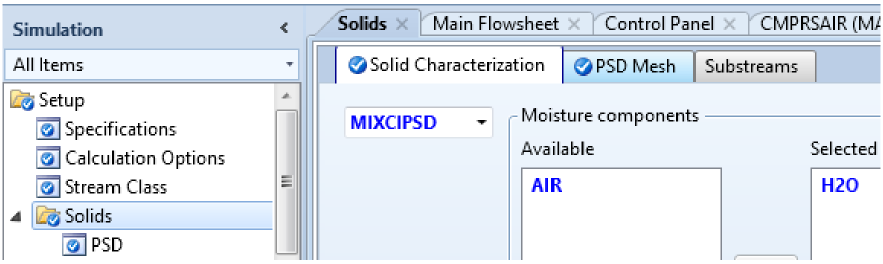


Figure 14.19 The process flowsheet for KCl drying using a compressed hot dry air.

Under "**Solids**" folder, select water as the moisture component, as shown in Figure 14.20.



MIXCIPSD

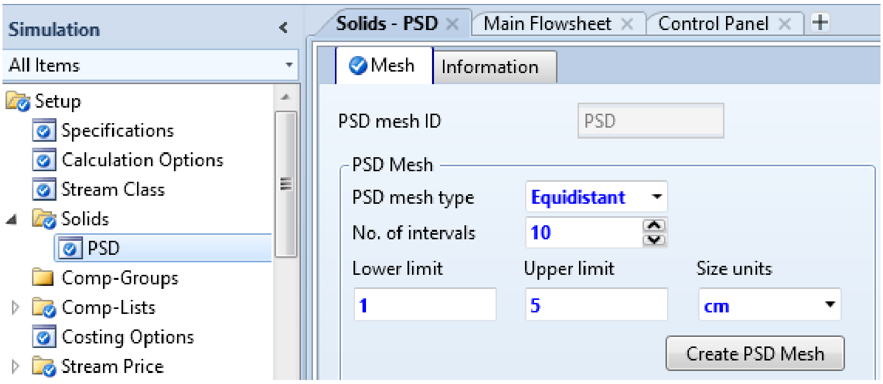
Moisture components

Available: AIR

Selected: H2O

Figure 14.20 Selection of water as the moisture component.

Figure 14.21 shows the creation of a simulation PSD mesh for monitoring the effect of drying on the particle size distribution of the substance being dried.



PSD mesh ID: PSD

PSD Mesh

PSD mesh type: Equidistant

No. of intervals: 10

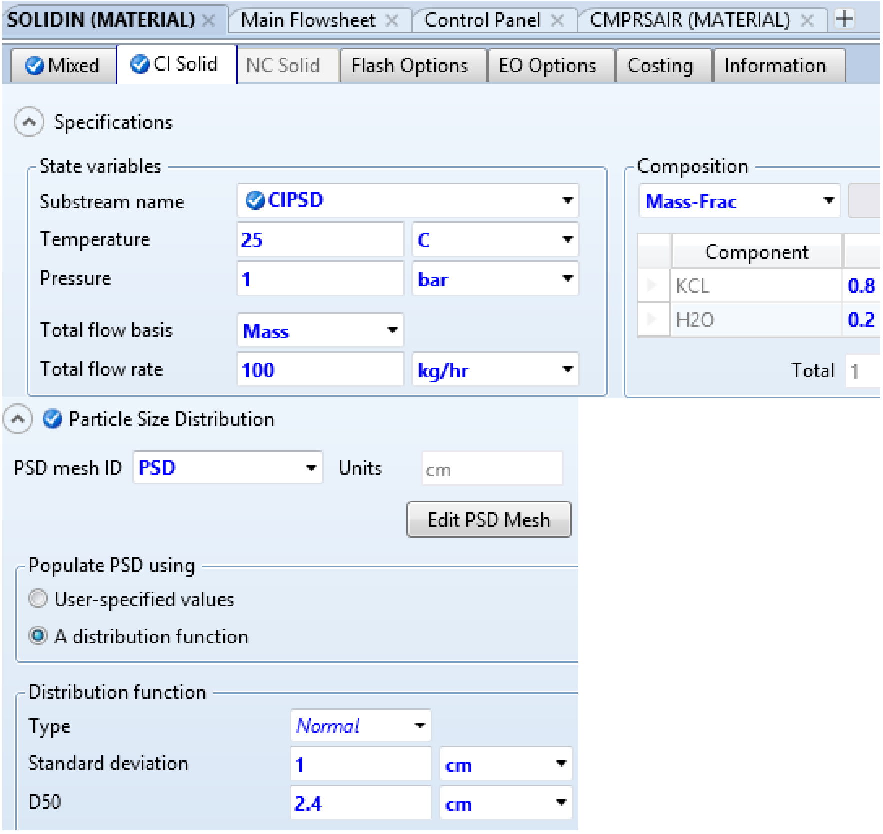
Lower limit: 1

Upper limit: 5

Size units: cm

Figure 14.21 Creation of a simulation PSD mesh to monitor the outlet stream PSD results.

Figure 14.22 shows the solid inlet stream properties in terms of *P*, *T*, compositional flow rate, and PSD.



Specifications

State variables

Substream name: CIPSD
Temperature: 25 C
Pressure: 1 bar
Total flow basis: Mass
Total flow rate: 100 kg/hr

Composition: Mass-Frac

Component	
KCL	0.8
H2O	0.2
Total	1

Particle Size Distribution

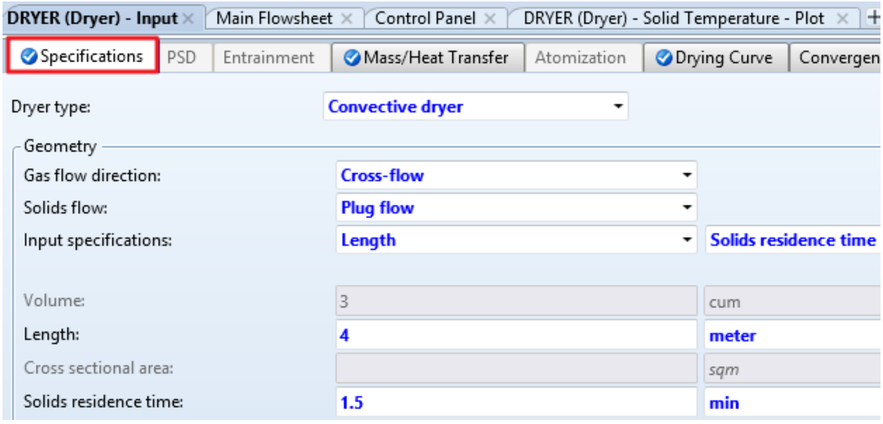
PSD mesh ID: PSD
Units: cm

Populate PSD using
○ User-specified values
● A distribution function

Distribution function
Type: Normal
Standard deviation: 1 cm
D50: 2.4 cm

Figure 14.22 “**SOLIDIN**” stream properties in terms of *P*, *T*, compositional flow rate, and PSD.

The inlet air stream enters the compressor at a flow rate of 3000 kg/h at room temperature and pressure and will leave it at 6 bar. The dryer specifications are shown in Figure 14.23.



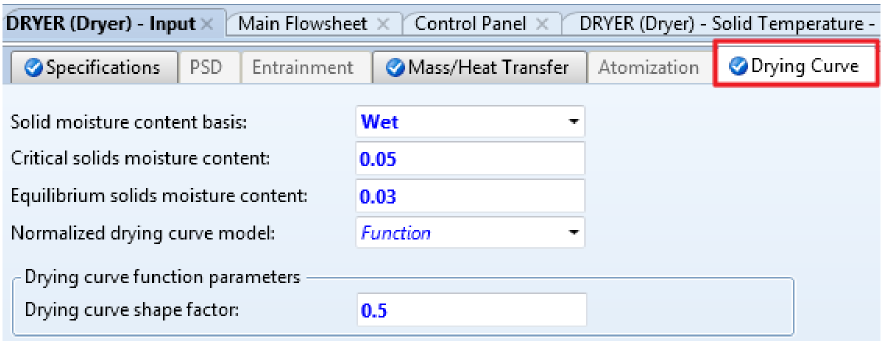
Dryer type: Convective dryer

Geometry
Gas flow direction: Cross-flow
Solids flow: Plug flow
Input specifications: Length | Solids residence time
Volume: 3 cum
Length: 4 meter
Cross sectional area: sqm
Solids residence time: 1.5 min

Figure 14.23 The dryer specifications where the “**Dryer type**” is selected as “*Convective dryer*”.

Notice that the “**Shortcut**” is simpler than the “**Convective dryer**” method in terms of input requirements, nevertheless, less rigorous.

The drying curve characteristics are shown in Figure 14.24. Notice that the **critical solids moisture content** is the moisture content at which further evaporation is mass-transfer limited and the second drying phase begins, and the **equilibrium solids moisture content** is the ultimate moisture content at which point no further drying is possible. See Aspen Plus built-in help: “**Drying Curve Function**” to have more information on “**Drying curve shape factor**”.



Solid moisture content basis: Wet
Critical solids moisture content: 0.05
Equilibrium solids moisture content: 0.03
Normalized drying curve model: *Function*

Drying curve function parameters
Drying curve shape factor: 0.5

Figure 14.24 The drying curve characteristics in terms of critical and equilibrium moisture content.

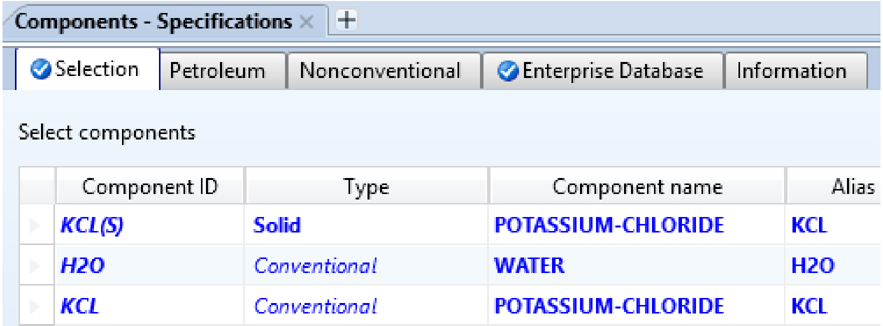
Report the outlet stream properties, dryer properties, and solid temperature profile within the dryer as a function of axial length (m).

HOMEWORK/CLASSWORK 14.2 (KCL CRYSTALLIZATION)

Consider the process of KCl crystallization from KCl solution using heat to evaporate the water and result in a supersaturated solution that will be the cause for solid precipitation at the bottom of the mother liquor.

Using Aspen Plus, start a new simulation by choosing the “**Solids**” category and selecting “**Solids with Metric Units**” template to create a steady-state flowsheet. Notice that Aspen Plus does not assign a default property method. So, we will set it to “**SOLIDS**”.

In “**Navigation**” pane menu tree, go to “**Components**” | “**Specifications**” | “**Selection**” sheet. Add KCl twice once as “*Solid*” (i.e., “**KCL(S)**”) and another as “Conventional” (i.e., “**KCL**”) to the list of components and add water as well, as shown in Figure 14.25.



Select components

Component ID	Type	Component name	Alias
KCL(S)	Solid	POTASSIUM-CHLORIDE	KCL
H2O	*Conventional*	WATER	H2O
KCL	*Conventional*	POTASSIUM-CHLORIDE	KCL

Figure 14.25 Entering KCl twice once as “*Solid*” and another as “*Conventional*” and H_2O.

Click on “**Next**” button, run the simulator, and monitor warning and errors (if any) via the “**Control Panel**”. Once you successfully manage to complete the property analysis step, switch to “**Simulation**” environment. From “**Model Palette**”, select “**Solids**” tab, click on “**Crystallizer**” icon, and add the crystallizer icon to the flowsheet area. In addition, add the proper input and output streams, as shown in Figure 14.26.

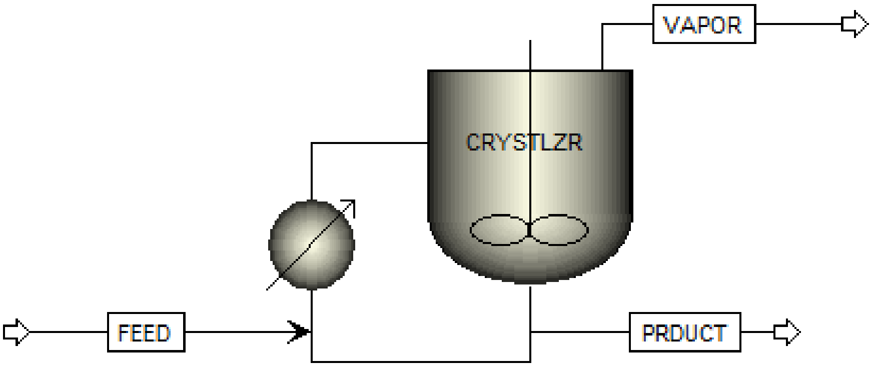
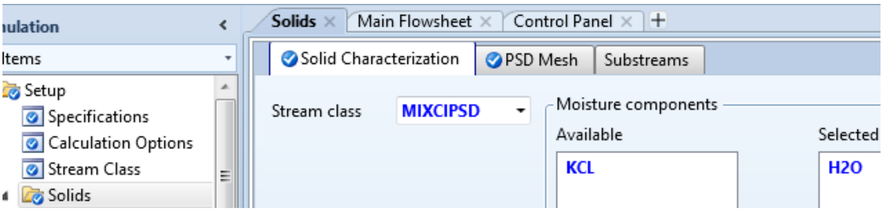


Figure 14.26 The process flowsheet for KCl crystallization using water evaporation.

Under “**Solids**” folder, select water as the moisture component, as shown in Figure 14.27.



Stream class MIXCIPSD

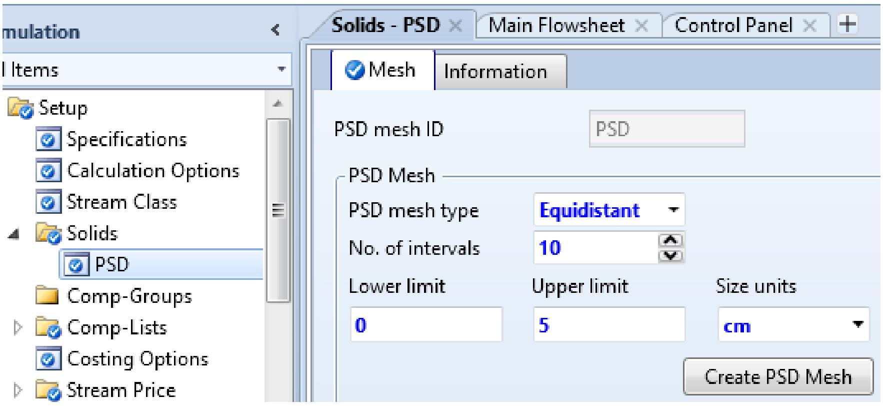
Moisture components

Available: KCL

Selected: H2O

Figure 14.27 Selection of water as the moisture component.

Figure 14.28 shows the creation of a simulation PSD mesh for monitoring the effect of water evaporation on the particle size distribution of the substance being crystallized.



PSD mesh ID: PSD

PSD Mesh

PSD mesh type: Equidistant

No. of intervals: 10

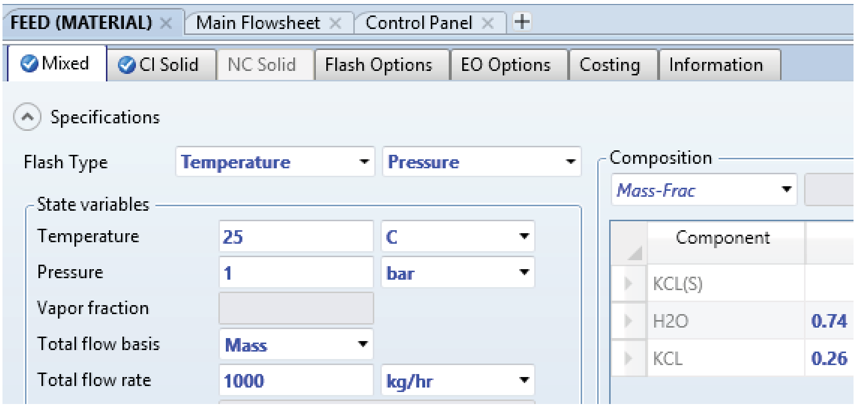
Lower limit: 0

Upper limit: 5

Size units: cm

Figure 14.28 Creation of a simulation PSD mesh to monitor outlet stream PSD results.

Figure 14.29 shows the feed stream properties in terms of P, T, and compositional flow rate. There will be no need for PSD specification because the feed stream is a saturated aqueous KCl solution entering at the maximum solubility, which is 35 g KCl/100 g water (amounts to KCl mass fraction of 0.26).



Flash Type: Temperature | Pressure

State variables

Temperature: 25 C

Pressure: 1 bar

Vapor fraction:

Total flow basis: Mass

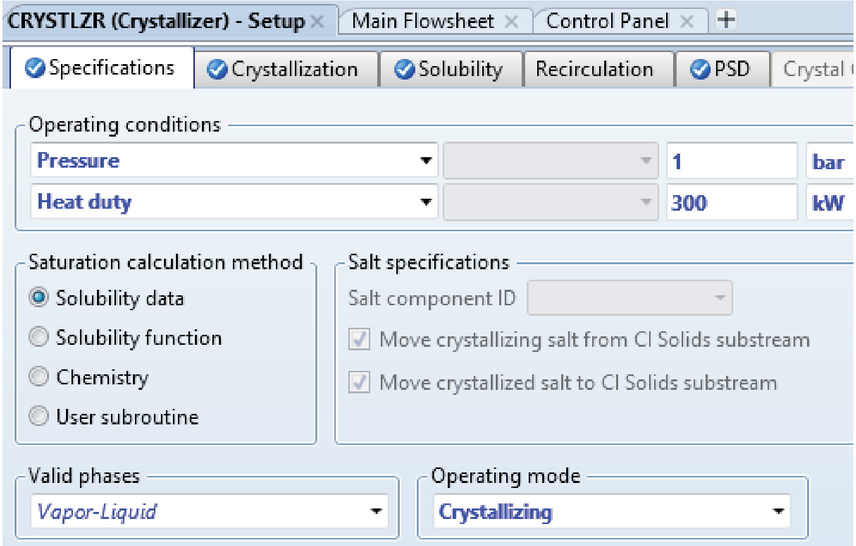
Total flow rate: 1000 kg/hr

Composition: Mass-Frac

Component	
KCL(S)	
H2O	0.74
KCL	0.26

Figure 14.29 The feed stream properties in terms of P, T, and compositional flow rate. There will be no PSD requirement as this is a saturated aqueous KCl solution.

Figure 14.30 shows the "**Specifications**" tab window for the crystallizer. A heat duty of 300 kW will be supplied to evaporate water (the solvent) and concentrate KCl solution. The "**Operating mode**" is set to "*Crystallizing*". Under this mode, the amount of crystals should increase in the flow and a warning will be issued if the crystal product flow rate is



Operating conditions

Pressure: 1 bar

Heat duty: 300 kW

Saturation calculation method

● Solubility data

○ Solubility function

○ Chemistry

○ User subroutine

Salt specifications

Salt component ID

☑ Move crystallizing salt from CI Solids substream

☑ Move crystallized salt to CI Solids substream

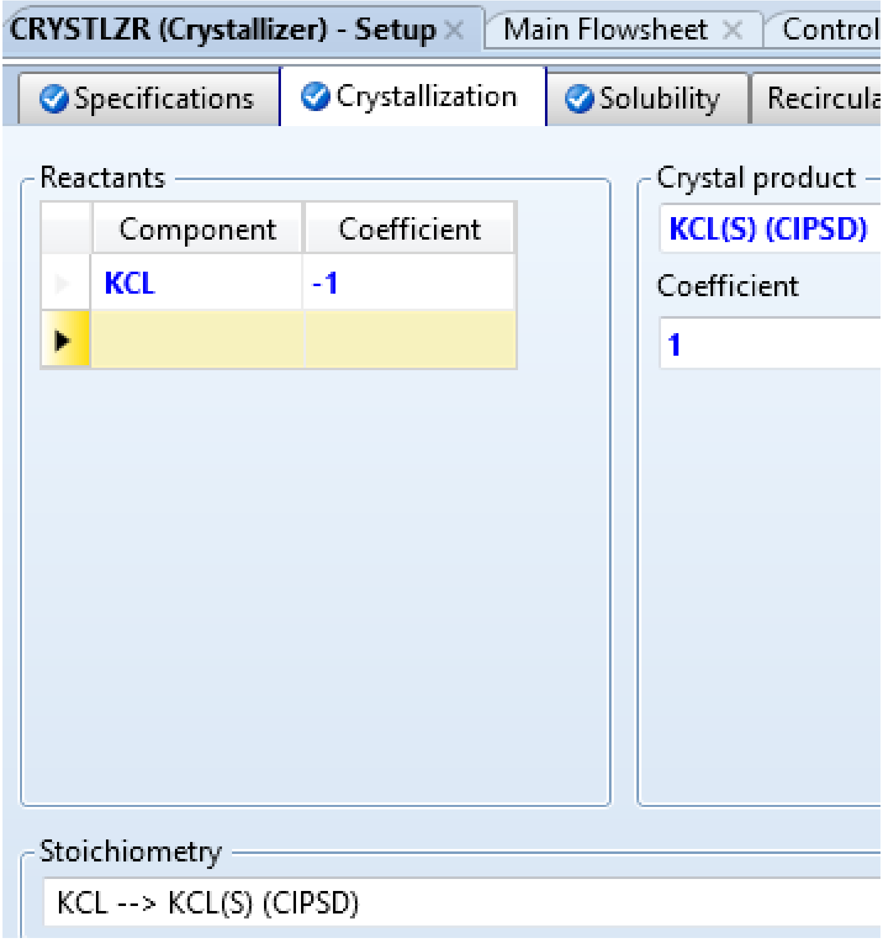
Valid phases: Vapor-Liquid

Operating mode: Crystallizing

Figure 14.30 The crystallizer specifications with the "**Operating mode**" set to "*Crystallizing*".

zero or smaller than that of the inlet. The opposite is true for the "*Dissolving or melting*" mode. No warning will be issued if the mode is set to "*Either*".

Figure 14.31 shows the "**Crystallization**" tab window where we define the sort of speaking "physical" reaction:KCl(aq) → KCl(S).



Reactants

	Component	Coefficient
	KCL	-1

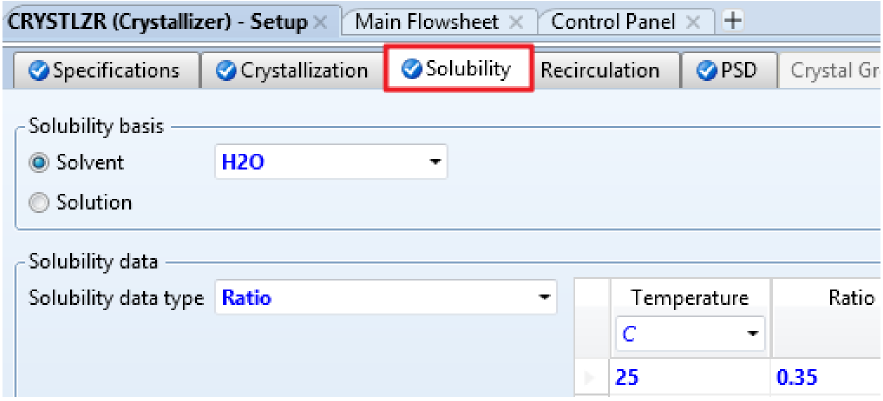
Crystal product: KCL(S) (CIPSD)

Coefficient: 1

Stoichiometry: KCL --> KCL(S) (CIPSD)

Figure 14.31 The crystallization "physical" reaction (i.e., transformation from dissolved into solid form).

Figure 14.32 shows the "**Solubility**" tab window where we enter the solubility data for KCl in water at room temperature. In the literature, it is reported as 35 g KCl per 100 g H_2O.



Solubility basis

● Solvent: H2O

○ Solution

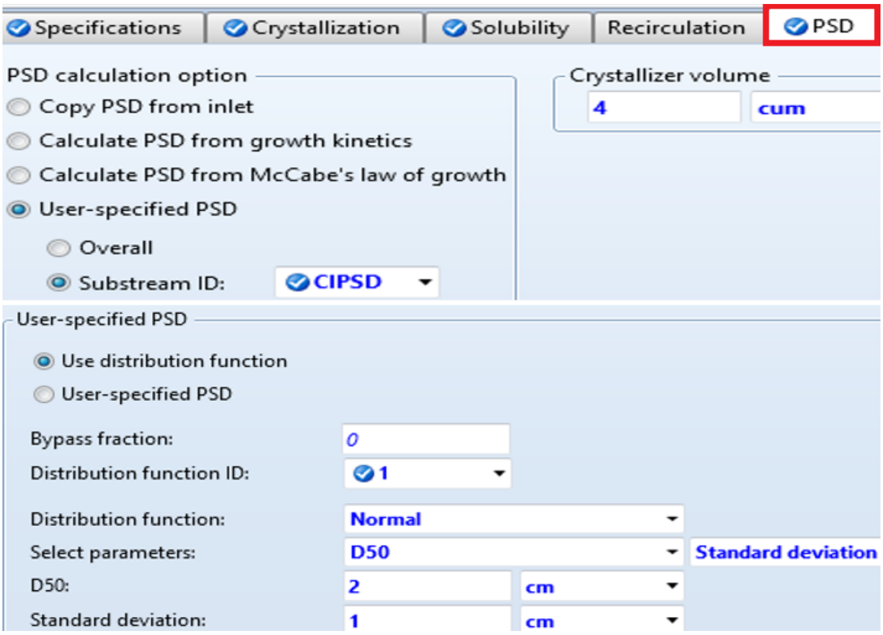
Solubility data

Solubility data type: Ratio

Temperature	Ratio
C	
25	0.35

Figure 14.32 The solubility data for KCl in water at room temperature.

Figure 14.33 shows the "**PSD**" tab window where the outlet PSD is defined in terms of a built-in known distribution function; namely, the normal distribution.



PSD calculation option

○ Copy PSD from inlet

○ Calculate PSD from growth kinetics

○ Calculate PSD from McCabe's law of growth

● User-specified PSD

○ Overall

● Substream ID: CIPSD

Crystallizer volume: 4 cum

User-specified PSD

● Use distribution function

○ User-specified PSD

Bypass fraction: 0

Distribution function ID: 1

Distribution function: Normal

Select parameters: D50 Standard deviation

D50: 2 cm

Standard deviation: 1 cm

Figure 14.33 The outlet PSD is expressed as a normal distribution function.

a) **Report the crystallizer summary of results, the outlet stream properties in terms of P, T, compositional flow rate, and particle size distribution (PSD).**
b) **Change the heat duty of the crystallizer from 300 to 500 kW and recalculate the crystallizer and product stream properties. How is the added energy mainly consumed?**

APPENDIX 14.A SOLIDS UNIT OPERATIONS

Aspen Plus has three categories of solids unit operations:

APPENDIX 14.A.1 Unit Operation Solids Models

Unit operations models used to describe treatment steps carried out on solids in the form of formation, size modification, size-based separation, washing, drying, and fluidization. Aspen Plus built-in unit operation solid models are (Figure 14.A.1):

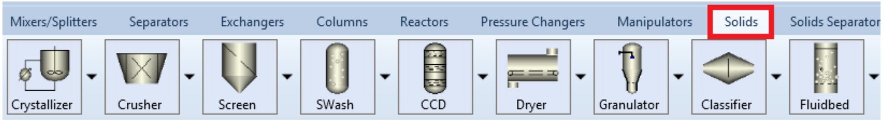


Figure 14.A.1 Different unit operation solids models are available in "**Model Palette**".

1. **Crystallizer:** produces crystals from solution based on solubility.
2. **Crusher:** breaks down solid particles to a smaller size.
3. **Screen:** separates solid particle based on their particle size.
4. **Swash:** separates solid particles from an entrained liquid of a solids stream using a washing liquid.
5. **CCD:** separates solid particles from an entrained liquid of a solids stream using a washing liquid in a countercurrent decanter or a multistage washer.
6. **Dryer:** evaporates volatile moisture components from wet solids.
7. **Spray Dryer:** evaporates moisture to form particles from sprinkled droplets.
8. **Granulator:** increases the size of solid particles.
9. **Classifier:** separates solid particles based on settling velocity.
10. **Fluidized Bed:** considers both chemical reactions and fluid mechanics.

APPENDIX 14.A.2 Solids Separators Models

Unit operation models for separating solids from gases and/or liquids are shown in Table 14.A.1.

TABLE 14.A.1 Unit Operation Models for Solid/Liquid and/or Solid/Gas Separation.

Model	Description	Purpose	Use For
Cyclone	Cyclone separator	Separates solids from gas using gas vortex in a cyclone	Rating and sizing cyclones
VScrub	Venturi scrubber	Separates solids from gas by direct contact with an atomized liquid	Rating and sizing venturi scrubbers
CFuge	Centrifuge filter	Separates solids from liquid using a rotating basket	Rating or sizing centrifuges
Filter	Rotary vacuum filter	Separates solids from liquid using a continuous rotary vacuum filter	Rating or sizing rotary vacuum filters
HyCyc	Hydrocyclone	Separates solids from liquid using liquid vortex in a hydrocyclone	Rating or sizing hydrocyclones
FabFl	Fabric filter	Separates solids from gas using fabric filter baghouses	Rating and sizing baghouses
ESP	Electrostatic precipitator	Separates solids from gas using an electric charge between two plates	Rating and sizing dry electrostatic precipitators

APPENDIX 14.A.3 Solids Handling Models

Pneumatic conveyance of granular solid materials over short and long distances through pipes. This includes solids transport through a single pipe or pipeline network.

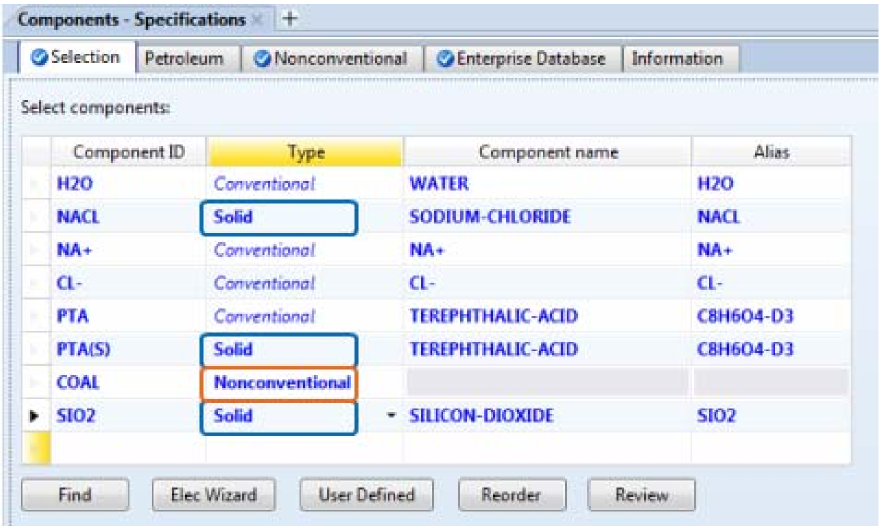
APPENDIX 14.B SOLIDS CLASSIFICATION

Solids are classified by Aspen Plus as shown in Table 14.B.1.

TABLE 14.B.1 Solids Classification Based on Knowledge of Molecular Structure and Chemical Reactivity.

Class	Type	Characteristics	Example
Conventional (a solid with a well-defined molecular structure)	Salts	Participates in phase equilibrium thus defined through chemistry	NaCl(s), ice, and purified terephthalic acid (pTA(s))
	Conventional Inert Solids (CISOLIDS)	An inert solid phase and does not participate in phase equilibrium	SiO_2(s) and urea(s)
Non-conventional (complex structure)	Non-conventional Solids (NCSOLIDS)	Characterized through component attributes (ultimate analysis) - special thermodynamic models	Coal and paper pulp

Figure 14.B.1 shows how one can define the same component using different types; hence, a different “**Component ID**” will be created each time. For example, if “**NACL**” is defined as “*Conventional*”, then it will be part of the aqueous medium (i.e., participates in phase equilibrium); on the other hand, if it is defined as “**NACL(S)**”, that is, “*Solid*”, then it will be treated as inert (i.e., will not be part of the aqueous medium). Silica being defined as “*Solid*” means it is with a known molecular structure; on the other hand, coal being defined as “*Nonconventional*” means that it has a complex structure.



Select components:

Component ID	Type	Component name	Alias
H2O	Conventional	WATER	H2O
NACL	Solid	SODIUM-CHLORIDE	NACL
NA+	Conventional	NA+	NA+
CL-	Conventional	CL-	CL-
PTA	Conventional	TEREPHTHALIC-ACID	C8H6O4-D3
PTA(S)	Solid	TEREPHTHALIC-ACID	C8H6O4-D3
COAL	Nonconventional		
SIO2	Solid	SILICON-DIOXIDE	SIO2

Figure 14.B.1 The same material can be defined in different ways, depending on whether the material will be chemically active or inert and whether or not it is of a known molecular structure.

APPENDIX 14.C PREDEFINED STREAM CLASSIFICATION

Stream classes are very useful when modeling solids because they can be used to differentiate between the properties of each substream in the simulation. Stream classes ease the integration of solids and fluids in one simulation. The stream class can either be created or selected from a predefined type. Upon one’s need, a predefined class can also be modified.

Aspen Plus predefined stream classes are in general sufficient for most applications. All unit operation models, except “**Extract**”, can handle stream classes with solid substreams. Table 14.C.1 shows different Aspen Plus built-in stream classes.

TABLE 14.C.1 Aspen Plus Built-In Stream Classes.

Stream Class	When
CONVEN	The simulation does not involve solids, or the only solids are electrolytes salts
MIXCISLD	Conventional inert solids are present, but there is no particle size distribution
MIXNC	Non-conventional solids are present, but there is no particle size distribution
MIXCINC	Both conventional inert and non-conventional solids are present, but there is no particle size distribution
MIXCIPSD	Conventional inert solids are present, with a particle size distribution
MIXNCPSD	Non-conventional solids are present, with a particle size distribution

The stream class can be changed to a different class using the stream class changer (manipulator) as shown in Figure 14.C.1.

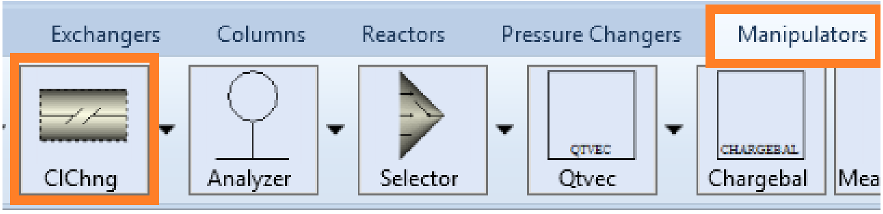


Figure 14.C.1 Transforming one stream class into another using "**ClChng**" manipulator.

NOTE #3: *For further information on how to use the stream class changer, refer to Chapter 18*: *TP #11*: *Using More Than One Property Method and Stream Class*: *Solid Catalyzed Direct Hydration of Propylene to Isopropyl Alcohol* (*IPA*).

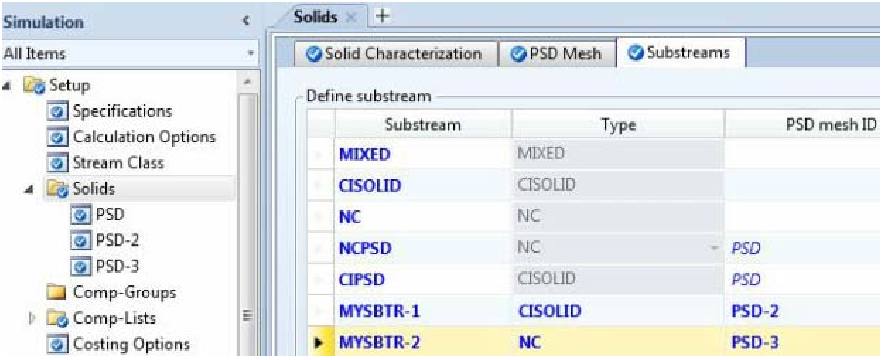
APPENDIX 14.D SUBSTREAM CLASSES

Substream classes are the building blocks of stream classes. They can either be predefined or customized. Predefined substream classes are shown in Table 14.D.1:

TABLE 14.D.1 Substream Classes for Solid-Bearing Streams.

#	Substream Class	Description
1	MIXED	Fluids only
2	CISOLID	Conventional inert solids that participate in reactions but do not participate in phase equilibria (except in the RGibbs model)
3	NC	Non-conventional solids
4	NCPSD	Non-conventional solids with PSD
5	CIPSD	Conventional inert solids with PSD

Notice that PSD can be specified for each substream in a stream class. Such an advantage permits the user to have different PSD functions for different streams or flowsheet sections. On the other hand, customized substream classes are additional substream types that can be created by the user to complement the existing predefined substreams. Customized substreams are usually used to ease the treatment of different solids in one simulation and permit the use of different PSDs for one predefined substream type, as shown in Figure 14.D.1.



Substream	Type	PSD mesh ID
MIXED	MIXED	
CISOLID	CISOLID	
NC	NC	
NCPSD	NC	PSD
CIPSD	CISOLID	PSD
MYSBTR-1	CISOLID	PSD-2
MYSBTR-2	NC	PSD-3

Figure 14.D.1 The ability to create new substreams and define different PSDs will grant the user the freedom to associate a PSD with a given substream.

APPENDIX 14.E PARTICLE SIZE DISTRIBUTION (PSD)

In Aspen Plus, particle size distribution (PSD) is represented by the weight fractions per particle size interval, given the number of intervals and the size range for each interval. In other words, a PSD describes the amount of particles in a sample of material with respect to size. The built in Aspen Plus particle size distribution has 10 predefined size intervals. The user can modify the built in particle size distribution by changing the number of intervals or the size ranges for the intervals. In some situations, he/she may want to have two or more particle size distribution definitions, with different size ranges. This will be useful if different sections of the flowsheet have different particle sizes.

In this regard, a PSD mesh is defined (i.e., a grid with size intervals over which the particle sizes will be described). The PSD is populated via experimental results (i.e., user-specified weight fractions) or utilizing built-in distribution functions. In Aspen Plus, there are simulation PSD meshes coined for a substream under which all the results for multiple streams will be presented and input stream PSD meshes that are defined for individual feed streams.

For **user-specified PSD meshes**, Aspen Plus provides four types: equidistant, geometric, logarithmic, and user-defined, where the user is required to enter the lower limit, upper limit, and size unit (i.e., mm, μm, angstrom, etc.). Depending on the selected type, the user may also have to enter the number of intervals. For the user-defined type, it is suited for experimental data where the user can copy and paste values from other spreadsheet packages such as Microsoft Excel sheet.

For **built-in distribution functions**, the user, however, must specify the function parameters that describe, in general, the mean or a reference datum and the degree of scatter around that mean or reference value, as in the following distributions:

1. **Gates–Gaudin–Schuhmann (GSS)**: It has two parameters: one for the maximum particle size (i.e., at which the cumulative mass fraction $Q(d) = 1$) and another for describing the profile (shape) of the distribution itself (i.e., narrow vs. broad). GGS is suited for coarse grinding.

2. **Rosin–Rammler–Sperling–Bennet (RRSB)**: It has two parameters: one for the particle size (i.e., at which the cumulative mass fraction $Q(d) = 0.632$) and another for describing the profile of the distribution itself (i.e., narrow vs. broad). RRSB is suited for fine grinding.
3. **Normal**: It has two parameters: one for the mean or median (at which the cumulative mass fraction $Q(d) = 0.5$) and another for describing the profile of the distribution itself (i.e., narrow vs. broad).
4. **Log Normal**: It has two parameters: one for the median (the median at which the cumulative mass fraction $Q(d) = 0.5$) and another for describing the profile of the distribution itself (i.e., narrow vs. broad). If particles are broken up at random, they will end up with such a distribution.

When viewing and analyzing the results for solid components, Aspen Plus provides sets of properties:

1. Median value (D50): the size at which 50% of particles are larger.
2. Mean particle size (D1_0): the sum over all intervals for the multiplication of the average particle size, in one interval, by the fraction.
3. Specific surface area (VSSA): the ratio of the surface area of a particle to its volume. For a completely spherical object, it is $4\pi r^2 / \frac{4}{3}\pi r^3 = \frac{3}{r} = \frac{6}{D}$. For other non-spherical objects, a shape or sphericity factor is used.
4. Sauter mean diameter (D3_2 or SMD): an average particle size. SMD is the diameter of spheres with the same volume/area ratio as the particle mixture. For example, if V is the total volume of particles and A is their total surface area, then $SMD = 6\,V/A = D_{particle}$. SMD is inversely proportional to VSSA. SMD is the characteristic diameter for a packed bed flow and is mainly used in fluidized bed calculations.

APPENDIX 14.F FLUIDIZED BEDS

The Aspen Plus fluidized bed model describes a bubbling or circulating fluidized bed and tackles five different aspects:

Entrainment of Particles: It takes into account the geometry of the vessel and additional gas supply and provides options to determine the minimum fluidization velocity, transport disengagement height, and distributor pressure drop for either a porous plate or bubble cap.

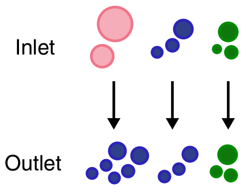
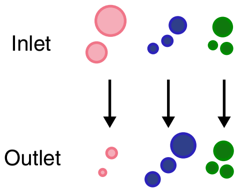
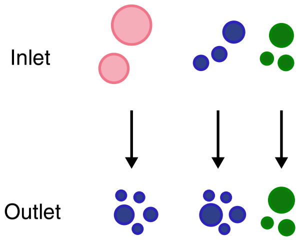
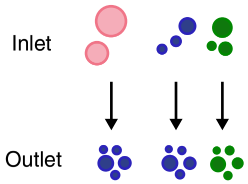
Chemical Reactions: After defining the reaction stoichiometry and its kinetics, the calculation method treats the gas as plug flow, the solids ideally mixed, and each balance cell is considered as CSTR (i.e., uniform in properties).

Fluid Mechanics: It assumes one-dimensional fluid mechanics and considers the impact of volume production/or reduction and heat exchange on fluid mechanics.

Change in PSD: Table 14.F.1 demonstrates different options of tackling the outlet PSD with respect to the inlet PSD.

Thermodynamics: Solids and vapors are in thermodynamic equilibrium while the model considers the impact of heat exchange and heat effect on bed temperature.

TABLE 14.F.1 **Different Approaches in Tackling the Outlet PSD For a Fluidized Bed.**

Keep PSD	Constant # of Particles	Overall PSD	PSD Per Particle Type
			
Particle types have the same PSD as the inlet and the new generated particle types have the overall PSD from the inlet. Total number of particles may change and inert particles will keep the same size	Total number of particles is fixed. The particle may shrink or grow, depending on the mass loss/gain of the particle type. Inert particles will keep the same size	Overall bed PSD is defined by the user. Total number of particles may change. Inert particles are allowed to change their size	Bed PSD is defined by the user on a particle-type basis. Total number of particles may change. Inert particles will keep the same size if PSD is defined only for the reacting species

Reaction: A ○ → B ●

Inert: C ●

The Aspen Plus fluidized bed model treats the bed as made of two zones. See Figure 14.F.1.

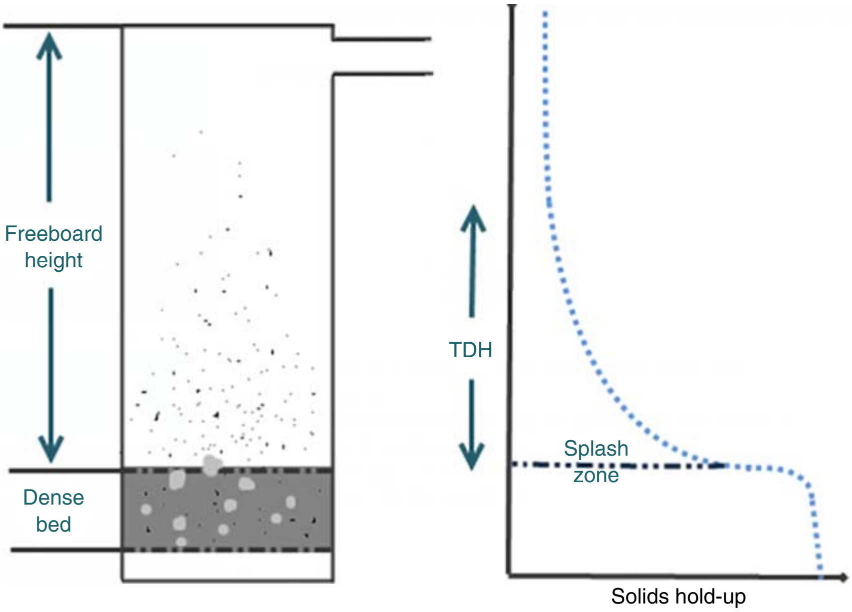


Figure 14.F.1 The fluidized bed is split into two zones the dense bed and the loose bed (freeboard). TDH stands for transport disengagement height.

The bottom zone (dense bed): High solids concentration and fluid mechanics is dealt with according to Werther and Wein [1], which considers the growth and splitting of bubbles. Bubble-related profiles (e.g., bubble diameter, bubble rise velocity, interstitial gas velocity, pressure, and solid volume concentration profiles can all be calculated.

The freeboard zone (loose bed): Relatively low solids concentration and fluid mechanics is dealt with according to Kunii and Levenspiel [2]. Using the selected entrainment correlation, the solids mass flow and PSD at the outlet condition can be calculated.

Overall, once the user defines bed inventory, by specifying the pressure drop or the solids hold-up, the height of the bottom zone and the freeboard can be determined.

15

ASPEN PLUS® DYNAMICS

15.1 INTRODUCTION

The goal of process control is to smoothly run the process in terms of keeping the controlled variable within control limits. Such limits usually represent constraints imposed on the process itself, in the form of environmental/governmental regulation, product quality or customer satisfaction, and the lower limit of profitability.

In an open-loop control, the controller output has no feedback from the process itself and the controller output is fixed at a value until it is manually changed by an operator. Keep in mind that many processes are stable in an open-loop control mode and will maintain the process variable at a value in the absence of disturbances. Disturbances are uncontrolled changes, caused by surroundings, which directly or indirectly affect the process variable to be controlled. In general, all processes suffer from disturbances, and with an open-loop control mode this will always result in deviations in the monitored process variable. Such deviations might be drastic, which will cause these processes to become unstable. Other deviations are mild such that the process inherently responds by what is called self-adjustment or self-regulation.

The deviation caused by a disturbance or set-point load is basically the dynamic response of a process that differs whether or not the controller is in action. If the controller is off, then the dynamics is denoted as "open loop". On the contrary, if the controller is on, then the dynamics is denoted as "closed loop". Under both modes, we need to understand the dynamic response of the process so that we are able to characterize it and thus better control it. In process control terminology, the dynamic response or behavior of process means how the measured process variable (PV) will respond over time to changes in the controller output (CO), disturbances (D), or both. The overall process gain as sensed by a controller is the product of the gains of the sensor, the final control element, and the process itself.

$$\text{Overall process gain} = \text{Gain}_{\text{Process}} \times \text{Gain}_{\text{Sensor}} \times \text{Gain}_{\text{Final control element}}$$

Aspen Plus®: Chemical Engineering Applications, First Edition. Kamal I.M. Al-Malah.

Companion Website: www.wiley.com/go/Al-Malah/AspenPlusApplications

The robustness of a controller is a measure of the range of process values over which the controller provides stable operation. The more non-linear a process is, the less aggressive the tuning approach will be in order to maintain robustness. The non-linear behavior of a process can stem from one or more of the inevitable happenings:

- Surfaces foul or corrode
- Mechanical elements, such as seals or bearings, wear
- Feedstock quality varies and catalyst activity decays
- Environmental conditions, such as heat and humidity, change.

The gain of a controller will be inversely proportional to the overall process gain that it sees or senses. In a social context, to have a family that is both happy and productive, the response of the dad/mom should be calm (robust) if the kids are bit nervous; vice versa, the dad/mom has to be more vigorous and enforcing if the kids are too cool or calm (i.e., lazy).

15.2 PROBLEM DESCRIPTION

The following kinetic data were quoted from [1]. Ethylene (**E**) reacts with benzene (**B**) to form the desired product ethylbenzene (**EB**). There is a consecutive reaction that produces the undesirable product diethylbenzene (**DEB**). A third reaction combines benzene and diethylbenzene to form ethylbenzene:

$$C_2H_4 + C_6H_6 \rightarrow C_8H_{10} \tag{15.1}$$

$$C_2H_4 + C_8H_{10} \rightarrow C_{10}H_{14} \tag{15.2}$$

$$C_6H_6 + C_{10}H_{14} \rightarrow 2C_8H_{10} \tag{15.3}$$

In symbolic notation:

$$\mathrm{E} + \mathrm{B} \rightarrow \mathrm{EB} \tag{15.4}$$

$$\mathrm{E} + \mathrm{EB} \rightarrow \mathrm{DEB} \tag{15.5}$$

$$\mathrm{B} + \mathrm{DEB} \rightarrow 2\mathrm{EB} \tag{15.6}$$

$$-r_1(\mathrm{kmol/m^3 \cdot s}) = 1.528 \times 10^6 \times \exp\left[-\frac{71.16 \times 10^3}{R} \times \left(\frac{1}{T}\right)\right] C_\mathrm{E} C_\mathrm{B} \tag{15.7}$$

$$-r_2(\mathrm{kmol/m^3 \cdot s}) = 2.778 \times 10^4 \times \exp\left[-\frac{83.68 \times 10^3}{R} \times \left(\frac{1}{T}\right)\right] C_\mathrm{E} C_\mathrm{EB} \tag{15.8}$$

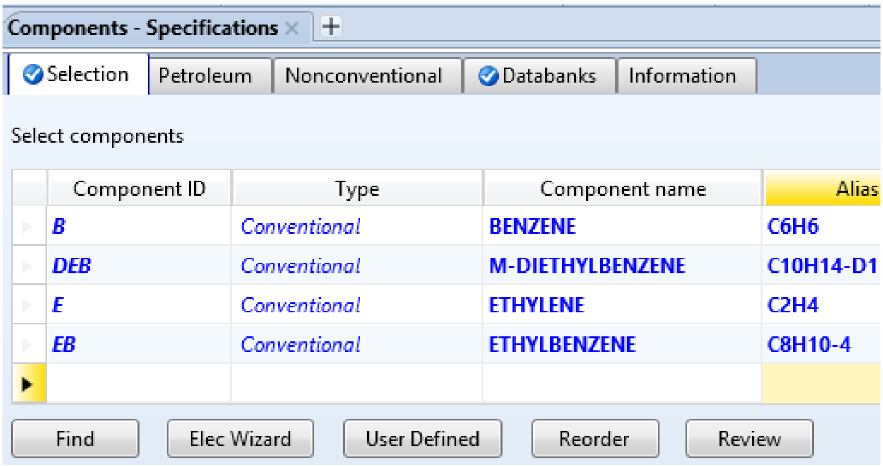
$$-r_3(\mathrm{kmol/m^3 \cdot s}) = 0.4167 \times \exp\left[-\frac{62.76 \times 10^3}{R} \times \left(\frac{1}{T}\right)\right] C_\mathrm{DEB} C_\mathrm{B} \tag{15.9}$$

The units of $\boldsymbol{k}$, for a second-order reaction, are$(\mathrm{m^3/kmol \cdot s})$. Concentrations have units of$(\mathrm{kmol/m^3})\ or (\mathrm{mol/l})$. Activation energies have units of *kJ/kmol*. Temperature is in degrees *Kelvin*. There are two feed streams to the reactor: 0.1 kmol/s of pure ethylene and 0.2 kmol/s of benzene. Compared with ethylene, benzene molar flow rate is above its stoichiometric value in order to keep low ethylene concentration so that the formation of *DEB* is minimized.

15.3 PREPARING ASPEN PLUS SIMULATION FOR ASPEN PLUS DYNAMICS (APD)

Using Aspen Plus, select the template: “**Chemicals with Metric Units**” Simulation. Under “**Setup**” | “**Specifications**” | “**Global**” tab window, change the units to “*SI*”.

Add the reacting components to the list of components as shown in Figure 15.1. *m*-DEB, among the three possible DEB isomers (*ortho*, *meta*, and *para*), is chosen to represent DEB, as it was found to be the most stable DEB isomer [2].



Select components

Component ID	Type	Component name	Alias
B	Conventional	BENZENE	C6H6
DEB	Conventional	M-DIETHYLBENZENE	C10H14-D1
E	Conventional	ETHYLENE	C2H4
EB	Conventional	ETHYLBENZENE	C8H10-4

Figure 15.1 Benzene (B), *meta*-diethylbenzene (DEB), ethylene (E), and ethylbenzene (EB) are added as components.

The default property method is “**NRTL**”; nevertheless, as the pressure is above 10 bar, a property method, such as “**PSRK**”, “**SRK**”, or “**SR-POLAR**”, can be used (as recommended by the “**Property Selection Method Assistant**”). “**PSRK**” will be chosen as the property method.

Click on “**Next**” button, run the show under “**Properties**” environment, and watch for any error or serious warning. After successfully completing the property analysis step, switch to “**Simulation**” environment.

In “**Setup**” | “**Report Options**” | “**Stream**” tab window, select the molar basis for expressing stream properties.

Let us create a simple process flowsheet for EB synthesis, as shown in Figure 15.2.

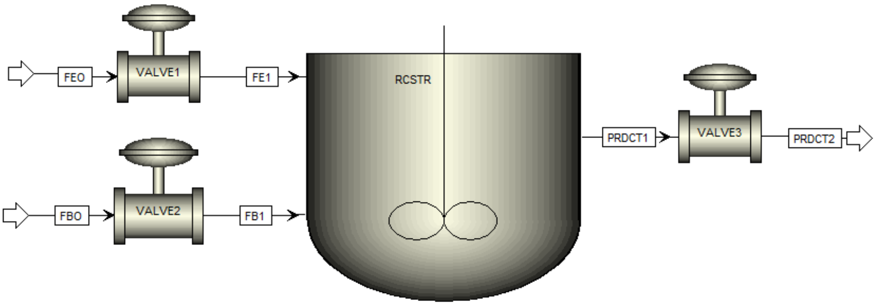
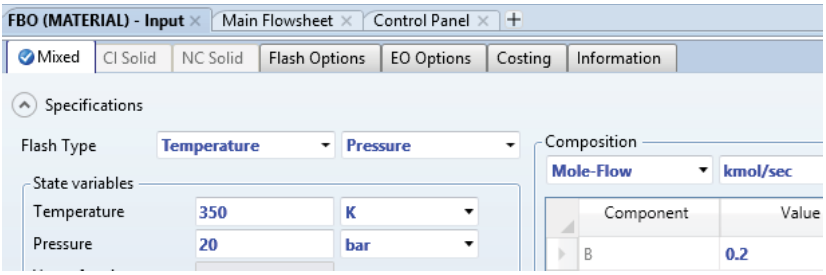


Figure 15.2 Three valves and one RCSTR are added to the process flowsheet.

Figure 15.3 shows liquid benzene inlet stream properties.



Flash Type: Temperature, Pressure

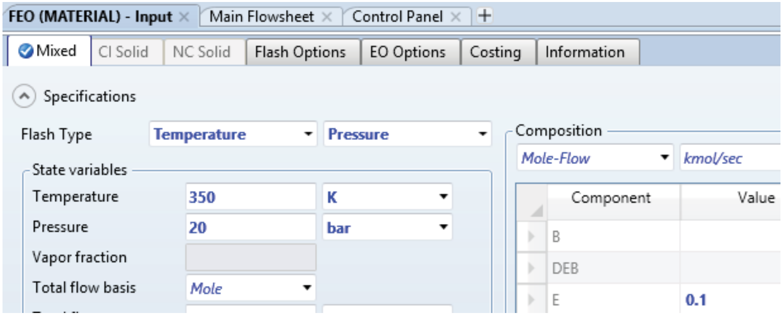
State variables
Temperature: 350 K
Pressure: 20 bar

Composition: Mole-Flow, kmol/sec

Component	Value
B	0.2

Figure 15.3 Liquid benzene inlet stream properties in terms of T, P, and compositional flow rate.

Figure 15.4 shows ethylene gas inlet stream properties.



Flash Type: Temperature, Pressure

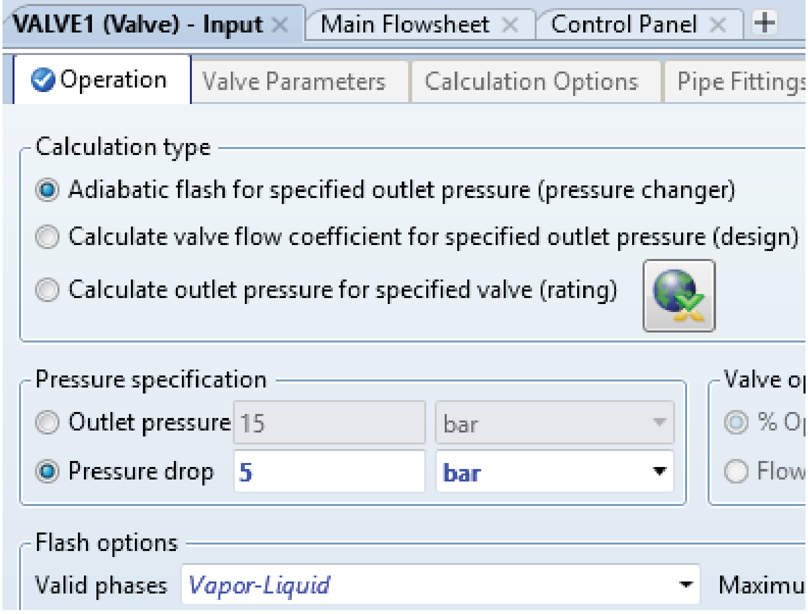
State variables
Temperature: 350 K
Pressure: 20 bar
Vapor fraction
Total flow basis: Mole

Composition: Mole-Flow, kmol/sec

Component	Value
B	
DEB	
E	0.1

Figure 15.4 Ethylene gas inlet stream properties in terms of T, P, and compositional flow rate.

Figure 15.5 shows "**VALVE1**" input specifications. "**VALVE2**" input specifications are same.



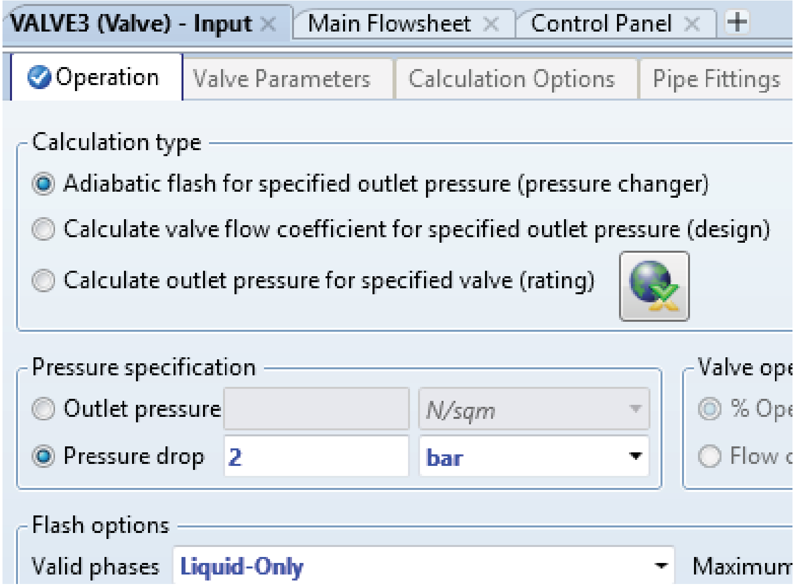
Calculation type
● Adiabatic flash for specified outlet pressure (pressure changer)
○ Calculate valve flow coefficient for specified outlet pressure (design)
○ Calculate outlet pressure for specified valve (rating)

Pressure specification
○ Outlet pressure 15 bar
● Pressure drop 5 bar

Flash options
Valid phases: Vapor-Liquid

Figure 15.5 "VALVE1" input specifications, where the pressure drop is set to 5 bar so that the outlet pressure is equal to that of the reactor.

Figure 15.6 shows specifications for “**VALVE3**” block, where a pressure drop of 2 bar is assumed and “**Valid phases**” is set to “*Liquid-Only*”. The selection was made to have a better simulation convergence.



Calculation type

● Adiabatic flash for specified outlet pressure (pressure changer)
○ Calculate valve flow coefficient for specified outlet pressure (design)
○ Calculate outlet pressure for specified valve (rating)

Pressure specification

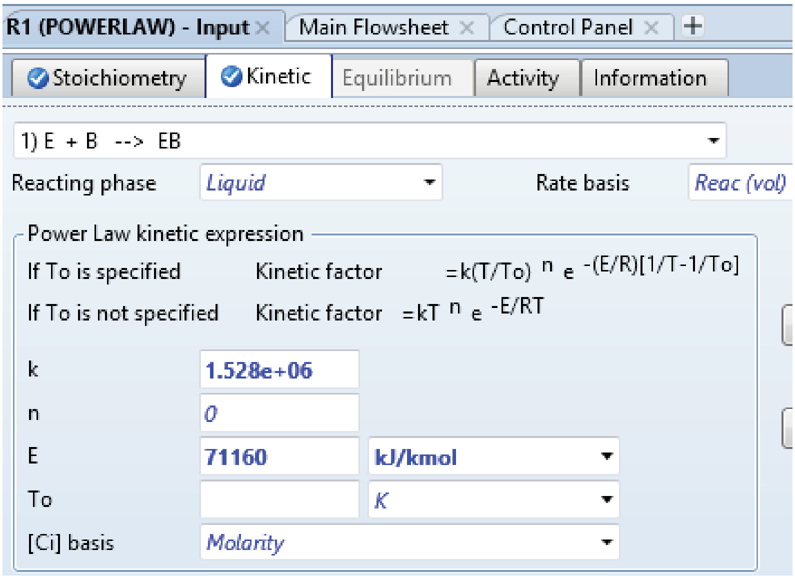
○ Outlet pressure | | N/sqm
● Pressure drop | 2 | bar

Flash options

Valid phases: Liquid-Only

Figure 15.6 “**VALVE3**” block specifications, where a pressure drop is set to 2 bar and “*Liquid-Only*” for “**Valid phases**” is used.

The three reaction rates are given in a power-law form (Eqs. 15.7–15.9), so “*POWERLAW*” type is selected. The reaction set “**R1**” describes the first reaction (Eq. 15.1, or 15.4 in symbolic notation), as shown in Figure 15.7. The kinetic parameters and reaction conditions are also shown.



1) E + B --> EB

Reacting phase: Liquid   Rate basis: Reac (vol)

Power Law kinetic expression

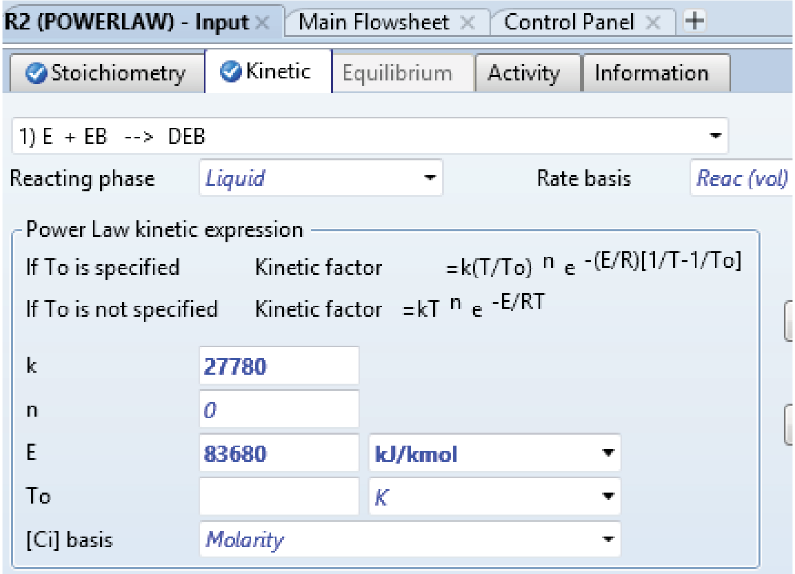
If To is specified   Kinetic factor $= k(T/To)^{n}\, e^{-(E/R)[1/T-1/To]}$

If To is not specified   Kinetic factor $= kT^{n}\, e^{-E/RT}$

k: 1.528e+06
n: 0
E: 71160 kJ/kmol
To: K
[Ci] basis: Molarity

Figure 15.7 Kinetic parameters associated with the first reaction. “*Liquid*” for “**Reacting phase**”; “*Reac(vol)*” for “**Rate basis**”; and “*Molarity*” for “**[Ci] basis**” are assigned.

The reaction set “**R2**” describes the second reaction (Eq. 15.2, or 15.5 in symbolic notation), as shown in Figure 15.8. The kinetic parameters and reaction conditions are also shown.



1) E + EB --> DEB

Reacting phase: Liquid

Rate basis: Reac (vol)

Power Law kinetic expression

If To is specified: Kinetic factor $=k(T/To)^{n}\ e^{-(E/R)[1/T-1/To]}$

If To is not specified: Kinetic factor $=kT^{n}\ e^{-E/RT}$

k: 27780

n: 0

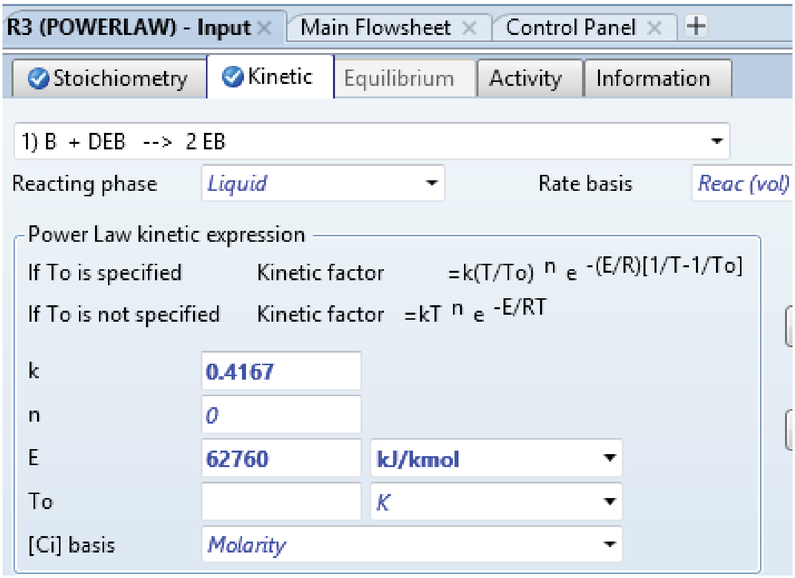
E: 83680 kJ/kmol

To: K

[Ci] basis: Molarity

Figure 15.8 Kinetic parameters associated with the second reaction. “*Liquid*” for “**Reacting phase**”; “*Reac(vol)*” for “**Rate basis**”; and “*Molarity*” for “**[Ci] basis**” are assigned.

The reaction set “**R3**” describes the third and last reaction (Eq. 15.3, or 15.6 in symbolic notation), as shown in Figure 15.9. The kinetic parameters and reaction conditions are also shown.



1) B + DEB --> 2 EB

Reacting phase: Liquid

Rate basis: Reac (vol)

Power Law kinetic expression

If To is specified: Kinetic factor $=k(T/To)^{n}\ e^{-(E/R)[1/T-1/To]}$

If To is not specified: Kinetic factor $=kT^{n}\ e^{-E/RT}$

k: 0.4167

n: 0

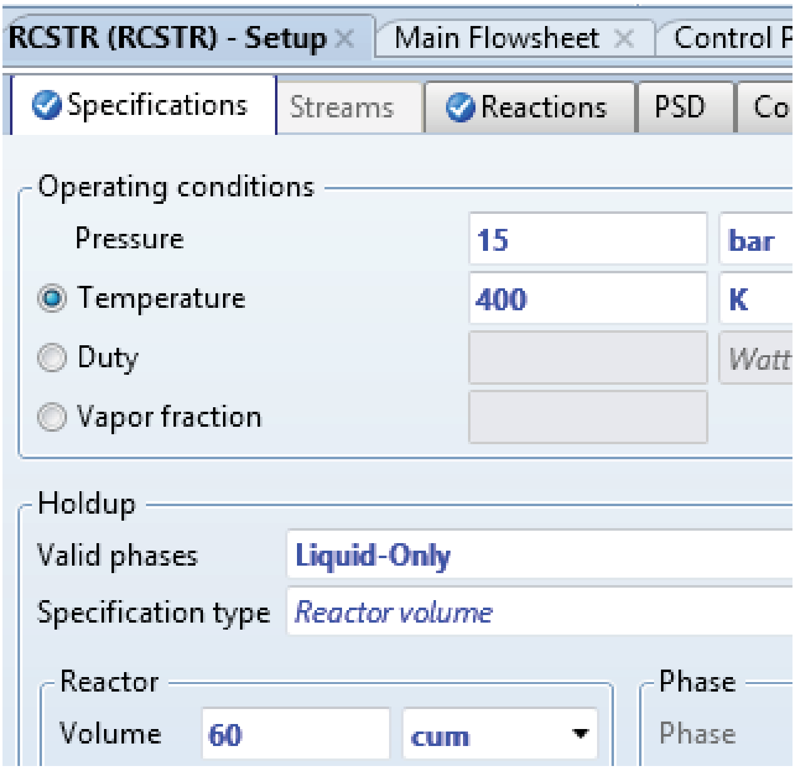
E: 62760 kJ/kmol

To: K

[Ci] basis: Molarity

Figure 15.9 Kinetic parameters associated with the third reaction. “*Liquid*” for “**Reacting phase**”; “*Reac(vol)*” for “**Rate basis**”; and “*Molarity*” for “**[Ci] basis**” are assigned.

The three reactions are now specified and can be associated with the reactor block (“**RCSTR**”). Finally, the reactor input specifications are as follows: “**Pressure**” = *15 bar*; “**Temperature**” = *400 K*; “**Valid phases**” = *Liquid-Only*; and “**Volume**” = $60\ m^3$, as shown in Figure 15.10.



Pressure 15 bar

● Temperature 400 K

○ Duty Watt

○ Vapor fraction

Valid phases Liquid-Only

Specification type Reactor volume

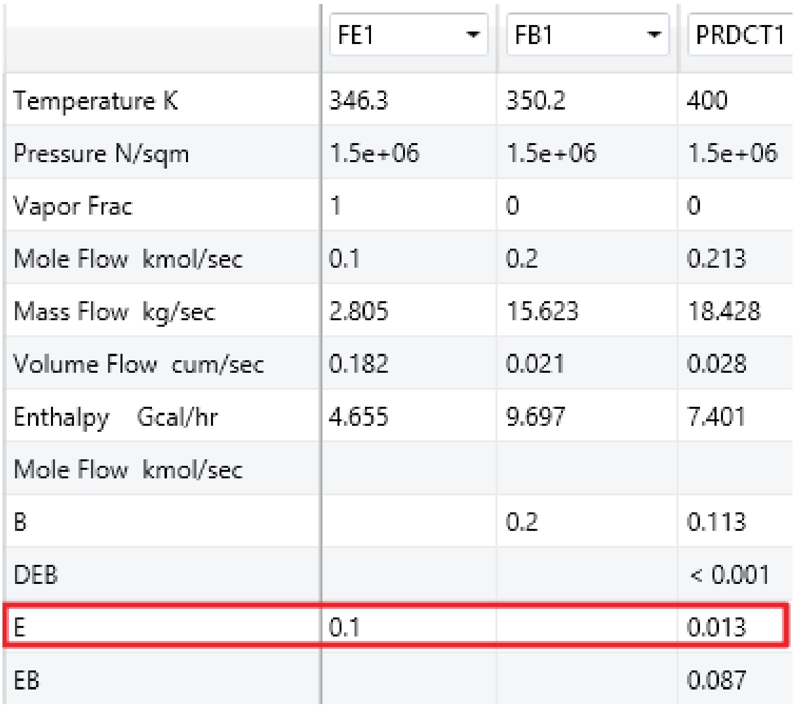
Volume 60 cum

Phase

Figure 15.10 Setting up reactor conditions: *P*, *T*, and volume. The holdup “**Valid phases**” option is set to “*Liquid-Only*”.

Do not forget to associate the three reaction sets defined earlier to “**RCSTR**” block under “**Reactions**” tab.

The simulator is now ready; run the show and watch out any simulation error or serious warning. Figure 15.11 shows the results of Aspen Plus simulator for “**RCSTR**” block. Based on the limiting reactant, which is ethylene in this case, the overall conversion is $(0.1 - 0.013)/0.1 = 0.87$.



	FE1	FB1	PRDCT1
Temperature K	346.3	350.2	400
Pressure N/sqm	1.5e+06	1.5e+06	1.5e+06
Vapor Frac	1	0	0
Mole Flow kmol/sec	0.1	0.2	0.213
Mass Flow kg/sec	2.805	15.623	18.428
Volume Flow cum/sec	0.182	0.021	0.028
Enthalpy Gcal/hr	4.655	9.697	7.401
Mole Flow kmol/sec			
B		0.2	0.113
DEB			< 0.001
E	0.1		0.013
EB			0.087

Figure 15.11 The simulation results showing the composition of the outlet stream of the reactor; where $\dot{n}_E$ is 0.013 kmol/s.

15.4 CONVERSION OF ASPEN PLUS STEADY-STATE INTO DYNAMIC SIMULATION

Figure 15.12 shows the “**Dynamics**” tab found in “**Top Toolbar**”. The user has to click on “**Dynamic Mode**” button to switch between the steady-state (i.e., static) and dynamic mode or, vice versa, to disable dynamic aspects of some blocks.

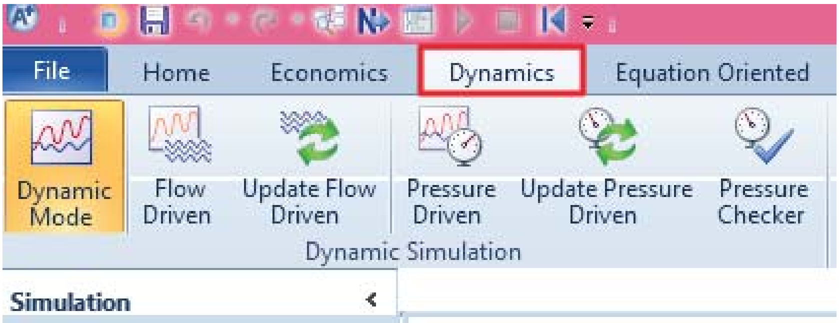
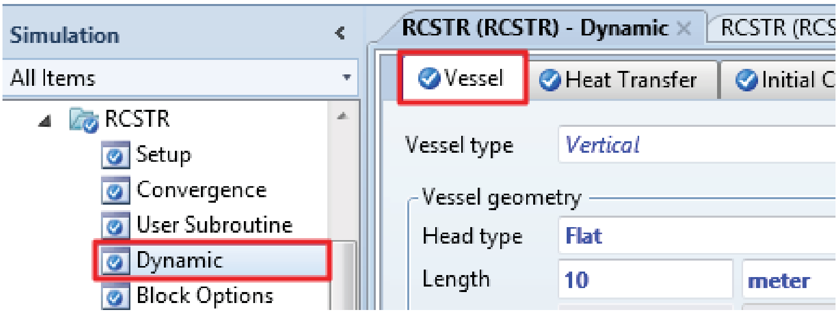


Figure 15.12 A portion of the top toolbar where it shows the “**Dynamics**” tab.

Figure 15.13 shows the activated "**RCSTR**" | "**Dynamic**" | "**Vessel**" tab sheet where it requires some input parameters. For example, enter "*10 meter*" for "**Length**" and "*Flat*" for "**Head type**".



Vessel type: Vertical

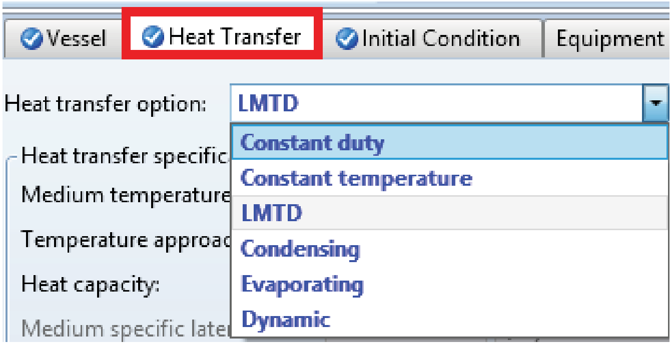
Head type: Flat

Length: 10 meter

Figure 15.13 Upon converting the steady-state (i.e., static) into dynamic simulation, the "**Dynamic**" sheet for **RCSTR** reactor becomes active, requiring some input parameters.

15.4.1 Modes of Dynamic CSTR Heat Transfer

Move to "**Heat Transfer**" tab window as shown in Figure 15.14.



Heat transfer option: LMTD

Figure 15.14 The six choices for "**Heat transfer option**".

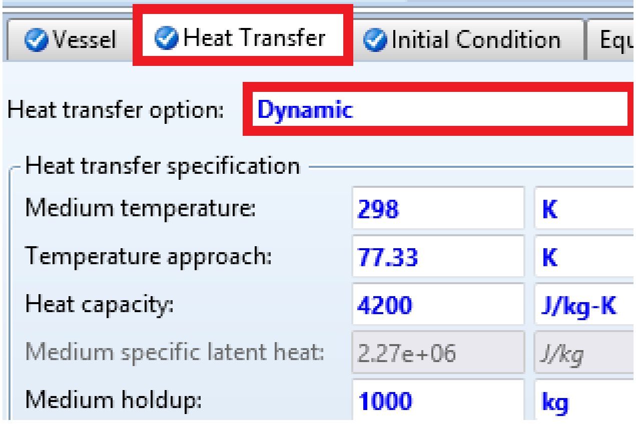
Each choice is explained in the following:

1. **Constant duty:** With this mode of heat transfer, the heat transfer rate is the manipulated variable. Duty is specified. It is initially equal to the steady-state value but can be manipulated during the simulation either manually or by using a controller. Constant duty is a useful first approximation for many situations. According to Aspen Plus sign convention, a negative heat duty means that heat will be removed and, vice versa, a positive heat duty means that heat must be supplied. The action of the temperature controller is reverse because an increase in temperature should force the controller to act in a way to remove more heat (i.e., the controller output signal is decreased or becomes more negative).

2. **Constant temperature:** Corresponds to the case where we have a condensing or boiling fluid exchanging its latent heat. With this mode of heat transfer, the temperature of the cooling medium is the manipulated variable. Aspen Plus calculates the steady-state **UA** for the given reactor temperature, coolant temperature, and heat transfer rate. The reactor temperature controller is reverse so that an increase in reactor temperature will decrease the coolant temperature.
3. **LMTD:** Corresponds to the case where we have a fluid whose temperature changes as it exchanges sensible heat. Initial medium flow rate is automatically calculated, but can be manipulated during the simulation either manually or by using a controller. The steady-state **UA** is used in Aspen Plus Dynamics. The manipulated variable is the flow rate of the cooling medium. The reactor temperature controller is direct so that an increase in reactor temperature will increase the coolant flow rate.
4. **Condensing:** Corresponds to the case when heating occurs due to "complete" condensation of the heating medium (e.g., latent heat from steam condensation). Initial flow rate of the medium is automatically calculated, but we can manipulate it during simulation either manually or using a controller. The manipulated variable is the flow rate of the condensing medium. Latent heat is assumed constant. The reactor temperature controller is reverse so that an increase in reactor temperature will decrease the condensing medium flow rate.
5. **Evaporating:** This is the reverse of the condensing mode. It corresponds to the case when cooling occurs due to "complete" evaporation of the cooling medium (e.g., cooling water/refrigerant evaporation). Initial flow rate of the medium is automatically calculated, but we can manipulate it during simulation either manually or using a controller. The manipulated variable is the flow rate of the evaporating medium. Latent heat is assumed constant. The reactor temperature controller is direct so that an increase in reactor temperature will increase the evaporating medium flow rate.
6. **Dynamic:** Corresponds to the case when you have a well-mixed heating/cooling jacket. The holdup of the coolant is specified, so the dynamics of the jacket, coil, or external heat exchanger are taken into consideration. If cooling is carried out, the manipulated variable can be the mass flow rate of the cooling medium and the reactor temperature controller is direct so that an increase in reactor temperature will increase the cooling medium flow rate. On the other hand, if heating is carried out, the manipulated variable can be the mass flow rate of the heating medium and the reactor temperature controller is reverse so that an increase in reactor temperature will decrease the heating medium flow rate.

NOTE #1: *It should be pointed out that none of these alternatives has a consideration of the actual heat transfer area or the heat transfer coefficient. The engineer must determine what area is required, using a realistic overall heat transfer coefficient.*

We will use the "*Dynamic*" option. The coolant (liquid water) "**Medium temperature**" is specified to enter at 298 K and leave at 343 K with a temperature approach about 77 K, as shown in Figure 15.15. The temperature approach is calculated as the two-terminal logarithmic mean temperature difference, assuming the reactor temperature is held at 400 K.



Heat transfer option: Dynamic

Medium temperature: 298 K

Temperature approach: 77.33 K

Heat capacity: 4200 J/kg-K

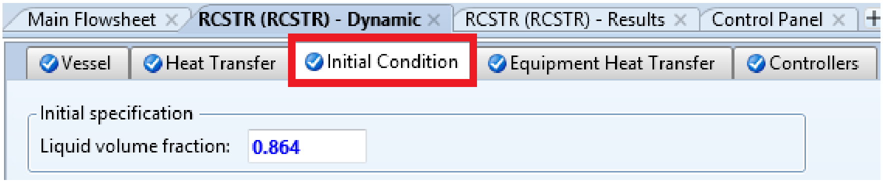
Medium specific latent heat: 2.27e+06 J/kg

Medium holdup: 1000 kg

Figure 15.15 The "*Dynamic*" option is chosen as the "**Heat transfer option**" with water as the cooling medium, entering at *298 K* and leaving at 343 K, with *LMTD = 77.33 K*.

$\mathrm{LMTD\,(K)} = [(400-298)-(400-343)]/\ln\left(\frac{102}{57}\right) = 77.33\,\mathrm{K}$. The heat capacity of water is 4200 J/(kg·K) and its hold-up in the jacket is 1000 kg.

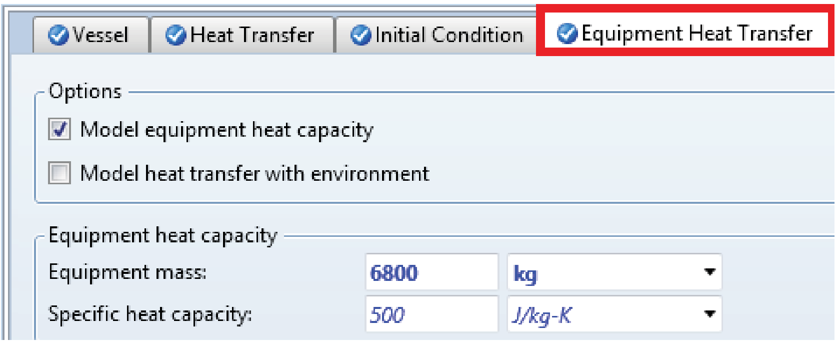
Figure 15.16 shows the "**Initial Condition**" tab window where the initial liquid volume fraction is set to 0.864. See Equation 15.15 for an explanation.



Liquid volume fraction: 0.864

Figure 15.16 The "**Initial Condition**" tab window where the initial liquid volume fraction is specified.

Figure 15.17 shows the "**Equipment Heat Transfer**" tab window where the equipment heat capacity will be modeled as stainless steel with the mass equal to $\mathrm{Area}_{\text{coiled jacket}} \times \mathrm{Thickness} \times \mathrm{Steel\ density} = 174.2 \times 0.005 \times 7800 \cong 6800\,\mathrm{kg}$. The steel heat capacity is about *500 J/(kg·K)*.



☑ Model equipment heat capacity

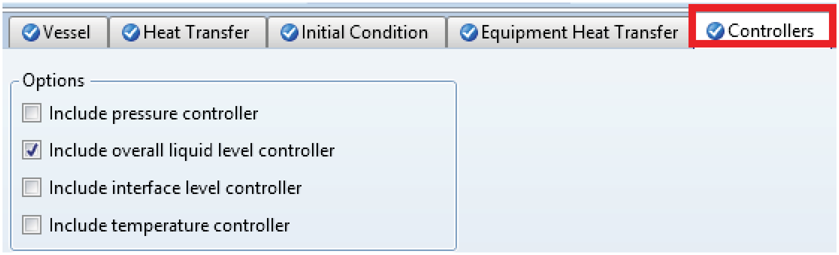
☐ Model heat transfer with environment

Equipment mass: 6800 kg

Specific heat capacity: 500 J/kg-K

Figure 15.17 Data for modeling of equipment heat transfer.

Figure 15.18 shows that an overall liquid level controller is selected in “**Controllers**” tab window.



Options

☐ Include pressure controller

☑ Include overall liquid level controller

☐ Include interface level controller

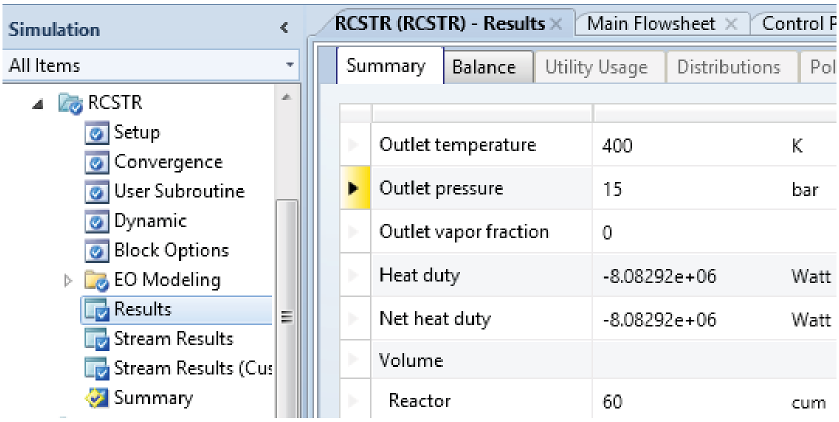
☐ Include temperature controller

Figure 15.18 Selection of an overall liquid level controller is done via “**Controllers**” tab window.

Finally, in “**Blocks**” | “**RCSTR**” | “**Convergence**” | “**Parameters**” tab window, change the default mass balance convergence solver from “*Broyden*” to “*Newton*”.

Reinitialize, rerun the show, and watch out for any error or serious warning. Figure 15.19 shows the results for “**RCSTR**” in terms of heat transfer requirement.

$$Q = UA\Delta T = 8.08292 \times 10^6 \mathrm{W} = UA \times \Delta T_{\mathrm{LM}} = UA \times 77.33\,\mathrm{K} \tag{15.10}$$



Outlet temperature	400	K
Outlet pressure	15	bar
Outlet vapor fraction	0	
Heat duty	-8.08292e+06	Watt
Net heat duty	-8.08292e+06	Watt
Volume		
Reactor	60	cum

Figure 15.19 The heat transfer requirement for “**RCSTR**”, which amounts to a heat removal of 8.08292 MW.

This means the value of UA must be 104,525 (W/K). If a typical value for the overall heat transfer coefficient, U, of 600 (W/(m^2·K)) is assumed [3], the area, required to transfer the 8.09288×10^6 W, will be 174.2 m^2. The jacket area is calculated as follows:

$$\text{Volume} = 60\,\mathrm{m}^3 = \pi\frac{D^2}{4}L = \pi\frac{D^2}{4} \times 10 \rightarrow D = 2.764\,\mathrm{m} \tag{15.11}$$

The maximum area that can be achieved assuming the reactor is full of process fluid:

$$\text{Area} = \pi DL = \pi \times 2.764 \times 10 = 86.83\,\mathrm{m}^2 \tag{15.12}$$

So, an additional area must be used. For example, the 174.2 m^2 surface area can be achieved using an external heat exchanger. Alternatively, an immersed coil inside CSTR itself can be installed, instead of an outside jacket. The total length of the coil is given by

$$\text{Lateral area} = 174.2\,\mathrm{m}^2 = \pi \times D_{\text{coil}} \times L_{\text{coil}} = \pi \times 0.1016\,\mathrm{m} \times L_{\text{coil}} \rightarrow L_{\text{coil}} = 545.8\,\mathrm{m} \tag{15.13}$$

The number of the coiled (i.e., helical) jacket loops can be given by

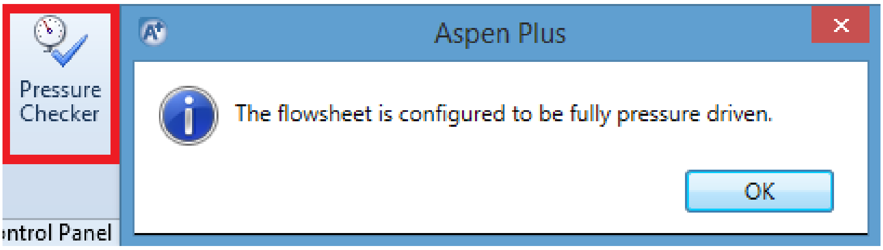
$$L_{\text{coil}} = N_{\text{loops}} \times \text{Length of a single loop} = N_{\text{loops}} \times \pi \times 0.95 \times D_{\text{tank}} \rightarrow N_{\text{loops}} \cong 66 \tag{15.14}$$

The factor 0.95 is used to leave a clearance between the reactor wall and the exterior surface of the coil. The vertical space allocated for the entire (multiloop) coil = $1.25 \times 0.1016 \times (66 + 2) = 8.64$ m, which means that the minimum height of reacting liquid medium has to be 8.64 m out of 10 m. The factor 1.25 is the clearance factor between one loop and another. Thus

$$\text{The liquid volume fraction} = 8.64/10 = 0.864 \tag{15.15}$$

NOTE #2: *If more heat transfer area is needed, then an external heat exchanger can be used. Alternatively, CSTRs in series (or in parallel) can be used, depending on the reaction order and kinetics, where each unit has its own cooling setup in terms of the cooling medium flow rate and temperature. Finally, a plug-flow multitubular reactor (PFR) can be used, instead of CSTR, for highly exothermic reactions. See HCW 15.3 for using PFR instead of CSTR.*

Click on the "**Pressure Checker**" button (see Figure 15.12), and if the plumbing has been correctly set up, the message shown in Figure 15.20 will appear.

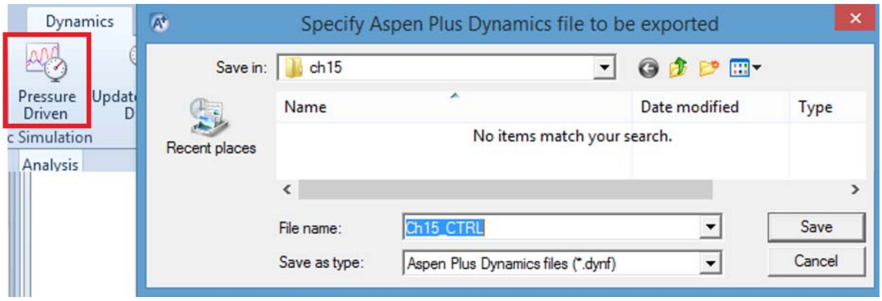


The flowsheet is configured to be fully pressure driven.

Figure 15.20 After the "**Pressure Checker**" button is clicked on and if the plumbing is correctly set up (i.e., process fluid flows downhill or down-hell), then the message assuring that the flowsheet is configured to be fully pressure driven will appear.

15.4.2 Creating Pressure-Driven Dynamic Files for APD

Click on “**Pressure Driven**” button found under “**Dynamics**” tab of the top toolbar. The window shown in Figure 15.21 will open up. Enter the file name to save the dynamic version of your project.



Save in: ch15

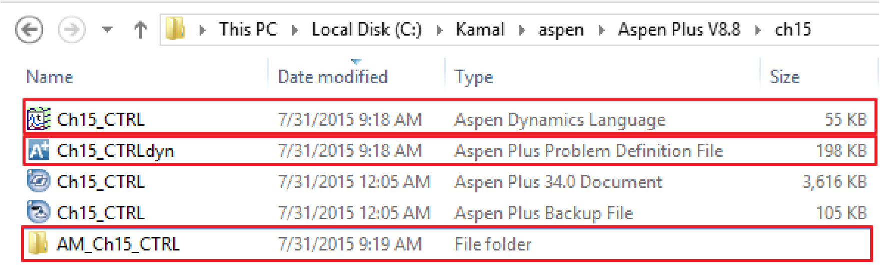
No items match your search.

File name: Ch15_CTRL

Save as type: Aspen Plus Dynamics files (*.dynf)

Figure 15.21 Saving the dynamic version of the flowsheet as: “**P Driven Dyn Simulation**”, with the file extension ***.dynf**.

As a result, two files and one folder are automatically created (Figure 15.22) and the Aspen Plus Dynamics simulator main window shows up (Figure 15.23). For example, if the filename is specified as “*Ch15_CTRL*”, then “*Ch15_CTRL.dynf*” file (The file “**Type**” is shown as “*Aspen Dynamic Language*” in Figure 15.22) will contain the details of the dynamic simulation including process units and controllers. On the other hand, “*Ch15_CTRLdyn.appdf*” file contains all the physical property information used by Aspen Plus Dynamics. On the other hand, the created folder will be used by APD to keep a record of user-customized settings, such as snapshots and screen layouts.



This PC ▸ Local Disk (C:) ▸ Kamal ▸ aspen ▸ Aspen Plus V8.8 ▸ ch15

Name	Date modified	Type	Size
Ch15_CTRL	7/31/2015 9:18 AM	Aspen Dynamics Language	55 KB
Ch15_CTRLdyn	7/31/2015 9:18 AM	Aspen Plus Problem Definition File	198 KB
Ch15_CTRL	7/31/2015 12:05 AM	Aspen Plus 34.0 Document	3,616 KB
Ch15_CTRL	7/31/2015 12:05 AM	Aspen Plus Backup File	105 KB
AM_Ch15_CTRL	7/31/2015 9:19 AM	File folder	

Figure 15.22 Creation of files needed to run the dynamic version by APD.

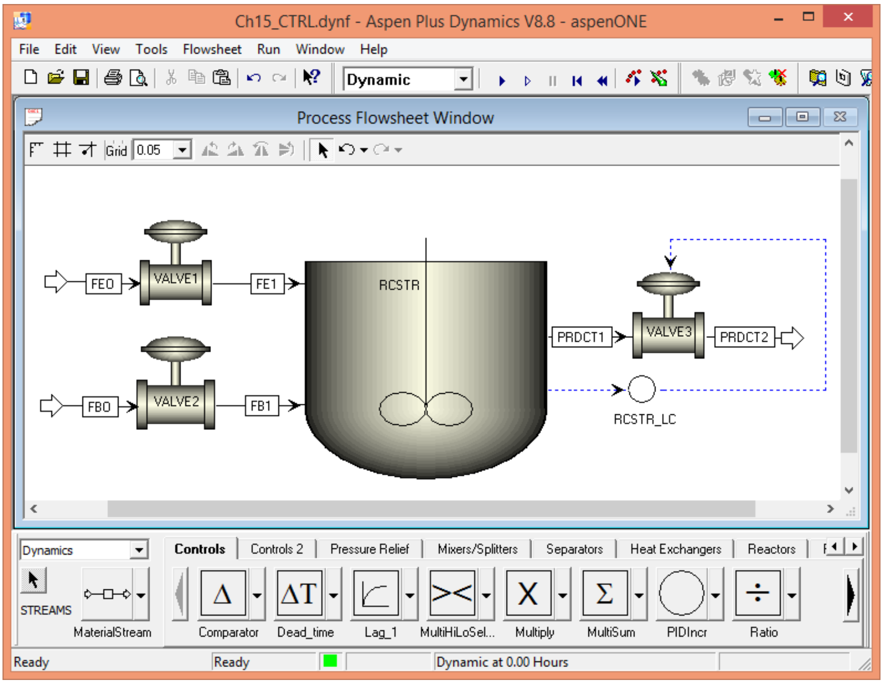


Figure 15.23 The main window of APD will pop up upon clicking on "**Pressure Driven**" button in "**Dynamics**" tab of Aspen Plus. The toolbar (top) and model libraries ribbon (bottom) are also shown.

Notice that in Figure 15.23, "**RCSTR_LC**" is an overall liquid level controller that is already instructed by the user as shown earlier in Figure 15.18. This level controller is imposed on the reactor to manipulate the product flow rate. The control loop is shown as a dotted line arrow issuing from the tank ("**RCSTR**"), passing by the level controller node, and terminating at the top of the third valve ("**VALVE3**"). Remember that the dotted line arrow can be displaced (i.e., moved up/down and right/left) in a way similar to a material stream (the solid line). So is the case with the location of the node itself in a way similar to any block. To do that, highlight the dotted line (or the node) and use the arrows keys and/or mouse to make any cosmetic change.

If for any reason you need to close the main window of APD, then see the next section to learn how to reopen a created dynamic file that pertains to the dynamic counterpart of the steady-state version of a process flowsheet.

Figure 15.23 shows that APD main window is titled as Ch15_CTRL.dynf, which means that such a file is already loaded into APD environment. This represents the "**Process Flowsheet**" window, which shows process components, such as CSTR, valves, connecting streams, and the control loop(s).

15.5 OPENING A DYNAMIC FILE USING APD

The APD can be opened via clicking on "**Microsoft Windows**" icon (bottom-left corner of the Windows 10/8.x desktop) and typing in the word "aspen" and Windows 8.x will provide you with Aspen-related applications. Select "**Aspen Plus Dynamics V8.8**" icon as shown in Figure 15.24.

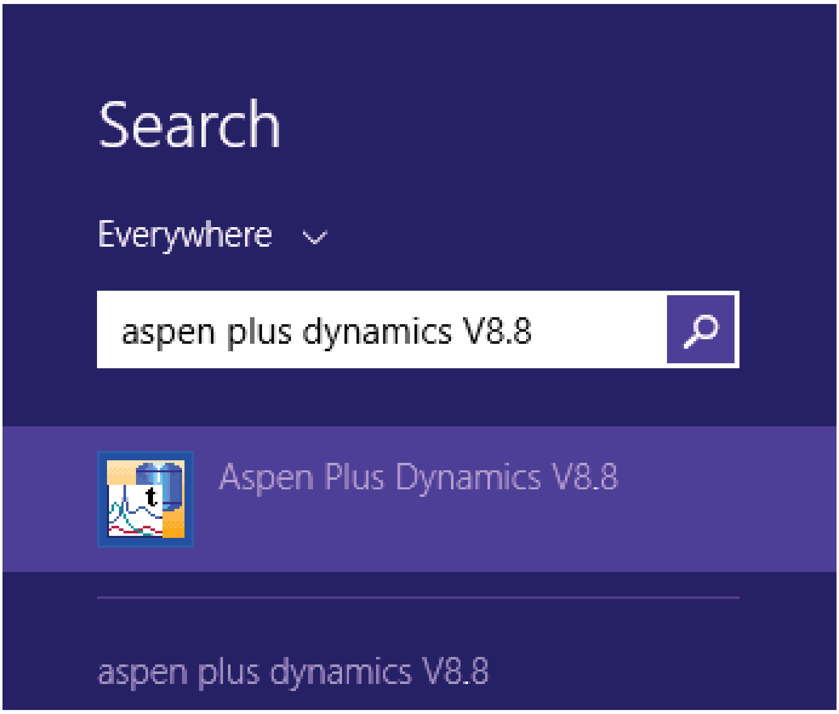


Figure 15.24 Selecting "**Aspen Plus Dynamics V8.8**" icon to open up the dynamic simulation file.

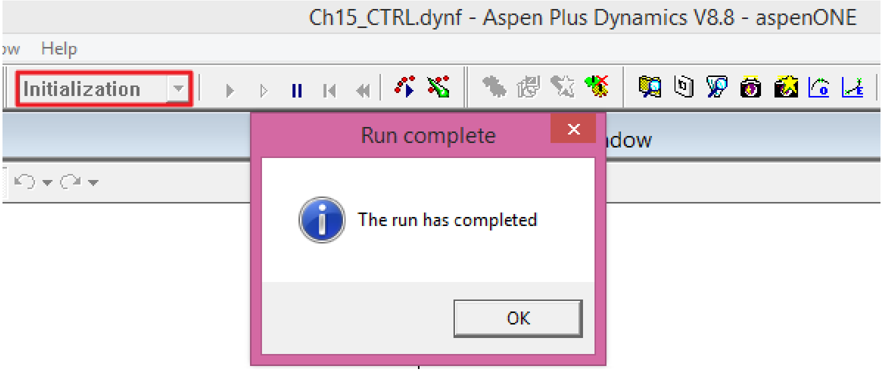
The main window of APD will show up and from its "**File**" menu, click on "**Open** … " button so that the "**Open**" dialog box will pop up, which then allows the user to select the *Aspen Plus Dynamic Language*-type of files (i.e., ***.dynf**). Locate the file that you have already created. In my case, it is found in "**C:\ProgramData\AspenTech\Aspen Plus V8.8\ch15**" folder. Select "*Ch15_CTRL.dynf*" and then click on "**Open**" button, the main window of APD, shown earlier in Figure 15.23, will pop up. The icons of toolbars and the objects of model libraries will be similar to those of Aspen Plus 8.x versions; however, their functions are to serve the dynamic aspects of a process. More features will be explored as we move on and off.

15.6 THE "SIMULATION MESSAGES" WINDOW

Before we add more control loops and carry out further analysis, let us start with the simple tasks. The "**Simulation Messages**" window can be invoked via clicking on "**View**" menu followed by "**Messages**" submenu. You can also close it and re-invoke another time using "**alt+F12**" key combination. It acts similar to "**Control Panel**" in Aspen Plus. The level of details for solver reporting can be tuned-up via right-clicking in **Simulation Messages** window and the shortcut context menu will pop up where you can adjust the level via selecting "**Solver Report Level**" submenu. You may clear the content of the "**Simulation Messages**" window as well.

15.7 THE RUNNING MODE: INITIALIZATION

The simplest task is to initialize the process, which means to assign values for some variables at time zero and reset the system to start. For example, the initial liquid volume fraction can be assigned, or it defaults to the supplied value borrowed from the steady-state solution. From the drop-down list found in the top toolbar, choose “*Initialization*” option as the “**Run Mode**” (instead of “*Dynamic*” option as shown in Figure 15.23, top middle) and run the simulator via clicking on the “**Run**” (▶) button. Figure 15.25 shows the pop-up informative window, telling the user that the initialization process is complete (i.e., successful).


Ch15_CTRL.dynf - Aspen Plus Dynamics V8.8 - aspenONE

Run complete

The run has completed

OK

Figure 15.25 Selecting “*Initialization*” option from the top toolbar drop-down list and running makes APD respond to the command via the pop-up informative window.

Let us try the second step, that is, “*Steady State*” option. So, select “*Steady State*” option from the drop-down list and click on the “**Run**” (▶) button. The pop-up informative window, similar to that shown in Figure 15.25, will tell you whether or not the steady-state solution is successful.

> **NOTE #3:** *The successful “Initialization” step is prerequisite for a successful “Dynamic” run. However, you may run the solver once under the “Steady State” mode for the first time to assure that everything is well done. Upon insertion of control loops, however, the “Steady State” may fail to converge, because the closed-loop dynamic response is not necessarily the same as that of the open-loop dynamic response. You may rewind to a previous successful “Initialization” step, if you wish, before you move to “Dynamic” run mode. Moreover, If you look at the “**Simulation Messages**” window while setting the “**Solver Report Level**” to at least “High”, you will notice that, for both “Initialization” and “Steady State” steps, Aspen Plus attempts to solve so many equations (sorted in different groups or sets by APD solver) where some of them are straightforward (i.e., explicit linear in terms of the variable or unknown term). On the other hand, other groups are not linear; hence, Newton’s method is invoked to solve such a set of implicit-type equations. The non-linear set may contain one or more non-linear equations that will be simultaneously solved.*

15.8 ADDING TEMPERATURE CONTROL (TC) UNIT

1. Referring to Figure 15.26, from "**Model Libraries**" ribbon, choose "**Controls**" tab and click on the "**PIDIncr**" item in the list, hold down the left mouse button, drag it to the flowsheet window, and release the mouse button. This drag and drop action will put a block called "**B1**" on the process flow diagram. Rename to "**TC**", temperature controller, as shown in Figure 15.26.

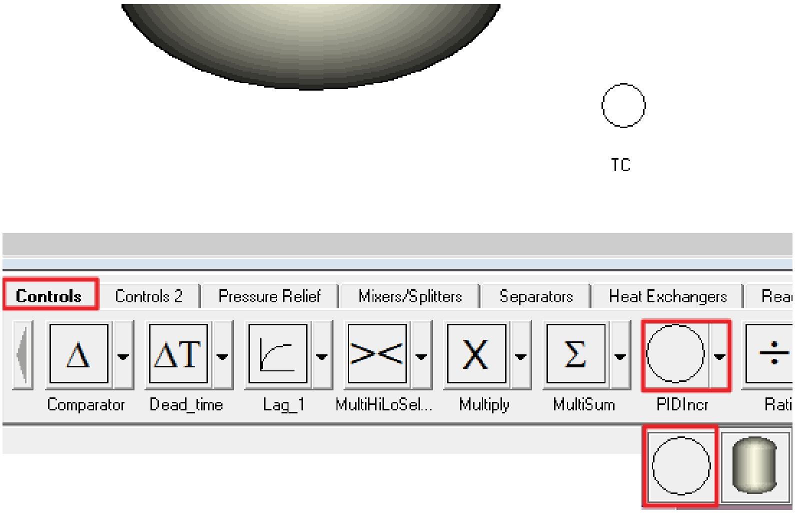
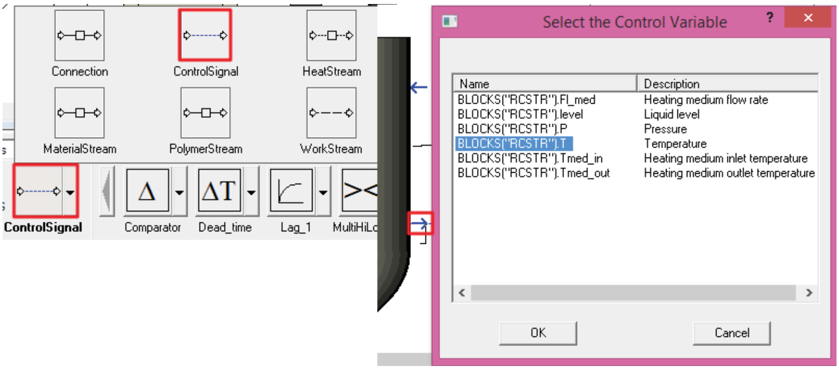


Figure 15.26 The procedure for installing a controller is to click on the "**PIDIncr**" icon under the "**Controls**" tab of the "**Model Libraries**" ribbon, hold down the left mouse button, drag it to the process flowsheet window, and release the mouse button. The default "**B1**" name was renamed to "**TC**" (i.e., temperature controller).

2. As seen in Figure 15.27 (*left*), from "**Model Libraries**" ribbon, click on "**Material Stream**" followed by "**ControlSignal**" icon from the list, and move your mouse to

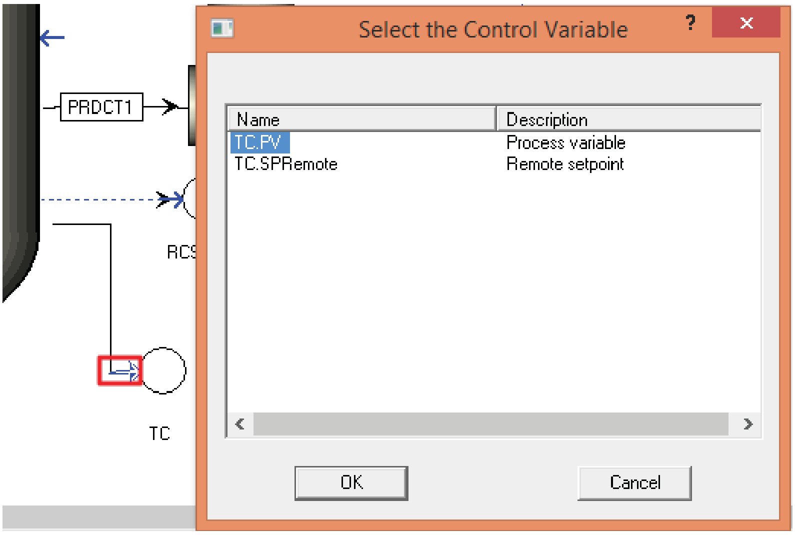


Name	Description
BLOCKS("RCSTR").Fl_med	Heating medium flow rate
BLOCKS("RCSTR").level	Liquid level
BLOCKS("RCSTR").P	Pressure
BLOCKS("RCSTR").T	Temperature
BLOCKS("RCSTR").Tmed_in	Heating medium inlet temperature
BLOCKS("RCSTR").Tmed_out	Heating medium outlet temperature

Figure 15.27 Selecting the "**ControlSignal**" icon (*left*) and placing the cursor on the arrow pointing out of the reactor (*right*), will open up a window that allows the user to select the block variable to be controlled. Here, the control signal will be hooked to the reactor temperature transmitter.

the flowsheet area where a number of arrows appear that indicate possible connections that can be made. Glide down on the arrow pointing out of the reactor and left-click the mouse over there. We want to control the temperature of the reactor, which is why we will place the cursor on the arrow pointing out of the reactor. The window shown in Figure 15.27 (*right*) will open up and indicate six possible choices. Clicking on "**BLOCKS("RCSTR").T**" choice will attach the control signal to the reactor temperature transmitter. Click on "**OK**" button to close the "**Select the Control Variable**" window.

3. Move the cursor to the arrow pointing into the temperature controller "**TC**" and click on the mouse. The window shown in Figure 15.28 will open up, from which we select "**TC.PV**" (the **P**rocess **V**ariable signal to this controller) option. Click on "**OK**" button to close the window. Keep in mind that you can displace (via mouse and arrows keys) the newly created dotted line arrow the way you like such that it does not interfere with any other material streams, blocks, or control loops.

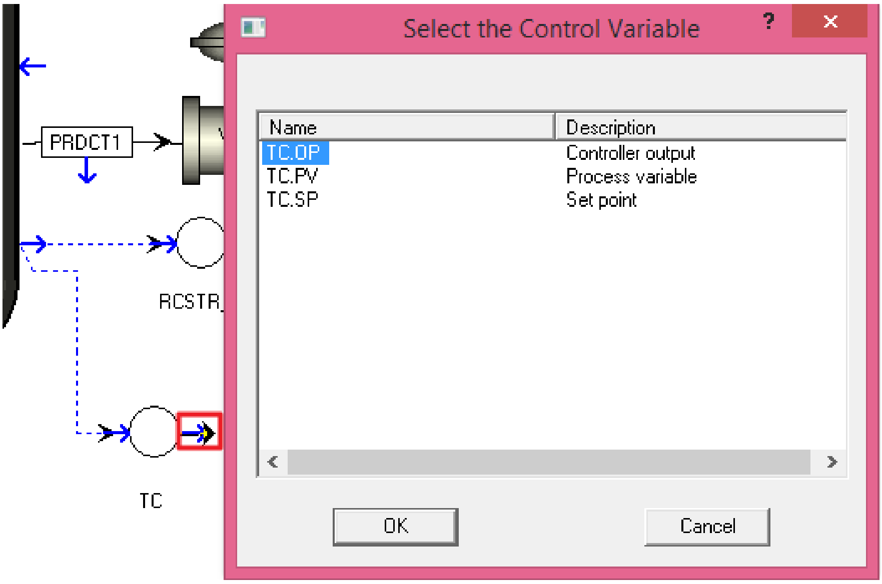


Name	Description
TC.PV	Process variable
TC.SPRemote	Remote setpoint

Figure 15.28 Moving the cursor to the arrow pointing into the temperature controller "**TC**" and clicking on the mouse will open up the window where the user will be able to pick up "**TC.PV**" as it represents the **P**rocess **V**ariable signal to "**TC**" controller.

4. In a similar fashion, from "**Model Libraries**" ribbon, click on "**MaterialStream**" and then on "**ControlSignal**" icon from the list, move your mouse to the arrow pointing out of the control node and left-click the mouse. Alternatively, you may hold down the left mouse button, drag it to the process flowsheet, but continue to hold down the mouse button, glide down on the arrow pointing out of the "**TC**" controller, and finally release the left mouse. Using either way will pop up a window as shown

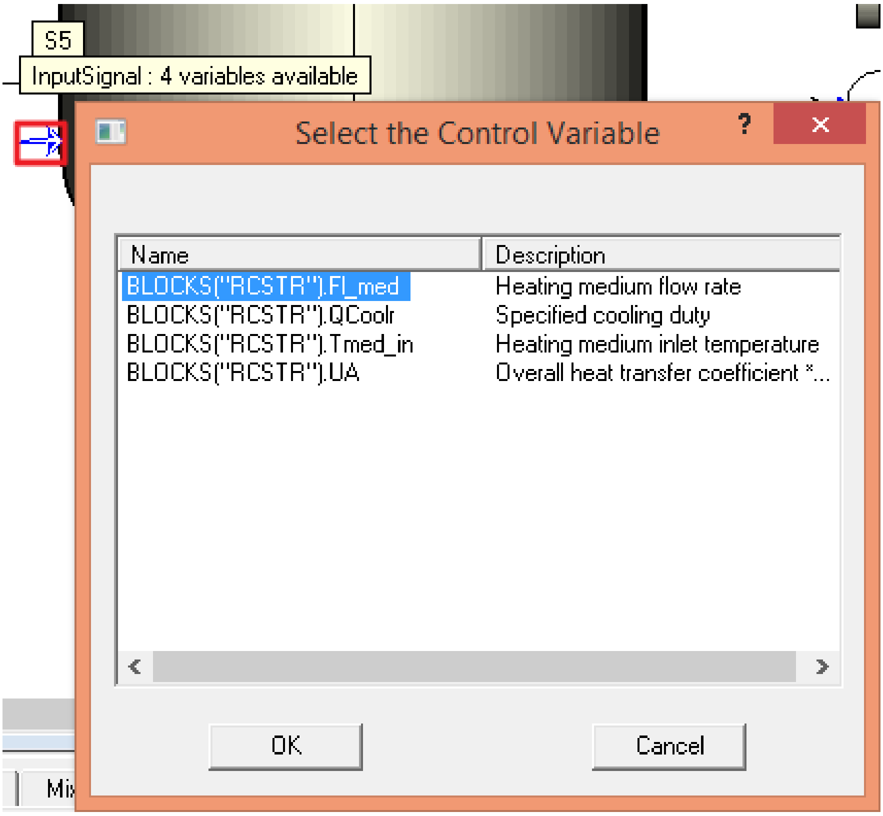
in Figure 15.29, where we select "**TC.OP**" (the **O**ut**P**ut signal from this controller) option. Click on "**OK**" button to close the window.



Name	Description
TC.OP	Controller output
TC.PV	Process variable
TC.SP	Set point

Figure 15.29 A control signal is added to the flowsheet and is hooked to the output of "**TC**" controller, which will open up the "**Select the Control Variable**" window, where the user will pick up "**TC.OP**" option as the controller output signal that will finally control the flow rate of the cooling medium as the latter represents the manipulated variable.

5. Move the cursor to the arrow pointing into reactor with a tooltip saying: "**InputSignal: 4 variables available**" and click/release the left mouse. The "**Select the Control Variable**" window will pop up, as shown in Figure 15.30, where you pick up the "**BLOCKS("RCSTR").Fl_med**" option, which symbolizes the manipulated or controlled variable. Click on "**OK**" button to close the window.



Name	Description
BLOCKS("RCSTR").Fl_med	Heating medium flow rate
BLOCKS("RCSTR").QCoolr	Specified cooling duty
BLOCKS("RCSTR").Tmed_in	Heating medium inlet temperature
BLOCKS("RCSTR").UA	Overall heat transfer coefficient *...

Figure 15.30 The "**ControlSignal**" stream type is hooked to the inlet of the cooling/heating medium stream, where "**BLOCKS("RCSTR").Fl_med**" option is selected from the list of possible controlled variables.

6. Finally, double-click on "**TC**" node to open its associated faceplate, click on "**Configure**" button (third yellow button from top right of the faceplate) to open "**TC.Configure**" | "**Tuning**" tab form. Click on "**Initialize Values**" button at the bottom of the last form to reset the temperature controller signal values to their initial values borrowed from the steady-state Aspen Plus simulator.

NOTE #4: *The "TC" node can be flipped right/left in a way to suit the user's needs. You may carry out some cosmetic changes by displacing or relocating the control loops; you can highlight the control loop icon, right-click the mouse, and select one out of many options, such as rotate left, rotate right, flip right/left, and flip up/down. In addition, you may displace the start or end of the control signal (i.e., dashed line) the way it is dealt with a material stream (i.e., solid line) (see Section 2.6).*

The process flowsheet, with the installed two controllers, is shown in Figure 15.31.

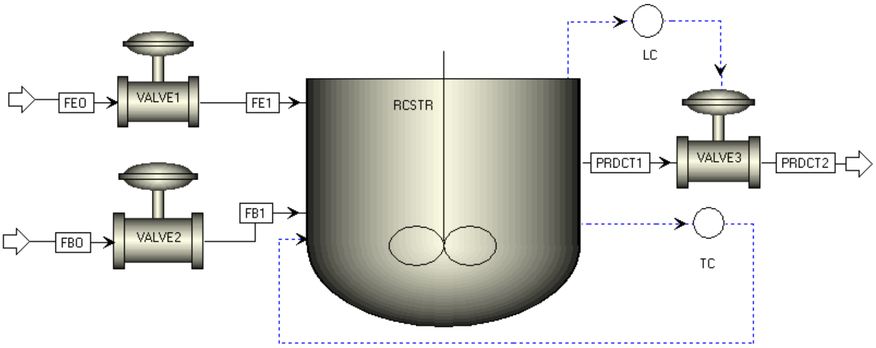


Figure 15.31 Both the closed-loop level control ("**LC**") unit and the closed-loop temperature control ("**TC**") unit are now installed on the process.

15.9 SNAPSHOTS MANAGEMENT FOR CAPTURED SUCCESSFUL OLD RUNS

At this stage, with the two controllers in place, let us check whether what we have done so far dynamically makes sense, at least, for APD. Carry out the first step: "*Initialization*". If the run is successful, then you will be informed by APD that the run has completed. Nevertheless, at this stage, if we attempt to run the solver under "*Steady State*" mode, the system will fail to converge to a solution (see **NOTE #3**). At this stage, click on "**Take Snapshot**" button (📷) found at the top toolbar, or use "**alt+F7**" key combination, where "**Enter snapshot description**" window will pop up asking you to enter a name for the snapshot to be taken for the current state of the dynamic flowsheet. All parameters and specifications will be saved to this captured snapshot and you can rewind your dynamic flowsheet to the saved captured state. This will save you a lot of headache in case things do not work fine (i.e., APD starts telling you that there are errors somewhere when you attempt to run it under "*Dynamic*" mode). The saved or captured snapshot will appear in "**Snapshot Management**" window (discussed later) and you can highlight it and rewind to this state any time should you get stuck later.

Let us switch the "**Run Mode**" to "*Dynamic*". Click on **Run** (▶) button on the top toolbar. You should be able to see the dynamic time counter at the right bottom of the main window expressing the dynamic time in the proper unit of time. You may pause the dynamics at a certain time using the **Pause** (⏸) button. You can also restart the run using the **Restart** (⏮) button. If things go wrong (i.e., the "*Dynamic*" mode no longer functions well) for any reason due to the insertion of improper input parameters for the unit, stream, or for any control loop object, then to save your neck, you may use the **Rewind** (⏪) button. This will give you the chance to revert to one of old successful captured states. This is a very useful feature that allows the user to mingle with and tweak APD settings so as to explore its hidden features without having to suffer a lot.

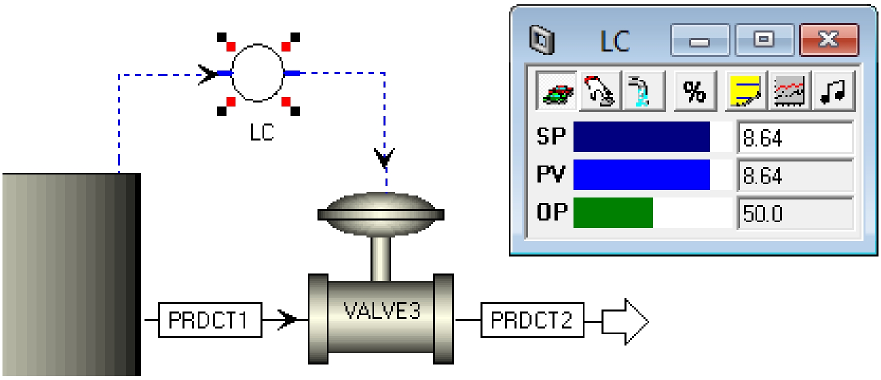
Furthermore, you may open "**Snapshot Management**" window using "**Snapshots**" (📷) button found at the top toolbar. Alternatively, you may go to "**Tools**"|"**Snapshots …** " (Shortcut key: "**alt+F3**") and open the "**Snapshot Management**" window. This will give you the chance to look at and manage old successful captured (i.e., snapshot) states. For example, you may highlight one old successful captured state and export it to a file so that you may import it later into the "**Snapshot Management**" window. If an old successful "*Initialization*" run is highlighted you may copy values from using "**Copy Values**" button. Moreover, if an old successful "**Rewind**" run is highlighted you may either rewind using "**Rewind**" button, or copy values from using "**Copy Values**" button, subject to whether the highlighted event is active (recent) or inactive (old).

NOTE #5: *It is recommended that after you open a dynamic file into APD, immediately run the "Initialization" step, assure that it successfully completes, go to "**Snapshots Management**" window, and then save such a step to a snapshot (***.asnp**) file. You may then import such a file into "**Snapshots Management**" window once you need it later. Of course, this will give you the chance to revert to the original values if you later mess up with any parameter or setting value and end up with a fail "Initialization" step.*

In the worst scenario, if there is a nagging problem that prevents running the simulation under "*Dynamic*" mode, you will have to go back to Aspen Plus Version 8.x and reexport the file to APD environment. Do not forget to watch out Aspen Plus "**Control Panel**" warning/error if any and later the APD "**Simulation Messages**" window to diagnose the source of error for the pressure-driven flow process.

15.10 THE CONTROLLER FACEPLATE

Let us dig deeper in the world of control. So far, we have prepared the stage for control testing and analysis. Double-clicking on "**LC**" controller icon will open up a controller faceplate, as shown in Figure 15.32. The controller faceplate is where all the features of the controller can be examined and adjusted. There are *seven buttons* at the top of the faceplate. The *first three buttons* at the top level enable you to switch between auto (the two car icon), manual (the hand icon), and cascade (the water fountain icon) mode, respectively. When APD is in auto mode (as shown in Figure 15.32), the value for "**SP**" has a white background (as opposed to off-white), which means you can



SP 8.64

PV 8.64

OP 50.0

Figure 15.32 The controller faceplate where the set point ("**SP**"), process variable ("**PV**"), and controller output ("**OP**") signals are displayed at the bottom left part as three horizontal bars, with numerical values given in the boxes. *See Plate section for color representation of this figure.*

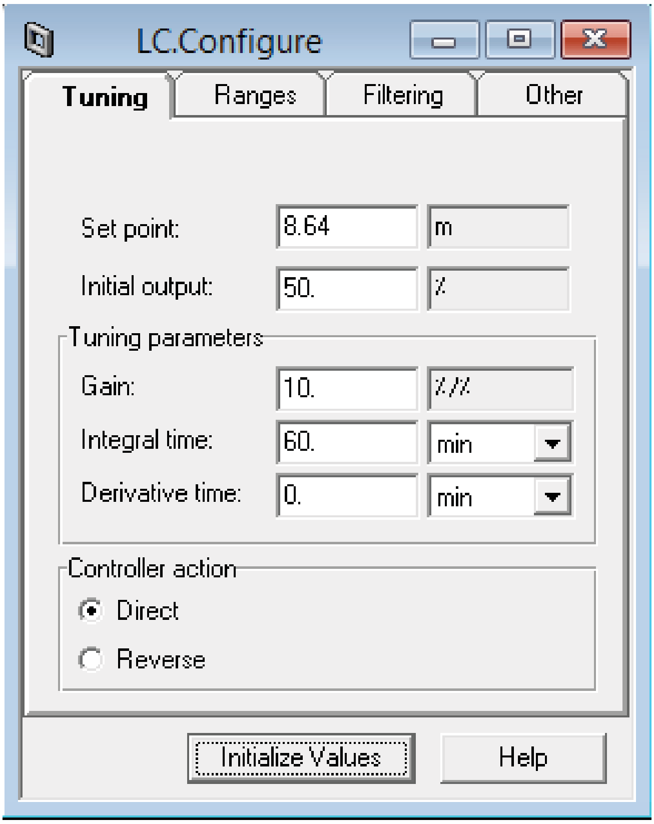
type a new value. On the other hand, when it is in manual mode, the value for "**OP**" will have a white background, which means you can change the value.

The *fourth button* enables us to switch between viewing values in process units or percentages of range. The last three buttons will be explained shortly.

Notice that the value *8.64* has units of *m*, which represents the set point ("**SP**") of liquid level inside the reactor and so does the "**PV**" value. This represents the initial liquid level, which corresponds to a liquid volume fraction of 0.864 (see Eq. 15.15). "**OP**" has a value of 50% of the range, which means that "**OP**" value is set at the middle-point between the minimum and maximum value, expressed in mV/mA for an electronic signal, or in units of pressure for a pneumatic signal.

NOTE #6: *To see the process units, you can hold the mouse pointer over the label "OP", "PV", or "SP". To switch the display of "OP", "PV", or "SP" between process units and percent, right-click on the label and select the required options from the pop-up menu.*

The *fifth (the yellow button in Figure* 15.32*) button from left* is the "**Configure**" button. Clicking on this button will open the "**Configure**" form so that you can easily change configuration parameters, as shown in Figure 15.33. The "**Tuning**" tab window shows the



Set point: 8.64 m

Initial output: 50. %

Tuning parameters

Gain: 10. %/%

Integral time: 60. min

Derivative time: 0. min

Controller action

● Direct

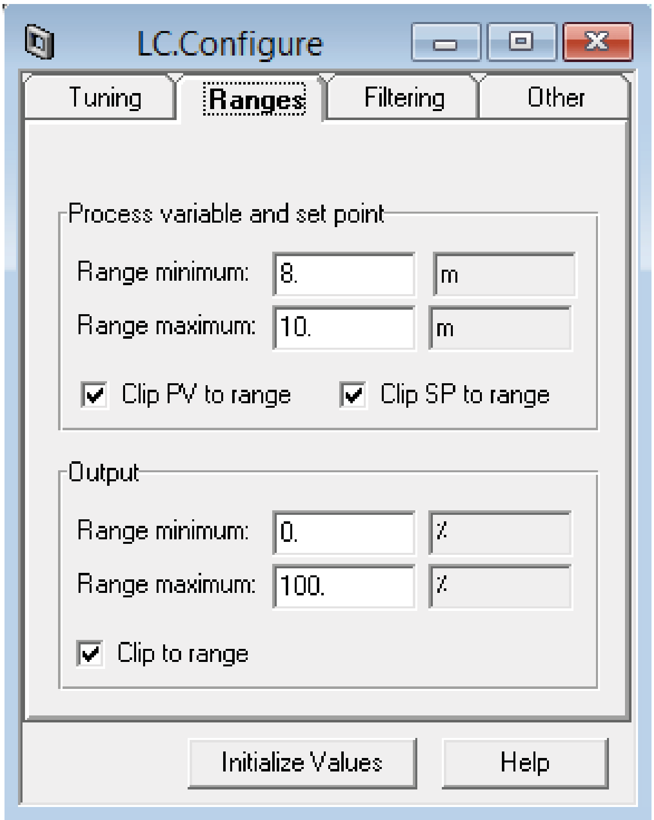
○ Reverse

Figure 15.33 The "**LC.Configure**" window with four tabs. The "**Tuning**" tab window shows the default values for "**SP**" and "**OP**", in addition to controller parameters and action.

default values. Here, we have a proportional-integral (“*PI*”) type of a controller with the derivative time set to zero and the control action is direct (i.e., the higher the measured level signal, the higher will be the output signal), which will increase the opening area of the valve to increase the product flow rate so as to offset the increase in liquid level inside the reactor. Notice that APD has already assumed that the liquid-level controller is of PI type and it has already shown the estimated parameters of the gain, integral time, and derivative time (i.e., zero τ_D for PI type). You may, however, change such values if you carry out your own analysis as will be explained later in controller tune-up test sections.

If you perturb either the set point or the initial output value and click on the “**Initialize Values**” button at the bottom of the form, the “**OP**”, “**PV**”, and “**SP**” signals will revert to their initial values. Moreover, the level controller, which manipulates the outflow from the vessel, is usually of proportional-only type. This can be done by setting the integral time (τ_I) to a very large value, say *1,000,000* min.

Clicking on the “**Ranges**” tab will open up the window shown in Figure 15.34. APD inserts default values for the range of the “**PV**” and “**OP**” signal. You may, however, change the level range to a more realistic range. In this case, a range from 8 to 10 m is selected for the “**PV**” signal (liquid level).



Process variable and set point

Range minimum: 8. m

Range maximum: 10. m

☑ Clip PV to range ☑ Clip SP to range

Output

Range minimum: 0. %

Range maximum: 100. %

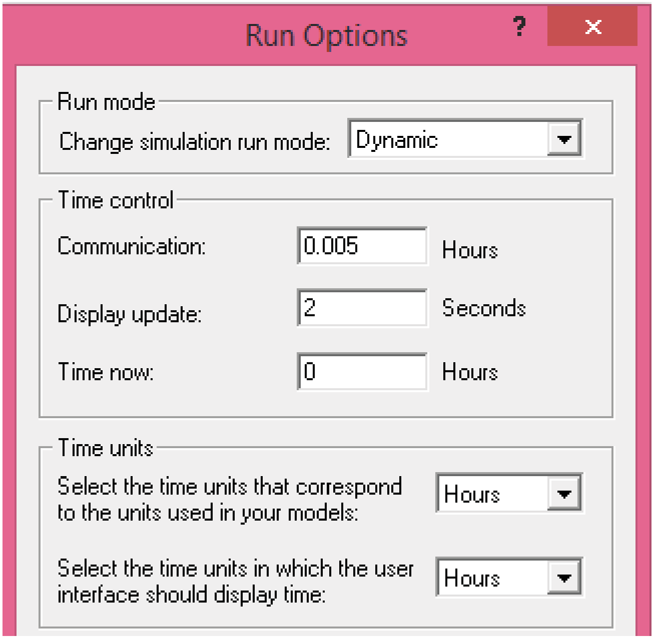
☑ Clip to range

Figure 15.34 The “**Ranges**” tab window where the user may set the range for both “**PV**” and “**SP**” signal.

For the “**Filtering**” tab window, it is ok to stick to the default assigned values. Finally, for the “**Other**” tab window, the user has the choice to pick up the type of controller algorithm. For example, the “*Ideal*” type is the classical form normally found in process control textbooks; “*Series*” is the interacting or analog algorithm; “*Parallel*” is the ideal parallel or non-interacting algorithm; and the last three are commercial brands of companies well-known in control systems, namely “*Foxboro*”, “*Honeywell*”, and “*Yokogawa*”. The “*Ideal*” type is selected for simplicity.

15.11 COMMUNICATION TIME FOR UPDATING/PRESENTING RESULTS

Let us change the “**Communication**” time, which is the sampling period for sending information to the strip-chart recorder. The default value (0.01 h, 36 s) is a bit long to get a high-resolution plot, so it is better to change to 0.005 h (18 s) by clicking on “**Run**” menu in the top toolbar and selecting “**Run Options** … ” submenu. The window shown in Figure 15.35 opens, whereby the “**Communication**” value is set to *0.005 h*.



Change simulation run mode: Dynamic

Communication: 0.005 Hours

Display update: 2 Seconds

Time now: 0 Hours

Select the time units that correspond to the units used in your models: Hours

Select the time units in which the user interface should display time: Hours

Figure 15.35 “**Run**” | “**Run Options**” window where the user may change the “**Communication**” time between control unit and the strip-chart recorder.

15.12 THE CLOSED-LOOP AUTO-TUNE VARIATION (ATV) TEST VERSUS OPEN-LOOP TUNE-UP TEST

The *sixth button* is called “**Plot**” button that is used for presenting some selected variables, such as “**OP**”, “**PV**”, and “**SP**” as a function of dynamic time. More on this button will be discussed shortly.

The *seventh and last button* is called "**Tune**" button that is used to tune-up controller parameters, using either a closed-loop or open-loop dynamic test.

The "**Tune**" tab form provides access to automatic tuning capabilities, which you can use to determine suitable values for the controller tuning parameters. This technique is useful when designing control systems for new processes or improving those for existing processes. To obtain good results that can be transferred to a real control system, it is important that you accurately model the loop dynamics. This means modeling the sensor and actuator dynamics if they have a significant effect on the overall loop dynamics.

The controller is tuned for handling both a set-point and load disturbance using the auto-tuner. The auto-tuner test identifies the process between the "**OP**" and the "**PV**" (estimates the gain, dead time, and time constant for the open-loop test, or the ultimate gain and ultimate period for the closed-loop ATV test).

These values are then used to calculate the tuning parameters for the controllers using tuning rules (i.e., Ziegler–Nichols, Cohen–Coon, and so on, for the open-loop test, and Ziegler–Nichols or Tyreus–Luyben for the closed-loop ATV test). The Ziegler–Nichols closed-loop technique is one of the most popular methods for tuning controllers. This technique gives approximate values of the controller's gain, integral time, and derivative time required to obtain a one-quarter amplitude response.

For a closed-loop ATV test, the controller operates as a relay controller to create a limit cycle in the "**PV**". For a direct acting controller, when the "**PV**" is greater than the set point ("**SP**"), the controller moves the output to the initial output plus the relay amplitude that you specify. When the "**PV**" is less than the set point ("**SP**"), the controller moves the output to the initial value minus the amplitude. Vice versa will be the case for the controller action if it is reverse. It is important that you select the correct controller action before running this test. The size and period of the limit cycle in the "**PV**" is used to determine the ultimate gain and ultimate period of the process.

For an open-loop test, the controller is set to manual and the output is stepped. You can specify whether the step is up or down, and the size of the step as a percentage of output range. This approach assumes that the process can be approximated by a first-order lag plus dead time. The response of the "**PV**" is used to estimate an open-loop gain, time constant, and dead time for the process.

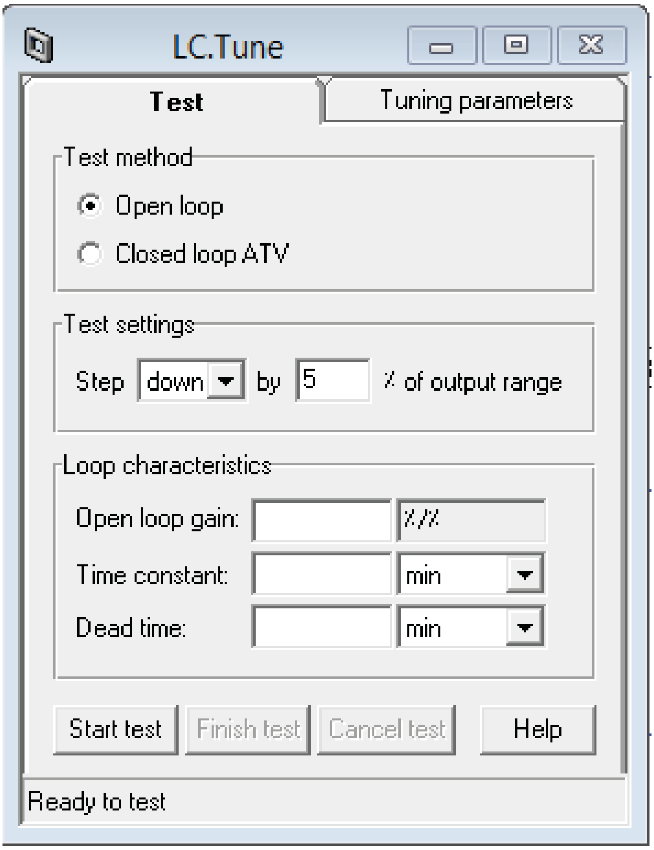
NOTE #7:

- *It is particularly important to model dead times in the control loop. The dead time will be introduced in "**TC**" controller tune-up. The closed-loop ATV test method is only effective if you have some dead time in the control loop. If the loop dead time is not accounted for, then you should use the open-loop test method.*
- *The dead time is the sum of transportation lag (i.e., the time it takes for a material to travel from one point to another), sample or instrument lag (i.e., the time it takes to collect, analyze, or process a measured PV sample), and the lag due to the sluggish behavior of higher-order processes.*
- *The Ziegler–Nichols closed-loop method is suitable for many single-loop controllers. For processes that contain interacting loops, open-loop tuning methods are preferred. For more information on open-loop tuning, refer to a text book on controller tuning.*
- *You can try different step directions and sizes to see how such causes of disturbance affect the results. The more non-linear the process, the greater the differences will be.*

15.13 THE OPEN-LOOP (MANUAL MODE) TUNE-UP FOR LIQUID LEVEL CONTROLLER

The following steps serve as a general guide for the open-loop tune-up procedure:

1. Double-click on “**LC**” node, which will open its controller faceplate (see Figure 15.32).
2. Make sure that the “**Manual**” (the hand icon) button is clicked on but not the “**Auto**” (the two car icon) button.
3. On the same faceplate, click on “**Tune**” (♫) button (first button from right top) and “**LC.Tune**” window will show up as shown in Figure 15.36. Since we did not account for the loop dead time for **LC** unit, we will use the open-loop test method (see **NOTE #7**). Click on the “**Open loop**” bullet. The default step down value is 5% of the output range. You can change it if you wish, depending on the expected variation in cause of disturbance for the level. If L range is 1 m then 5% will be 0.05 m (or 5 cm). Let us keep the default value.



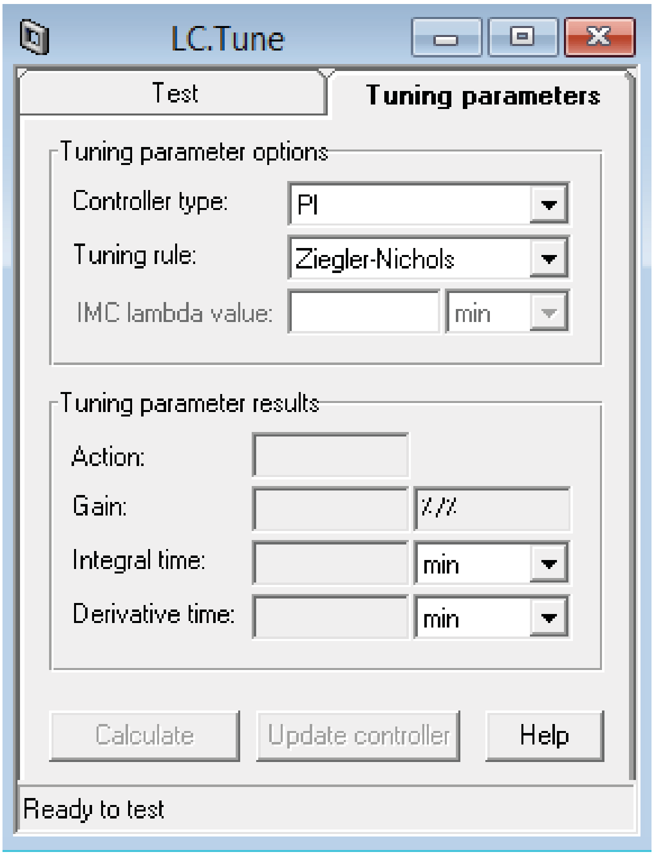
Test method: ● Open loop ○ Closed loop ATV

Step down by 5 % of output range

Ready to test

Figure 15.36 “**LC.Tune**” | “**Test**” tab window for selecting the “**Test method**” and for stepping up/down the output (“**OP**”) value.

4. Click on "**Tuning parameters**" tab window to select the type of controller as shown in Figure 15.37. As mentioned earlier, a proportional-only controller is usually used for liquid level control; however, for the sake of learning the tune-up procedure, we will use "*PI*" controller type and the tuning rule is "*Ziegler–Nichols*". Notice that both "**Calculate**" and "**Update controller**" button are currently disabled; they will become active upon finishing the test so that you can calculate the gain and integral time for "*PI*" controller and also update the controller itself (i.e., change its settings to the newly calculated values).



Tuning parameter options

Controller type: PI

Tuning rule: Ziegler-Nichols

IMC lambda value: min

Tuning parameter results

Action:

Gain: %/%

Integral time: min

Derivative time: min

Ready to test

Figure 15.37 The "**LC.Tune**" | "**Tuning parameters**" tab window for selecting the "**Controller type**" and the "**Tuning rule**" option.

5. Open "**LC.ResultsPlot**" plot, as shown in Figure 15.38, by clicking on the "**Plot**" (second button from right top) button, in order to monitor liquid level profile. It is preferred that you also open "**LC.Configure**" window, shown in Figure 15.33, just to assure that the control action is in direct mode and also watch the latest controller tuning parameters.

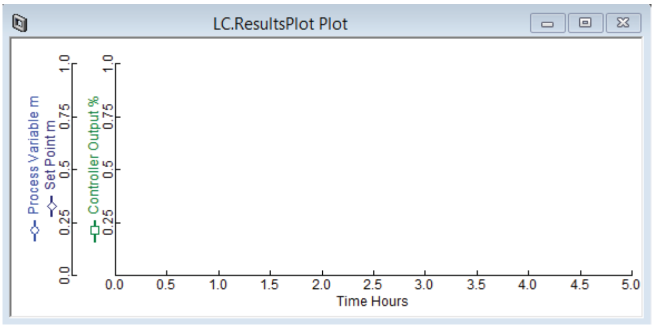


Figure 15.38 The "**LC.ResultsPlot**" plot, used for plotting "**OP**", "**PV**", and "**SP**" as a function of dynamic time.

6. Start APD under "*Initialization*" mode. Assure that the run is complete via the confirming message telling the user that the run has completed. Running the "*Steady State*" mode is not required for "*Dynamic*" mode.

7. Switch to "*Dynamic*" mode and start APD by clicking on the run (▶) button. Let it run for a sufficient time just to assure that everything is perfectly running (i.e., the controller "**OP**" and "**PV**" values are stable), which can be monitored via the "**LC.ResultsPlot**" plot. Then, click on the "**Start test**" button (see Figure 15.36) to start the test.

8. Continue the test. For an open-loop tune-up test, press the "**Finish test**" button (see Figure 15.36) when the "**PV**" stops changing significantly. On the other hand, for a closed-loop ATV test, it is finished when each cycle looks the same as the previous one. Figure 15.39 shows the plot window for "**OP**", "**PV**", and "**SP**" as a function

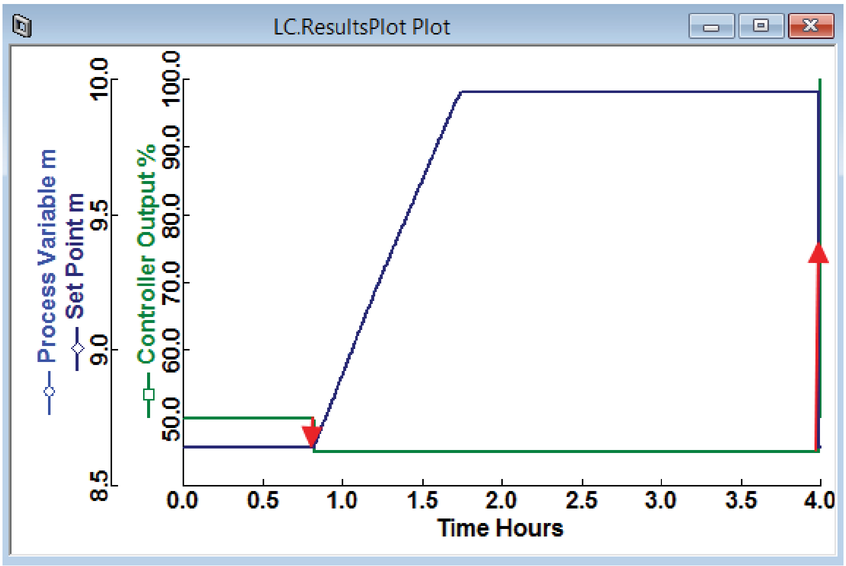
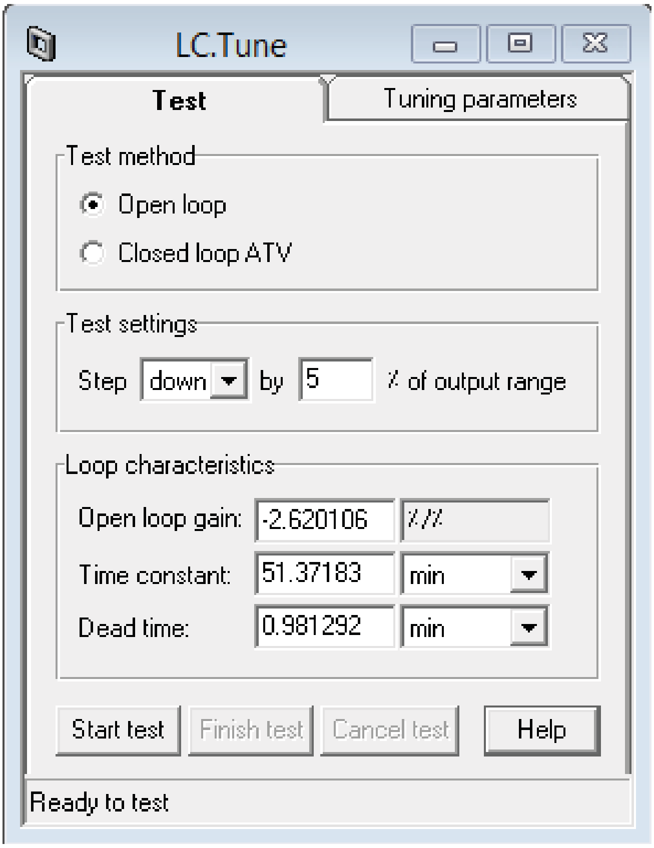


Figure 15.39 The plot of the three variables for the step-down open-loop test: "**OP**", "**PV**", and "**SP**" as a function of time while showing the start-up (the down arrow) and termination (the up arrow) of the tune-up test period.

of time. Notice that the down arrow indicates when we started the tune-up test and the up arrow when we finished the test. Both events occurred after achieving a stable "**OP**" and "**PV**" value with time.

9. Figure 15.40 shows the estimated control loop characteristics in terms of the gain, time constant, and dead time, carried out under the open-loop test.



Test method

● Open loop

○ Closed loop ATV

Test settings

Step down by 5 % of output range

Loop characteristics

Open loop gain: -2.620106 %/%

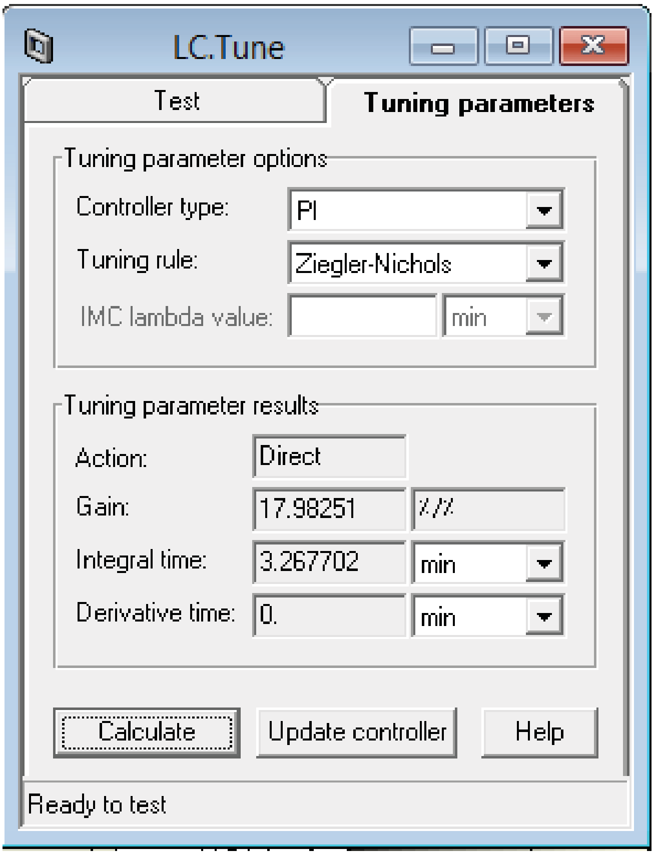
Time constant: 51.37183 min

Dead time: 0.981292 min

Ready to test

Figure 15.40 The estimated control loop characteristics in terms of the gain, time constant, and dead time.

10. Figure 15.41 shows both the gain constant (K_C) and the integral time (τ_I) for "*PI*" controller after clicking on the "**Calculate**" button at the bottom of the "**Tuning parameters**" window of "**LC.Tune**" form. Of course, τ_D is zero for a PI controller.



Controller type: PI

Tuning rule: Ziegler-Nichols

IMC lambda value: min

Action: Direct

Gain: 17.98251 %/%

Integral time: 3.267702 min

Derivative time: 0. min

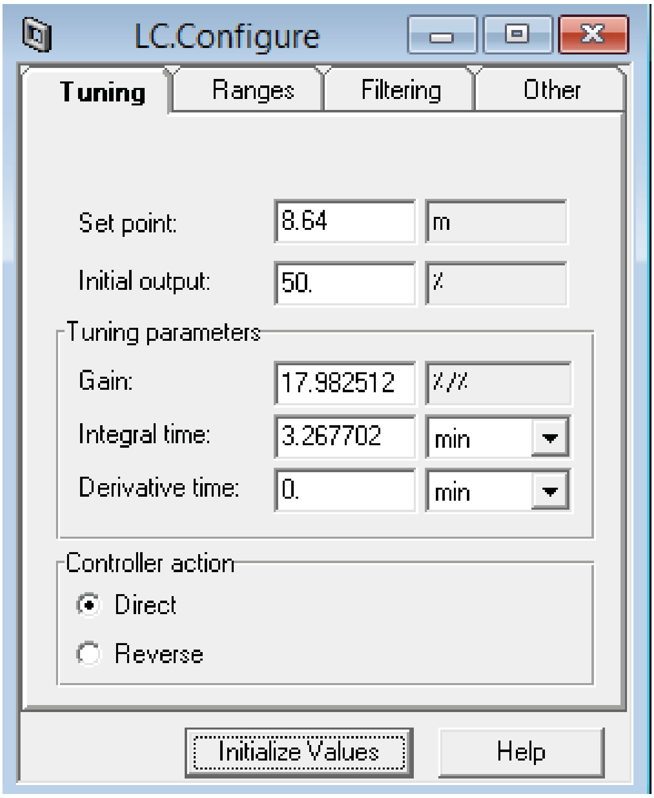
Ready to test

Figure 15.41 The tuning parameter results for a "*PI*" controller after finishing the open-loop tune-up test and clicking on the "**Calculate**" button.

11. After restarting the simulation using (⏮) button, you may now click on "**Update controller**" button so that the new settings take effect. You can carry out both a set point and load disturbance test on the process and see how the closed-loop dynamic response will be with the new settings. Figure 15.42 shows that after restarting the simulation and clicking on the "**Update controller**" button, the new "*PI*" controller settings are now taking into effect.

On the other hand, if the open-loop test is selected with "*Step up by 5%*", instead of "*Step down by 5%*" of the output range, as shown earlier in Figure 15.36, the open-loop dynamic response of the process on the right side (step up) is not necessarily the same as that on the left side (step down) of the initial output. Figure 15.43 shows the dynamic response of three signals "**OP**", "**PV**", and "**SP**".

See Section 15.20 for further information.



Set point: 8.64 m

Initial output: 50. %

Tuning parameters

Gain: 17.982512 %/%

Integral time: 3.267702 min

Derivative time: 0. min

Controller action

● Direct

○ Reverse

Figure 15.42 The newly estimated "*PI*" controller parameters as a result of the open-loop tune-up test.

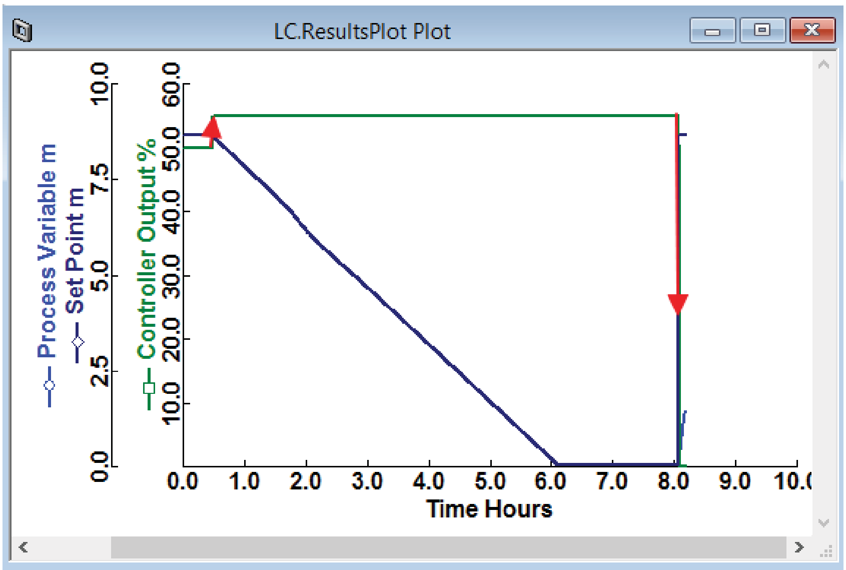
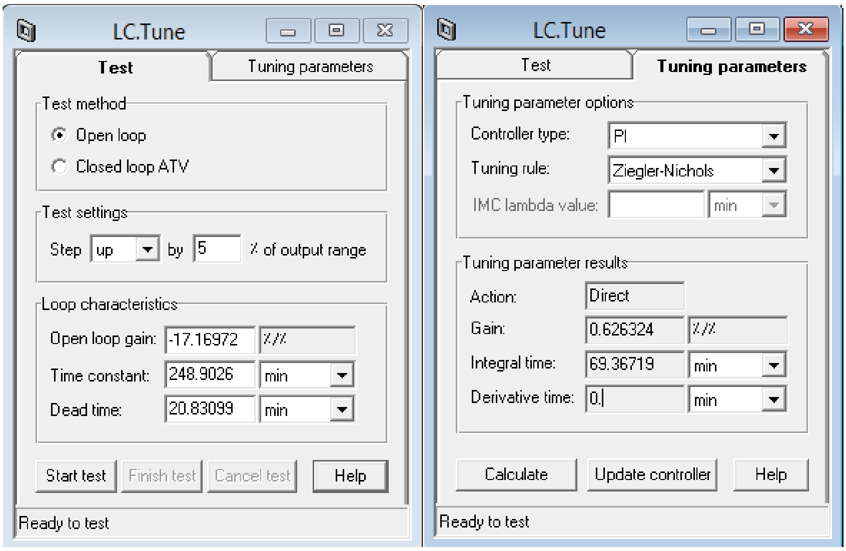


Figure 15.43 The plot of the three variables for the step-up open-loop test: "**OP**", "**PV**", and "**SP**" as a function of time while showing the start-up (the up arrow) and termination (the down arrow) of the tune-up test period.

Figure 15.44 shows the Ziegler–Nichols tuning rule-based “*PI*” estimated controller parameters for the step-up open-loop test. Notice that the estimated parameters are different from those of step-down open-loop test.



Test method
● Open loop
○ Closed loop ATV

Test settings
Step up by 5 % of output range

Loop characteristics
Open loop gain: -17.16972 %/%
Time constant: 248.9026 min
Dead time: 20.83099 min

Ready to test

Tuning parameter options
Controller type: PI
Tuning rule: Ziegler-Nichols
IMC lambda value: min

Tuning parameter results
Action: Direct
Gain: 0.626324 %/%
Integral time: 69.36719 min
Derivative time: 0. min

Ready to test

Figure 15.44 The Ziegler–Nichols tuning rule-based “*PI*” estimated controller parameters for the step-up open-loop test.

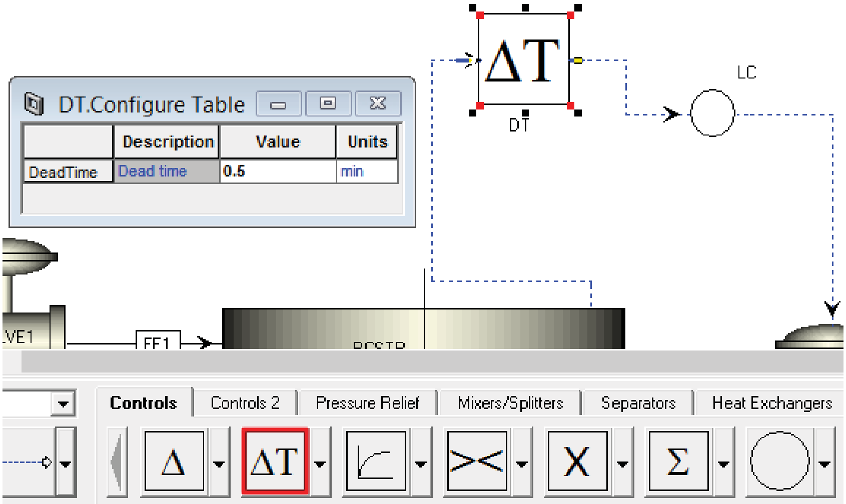
NOTE #8:

1. *To have a better description of the process dynamics, it is recommended that the tune-up test is repeated many times for different step up/down magnitudes and consider only the cases where stable “**OP**”, “**PV**”, and “**SP**” values are obtained. Taking the average value for gain, time constant, and dead time is expected to give a better resolution about the dynamics of the process.*
2. *After restarting (* ⏮ *) the simulation and clicking on the* “**Update controller**” *button, the controller parameters (i.e., the new settings) become effective unless you rewind to a different old successful captured state. You may save, however, the new settings via taking a snapshot to the current values and rewind to it later upon your request. Alternatively, you may manually edit the controller settings using* “**Tuning**” *tab window found in* “**LC.Configure**” *form.*
3. *The open-loop test assumes that the process can be approximated by a first-order lag plus dead time. The response of the* “**PV**” *is used to estimate an open-loop gain, time constant, and dead time for a given process. Thus, the* open-loop test *is useful for approximating unknown complex dynamics system. On the other hand, the* closed-loop ATV test *better describes the controlled process and reveals more reliable tuned-up controller parameters.*

4. *Consequently, the estimated open-loop test parameters for* “**LC**” *unit will not be used further. We present the open-loop test and its results for the sake of learning how to use such a test. The closed-loop ATV test tuning parameters will be used instead. For* “**TC**” *unit, we will also use the* closed-loop ATV test *as we take into account the time delay incurred in temperature measurement and manipulation.*
5. *APD allows the user to capture any current screen layout so that he/she can reuse the layout in future analysis and testing. To capture the screen layout, click on* “**Capture layout**” (★) *button in the top tool bar, and the* “**Capture Screen Layout**” *window will pop up asking the user to enter a name for the captured layout. Enter a name (e.g., CSL1) and close the window. To recall the layout by name, click on* “**Flowsheet**” | “**Scripts**” | “**CSL1**” *submenu and APD will execute the script and revert to the saved screen layout. Remember that the screen layout can have more than one opened window at the same time, such as the* “**Plot**”, “**Faceplate**”, “**Tune**”, and “**Configure**” *window. Notice that the* “**Flowsheet**” *menu will not be available unless the main window that contains the flowsheet is active.*

15.14 THE CLOSED-LOOP DYNAMIC RESPONSE FOR LIQUID LEVEL LOAD DISTURBANCE

First, a dead-time control element has to be inserted within the level controller loop to account for the time delay incurred in level measurement and flow manipulation. The dead time is set to 0.5 min, which can be accessed via right-clicking on the “**DT**” icon and selecting “**Forms**” | “**Configure**” submenu item, as shown in Figure 15.45 (see Section 15.16).



DT.Configure Table

	Description	Value	Units
DeadTime	Dead time	0.5	min

Figure 15.45 Insertion of a dead-time control element within the level controller loop to account for dead time elapsing between measured liquid level and final control element signal.

Second, a closed-loop ATV test is carried out with a relay amplitude of 5% of the output range using Ziegler–Nichols tuning rule. More details on the closed-loop ATV test are presented in Section 15.17. The start-up and the end of the test are maintained for a period such that a repetitive pattern (i.e., sinusoidal cyclic behavior) persists as shown in Figure 15.46.

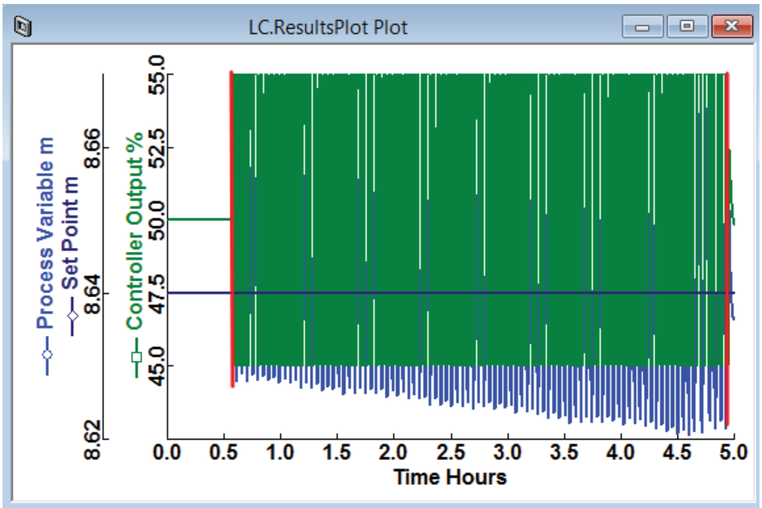
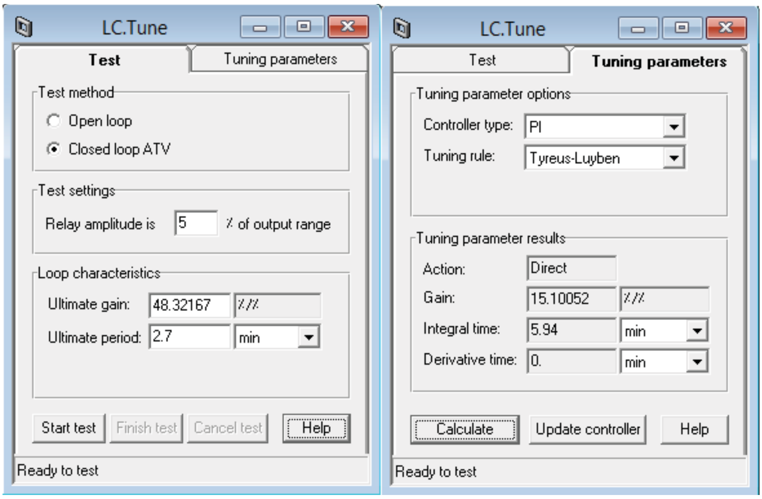


Figure 15.46 The closed-loop ATV test for tuning-up “**LC**” controller, where the test period lies between the two red lines. *See Plate section for color representation of this figure*.

As shown in Figure 15.47, it is found that $K_C = 15.1$ and the integral time constant, $\tau_I = 5.94$ min. After restarting (⏮) the simulation and clicking on the “**Update controller**” button, the controller parameters (i.e., with the new settings) become operational.



Test method
○ Open loop
● Closed loop ATV

Test settings
Relay amplitude is 5 % of output range

Loop characteristics
Ultimate gain: 48.32167 %/%
Ultimate period: 2.7 min

Ready to test

Tuning parameter options
Controller type: PI
Tuning rule: Tyreus-Luyben

Tuning parameter results
Action: Direct
Gain: 15.10052 %/%
Integral time: 5.94 min
Derivative time: 0. min

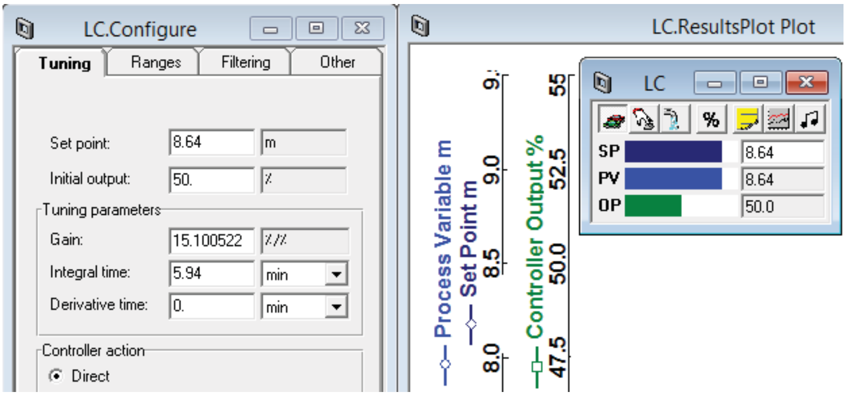
Ready to test

Figure 15.47 The “Closed-loop ATV test” tune-up results for “*PI*” level controller.

Let us cause a load disturbance to the system and see how the system will respond to that, of course, with a control action by the “**LC**” proportional-integral (“*PI*”) controller being effective.

The disturbance can be done by either changing the initial output level (“**OP**”), which is called load disturbance, or by the set point (“**SP**”), which is called set-point disturbance. Moreover, the change can be either positive or negative relative to the steady-state value. Here are the steps to follow in order to cause a disturbance for the initial output level (“**OP**”) and to monitor the closed-loop control dynamic response:

1. Double-click on “**LC**” node; this will open up the level controller faceplate (see Figure 15.32).
2. On the same faceplate, click on the “**Plot**” (second right top) button to open “**LC.ResultsPlot**” plot, shown earlier in Figure 15.38, to monitor the level profile.
3. On the same faceplate, click on the “**Configure**” (yellow button) button to open “**LC.Configure**” window, shown earlier in Figure 15.42, just to assure that the control action is in direct mode.
4. Run APD under “*Initialization*” mode. Assure that the run is complete via the confirming message telling the user that the run has completed. It is better that you rewind (⏪) to an old successful state such that “**OP**”, “**PV**”, and “**SP**” values are as shown in Figure 15.48. Alternatively, you may use the “**Snapshots Management**” window and revert to an old successful captured “*Initialization*” run. Figure 15.48 shows the numerical values of “**LC**” controller-related parameters. After all, if the controller tuning parameters are not refreshed by the desired values, then after carrying out the initialization step, the gain constant and integral time can be manually adjusted via “**LC.Configure**” | “**Tuning**” tab window.
5. Run the simulator under “*Dynamic*” mode and you will see how level signals change as a function of time. All the three opened windows, shown in Figure 15.48, will update the user by the level signals as *f(time)*. Continue running the dynamic mode until the value of “**OP**” reaches a steady-state (or stable) condition. Figure 15.49 shows the “*Dynamic*” run is paused (⏸) after stable values of “**OP**”, “**PV**”, and “**SP**” signal are reached.



Set point: 8.64 m

Initial output: 50. %

Tuning parameters

Gain: 15.100522 %/%

Integral time: 5.94 min

Derivative time: 0. min

Controller action

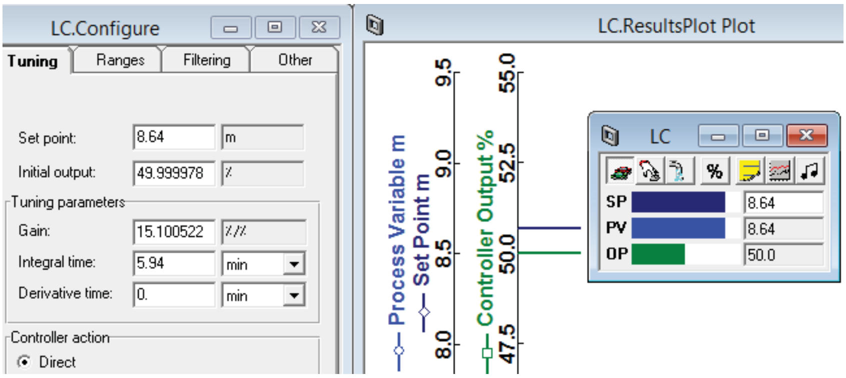
● Direct

SP 8.64

PV 8.64

OP 50.0

Figure 15.48 APD stage is ready for the running under “*Dynamic*” mode and carrying out the load and set point disturbance test.

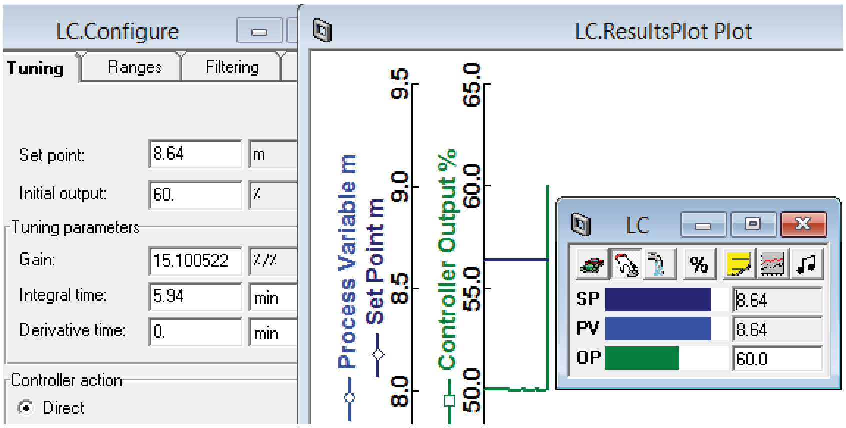


Set point: 8.64 m
Initial output: 49.999978 %
Gain: 15.100522 %/%
Integral time: 5.94 min
Derivative time: 0. min
Controller action: ● Direct

SP 8.64
PV 8.64
OP 50.0

Figure 15.49 The "*Dynamic*" mode is run until a steady-state condition is attained as indicated by stable values of "**OP**", "**PV**", and "**SP**" signal.

6. While in pause mode, switch "**LC**" to manual mode using the "**Manual**" (the hand icon) button shown at the top of the faceplate. Manually, enter the value of "**OP**" as *60* in "**OP**" edit box in the faceplate and click enter button. Figure 15.50 shows the result of imposing a positive step change in "**OP**" value. Notice that the "**Initial output**" value in "**Tuning**" tab window is automatically updated to *60%*.

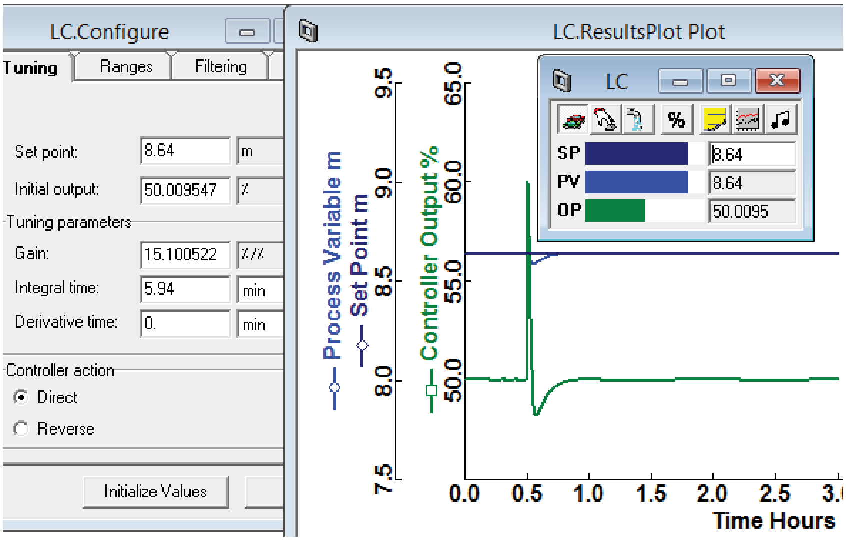


Set point: 8.64 m
Initial output: 60. %
Gain: 15.100522 %/%
Integral time: 5.94 min
Derivative time: 0. min
Controller action: ● Direct

SP 8.64
PV 8.64
OP 60.0

Figure 15.50 Imposing a positive step change in "**OP**" value where it is increased from 50.0 to 60%.

7. While still in pause mode, switch "**LC**" back to auto mode using the "**Auto**" (the two car icon) button shown at the left top of the faceplate.
8. Resume the "*Dynamic*" mode. Continue until a steady-state condition is reached then pause the "*Dynamic*" run. Figure 15.51 shows that with a control action, the process reverts to the original steady-state as it is before the load disturbance takes place.



LC.Configure

Tuning | Ranges | Filtering

Set point: 8.64 m

Initial output: 50.009547 %

Tuning parameters

Gain: 15.100522 %/%

Integral time: 5.94 min

Derivative time: 0. min

Controller action

● Direct

○ Reverse

LC

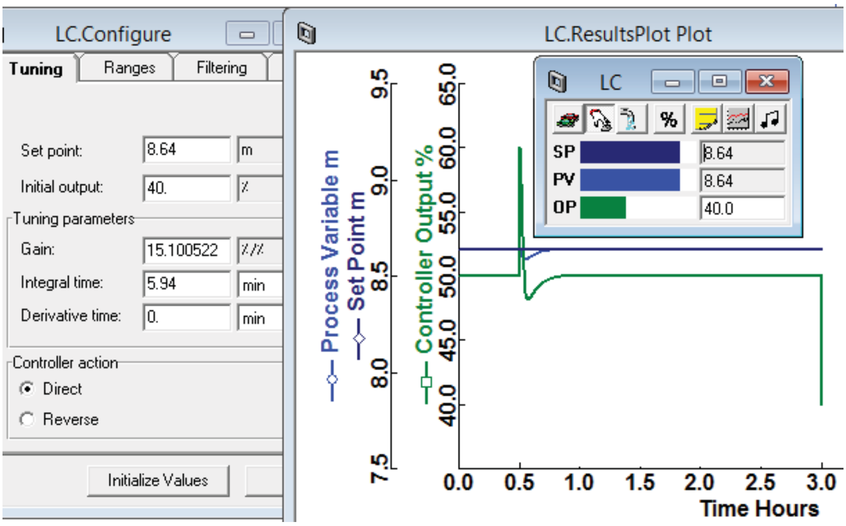
SP 8.64

PV 8.64

OP 50.0095

Figure 15.51 Under the load disturbance caused by a positive step change, the control action of "*PI*" controller will make the process revert to the original "**OP**", "**PV**", and "**SP**" signal values, as they prevail before the load disturbance takes place.

9. While in pause mode, switch "**LC**" to manual mode using the "**Manual**" (the hand icon) button shown at the top of the faceplate. Manually enter the value of "**OP**" as *40* in "**OP**" edit box in the faceplate and click enter button. Figure 15.52 shows the result of imposing a negative step change in "**OP**" value. Notice that the "**Initial output**" value in "**Tuning**" tab window is automatically updated to *40%*.



LC.Configure

Tuning | Ranges | Filtering

Set point: 8.64 m

Initial output: 40. %

Tuning parameters

Gain: 15.100522 %/%

Integral time: 5.94 min

Derivative time: 0. min

Controller action

● Direct

○ Reverse

LC

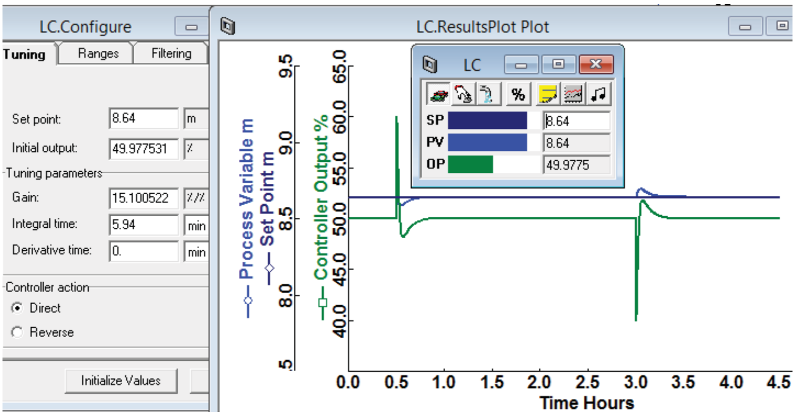
SP 8.64

PV 8.64

OP 40.0

Figure 15.52 Imposing a negative step change in "**OP**" value where it is decreased from 50.0 to 40%.

10. While still in pause mode, switch “**LC**” back to auto mode using the “**Auto**” (the two car icon) button shown at the left top of the faceplate.
    Resume the “*Dynamic*” mode. Continue until a steady-state condition is reached then pause the “*Dynamic*” run. Figure 15.53 shows that with a control action, the process reverts to the original steady state as it is before the load disturbance takes place.



Set point: 8.64 m
Initial output: 49.977531 %
Tuning parameters
Gain: 15.100522 %/%
Integral time: 5.94 min
Derivative time: 0. min
Controller action
● Direct
○ Reverse

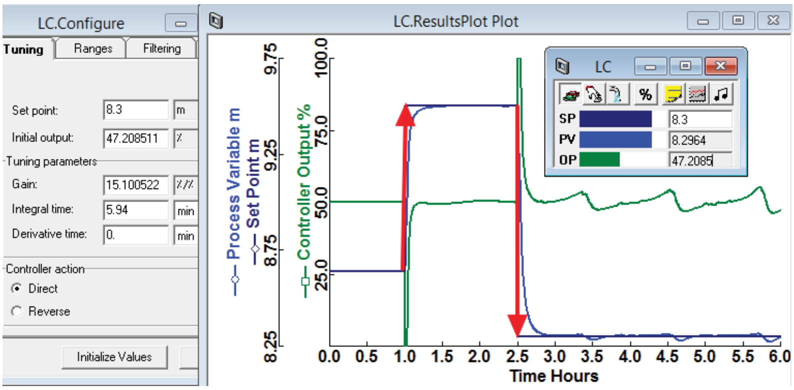
SP 8.64
PV 8.64
OP 49.9775

Figure 15.53 Under the load disturbance caused by a negative step change, the control action of “*PI*” controller will make the process revert to the original “**OP**”, “**PV**”, and “**SP**” signal values, as they prevail before the load disturbance takes place.

11. Upon finishing from the test, reset to zero time using the restart (⏮) button.

15.15 THE CLOSED-LOOP DYNAMIC RESPONSE FOR LIQUID LEVEL SET-POINT DISTURBANCE

The same procedure, outlined in the previous section, is traced here except that we cause a positive step change for the set point “**SP**” from an old (“**SP**” = 8.6 m) to a new value (“**SP**” = 9.5 m) followed later by a negative step change from the latter to a new value (“**SP**” = 8.3 m), as shown in Figure 15.54. Notice that the set-point disturbance is carried out in “**Auto**” mode (i.e., the two car icon button is clicked). As a result of PI controller action, the system evolves from the old to the new, imposed steady-state condition as far as the liquid level inside the tank is concerned. The word “steady-state” here means, with the aid of a controller action, the liquid level signal values remain invariant with time and steadiness in this regard does not necessarily reflect the “genuine” steady-state condition with no control action in effect.



Set point: 8.3 m

Initial output: 47.208511 %

Tuning parameters

Gain: 15.100522 %/%

Integral time: 5.94 min

Derivative time: 0. min

Controller action

● Direct

○ Reverse

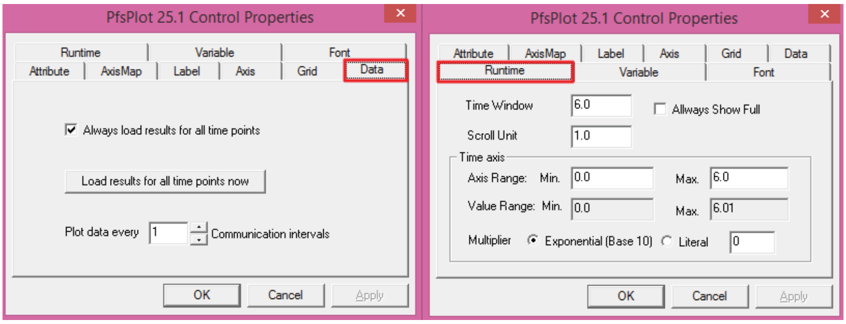
SP 8.3

PV 8.2964

OP 47.2085

Figure 15.54 A set-point disturbance for the process with "*PI*" level controller in action. Both positive and negative step change in the set point ("**SP**") of liquid level are executed at $t = 1.0$ and at $t = 2.5\ h$, respectively. Notice how "**PV**" chases "**SP**" signal with a control action in effect.

<u>NOTE #9:</u> *The plot can be customized for many of its features, such as the x- and y-axis range; the font type and size; x- and y-label; and grid interval. While the mouse hovers over the plot area, right-click and a shortcut (context) menu will pop up where you select "**Properties** … " submenu. A window will then pop up where you can carry out many cosmetic changes to the current plot and make it look more expressive, thus more impressive. For example, in "**Data**" tab window, if not all the data are shown for the entire time range, then here you can ask APD to load all results for all time data points to the current plot (see Figure* 15.55 *left). In addition, the time-axis range can be adjusted in "**Runtime**" tab form (see Figure* 15.55 *right). Finally, from the previous shortcut (context) menu, you can select "**Redraw**" submenu to refresh the plot if it is not already refreshed.*



☑ Always load results for all time points

Plot data every 1 Communication intervals

Time Window 6.0

☐ Allways Show Full

Scroll Unit 1.0

Time axis

Axis Range: Min. 0.0 Max. 6.0

Value Range: Min. 0.0 Max. 6.01

Multiplier ● Exponential (Base 10) ○ Literal 0

Figure 15.55 Cosmetic changes for the plot itself are made feasible via right-clicking the mouse over the plot area and selecting the proper submenu item.

15.16 ACCOUNTING FOR DEAD/LAG TIME IN PROCESS DYNAMICS

To obtain good results that can be transferred to a real control system, it is important that you accurately model the loop dynamics. This means modeling the sensor and actuator dynamics if they have a significant effect on the overall loop dynamics. It is particularly important to model dead times in the control loop. The tuning of the temperature controller involves inserting a dead-time element in the loop to account for the dynamic lags that are always present in any real controller. Temperature measurement lags are not negligible (about 30–60 s). In addition, changing the medium temperature cannot be instantly achieved. Therefore, a typical one-minute dead time is usually used.

We have already inserted the "**Dead_time**" control element in the liquid-level control loop (Figure 15.45). With a temperature control loop, we would also like to position the "**Dead_time**" element between the reactor outlet and the controller input. From "**Model Libraries**" ribbon and under "**Controls**" tab, drag once the "**Dead_time**" icon to the flowsheet area and release the mouse. Rename the block to "**DT2**".

Click on (i.e., highlight) the signal dashed line going out of the reactor, click the right mouse button, and select "**Reconnect Destination**" submenu item. Position the cursor on the arrow pointing to "**DT2**" element and click. Figure 15.56 shows this connection. From "**Model Libraries**" ribbon and under "**MaterialStream**" tab, add a control signal line which will connect the outlet of "**DT2**" element to the inlet of "**TC**" node (i.e., **PV** signal). Figure 15.56 shows the inserted "**Dead_time**" control element within the temperature control loop, in addition to that of the liquid-level control loop.

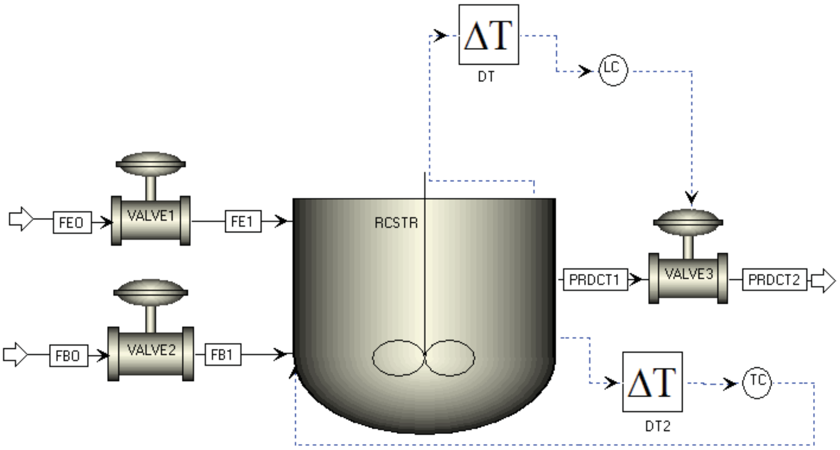


Figure 15.56 The insertion of the "**Dead_time**" control element between the temperature transmitter and "**TC**" control node.

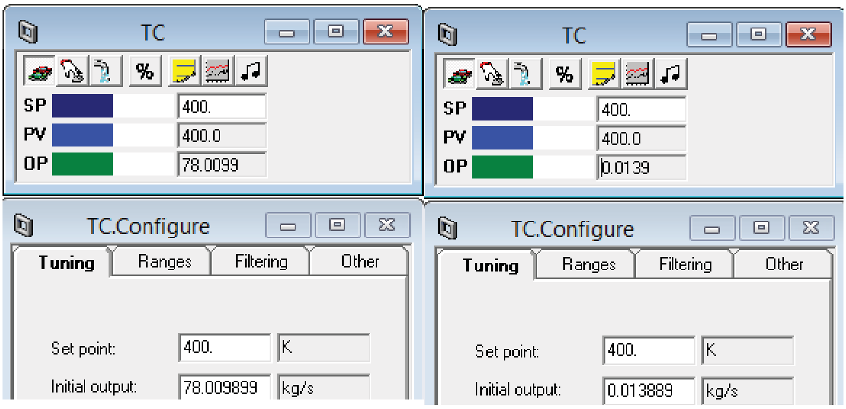
To assign the dead-time value with the proper unit, click on "**DT2**" icon, right-click the mouse, select "**Forms**" followed by "**Configure**" submenu item, and the "**DT2.Configure Table**" form will pop up where you can set the length of its dead time and decide on its unit. A value of 1 min is assigned to the duration of the dead time.

15.17 THE CLOSED-LOOP (AUTO MODE) ATV TEST FOR TEMPERATURE CONTROLLER (TC)

In the past, many of the controllers were analog; however, recent controllers use digital signals and computers. When a mathematical model of a system is known, the parameters of the controller can be explicitly determined. However, when a mathematical model is unknown, then parameters must be experimentally determined. *Controller tuning is the process of determining the controller parameters that produce the desired output. Controller tuning allows for optimization of a process via minimization of the error between the variable of the process and its set point*.

In this section, we follow the steps that were shown in Section 15.13 and show things that are different from the liquid level control case.

Double-click on "**TC**" node and "**TC**" controller faceplate will show up (see Figure 15.57 *left*). Notice that "**OP**" signal represents the mass flow rate of cooling water on the coiled jacket side of the heat exchanger. Be sure that Step #6 in Section 15.8 is properly executed and gives the right flow rate of cooling water, that is, 78.0099 kg/s; else, you may end up with cooling water mass flow rate equal to 0.013889 kg/s as shown in Figure 15.57 *right*.



Left:

SP 400.
PV 400.0
OP 78.0099

Set point: 400. K
Initial output: 78.009899 kg/s

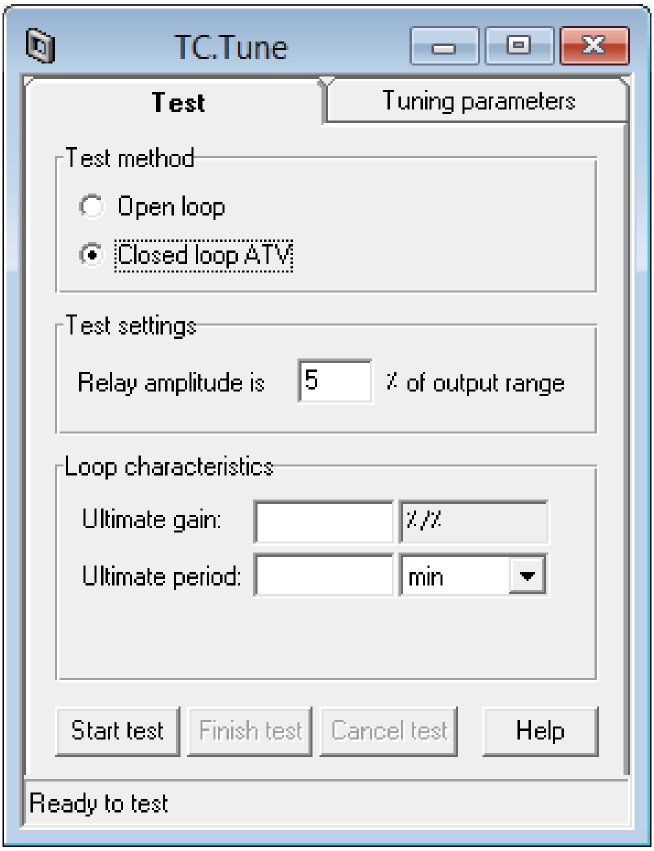
Right:

SP 400.
PV 400.0
OP 0.0139

Set point: 400. K
Initial output: 0.013889 kg/s

Figure 15.57 "**TC**" controller faceplate showing "**PV**" and "**SP**" initialized values in (K) and the right "**OP**" value (*left*) and wrong "**OP**" value (*right*) in (kg/s).

On the same faceplate, click on "**Tune**" (♫) button. "**TC.Tune**" window will show up as shown in Figure 15.58. Since we have already accounted for the time delay via insertion of a dead-time block within our temperature control loop, we will choose the closed-loop ATV test (see **NOTE #7**). Select the "**Closed loop ATV**" bullet. The "**Relay amplitude**" value, by default, is 5% of the output range. You can change it if you wish, depending on the maximum variation of disturbance in cooling water flow rate. Let us stick to the default value. Moreover, open "**TC.ResultsPlot**" plot to monitor the temperature profile.



Test method

○ Open loop

● Closed loop ATV

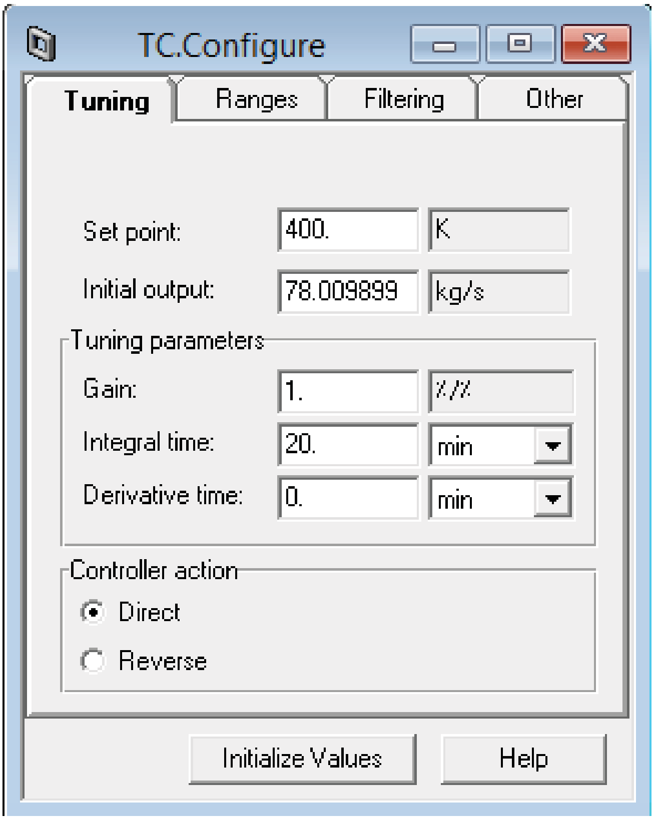
Test settings

Relay amplitude is 5 % of output range

Ready to test

Figure 15.58 The "**TC.Tune**" | "**Test**" tab window for selecting the test type and the relay amplitude.

Open "**TC.Configure**" window just to assure that the control action is in "*Direct*" mode and also to see the assigned controller tuning parameters before carrying out the test, as shown in Figure 15.59. Keep in mind that controller tuning parameters are initially estimated by APD. The user may change them, however, if he/she finds them inappropriate and do not precisely reflect the closed-loop (i.e., with a control action) dynamic response of the process.



Set point: 400. K

Initial output: 78.009899 kg/s

Tuning parameters

Gain: 1. %/%

Integral time: 20. min

Derivative time: 0. min

Controller action

● Direct

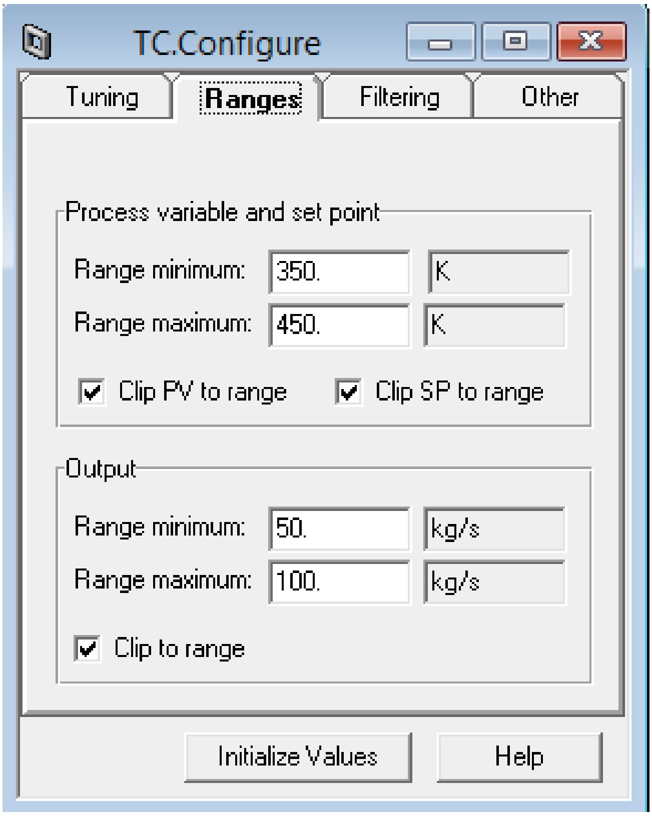
○ Reverse

Figure 15.59 The "**Tuning**" tab window of "**TC.Configure**" form, where it shows the default "**OP**" and "**SP**" value, in addition to APD initially estimated controller tuning parameters.

Click on "**Ranges**" tab window, and change the ranges to more realistic values, as shown in Figure 15.60.

Run APD under "*Initialization*" mode. Assure that the run is successfully complete via the confirming message telling the user that the run has completed. Watch out that the default settings are the same as those shown in Figure 15.59. APD platform is now ready for ATV test.

Switch to "*Dynamic*" mode and run APD by clicking the run (▶) button. Let it run just to assure that everything is running perfect and all three variables exhibit stable values with time.



Process variable and set point

Range minimum: 350. K

Range maximum: 450. K

☑ Clip PV to range ☑ Clip SP to range

Output

Range minimum: 50. kg/s

Range maximum: 100. kg/s

☑ Clip to range

Figure 15.60 In “**Ranges**” tab window, “**OP**”, “**PV**”, and “**SP**” range are changed to more realistic values.

Push “**Start test**” button shown in Figure 15.58, which temporarily sets the feedback controller as an On/Off (or relay) controller and the controlled variable exhibits a sustained oscillation that is characteristic of an On/Off controller. Figure 15.61 shows the result after starting the test, keeping it running for a while, then stopping the test using “**Finish test**” button (shown in Figure 15.58).

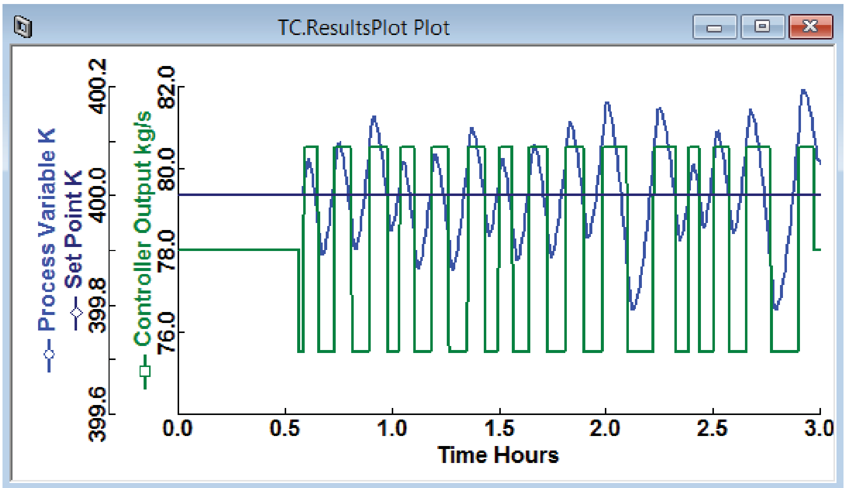
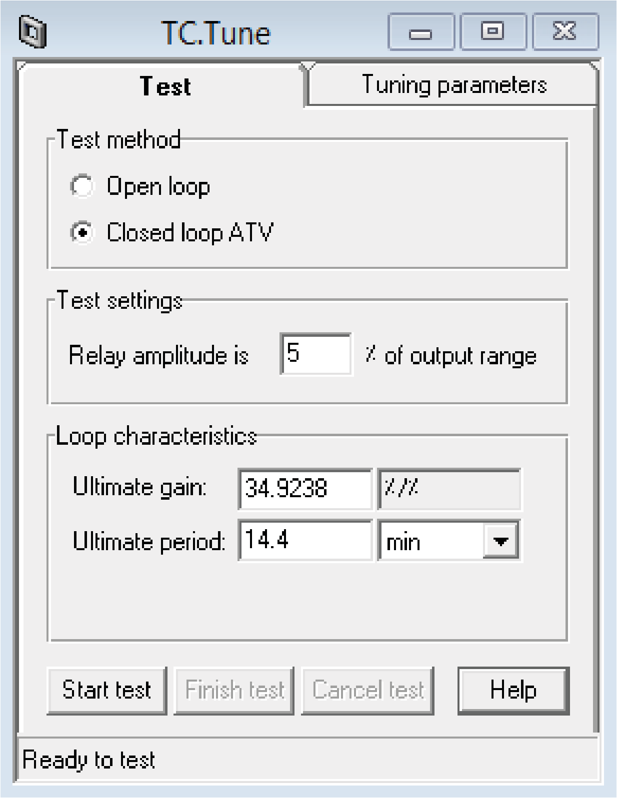


Figure 15.61 The sinusoidal oscillation behavior can be seen for both “**OP**” and “**PV**” signal during the period of “**Closed-loop ATV**” test which sets the controller type as On/Off (relay).

Moreover, Figure 15.62 shows the calculated ultimate gain (***K****$_U$*) and the ultimate period (***P****$_U$*) based on the “**Closed-loop ATV**” test.



Test method

○ Open loop

● Closed loop ATV

Test settings

Relay amplitude is 5 % of output range

Loop characteristics

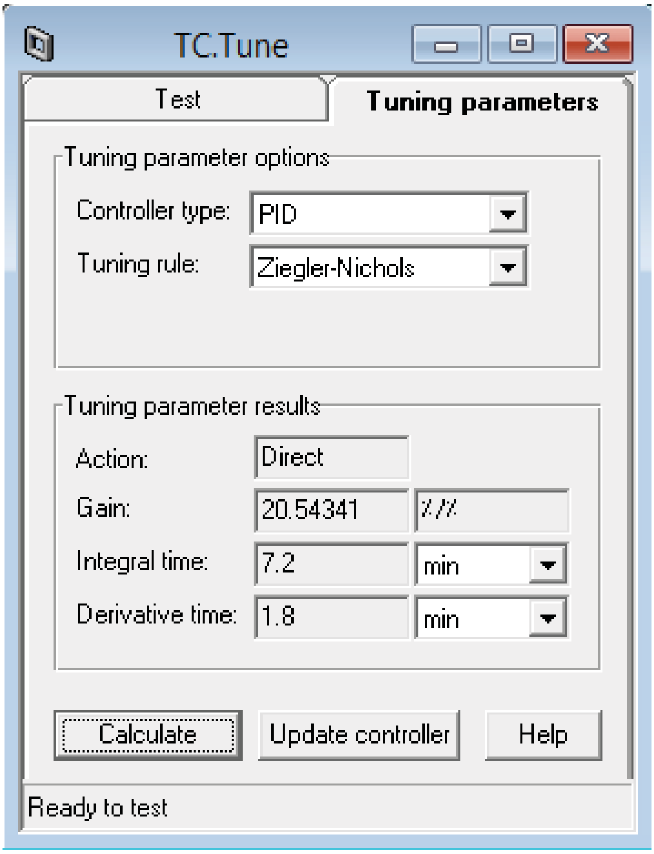
Ultimate gain: 34.9238 %/%

Ultimate period: 14.4 min

Ready to test

Figure 15.62 Calculation of the ultimate gain (***K****$_U$*) and the ultimate period (***P****$_U$*) based on the “**Closed-loop (Auto Mode) ATV**” test.

After finishing the test, go to “**Tuning parameters**” tab window. After selecting the tuning rule and controller type, click on “**Calculate**” button (it becomes active after the test) to calculate the controller tuned-up parameters. Figure 15.63 shows the “*Ziegler–Nichols*” tuning rule case with $K_C = 20.54$, $\tau_I = 7.2$ min, and $\tau_D = 1.8$ min for a “*PID*”-type temperature controller.



Controller type: PID

Tuning rule: Ziegler-Nichols

Action: Direct

Gain: 20.54341 %/%

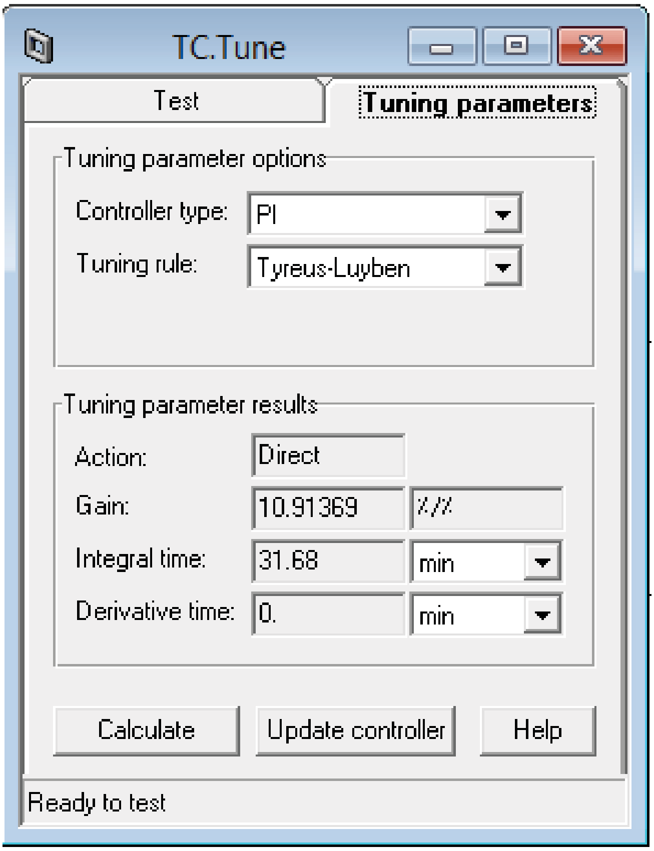
Integral time: 7.2 min

Derivative time: 1.8 min

Ready to test

Figure 15.63 Using the “*Ziegler–Nichols*” tuning rule, $K_C = 20.54$, $\tau_I = 7.2$ min, and $\tau_D = 1.8$ min are calculated for a “*PID*”-type temperature controller.

For the same test and while you are still in “**Tuning parameters**” tab window, you may change the “**Controller type**” to “*PI*” and the “**Tuning rule**” to “*Tyreus–Luyben*” and ask APD to calculate the gain, K_C, and the integral time, τ_I, as shown in Figure 15.64.



TC.Tune

Tuning parameter options

Controller type: PI

Tuning rule: Tyreus-Luyben

Tuning parameter results

Action: Direct

Gain: 10.91369 %/%

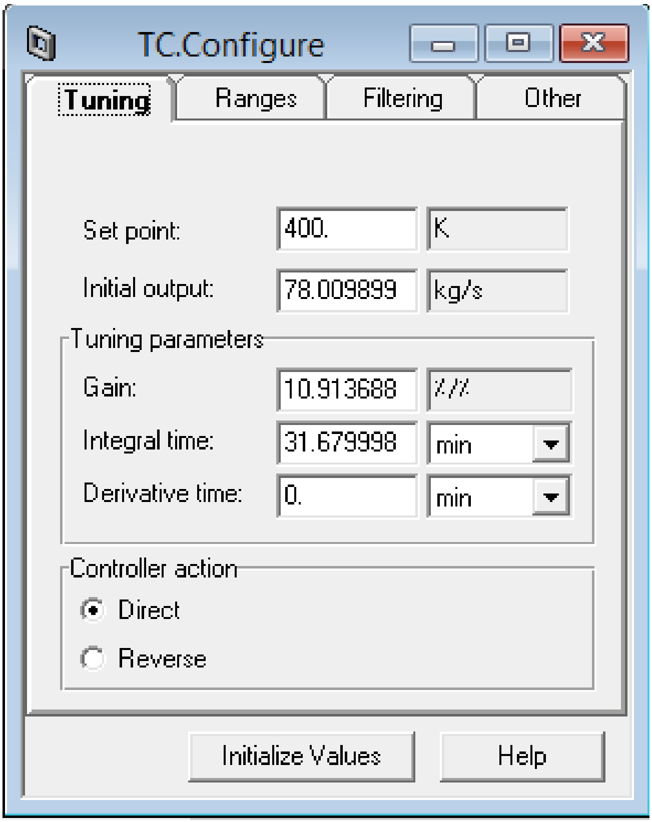
Integral time: 31.68 min

Derivative time: 0. min

Ready to test

Figure 15.64 Using the “*Tyreus–Luyben*” tuning rule, $K_C = 10.91$, $\tau_I = 31.68$ min, and $\tau_D = 0.0$ min are calculated for a “*PI*”-type temperature controller.

The calculated tuned-up parameters can be used in the controller by restarting (⏮) the simulation, first, and clicking on the “**Update controller**” button (shown in Figure 15.64), second, depending whether we would like to go with "*PID*" or "*PI*" case. Figure 15.65 shows "**TC.Configure**" | "**Tuning**" tab window, where the "*PI*" controller is now augmented by "*Tyreus–Luyben*"-based, newly calculated parameters.



Set point: 400. K

Initial output: 78.009899 kg/s

Tuning parameters

Gain: 10.913688 %/%

Integral time: 31.679998 min

Derivative time: 0. min

Controller action

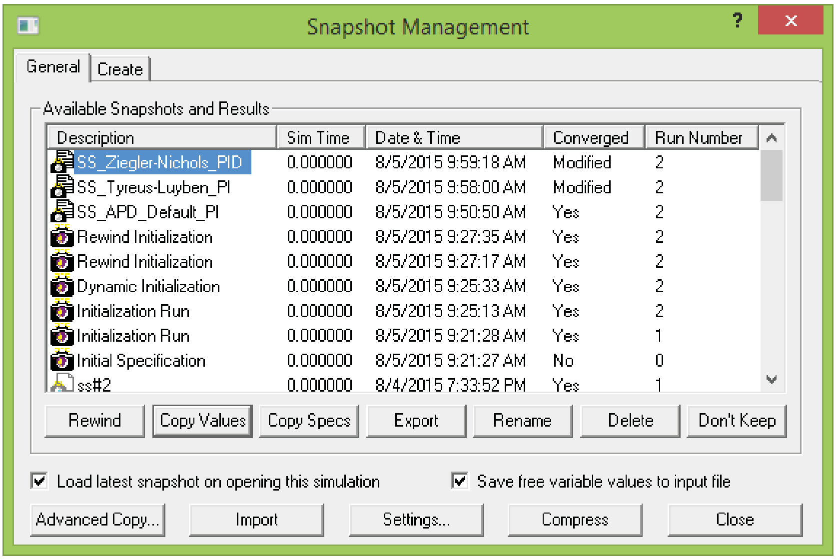
● Direct

○ Reverse

Figure 15.65 "**TC**" control unit will acquire the new parameters once you restart the simulation and then push the "**Update controller**" button at the bottom of "**TC.Tune**" | "**Tuning parameters**" tab window.

NOTE #10: *To have more flexibility, carry out a successful "Initialization" step and manually change the set of controller parameters (via "**TC.Configure**" | "**Tuning**" tab form), then save each set of controller tune-up parameters to a different captured snapshot so that you can rewind to a particular set of controller tune-up parameters without having to manually enter them each time you want to run the process dynamics with particular controller tune-up parameters. I noticed that if I rewind to another state not all controller tuning parameters will be updated; however, if I close APD, open, and then rewind to any saved state, it will do the job (i.e., it will correctly update all records). To be on the safe side, always open "**TC.Configure**" | "**Tuning**" tab form (It also applies to level controller, as well) and be sure that when you rewind to a particular set of controller tune-up parameters, all of them are updated by the correct (or desired) values.*

Figure 15.66 shows the "**Snapshot Management**" window where three different successful "*Initialization*" steps are carried out each time with a different set of controller tune-up parameters and then are saved as captured snapshots: one for the default APD-supplied "*PI*" case (a snapshot of the first successful "*Initialization*" step right after installing the two control units and before doing any closed-loop tune-up test), a second one for Tyreus–Luyben-based "*PI*" controller case, and a third one for Ziegler–Nichols-based "*PID*" controller case. Once you highlight any case, you can click on the "**Rewind**" button at the bottom of the window and APD will revert to that case. Always check that the controller acquires the required (or desired) tune-up parameters, upon carrying out a rewind step (see **NOTE #10**).



Available Snapshots and Results

Description	Sim Time	Date & Time	Converged	Run Number
SS_Ziegler-Nichols_PID	0.000000	8/5/2015 9:59:18 AM	Modified	2
SS_Tyreus-Luyben_PI	0.000000	8/5/2015 9:58:00 AM	Modified	2
SS_APD_Default_PI	0.000000	8/5/2015 9:50:50 AM	Yes	2
Rewind Initialization	0.000000	8/5/2015 9:27:35 AM	Yes	2
Rewind Initialization	0.000000	8/5/2015 9:27:17 AM	Yes	2
Dynamic Initialization	0.000000	8/5/2015 9:25:33 AM	Yes	2
Initialization Run	0.000000	8/5/2015 9:25:13 AM	Yes	2
Initialization Run	0.000000	8/5/2015 9:21:28 AM	Yes	1
Initial Specification	0.000000	8/5/2015 9:21:27 AM	No	0
ss#2	0.000000	8/4/2015 7:33:52 PM	Yes	1

☑ Load latest snapshot on opening this simulation

☑ Save free variable values to input file

Figure 15.66 Saving more than one captured snapshot for a successful "*Initialization*" step will save the user a lot of headache when he/she attempts to move from one to another case.

15.18 THE CLOSED-LOOP DYNAMIC RESPONSE: "TC" RESPONSE TO TEMPERATURE LOAD DISTURBANCE

Notice that we follow the same procedure, outlined in Section 15.14; however, we present results related to temperature control. Let us cause a disturbance to the system and see how the system responds to that. Three cases are handled here.

The first case represents the "*PI*" of "**TC**" control unit using initially APD-estimated gain constant ($K_C = 1.0$), integral time constant ($\tau_I = 20$ min), and derivative time constant ($\tau_D = 0.0$ min). Figure 15.67 shows the dynamic response of the controlled process to a load disturbance caused by a negative step change in "**OP**" from the default initial value of 78.01 kg/s of cooling water down to 70 kg/s (at about $t = 1.0\,h$), waiting for the process to offset the impact of the negative load disturbance by the watching dog (i.e., controller action), followed by a positive step change from 78.01 up to 88 kg/s (at about $t = 16.0\,h$),

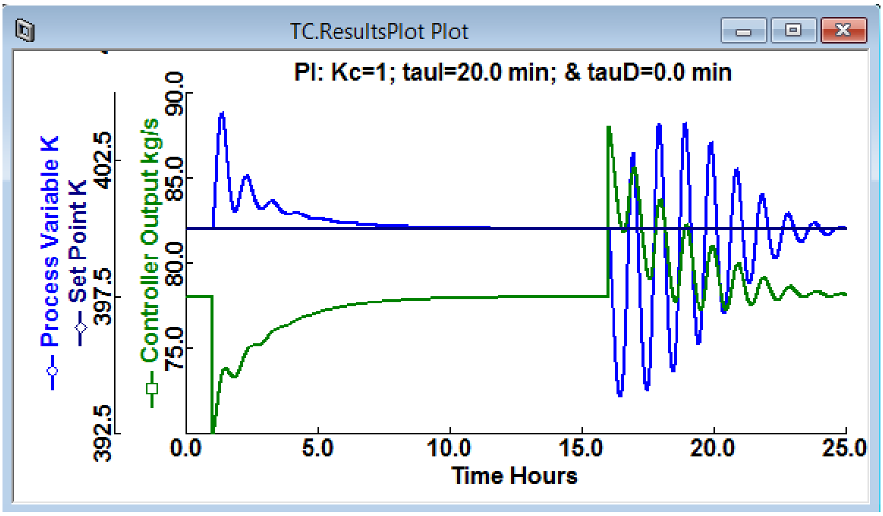


Figure 15.67 Imposing a negative step change in the initial output (“**OP**”) where it is dropped from 78.01 down to 70 kg/s (at about $t = 1.0\,h$), letting the process recover, imposing a positive step change (at about $t = 16.0\,h$) from 78.01 up to 88 kg/s, and letting the process recover again. The initially APD-estimated “*PI*” controller parameters are used.

and finally letting the process to offset the impact of the positive load disturbance by the virtue of the controller vigilance.

The second case represents the PID controller of “**TC**” control unit using the Ziegler–Nichols-based tune-up parameters (see Figure 15.63) with gain constant $K_C = 20.54$, $\tau_I = 7.2$ min, and $\tau_D = 1.8$ min. Figure 15.68 shows the dynamic response of the controlled

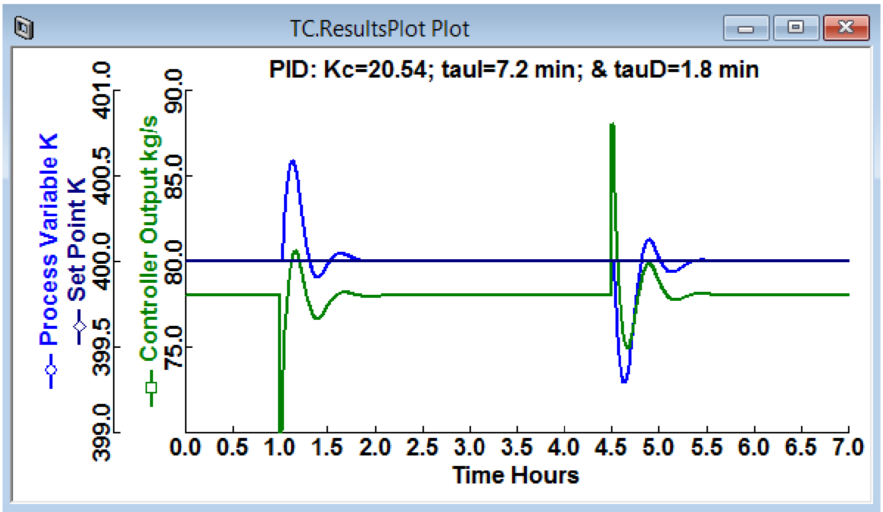


Figure 15.68 Imposing a negative step change in the initial output (“**OP**”) where it is dropped from 78.01 down to 70 kg/s (at about $t = 1.0\,h$), letting the process recover, imposing a positive step change (at about $t = 4.5\,h$) from 78.01 up to 88 kg/s, and letting the process recover again. The Ziegler–Nichols-based “*PID*” controller tune-up parameters are used.

process to a load disturbance caused by a negative step change in "**OP**" from the default initial value of 78.01 kg/s of cooling water down to 70.0 kg/s (at about $t = 1.0\,h$) and to a positive step change from 78.01 up to 88 kg/s (at about $t = 4.5\,h$).

The third case represents the "*PI*" controller of "**TC**" control unit using the Tyreus–Luyben-based tune-up parameters (see Figure 15.64) with gain constant $K_C = 10.91$, $\tau_I = 31.68$ min, and $\tau_D = 0.0$ min. Figure 15.69 shows the dynamic response of the controlled process to a load disturbance caused by a negative step change in "**OP**" from the default initial value of 78.01 kg/s of cooling water down to 70.0 kg/s (at about $t = 1.0\,h$) and to a positive step change from 78.01 up to 88 kg/s (at about $t = 6.0\,h$).

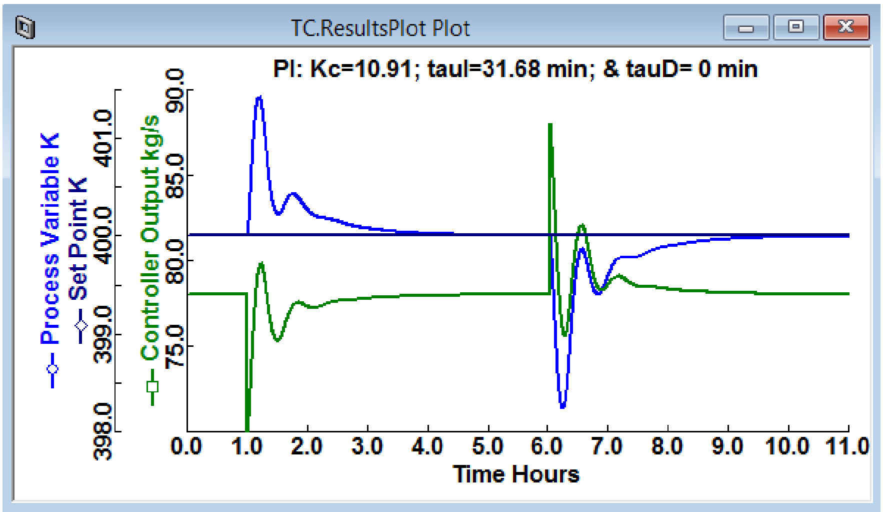


Figure 15.69 Imposing a negative step change in the initial output ("**OP**") where it is dropped from 78.01 down to 70 kg/s (at about $t = 1.0\,h$), letting the process recover, imposing a positive step change (at about $t = 6.0\,h$) from 78.01 up to 88 kg/s, and letting the process recover again. The Tyreus–Luyben-based "*PI*" controller tune-up parameters are used.

Notice that the dynamic response in the second case is the fastest among all and in the first case is the slowest among all in terms of regaining the original steady-state condition, hence offsetting the impact of a load disturbance. The first case is considered to be sluggish, characterized by a low K_C and relatively a medium integral time constant (τ_I). Notice that the "*PID*" controller calculation algorithm involves three separate constant parameters: proportional, integral, and derivative, denoted as *P*, *I*, and *D*, respectively. Such values can be related to the error, which is the difference between "**PV**" and "**SP**" signal. *P* depends on (i.e., proportional with) the present error, *I* on the accumulation (integral) of past errors, and *D* is a prediction of future errors, based on the current rate of change (i.e., derivative). The weighted sum of these three actions is used to adjust the process via the final control (manipulated) element, such as the position of a control valve. Consequently, "*PID*" controller has more freedom and luxury to entertain the process of regaining the old steady-state condition faster than "*PI*" type of controller, for almost the same order of magnitude of K_C and τ_I values.

Moreover, in the first case, the dynamic response of the controlled process/system exhibits the most oscillatory behavior towards reaching the final, steady-state condition, hence the longest time to offset the difference between the set point ("**SP**") and process variable ("**PV**") value. Such a response is denoted as underdamped response, which means that as time goes on, the amplitude (i.e., the peak height or valley depth relative to the zero datum) dips down until the peak height (or valley depth) completely diminishes. A real-life example is if someone releases a rubber ball on the floor, the ball will keep hitting and bouncing off the floor but each time it bounces off the ground it will not reach the same height it has already reached in the previous cycle until eventually the ball resides on the floor. This damping effect, in principle, is mainly due to the non-elastic collision with the floor and the presence of air resistance (viscous effect). If the collision with floor is completely elastic and there is no air resistance, then the ball will exhibit an undamped, perpetual oscillation and will not stop dancing at all.

In general, for a "PI" controller, as K_C increases or τ_I decreases, the closed-loop dynamics will pass through overdamped, critically damped, underdamped (i.e., oscillatory), sustained oscillations, and finally unstable oscillations. On the other hand, a "PID"-controlled process will dynamically exhibit the same behavior with varying K_C and τ_I as that observed for a "PI"-controlled process. The derivative action tends to reduce the oscillatory nature of the response and results in faster settling for systems, particularly, for those characterized by larger dead time to process time constant (τ_D/τ_P) ratios. So, in the presence of the derivative action, "PID" controller tends to settle down (or offset) earlier than pure "PI" controller with no derivative action.

15.19 INTERACTIONS BETWEEN "LC" AND "TC" CONTROL UNIT

Let us see if we cause a set-point disturbance for the liquid level, how "**TC**" control unit will respond to that. Figure 15.70 shows that at $t = 1.0\,h$, a positive step change is carried out from 8.6 to 9.6 m. The "**PV**" signal will adjust to the new "**SP**" accordingly. K_C and τ_I for "PI" level controller are set to 15.1 and 5.94 min, respectively (see Figure 15.47).

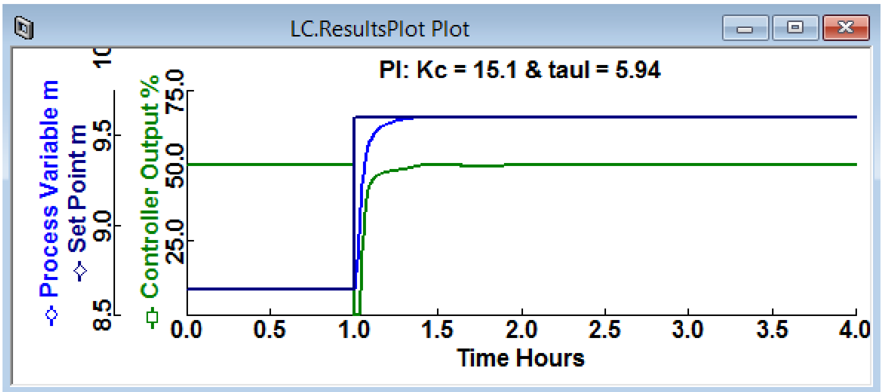


Figure 15.70 The controlled dynamic response due to a positive step change in "**SP**" for the liquid level from 8.6 to 9.6 m.

Figure 15.71 shows how the temperature of the reactor rose up to 402 K in response to the immediate increase of liquid hold-up inside the reactor, which means more liquid volume, hence, a longer residence time, a higher conversion, and more heat duty, where the latter effect leads to a temporary jump in temperature. Consequently, “PID” controller of “**TC**” control unit will act in a way to eliminate the offset and let the process revert to the original steady-state temperature (i.e., $T = 400$ K). This is achieved via temporarily increasing the cooling water flow rate from 78.01 to 100 kg/s, which is then reduced to a new steady-state value (i.e., 82.71 kg/s) that is compatible with the new steady-state of liquid level ($L_{SP} = 9.6$ m) inside the reactor.

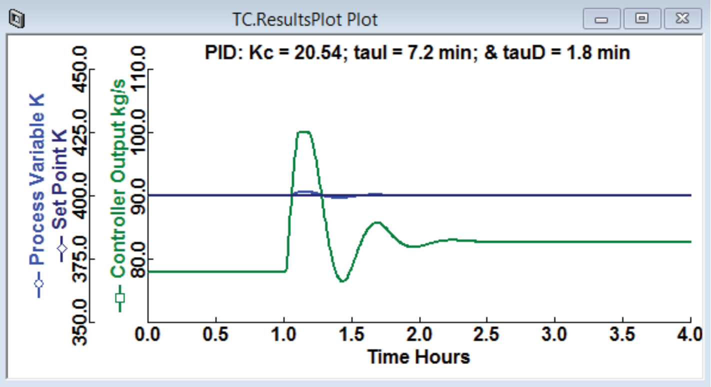


Figure 15.71 The reactor temperature immediately jumped up following the positive step change in “**SP**” value for the liquid level. T offset is then eliminated by the control action of “*PID*” controller.

On the other hand, Figure 15.72 shows that at $t = 1.0\,h$, a positive step change in “**SP**” is carried out from 400 to 408 K. The “**PV**” signal will adjust accordingly and reach the new steady-state value (i.e., $T = 408$ K). Notice that the new steady-state value of cooling water flow rate is 60.55 kg/s, which is less than the old value (i.e., 78.01 kg/s). Thus, T will attain the new steady-state value by reducing the mass flow rate of cooling water from 78.01 down to 60.55 kg/s.

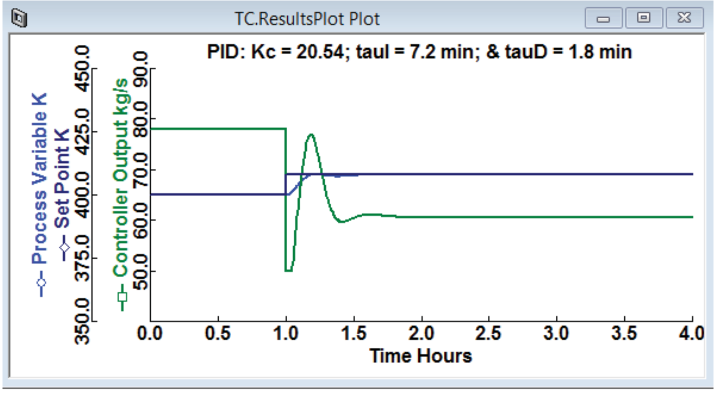


Figure 15.72 The closed-loop dynamic response of “*PID*” temperature controller in response to a positive step change in “**SP**” from 400 to 408 K via adjusting the cooling water flow rate down to 60.55 kg/s.

Figure 15.73 shows the liquid level three signals as a function of time. Obviously, "**PV**" signal coincides with "**SP**" signal, indicating that neither the process liquid hold-up inside the reactor (i.e., **PV**) nor its flow rate out of the tank (i.e., "**OP**") is affected by the step change in temperature.

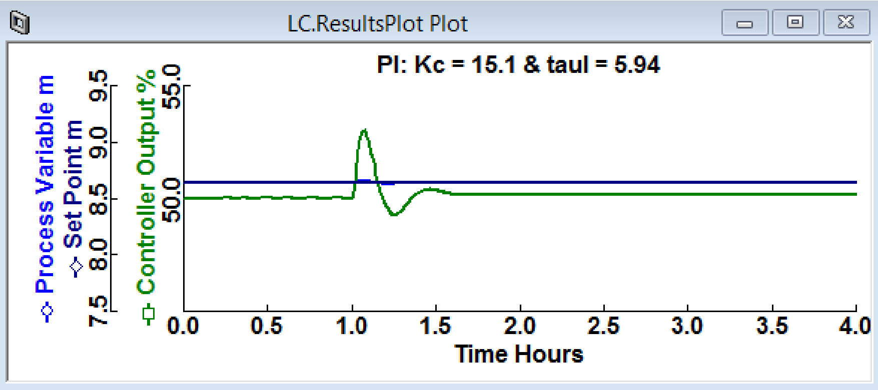
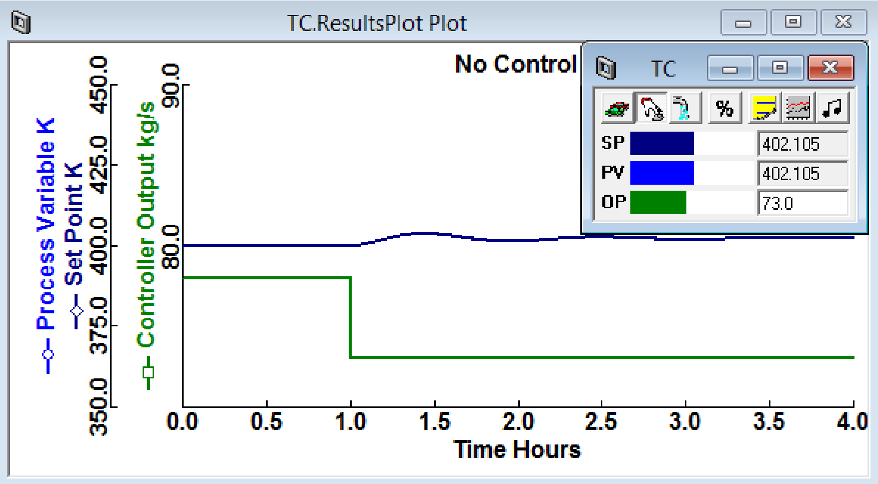


Figure 15.73 The liquid hydrodynamics is not affected by the step change in reactor temperature.

15.20 THE STABILITY OF A PROCESS WITHOUT CONTROL

Let us analyze our CSTR and show how it responds to a step change in the cooling water flow rate in both directions with no control action (i.e., the run will be carried out while the "**Manual**" button is clicked on for both level and temperature faceplate).

Figure 15.74 shows that at $t = 1.0\,h$, we manually perturbed the process by changing the input flow rate of cooling water from 78.01 down to 73.0 kg/s. Accordingly, the

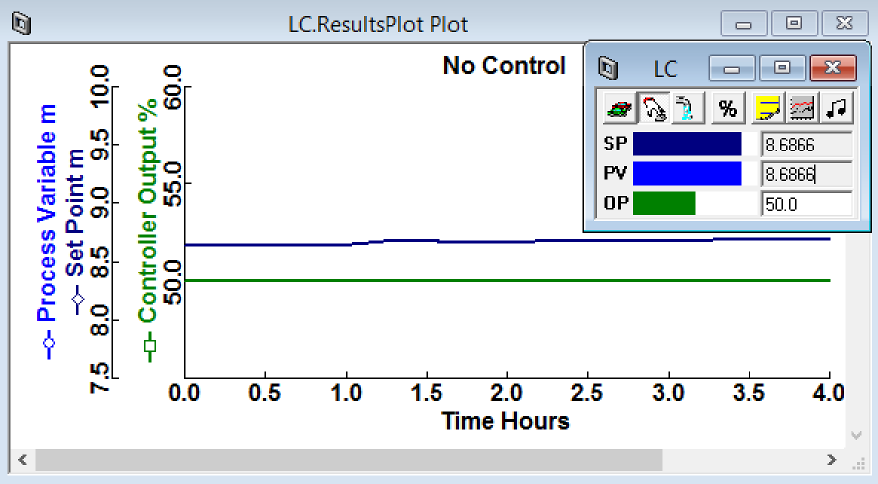


SP 402.105
PV 402.105
OP 73.0

Figure 15.74 The uncontrolled (open-loop) dynamic response of the process to a negative step change in the input flow rate of cooling water from 78.01 down to 73 kg/s.

temperature of the reactor (i.e., “**PV**” signal) will increase and show this kind of an up and down loose oscillatory but stable behavior and eventually levels off to 402.1 K. Notice that all dramatic events take place while the “*PID*” controller (the watching dog) is in sleep mode; that explains why the “**Manual**” (the hand icon) button is clicked on. So, a step decrease in cooling water flow rate from 78.01 down to 73 kg/s will make the uncontrolled process evolve to a new steady-state condition; in this regard, it is a self-regulatory process.

Figure 15.75 shows the liquid-level behavior with time where it shows that the process evolved from the old steady-state (8.6 m) to a negligibly different new steady-state level (8.687 m). There is no reason why it should evolve from the old to any new steady-state condition because the process (organic) fluid is not hydrodynamically perturbed by any means. One may explain, in part, that the increase in liquid volume is a direct result of the thermal volume expansion effect (i.e., increase of volume with increasing temperature from 400 to 402.1 K). Another part may have to deal with the virtual not real picture of the process (see Section 15.23).



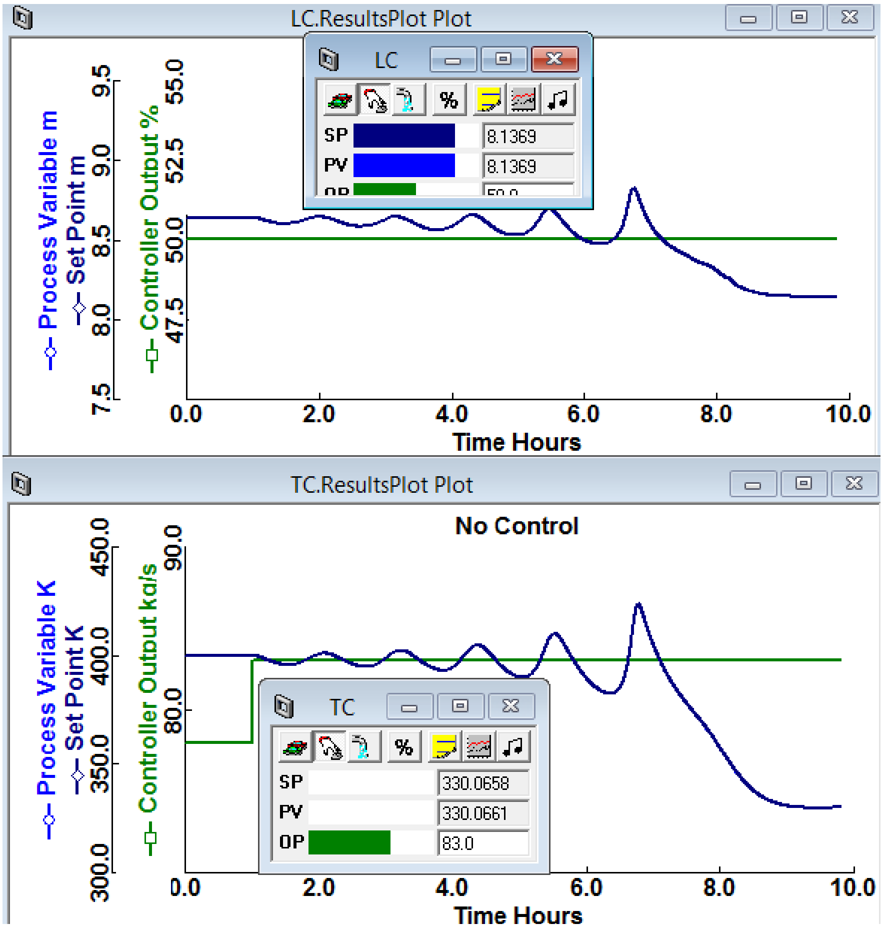
SP 8.6866

PV 8.6866

OP 50.0

Figure 15.75 The open-loop dynamic response of the liquid level as a result of a negative step change in the cooling water flow rate.

On the other hand, Figure 15.76 shows how the process behaves when we manually adjust the input flow rate of cooling water from 78.01 up to 83 kg/s. Both the liquid signal (Figure 15.76 *top*) and the reactor temperature, that is, “**PV**” signal, (Figure 15.76 *bottom*) start this kind of an oscillatory but unstable behavior until the temperature hits a floor value (i.e., $T = 330.07$ K). This value lies between the temperature of the entering ($T = 300$ K) and leaving ($T = 343$ K) cooling medium stream. This condition is called “runaway condition” where a small drift in temperature causes the process to erroneously run a way down to practically the quenching (i.e., no reaction) zone. The following quote is taken from Peacock [4]. “*A small minority of processes are neither self-regulating nor integrating and, rather unhelpfully, are unstable under open-loop control. That is, if you switch the controller to manual, the PV will continue to rise (or fall), possibly in an exponential fashion, until*



LC
SP 8.1369
PV 8.1369
OP 50.0

TC
SP 330.0658
PV 330.0661
OP 83.0

Figure 15.76 The uncontrolled (open-loop) dynamic response of the process to a positive step change in the input flow rate of cooling water from 78.01 up to 83 kg/s. The liquid level signal (*top*) and the reactor temperature (*bottom*).

some physical, possibly disastrous, limit is reached. These are called runaway processes. The most common of these processes is the exothermic reactor with cooling jacket".

On the other hand, the liquid level dropped down to 8.14 m for the same 10-h period. Again, one may explain this, in part, due to the decrease of volume with decreasing temperature. The other reason has to deal with how good the virtual describes the real process.

15.21 THE CASCADE CONTROL

A cascade control structure is made of a master (or main) control loop and a slave (or auxiliary) control loop such that in addition to the main process variable (reactor temperature), more system variables are also measured and fed back as auxiliary process variables (outlet cooling medium temperature and the valve position of the cooling/heating medium).

Cascade control is one of the most common control system structures in process plants. Figure 15.77 shows a general schematic for the concept of cascade control structure, where the controller output (CO) of the master controller is connected as an external set point for the slave controller so that both control loops are nested.

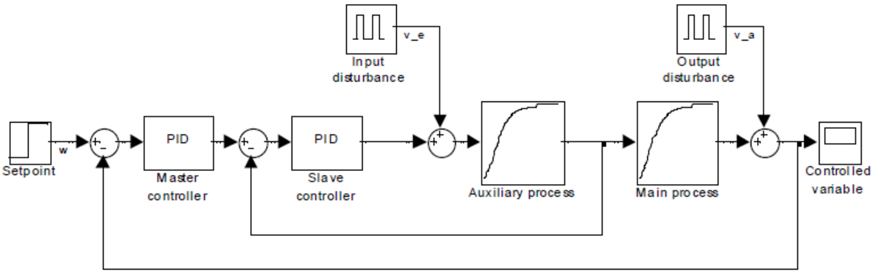


Figure 15.77 A schematic for the cascade control structure. The output of the master (outer) controller acts as the set point for the slave (inner) controller, where the latter manipulates variables (the jacket temperature and valve position) that affect the outer controlled variable (reactor temperature). (Reference: Configuration of Cascade Control SIMATIC PCS 7, Service Portal of Siemens AG, Industry Automation and Drives Technologies, http://support.automation.siemens.com/WW/view/en/43033319. Reprinted with permission).

Figure 15.78 shows a schematic for a cascade control structure that applies to our case. The reactor temperature (external loop) is measured and fed to the master PID controller that holds responsible for reactor temperature. The measured value is compared with an external set point (i.e., history record) and the controller output acts as a set point, but this time, for the slave PID controller that holds responsible for the jacket temperature. The

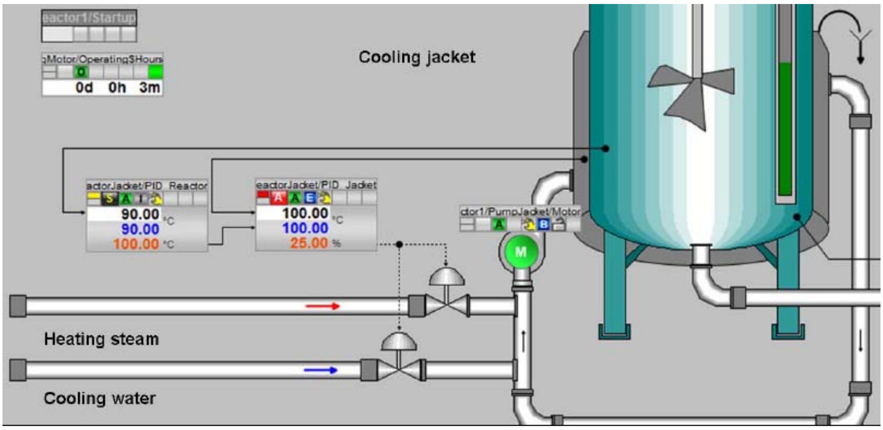


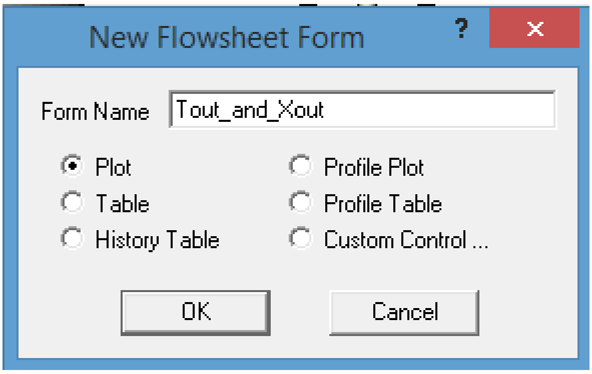
Figure 15.78 A schematic showing how the reactor temperature is controlled via two controllers: the master that holds responsible for the reactor temperature and the slave that holds responsible for the jacket temperature. (Reference: Configuration of Cascade Control SIMATIC PCS 7, Service Portal of Siemens AG, Industry Automation and Drives Technologies, http://support.automation.siemens.com/WW/view/en/43033319. Reprinted with permission).

output from the slave controller will in turn manipulate the valve position of either the cooling or heating medium, often in combination with a split-range at the slave controller to switch between heating and cooling mode.

NOTE #11: *It is common practice that the inner (slave) loop is characterized by a fast dynamic response, as opposed to the outer (master) loop, which is slow in dynamic response. For example, flow change-driven dynamics is faster than temperature change-driven dynamics and the latter is faster than composition change-driven dynamics. Historically, keep in mind that a master (or a boss in work) can be slow and lazy (i.e., the outer loop), whereas a slave (or an employee) must be active and energetic (i.e., the inner loop). The energetic master cannot tolerate a lazy slave; on the other contrary, the energetic slave can survive with a lazy master.*

15.22 MONITORING OF VARIABLES AS FUNCTIONS OF TIME

Let us show how to monitor a dependent variable or a set of variables as a function of time upon causing a change in a certain input variable. The variables to be monitored can be shown in the form of a plot. A plot is created by selecting "**Tools**" | "**New**" → "**New Form** … ". Alternatively, click on the "**New form**" ( ) button at the top toolbar, and the "**New Flowsheet Form**" window will pop up as shown in Figure 15.79.



New Flowsheet Form

Form Name: Tout_and_Xout

● Plot
○ Table
○ History Table
○ Profile Plot
○ Profile Table
○ Custom Control ...

Figure 15.79 Creation of a new flowsheet form.

Provide an appropriate name and click on "**OK**" button. The plot shown in Figure 15.80 will open.

NOTE #12: *You can bring to front any form you create via clicking anywhere on the flowsheet window and then go to "**Flowsheet**" menu followed by "**Forms**" submenu and finally select the name of the form.*

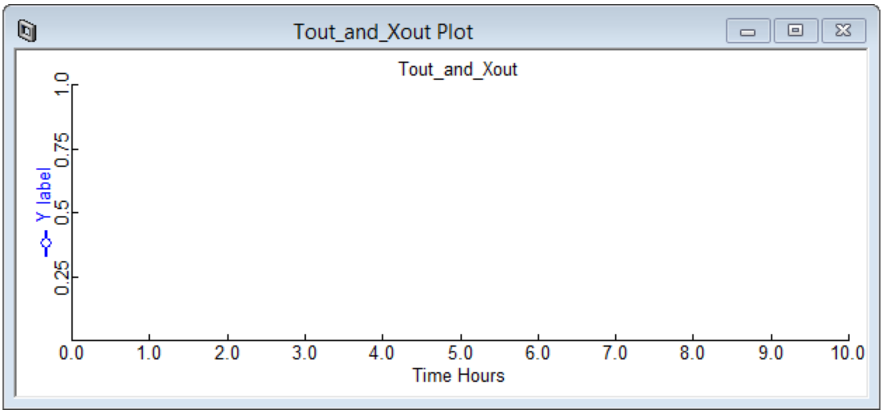


Figure 15.80 The form (window) where we can monitor selected variables as a function of input variable.

To plot the mole fraction of benzene (“**B**”), ethylbenzene (“**EB**”), and diethylbenzene (“**DEB**”), click on the reactor outlet stream, click the right mouse button, and select “**Forms**” | “**AllVariables**” submenu, as shown in Figure 15.81.

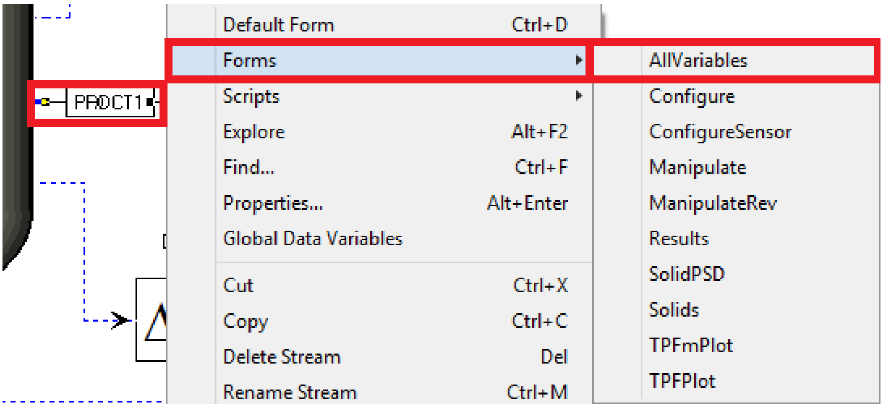
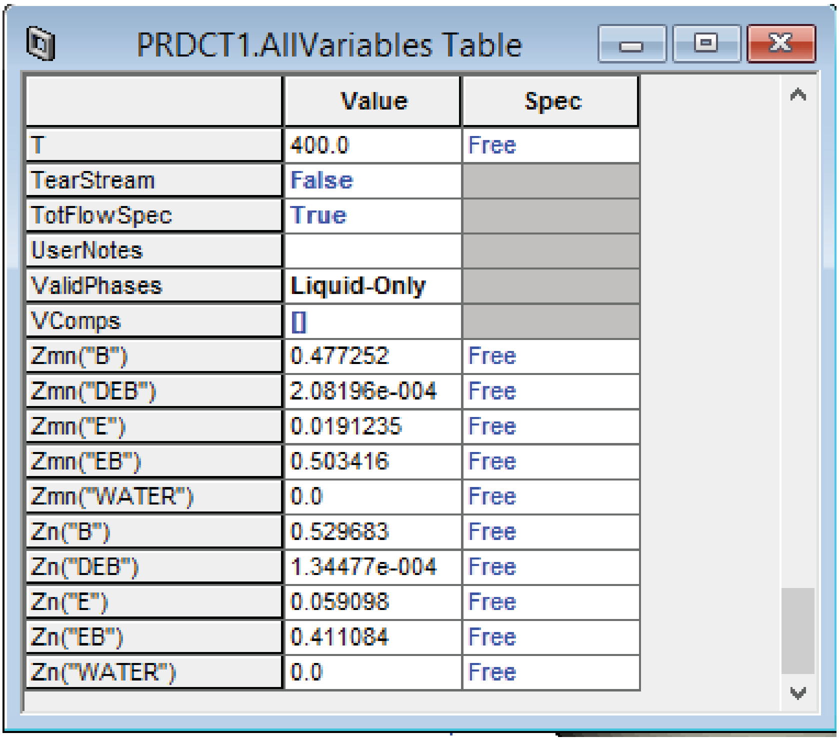


Figure 15.81 Right-click on the highlighted “**PRDCT1**” stream and choose “**Forms**” | “**AllVariables**” submenu to pick up the variables to be plotted in the “**Tout_and_Xout**” form as functions of time.

The window shown in Figure 15.82 will open. Position the cursor on “**Zn(“B”)**” and click. Then, left-click and hold the left mouse button pressed (i.e., drag mode), drag it to the plot window and release the mouse button over there. The procedure is repeated for the other two mole fractions and for the reactor temperature (*T*), as shown in Figure 15.83. Notice that “**Zn**” represents the mole fraction and “**Zmn**” the mass fraction of a substance.

Refer to **NOTE #9** and Figure 15.55 if you wish to carry out some cosmetic changes such that the plot becomes more expressive for itself and more impressive for the one who looks at (the beauty is in the eye of the beholder).



	Value	Spec
T	400.0	Free
TearStream	False	
TotFlowSpec	True	
UserNotes		
ValidPhases	Liquid-Only	
VComps	[]	
Zmn("B")	0.477252	Free
Zmn("DEB")	2.08196e-004	Free
Zmn("E")	0.0191235	Free
Zmn("EB")	0.503416	Free
Zmn("WATER")	0.0	Free
Zn("B")	0.529683	Free
Zn("DEB")	1.34477e-004	Free
Zn("E")	0.059098	Free
Zn("EB")	0.411084	Free
Zn("WATER")	0.0	Free

Figure 15.82 "**PRDCT1.AllVariables Table**" form that shows all product stream variables, including the mole fraction of "**B**", "**DEB**", "**EB**", and the reactor temperature (*T*).

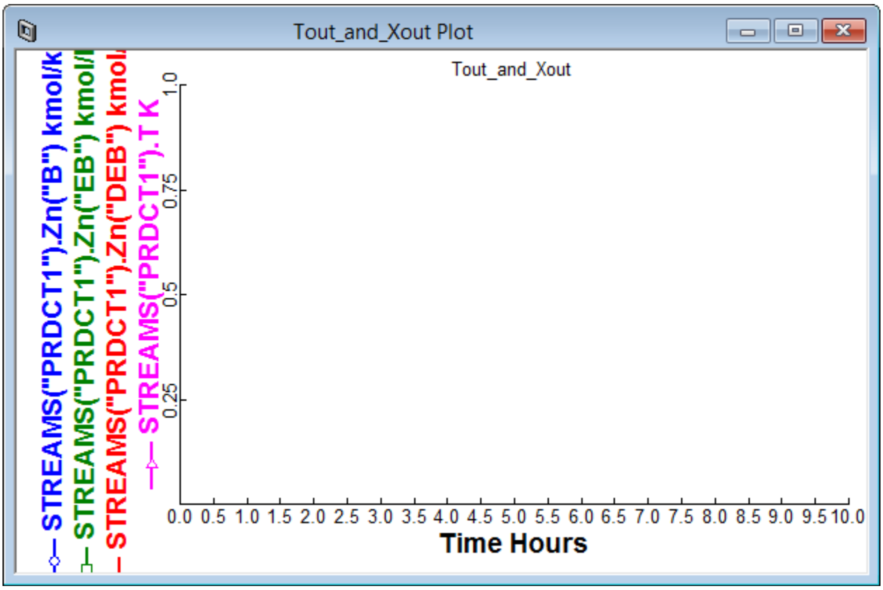


Figure 15.83 Selection of three component mole fractions and the reactor temperature to be each monitored as a function of time.

Double-click “**TC**” node to open its faceplate. Reinitialize APD to any previous successful captured snapshot. It will be better to open “**TC.Configure**” form to see what K_C, τ_I, and τ_D are assigned to “*PID*” temperature controller. Start APD under “*Dynamic*” mode. Let it run for a while until steady-state values are achieved and pause the run. At about 1 h of simulation, make a step change (from 400 to 405 K) in the set-point temperature to see how T affects the mole fraction of the products.

Resume the run, after causing a step-change disturbance. Let the dynamic run continue until new steady-state values are achieved. Figure 15.84 shows the new steady-steady state values for the mole fraction of “**B**”, “**EB**”, and “**DEB**”. Notice that both “**EB**” and “**DEB**” mole fraction increased with increasing T while “**B**” mole fraction decreased. Since “**DEB**” is considered as undesired by-product, the optimum T will be the one with the maximum yield and selectivity. This can be found using the “**Model Analysis Tools**” of Aspen Plus, which will maximize the objective function, the selectivity in this case, as a function of temperature. Notice that if not all four curves appear, then right-click the mouse over the plot area, select “**Properties** … ” submenu followed by “**AxisMap**” tab form and click on “**One for Each**” button.

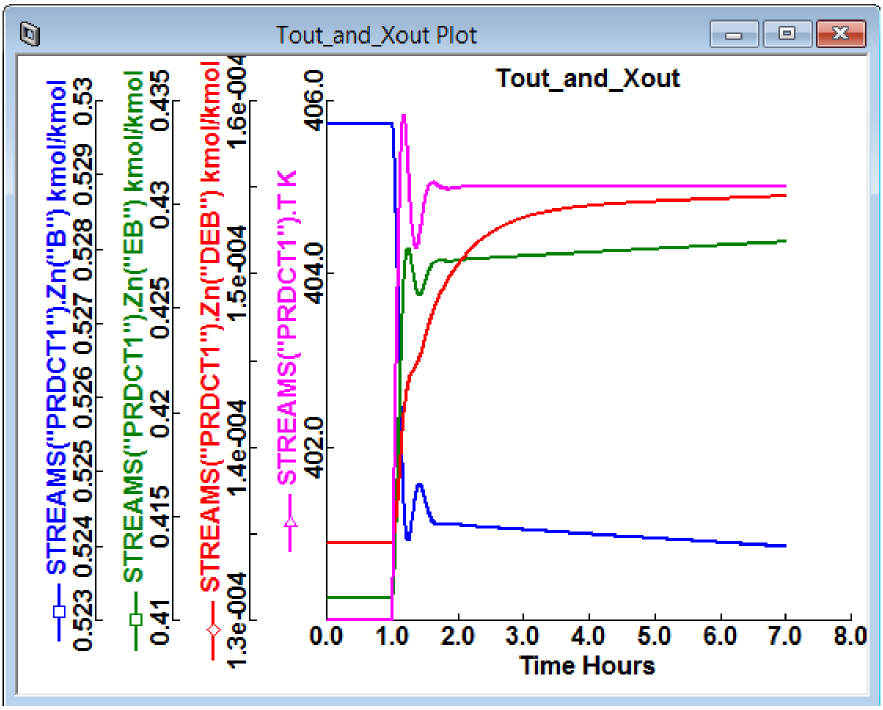
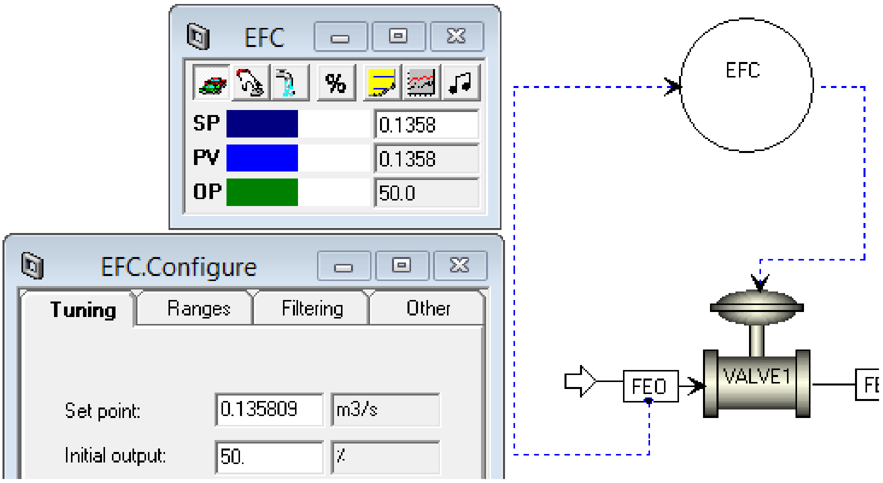


Figure 15.84 A positive step change in reactor T (first top curve) causes an increase in mole fraction of “**DEB**” (second top curve) and “**EB**” (third top curve) while a decrease in “**B**”. (bottom curve)

Finally, a flow rate controller can be installed on both feed streams so that it gives the user the luxury to entertain analyzing the load and set point disturbance of the entering feed on the reactor performance manifested via measurement of the mole fraction (or the selectivity) of the desired product (i.e., “**EB**”). Figure 15.85 shows a flow controller on



SP 0.1358
PV 0.1358
OP 50.0

Set point: 0.135809 m3/s
Initial output: 50. %

Figure 15.85 Installing a flow-rate controller for ethylene stream where the valve position is adjusted based on the desired set point for the feed flow rate. The "**SP**" and "**PV**" have units of m^3/s.

ethylene stream is installed where the user can cause a load or set-point disturbance on the volumetric flow rate of ethylene and see how it affects some downstream reactor properties.

15.23 FINAL NOTES ON THE VIRTUAL (DRY) PROCESS CONTROL IN APD

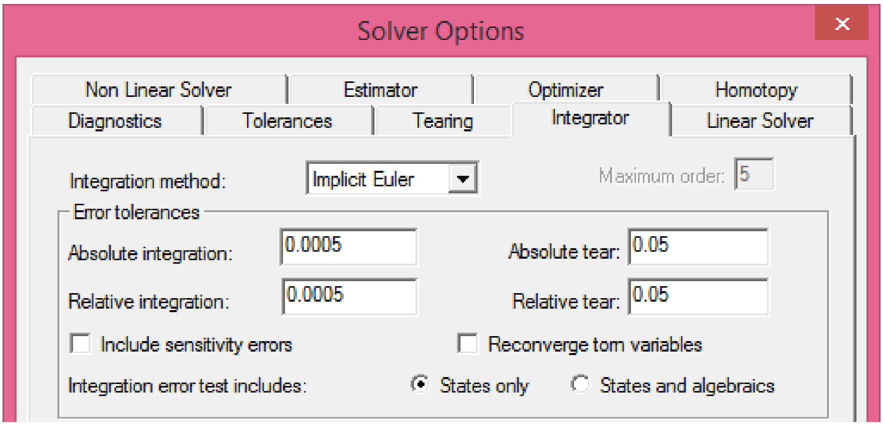
At the end of this episode, I would like to enlighten the user with the virtual (dry) life of process control.

APD attempts to solve a set of non-linear differential/algebraic equations using the common techniques and methods found in standard numerical methods. In general, such methods involve approximation, hence inherent errors, in solving either a non-linear algebraic and/or differential equation. For example, finding the root of a non-linear algebraic equation requires an assumption for the root, while solving an ordinary non-linear differential equation requires an assumption for the step change in time domain. Both steps end up, in general, with an approximate solution that will yield to propagation of errors via iterative (i.e., trial-and-error) techniques and in part contributes to the destabilization of the numerical solution. Moreover, the set of non-linear differential/algebraic equations describing the dynamics of systems, such as a non-isothermal PFR or CSTR case, most likely ends up with what is called a stiff set of differential equations. I quote here from Chapter 7 of my published book [5]:

> A stiff equation is a differential equation for which certain numerical methods for solving the equation are numerically unstable, unless the step size is taken to be extremely small. The main idea is that the equation includes some terms that can blow up the solution (i.e., the values of the dependent variable become infeasible or physically non-sense). When integrating a differential equation numerically, one would expect the suggested step size to be relatively small in a region where the solution curve displays much variation and to be relatively large where the solution curve straightens out to approach a line with slope nearly zero. Unfortunately, this

is not always the case. The ODEs that make up the mathematical models of most chemical engineering systems usually represent a collection of fast and slow dynamics. For instance, in a typical distillation tower, the liquid mechanics (e.g. flow, hold-up) is considered as fast dynamics (time constant ≈ seconds), compared with the tray composition slow dynamics (time constant ≈ minutes). Systems with such a collection of fast and slow ODEs are denoted *stiff systems*.

To make things clearer, let us look at the solver options of APD. Click on the “**Solver Options**” ( ) button (Alternatively, go to “**RUN**” | “**Solver Options** … ” submenu). You will notice that there are different tabs where each tab represents a set of default tuning-up parameters that have to deal with the virtual (dry) life of process control, that is, the simulation or solution of the set of algebraic/differential equations describing the dynamic response of either the open-loop or closed-loop process, as shown in Figure 15.86. Under each tab, there are numerous sets of parameters, which can be modified by the user; however, you need to be aware how each parameter affects the performance of the simulation process.



Integration method: Implicit Euler

Maximum order: 5

Error tolerances

Absolute integration: 0.0005

Absolute tear: 0.05

Relative integration: 0.0005

Relative tear: 0.05

☐ Include sensitivity errors

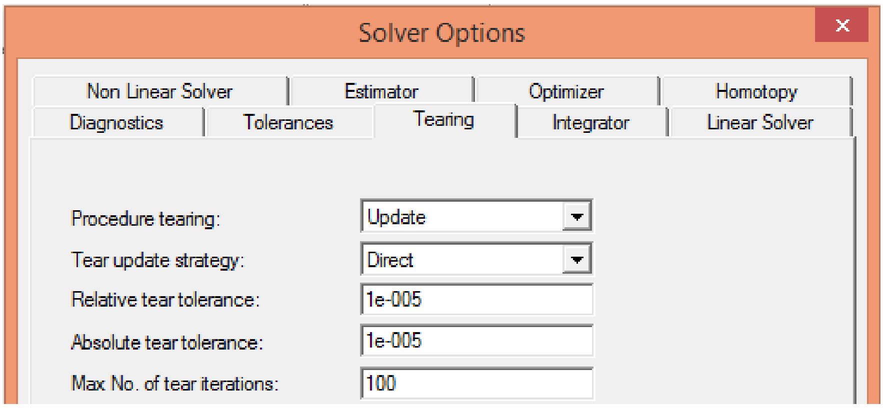
☐ Reconverge torn variables

Integration error test includes: ● States only ○ States and algebraics

Figure 15.86 The “**Solver Options**” form that contains many tabs where each tab window allows the user to modify some parameters that affect the performance of APD solver (i.e., simulator).

Out of such tabs, we have the “**Tearing**” tab, shown in Figure 15.87, which represents the “**Tearing**” method that enables the user to control the options for tearing procedure. “Aspen Modeler” is an equation-based simulator. For example, for steady-state or initialization simulations, and for reinitializations with the “**Gear**” integrator, all the simulation equations are solved simultaneously. To make this task easier, “Aspen Modeler” applies decomposition to break down the sets of equations into groups. Each equation group is then solved in sequence. The degree to which the equations can be broken down into groups depends on the nature of the simulation. Typically, simulations of processes with recycles require that more of the equations be solved together in one large group. This is more difficult than solving many smaller groups.

Consequently, the tearing procedure enables you to influence the way a simulation is solved and to improve the decomposition by decoupling the procedure inputs and outputs.



Procedure tearing: Update

Tear update strategy: Direct

Relative tear tolerance: 1e-005

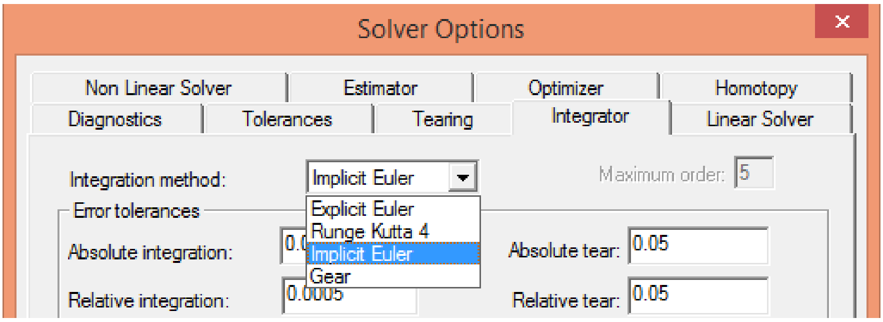
Absolute tear tolerance: 1e-005

Max No. of tear iterations: 100

Figure 15.87 Selection of the type of tearing procedure tells Aspen Plus how to deal with the set of algebraic/differential equations in terms of splitting them into subgroups or keeping them as one unity.

Use "**Procedure tearing**" drop-down list to break the simulation down into smaller groups of equations. The "*Update*" (default) torn procedures are calculated throughout solution of decomposed runs; the "*Start*" torn procedures are calculated once at the start of the simulation, and "*Complete*" torn procedures are never calculated (i.e., all equations are dealt with as one large group).

A second tab window has to deal with the numerical integration method (Integrator) being used for solving a set of ordinary differential equations, as shown in Figure 15.88. The "**Integrator**" tab form enables you to choose the integrator you use for your simulation. The integrator you choose depends on the type of models you have in the flowsheet and the objective of the run. It is a decision to be made by the user to trade-off between speed (i.e., less accurate) and robustness (i.e., more accurate). See Table 15.1 for the four different types of integrator available in APD and their recommended applications. Notice that other tab windows are also important and do have adjustable parameters that can be modified and, in general, will affect the solver performance in terms of speed versus accuracy.



Integration method: Implicit Euler

Maximum order: 5

Error tolerances

Absolute integration: 0.0

Relative integration: 0.0005

Absolute tear: 0.05

Relative tear: 0.05

Figure 15.88 The selection of numerical integration method (Integrator) being used for solving a set of ordinary differential equations, where a compromise is made between speed (but less accurate) and robustness (but more accurate).

TABLE 15.1 The Four Types of Integrator (Under "Integrator" Tab) and Their Applications.

Integrator	Application
Explicit Euler	Explicit first-order method. Fastest integration method with consistent speed but can become unstable. Often requires a very small step size to maintain stability.
Runge–Kutta 4	Fourth-order Explicit method. Suitable for some stiff systems. Variable step size is used to maintain error. It can be good for problems with a large number of disturbances.
Implicit Euler	First-order Implicit Euler method. Step size can be variable (to control integration error) or fixed (integration error ignored). A fixed step method can be used for simple flowsheets where a reliable, predictable integration is needed. A variable step method (the default) should be used where the error must be controlled.
Gear	Variable order, variable step backward difference implicit method. Uses decomposition and obeys procedure tearing. You can define the behavior of the method for model discontinuities and variable step changes. Use when high accuracy is required.

Figure 15.89 shows the closed-loop dynamic response of the process to a negative step change in set point from 400 down to 395 K while using the default solver settings.

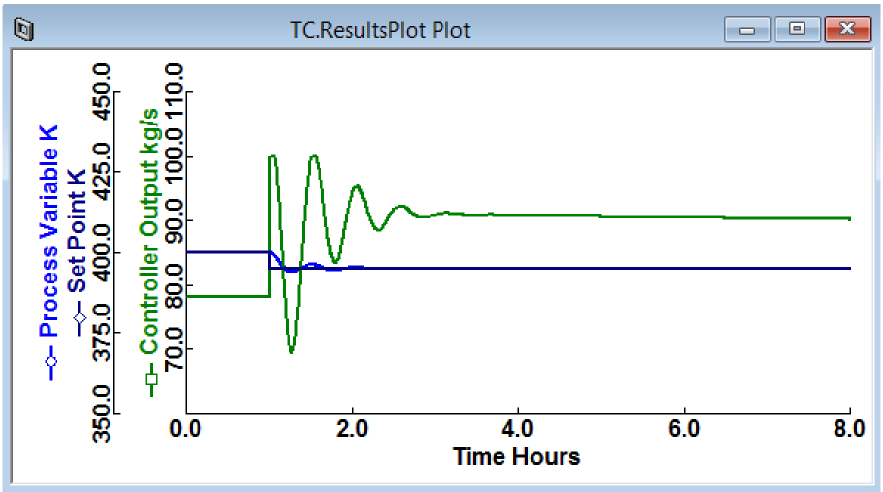


Figure 15.89 The closed-loop dynamic response of the process to a negative step change from 400 down to 395 K while using the default APD solver settings. A "*PID*" controller, with $K_C = 20.54$ and $\tau_I = 7.2$ min, and $\tau_D = 1.8$ min, is used.

Figure 15.90 shows the same response for the same magnitude of set-point disturbance; however, some solver settings are made tighter "more conservative" in terms of accuracy,

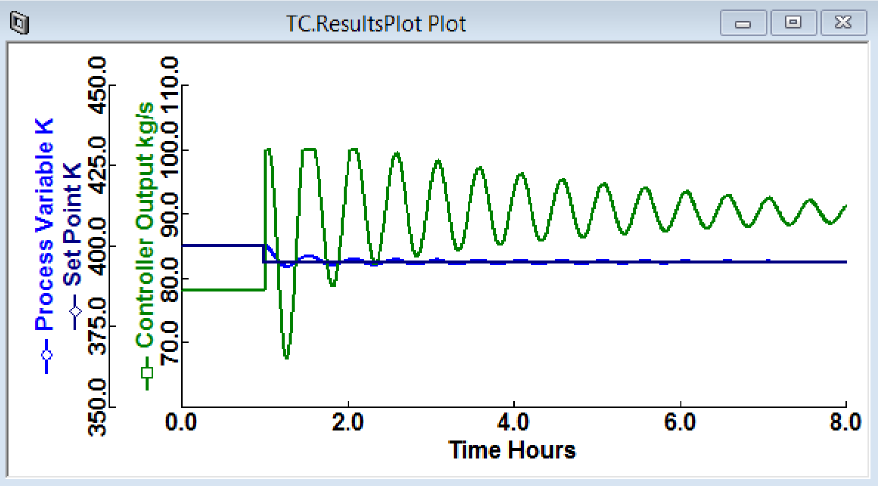
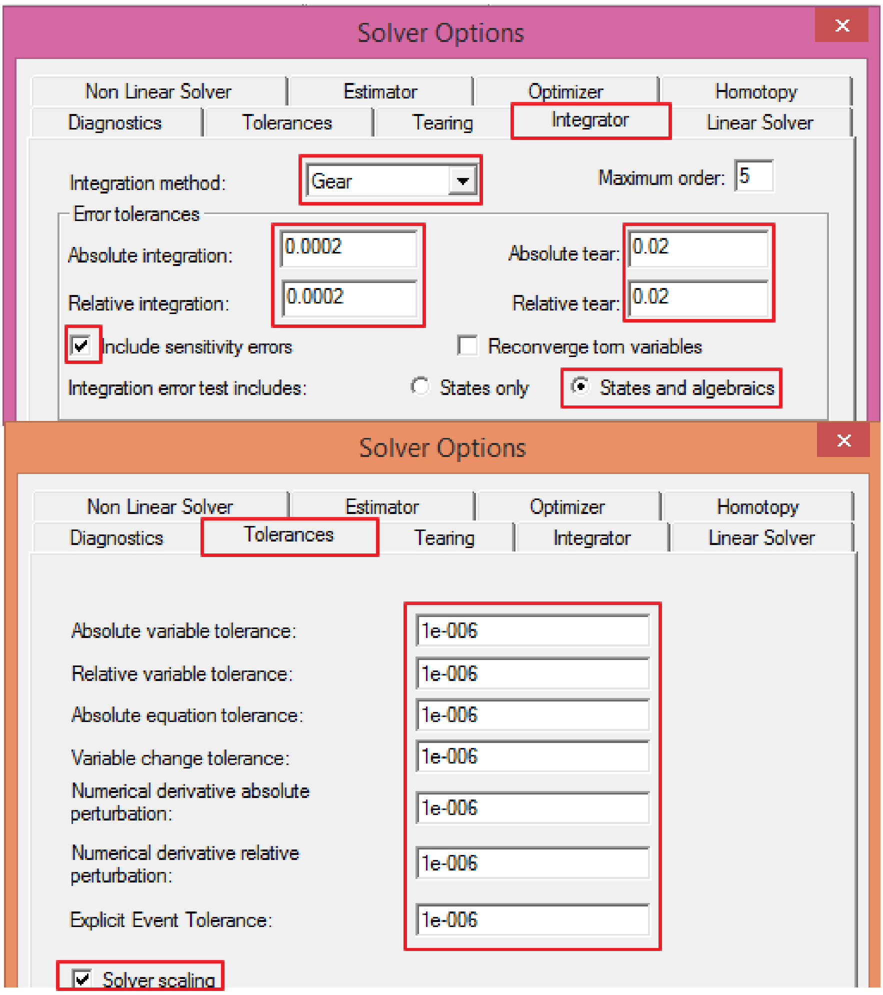


Figure 15.90 The closed-loop dynamic response of the process to a negative step change from 400 down to 395 K while making APD solver settings more “conservative” in terms of accuracy. A “*PID*” controller, with $K_C = 20.54$ and $\tau_I = 7.2$ min, and $\tau_D = 1.85$ min, is used.

as shown in Figure 15.91. Obviously, the “virtual” process becomes more sensitive (or vulnerable) to the disturbance or perturbation caused by the set-point change given that both controller output (“**OP**”) and process variable (“**PV**”) signal exhibit such a pronounced oscillatory behavior toward reaching the new final steady-state temperature. If a person is so sensitive and extra delicate, then he/she will be more sensitive, hence vulnerable to background noise and disturbance to the point that he/she may end up with a nervous breakdown (i.e., an unstable behavior).

On the other hand, it is worth mentioning here that there is no significant difference in the closed-loop dynamic response of the process carried out under “default” and “conservative” APD solver settings for the positive step change in the set point from 400 up to 405 K,



Integration method: Gear

Maximum order: 5

Error tolerances

Absolute integration: 0.0002

Relative integration: 0.0002

Absolute tear: 0.02

Relative tear: 0.02

☑ Include sensitivity errors

☐ Reconverge torn variables

Integration error test includes: ○ States only ● States and algebraics

Absolute variable tolerance: 1e-006

Relative variable tolerance: 1e-006

Absolute equation tolerance: 1e-006

Variable change tolerance: 1e-006

Numerical derivative absolute perturbation: 1e-006

Numerical derivative relative perturbation: 1e-006

Explicit Event Tolerance: 1e-006

☑ Solver scaling

Figure 15.91 Some APD solver settings are made more “conservative” in terms of accuracy.

as shown in Figure 15.92. This also has to deal, to a large extent, with the uncontrolled (open-loop) but stable behavior on the right-side of the set point (see Figure 15.74) versus the uncontrolled but unstable behavior on the left side of the set point (see Figure 15.76).

In conclusion, the APD platform has to be tuned-up, first, for a given, highly intricate and interacting process (i.e., a system of coupled algebraic/differential equations) and controller tune-up tests can then be carried out, as well as, studying set-point and load disturbance effects on the process performance.

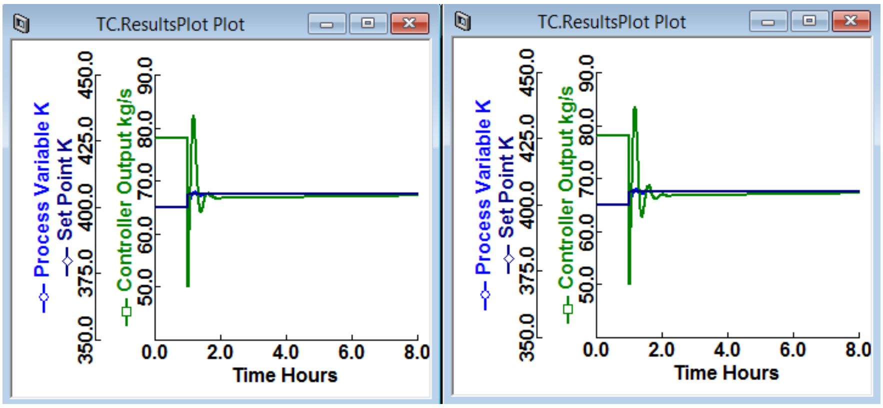


Figure 15.92 The closed-loop dynamic response of the process to a positive step change from 400 up to 405 K under default (*left*) and more conservative (*right*) APD solver settings, from accuracy standpoint. A "*PID*" controller, with $K_C = 20.54$ and $\tau_I = 7.2$ min, and $\tau_D = 1.85$ min, is used.

NOTE #13: *For all problems here, remember to run APD under "Initialization" mode each time you create a control loop made of control elements and control signals. Always check the default "OP", "PV", and "SP" signal values for each constructed control loop.*

Moreover, do not forget to periodically capture a snapshot for a successful simulation run and save it each time with a different name.

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HOMEWORK/CLASSWORK 15.1 (A CASCADE CONTROL OF A SIMPLE WATER HEATER)

Consider the flowsheet of a water heating process as shown in Figure 15.93:

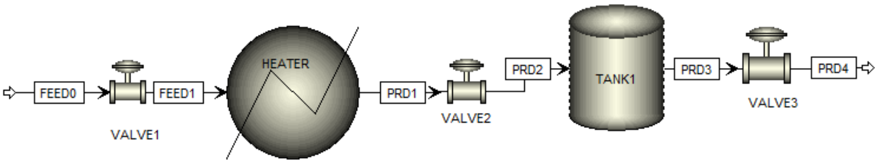


Figure 15.93 A simple water heating process made of a heater, storage tank, and flow-regulating valves.

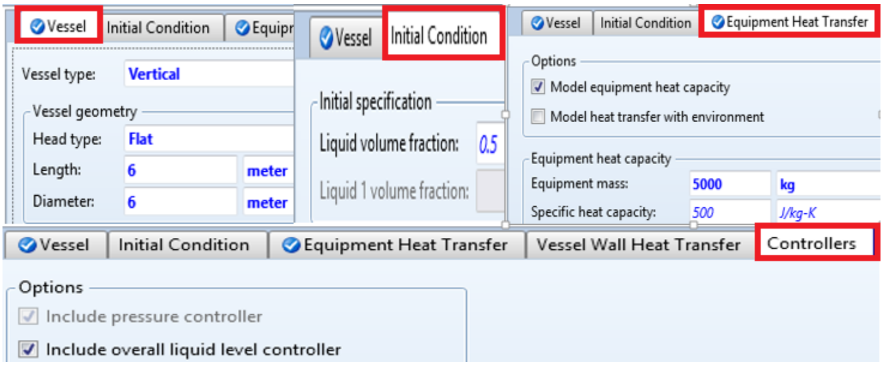
The process mainly consists of a heater, storage tank, and three flow-regulating valves. The process is made simple to tackle process dynamics and control aspects. The following is a portion of the created "**Input File**":

```
COMPONENTS
    H2O H2O
FLOWSHEET
    BLOCK VALVE1 IN=FEED0 OUT=FEED1
    BLOCK VALVE2 IN=PRD1 OUT=PRD2
    BLOCK HEATER IN=FEED1 OUT=PRD1
    BLOCK TANK1 IN=PRD2 OUT=PRD3
    BLOCK VALVE3 IN=PRD3 OUT=PRD4
PROPERTIES STEAMNBS FREE-WATER=STEAMNBS
ESTIMATE ALL
STREAM FEED0
    SUBSTREAM MIXED TEMP=300 K. PRES=5. <atm>
    MOLE-FLOW H2O 1 kmol/s.
BLOCK TANK1 MIXER
    PARAM PRES=3.7 <atm> NPHASE=1 PHASE=L
    BLOCK-OPTION FREE-WATER=NO
BLOCK HEATER HEATER
    PARAM TEMP=400 K. PRES=4.2 <atm> NPHASE=1 PHASE=L
    BLOCK-OPTION FREE-WATER=NO
BLOCK VALVE1 VALVE
    PARAM P-DROP=0.5 <atm>
BLOCK VALVE2 VALVE
    PARAM P-DROP=0.5 <atm>
BLOCK VALVE3 VALVE
    PARAM P-DROP=0.2 <atm> NPHASE=1 PHASE=L
    BLOCK-OPTION FREE-WATER=NO
```

As can be seen, the flowsheet is configured to be fully pressure driven (i.e., the flow is downhill from an upstream to downstream zone). First, run under "**Properties**" environment, assure that there is no error or serious warning, and once you successfully complete the properties analysis step, switch to "**Simulation**" environment. Run the solver under "**Steady-State**" mode and assure that there is no error/serious warning. Activate "**Dynamic**" mode using "**Dynamics**" | "**Dynamic Mode**" button.

On one hand, Figure 15.94 shows the different tab windows for entering options pertaining to the tank "**Dynamic**" sheet.

On the other hand, for the heater block dynamics, select the "**Heater type**" as "*Instantaneous*" in "**Blocks**" **|** "**HEATER**" **|** "**Dynamic**" **|** "**Heater Type**" tab form.



Vessel type: Vertical

Vessel geometry

Head type: Flat

Length: 6 meter

Diameter: 6 meter

Initial specification

Liquid volume fraction: 0.5

Liquid 1 volume fraction:

Options

☑ Model equipment heat capacity

☐ Model heat transfer with environment

Equipment heat capacity

Equipment mass: 5000 kg

Specific heat capacity: 500 J/kg-K

Options

☑ Include pressure controller

☑ Include overall liquid level controller

Figure 15.94 Options to be entered for tank “**Dynamic**” items.

After a successful run, click on the “**Dynamics**” | “**Pressure Checker**” button and assure that you get the message saying: “The flowsheet is configured to be fully pressure driven”.

Click on the “**Dynamics**” | “**Pressure Driven**” button to export the dynamic simulation into APD environment and give a name for the “**P Driven Dyn Simulation** (*.dynf)” type file, which can be later opened by APD. The imported flowsheet will be similar to that shown in Figure 15.95.

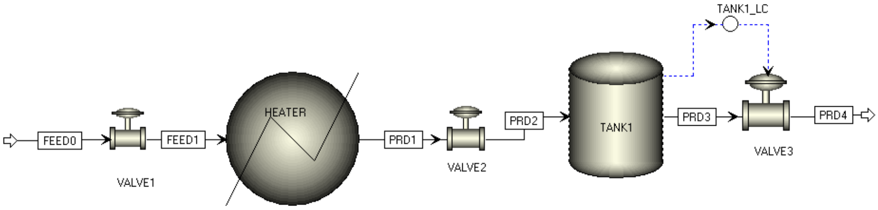


Figure 15.95 The flowsheet as imported to APD simulator with an installed liquid level controller.

A cascade control structure will be installed, as shown in Figure 15.96. The cascade structure consists of the temperature control master loop and level control slave loop. On

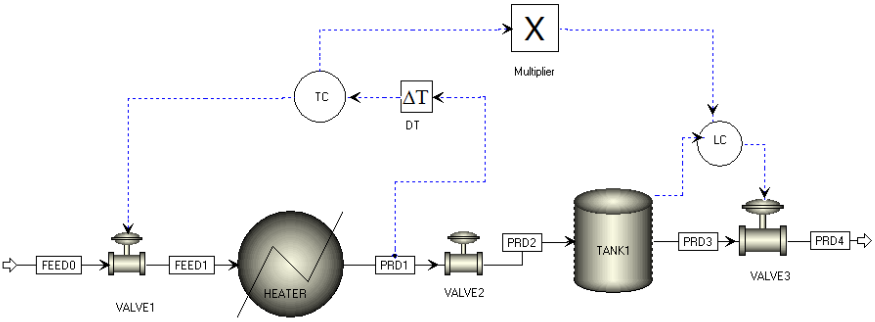
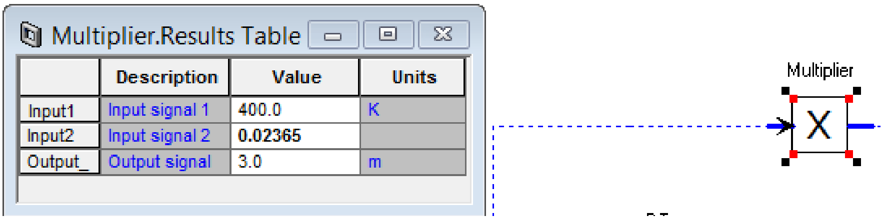


Figure 15.96 A cascade control structure with a master and slave loop. The master loop is the temperature control and the slave loop is the liquid level control.

one hand, the temperature control loop itself is made of a dead time ("**DT**") block, the temperature control element ("**TC**") and three connecting control signals (the dotted lines). On the other hand, the liquid level control loop is made of a level control element and two connecting control signals. Importantly, the connection between the master and slave loop is maintained via a connecting control signal, the multiplier ("**Multiplier**"), and another connecting control signal.

The multiplier is used to make the proper conversion factor between temperature and level signal. Figure 15.97 shows the "**Multiplier.Results Table**" form where it shows that this element receives the signal from the outer temperature control loop and using the adjustable parameter, that is, "**Input 2**", the "**Output_**" signal will be calculated and transmitted to the inner (slave) level control loop as a set point.



	Description	Value	Units
Input1	Input signal 1	400.0	K
Input2	Input signal 2	0.02365	
Output_	Output signal	3.0	m

Figure 15.97 The "**Multiplier.Results Table**" form where the signal from "**TC**" loop is multiplied by an adjustable parameter, that is, "**Input2**", and the "**Output_**" signal will be calculated and transmitted to "**LC**" loop as a set point. *See Plate section for color representation of this figure*.

NOTE: If "**Input1**" value, shown in Figure 15.97, is not set to 400 K, then you have to open "**TC.Configure**" window and click on "**Initialize Values**" button to reset the value to the steady-state temperature, borrowed from Aspen Plus steady-state simulator. To be on the safe side, run APD under "*Initialization*" mode once prior to any "*Dynamic*" test.

For the dead time ("**DT**") unit, set its "**DeadTime**" value as 1 min.

Notice that once you add a connecting stream signal, all possible blue arrows will show up where you can hook it either as a source or destination. For the "**TC**" output signals, there are two signals: One goes out as "**TC.OP**" controller output for manipulating the final control element, that is, the valve and another one acts as "**TC.SP**" set-point, which will go to the multiplier as "**Multiplier.Input1**" and be multiplied by an adjustable factor to convert it into a level signal so that the signal leaves the multiplier as "**Multiplier.Output_**" and at the same time enters into "**LC**" node as a remote set point ("**LC.SPRemote**") for the level controller.

Moreover, do not forget to change the "**Communication**" time to a more appropriate value, say 0.005 h (See Figure 15.35). Use the default APD-assigned parameters for both controllers. Set the range minimum and maximum to 350 and 450 K, respectively as far as "**PV**" and "**SP**" signal for temperature controller are concerned.

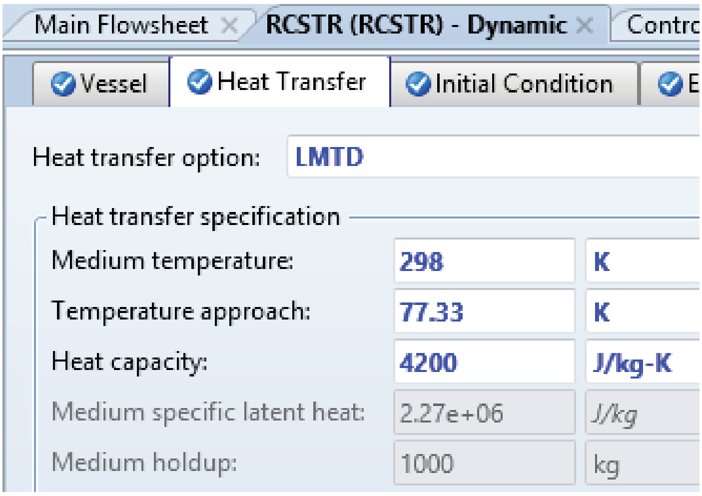
a) Carry out both an open-loop and closed-loop ATV test for "**TC**" unit. Using Ziegler–Nichols as the tuning rule, report "*PID*" controller tune-up parameter values. Notice that the closed-loop ATV test for temperature controller can be done under "**Auto**" or "**Cascade**" mode. After restarting the APD solver to time zero and carrying out a successful "*Initialization*" run, update the temperature controller tune-up parameters with those of the closed-loop ATV test.

b) The APD platform is now ready for carrying out a set-point and load temperature disturbance. Cary out both a set-point and load disturbance in both an increasing and decreasing direction. Change "**SP**" by ±10 K and "**OP**" by ±10%. Show the plot of temperature profile (i.e., "**OP**", "**PV**", and "**SP**" as f(dynamic time)) for the four cases.

Keep in mind that "**LC**" is always run under "**Cascade**" (third button of **LC** faceplate labeled with the water fountain icon) mode. For "**TC**" control unit, you must switch to automatic mode if you plan to change the set point (i.e., click "**Auto**" (first button of **TC** faceplate) button). On the other hand, if you plan to change the "**OP**" signal, then you need to momentarily switch to "**Manual**" (second button of **TC** faceplate) mode, make the "**OP**" step change, and then be back to "**Cascade**" mode.

HOMEWORK/CLASSWORK 15.2 (A CSTR CONTROL WITH "LMTD" HEAT TRANSFER OPTION)

Repeat the same tasks that are outlined in this chapter tutorial; however, in "**Heat Transfer**" tab window of "**CSTR**" block (see Figure 15.15) change the "**Heat transfer option**" from "*Dynamic*" to "LMTD" as shown in Figure 15.98. Notice that the difference between "*Dynamic*" and "*LMTD*" is in spelling out the medium hold-up of the cooling jacket. Other dynamic options remain the same as those shown in this chapter.



Heat transfer option: LMTD

Heat transfer specification

Medium temperature: 298 K

Temperature approach: 77.33 K

Heat capacity: 4200 J/kg-K

Medium specific latent heat: 2.27e+06 J/kg

Medium holdup: 1000 kg

Figure 15.98 The dynamic heat transfer option for "**CSTR**" block.

a) Reinitialize, run the show, and check for any simulation error or serious warning.

b) Check that the process is pressure driven via clicking the on "**Pressure Checker**" button.

c) Export the file to APD environment via clicking on "**Pressure Driven**" button and saving it as "**P Driven Dyn Simulation**" type file, with the file extension "***.dynf**".

d) Go to APD simulator main window. In addition to the existing "**LC**" control unit, add "**TC**" control unit augmented by the "**Dead_time**" element and assign a value of 1 min for the dead-time unit. Notice that the final control element will manipulate the cooling medium flow rate.

e) Open "**TC.Configure**" window and click on "**Initialize Values**" button to reset the value to the steady-state temperature borrowed from Aspen Plus steady-state simulator. To be on the safe side, run APD under "*Initialization*" mode once prior to any "*Dynamic*" test.

f) Change the "**Communication**" time to a more appropriate value, for instance, 0.005 h (see Figure 15.35). Use the default APD-assigned parameters for both controllers.

g) Open "**TC.Configure**" window. Under "**Ranges**" tab window, change "**PV**" and "**SP**" range to be limited between 350 and 450 K. Do not forget to select the check button to clip values to the assigned ranges for all T signals.

h) Open "**TC.Tune**" window. Under "**Test**" tab, use the default relay amplitude of 5% of the output range. Carry out a closed-loop ATV test**.** Using Ziegler–Nichols as the tuning rule, report "*PID*" controller parameter values.

i) Assign the closed-loop ATV test-estimated parameters to the "*PID*" temperature controller.

j) Cary out both a set-point and load disturbance in both an increasing decreasing direction. Change "**SP**" by ±10 K for the set-point disturbance and "**OP**" by 78.106 ± 8 kg/s for the load disturbance. Report how the civilized (controlled) process behaves in both directions.

k) Carry out uncontrolled (i.e., open-loop) dynamic response test by causing a load disturbance both in an increasing and decreasing "**OP**" direction. Change "**OP**" by 78.106 ± 8 kg/s. The "**Manual**" mode must be maintained before and after causing the load disturbance. Report how the wild (uncontrolled) process behaves in both directions.

HOMEWORK/CLASSWORK 15.3 (A PFR CONTROL FOR ETHYLBENZENE PRODUCTION)

Repeat the same tasks that are outlined in this chapter tutorial; however, using a plug flow reactor (PFR) instead of CSTR as shown in Figure 15.99.

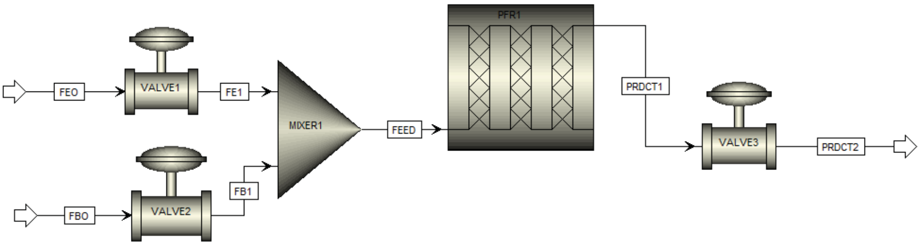
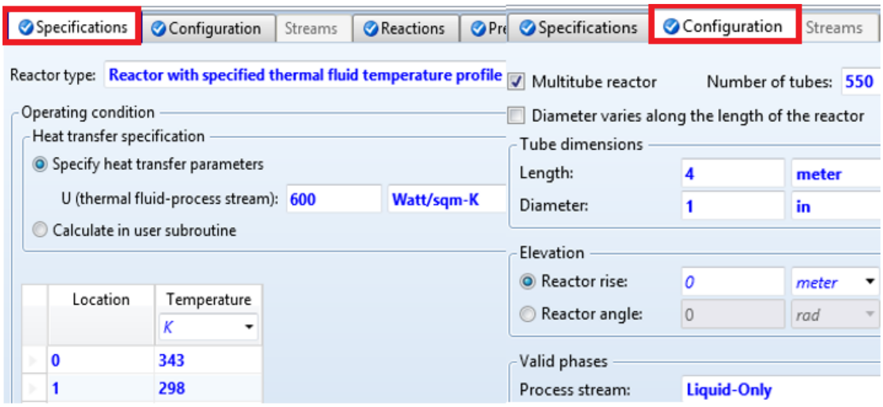


Figure 15.99 The flowsheet for "EB" production using a PFR, instead of CSTR.

The following settings are pertinent to PFR as shown in Figure 15.100.



Reactor type: Reactor with specified thermal fluid temperature profile

Operating condition

Heat transfer specification

● Specify heat transfer parameters

U (thermal fluid-process stream): 600 Watt/sqm-K

○ Calculate in user subroutine

Location	Temperature
	K
0	343
1	298

☑ Multitube reactor Number of tubes: 550

☐ Diameter varies along the length of the reactor

Tube dimensions

Length: 4 meter

Diameter: 1 in

Elevation

● Reactor rise: 0 meter

○ Reactor angle: 0 rad

Valid phases

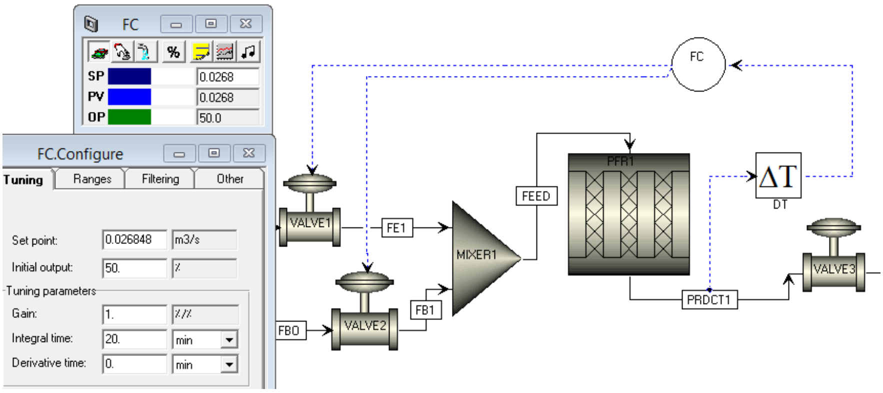
Process stream: Liquid-Only

Figure 15.100 PFR specifications that need to be entered by the user.

Run the simulation, check for any error or serious warning.

Switch to “*Dynamic*” mode using the “**Dynamic Mode**” button. For mixer dynamic, the vessel type will be set to “*Instantaneous*” and for PFR dynamic under “**Equipment Heat Transfer**” tab, select “**Model equipment heat capacity**”, with wall temperature being same as process stream temperature (i.e., neglecting the thermal inertia of metal wall) and the equipment mass is set to *7000 kg*.

Run the simulation under “*Dynamic*” mode and watch out any error or serious warning. Check that the process is fully configured to be pressure driven using “**Pressure Checker**” button. Export to APD environment using the “**Pressure Driven**” button. Add the following flow control “**FC**” loop to the flowsheet as shown in Figure 15.101. The “**Dead_time**” element is assigned one minute (1 min) for the dead-time value.



SP 0.0268

PV 0.0268

OP 50.0

Set point: 0.026848 m3/s

Initial output: 50. %

Tuning parameters

Gain: 1. %/%

Integral time: 20. min

Derivative time: 0. min

Figure 15.101 The flow control unit is imposed on the process, augmented by the dead-time control element.

The volumetric flow rate of the product stream will be measured and transmitted to the control unit and be compared with the set-point value and the controller output will be a function of the difference between measured and preset value, which will finally manipulate the position of the two feed valves.

Refer to the notes and previous two problem statements on how to prepare APD simulation environment for carrying out the closed-loop ATV test, assigning the tune-up parameters to "*PI*" controller, and finally carrying out the set-point and load disturbance test both in an increasing and decreasing direction. Report the result for the test and disturbance tests. Your job is also to select whether the controller should be run in "*Direct*" or "*Reverse*" mode. Moreover, for the same closed-loop ATV test try to use "*PID*" instead of "*PI*" flow controller and see how the controller type affects the performance or stability of the closed-loop dynamic response of the process.

16

SAFETY AND ENERGY ASPECTS OF CHEMICAL PROCESSES

16.1 INTRODUCTION

If there is another fossil fuel surplus, as is the case with oil and natural gas, it will probably be natural gas liquids (NGLs, not to be confused with liquefied natural gas (LNG)). Unconditioned NGLs usually contain about 28 wt% of C1–C4 hydrocarbons and the rest is C4+ hydrocarbons. There are many applications for NGLs, including nearly all sectors of the economy. NGLs are used as feedstock for petrochemical plants, burned for space heat and cooking, and blended into a vehicle fuel. A blend of propane and butane, sometimes referred to as "autogas", is a popular fuel in some parts of Europe, Turkey, and Australia. Natural gasoline (pentanes plus) can be blended into various kinds of fuel for combustion engines and is useful in energy recovery from wells and oil sands.

16.2 PROBLEM DESCRIPTION

The natural gas liquids (NGLs) produced from wells must be conditioned before they can be economically transmitted through pipelines. The conditioning process generally involves removal of brine (salt water), hydrogen sulfide, sand, and dissolved light gases. The high pressure liquid from field gathering lines is depressurized and sent through a knock-out drum with water boot to separate brine from the hydrocarbon liquid. The knock-out drum and the let-down valves can be modeled together by "**Flash2**" type block connected to water decant stream. Moreover, The stabilization is carried out in distillation column, which removes hydrocarbons lighter than butanes. The amount of butane allowed in the liquid product depends on the Reid vapor pressure specifications. The NGL and gas products are then pressurized to the pipeline pressure. The goal here is to demonstrate the safety

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Aspen Plus®: Chemical Engineering Applications, First Edition. Kamal I.M. Al-Malah.

Companion Website: www.wiley.com/go/Al-Malah/AspenPlusApplications

and energy aspects of such a petroleum process. Aspen Plus$^{®}$ provides “**ngl.bkp**” as an example (i.e., “**C:\Program Files (x86)\AspenTech\Aspen Plus V8.8\GUI\Examples**”), which can be reached via “**Examples**” button found in “**Resources**” ribbon.

16.3 THE “SAFETY ANALYSIS” ENVIRONMENT

I will not elaborate on the successful completion of the first two compulsory steps: “**Properties**” and “**Simulation**”, which are essential for any process flowsheet simulation. The components, the property method, and stream and block operating conditions are all given in the example. However, based on the warning messages issued by Aspen Plus, the following two databanks were added to the default selected databanks: “**ETHYLENE**” and “**NRTL-SAC**”. The property method is selected as “**RK-SOAVE**”. What you need to do is to save the file, in a separate folder, as an *.apw file, then run the file under “**Properties**” followed by “**Simulation**” environment. Let us switch to third environment, that is, “**Safety Analysis**”. Figure 16.1 shows the Aspen Plus under “**Safety Analysis**” environment.

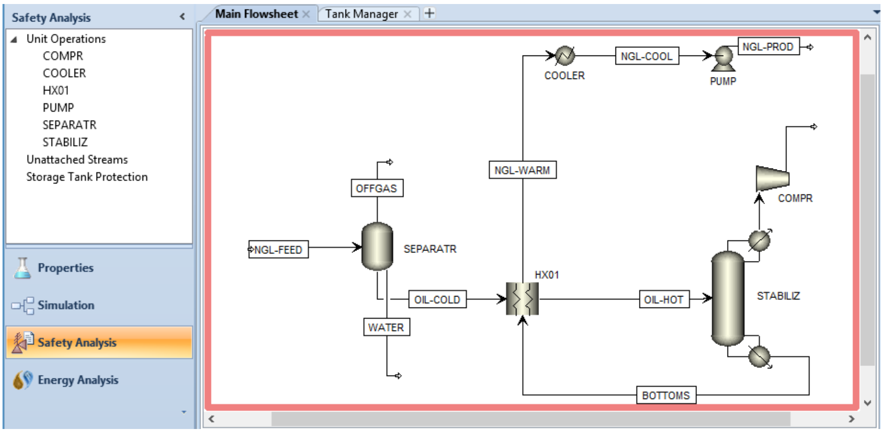


Figure 16.1 The process flowsheet for NGL conditioning made of “**Flash2**” separator, “**MHeatX**” exchanger, “**Heater**” exchanger, “**Pump**” pressure changer, “**RadFrac**” column, and “**Compr**” pressure changer. See “**Model Palette**” for such types of blocks.

NOTE #1: *The “**Safety Analysis**” environment requires that the “**Simulation**” environment is successfully completed. When you switch to the “**Safety Analysis**” environment, if the “**Simulation**” environment is incomplete then you will be informed of this issue. Moreover, Aspen Plus will allow you to move back and forth among different environments, upon successful completion of the prerequisite step(s).*

The “**Safety Analysis**” environment lets the user analyze overpressure scenarios, determine which contingencies require pressure relieving devices, size these devices according to appropriate standards, and generate appropriate documentation for analysis. **P**ressure **R**elieving **D**evices (**PRDs**) are critical components of the pressure relief and safety systems for chemical plants, refineries, and similar industrial applications. There are many types and designations of **PRD**s; some acronyms typically used in the domain are **P**ressure **R**elief **V**alves devices (**PRVs**), **P**ressure **S**afety **V**alves (**PSVs**), **R**elief **V**alves (**RVs**), **S**afety **R**elief **V**alves (**SRVs**), **S**afety **V**alves (**SVs**), **T**emperature **R**elief **V**alves (**TRVs**), or **T**emperature **S**afety **V**alves (**TSVs**). **PRDs** are attached to equipment in order to prevent overpressuring. Because the primary function of this equipment is safety, it is imperative that **PRDs** are designed properly. Process simulators can aid process engineers when analyzing overpressure scenarios and sizing **PSVs** as part of the pressure relief system in a plant.

With the "**Safety Analysis**" environment, the user can use the same properties and process data for both equipment design and overpressure analysis. He/she can use the familiar Aspen Plus flowsheet to visualize the process and simulation results to help the user perform rigorous overpressure scenario analysis. He/she can also use relief load calculation schemes for common contingencies (such as fire and exchanger tube rupture).

The "**Safety Analysis**" environment uses the latest API 520 and 521 pressure relieving device sizing equations (including **H**omogeneous **E**quilibrium **M**ethod, **HEM**) and performs design temperature and valve material checks in full accordance with API 526, resulting in better **PSV** types and flanges identification. It also provides the ability to calculate noise and reaction forces and perform line sizing calculations for single- and mixed-phase systems. The user can also use the "**Safety Analysis**" environment to create automatically generated documentation of relief devices with data used in sizing of **PSVs**.

Moreover, the "**Safety Analysis**" environment lets the user perform low-pressure storage tank calculations. Such a tank is designed to hold petroleum intermediates (gases or vapors) and finished products, as well as other liquid products commonly handled and stored by the various branches of the industry. The user can calculate thermal and liquid movement normal venting requirements in accordance with the latest API 2000 code and calculate emergency venting contingencies. The "**Safety Analysis**" environment provides the ability to quickly evaluate the requirement for normal and emergency venting for storage tanks. Tank design calculations fall under the scope of API 650 and 620, and pressure protection (overpressure and vacuum protection) calculations fall under the scope of API 2000. All accessory pressure parts, such as pipe fittings, valves, flanges, nozzles, welding necks, welding caps, manhole frames, and covers are taken into account to end up with a safe storage tank facility. This requires establishing procedures, methods, equipment, and other requirements to prevent or control the discharge of oil (i.e., oil spill) or gas release from vessels and facilities into the neighboring Mother Nature (as opposed to Father Artifact).

You can view the "**Tank Report**" summarizing the storage tank calculations by selecting the "**Calculation Sheet**" button on the "**Reports**" contextual ribbon. See Homework/Classwork 16.1.

In addition, the "**Safety Analysis**" environment also provides methods to quickly determine the orifice area required and the rated capacity of a rupture disk device. The user can change **PSVs** to rupture disks and rupture disks to **PSVs** after defining scenarios and sizes. The "**Safety Analysis**" environment can quickly determine multiple valve configurations. In "**Aspen Flare System Analyzer**" the user can import **PSV** information from Aspen Plus "**Safety Analysis**" environment.

16.4 ADDING A PRESSURE SAFETY VALVE (PSV)

Since the NGL process is a high-pressure process, then there will be no need to add a low-pressure storage tank but we will show how to add a **PSV**. Click on "**Add PSV**" button found in "**Home**" ribbon under "**Safety Analysis**" environment. Move the cursor over the material stream that you would like to add a **PSV** to and the cursor will change to "+" crosshairs. At such a point in time and space, you can release the dragged mouse and "**PSV**" icon shows up unto the flowsheet as shown in Figure 16.2. Alternatively, you may click on the "**Add PSV**" button once and release the mouse, move to the flowsheet area where the cursor will change to "+" crosshairs, and once you hover the mouse over any potential stream, a blue square will be shown toward the end of the candidate stream where now you can click on the blue square to add a PSV.

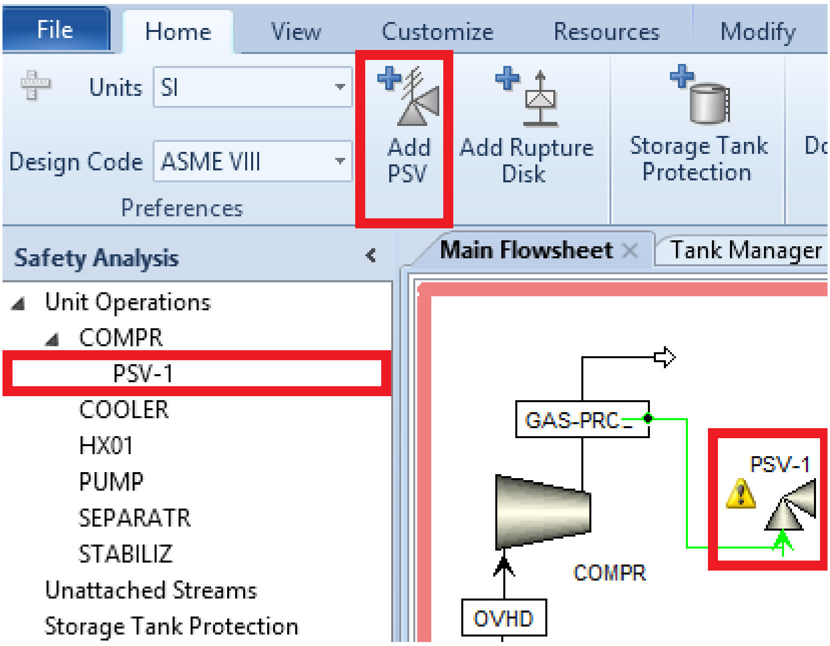
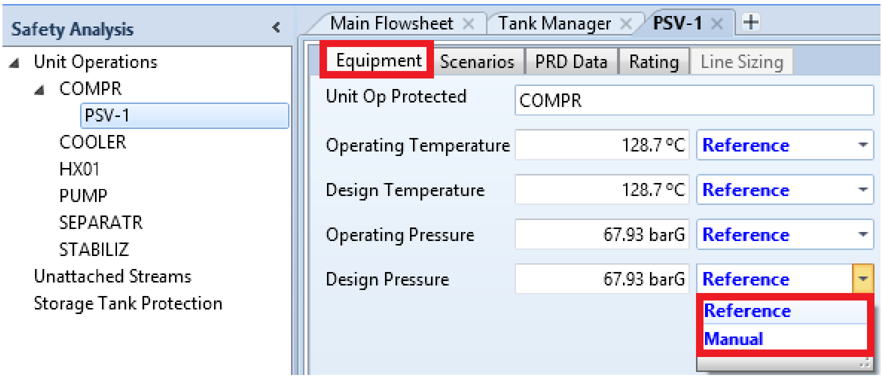


Figure 16.2 The insertion of a "**PSV**" block where it is hooked to the outlet stream of the compressor.

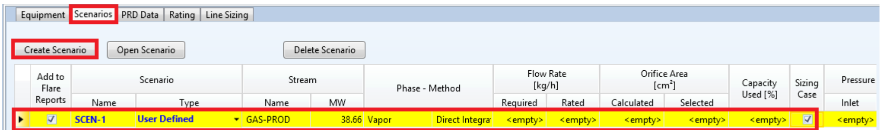
Next, we will customize the newly added PSV. From the "**Safety Analysis**" pane, click on "**PSV-1**" subfolder and "**Equipment**" tab form will show up as shown in Figure 16.3. You have the choice to enter the input data manually or by reference. To avoid yourself a headache, select the "**Reference**" option and Aspen Plus will complete the job.



Unit Op Protected	COMPR	
Operating Temperature	128.7 °C	Reference
Design Temperature	128.7 °C	Reference
Operating Pressure	67.93 barG	Reference
Design Pressure	67.93 barG	Reference

Figure 16.3 Entering specifications for the added PSV under "**Equipment**" tab.

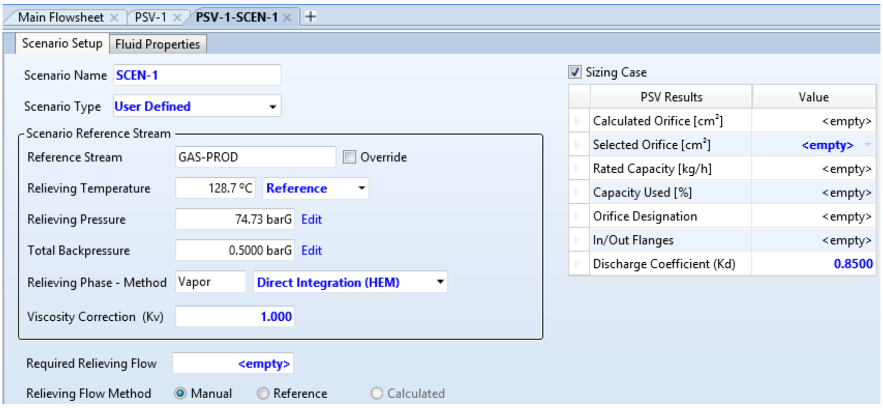
Click on "**Scenarios**" tab and then on "**Create Scenario**" button to create a new scenario and the newly created scenario will show up as in Figure 16.4. Highlight (i.e., select) the scenario and "**Open Scenario**" button will become active. Click on "**Open Scenario**" button to edit the selected scenario.



Add to Flare Reports	Scenario		Stream		Phase - Method		Flow Rate [kg/h]		Orifice Area [cm²]		Capacity Used [%]	Sizing Case	Pressure
	Name	Type	Name	MW			Required	Rated	Calculated	Selected			Inlet
☑	SCEN-1	User Defined	GAS-PROD	38.66	Vapor	Direct Integra	<empty>	<empty>	<empty>	<empty>	<empty>	☑	<empty>

Figure 16.4 The created scenario associated with PSV.

Figure 16.5 shows the "**Scenario Setup**" tab form with the "**Scenario Type**" as "*User Defined*".



Scenario Name SCEN-1

Scenario Type User Defined

Scenario Reference Stream

Reference Stream	GAS-PROD	☐ Override
Relieving Temperature	128.7 °C	Reference
Relieving Pressure	74.73 barG	Edit
Total Backpressure	0.5000 barG	Edit
Relieving Phase - Method	Vapor	Direct Integration (HEM)
Viscosity Correction (Kv)	1.000	

Required Relieving Flow <empty>

Relieving Flow Method ● Manual ○ Reference ○ Calculated

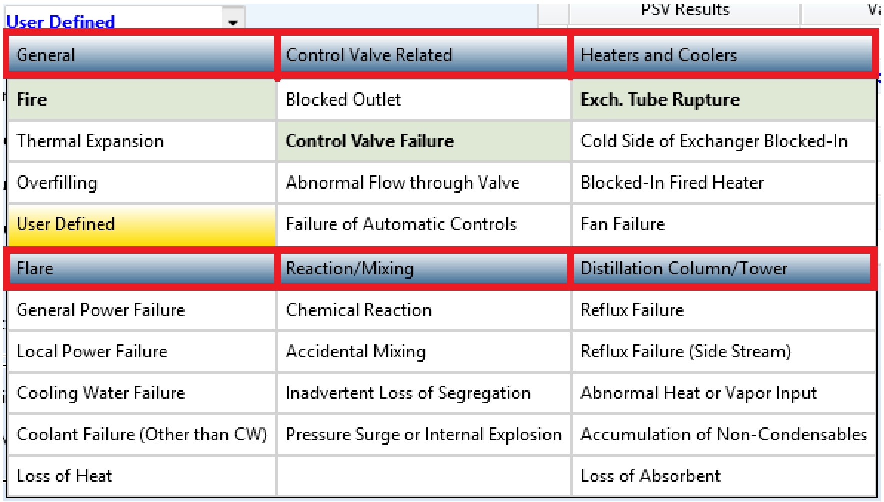
☑ Sizing Case

PSV Results	Value
Calculated Orifice [cm²]	<empty>
Selected Orifice [cm²]	<empty>
Rated Capacity [kg/h]	<empty>
Capacity Used [%]	<empty>
Orifice Designation	<empty>
In/Out Flanges	<empty>
Discharge Coefficient (Kd)	0.8500

Figure 16.5 The "**Scenario Setup**" tab form for selecting the scenario type.

NOTE #2: *For emergency scenario calculations, the fluid properties are obtained from a fluid with the same composition as the stream connected to the main PSV at the relieving conditions. Occasionally, a scenario will need a composition different from the default PSV stream. In that case, select the "**Override**" checkbox next to "**Reference Stream**" (see Figure* 16.5*) to override the reference stream in a specific scenario. A stream selection dialog box will appear and allow you to choose a new stream for the current scenario. Moreover, select the "**Sizing Case**" checkbox shown in Figure* 16.4.

Here, we can either define our own scenario via sticking to "*User Defined*" option or select from a drop-down menu, classified under different categories, as there are many possible scenarios to select from, as shown in Figure 16.6. Notice that Aspen Plus will notify the user if further information is required (a yellow strip at the bottom of the form) versus the information is complete (a green strip at the bottom).

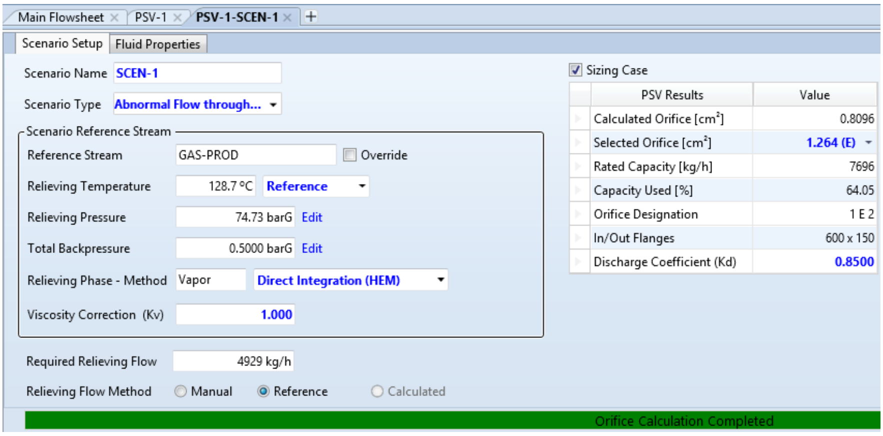


General	Control Valve Related	Heaters and Coolers
Fire	Blocked Outlet	**Exch. Tube Rupture**
Thermal Expansion	**Control Valve Failure**	Cold Side of Exchanger Blocked-In
Overfilling	Abnormal Flow through Valve	Blocked-In Fired Heater
User Defined	Failure of Automatic Controls	Fan Failure
Flare	Reaction/Mixing	Distillation Column/Tower
General Power Failure	Chemical Reaction	Reflux Failure
Local Power Failure	Accidental Mixing	Reflux Failure (Side Stream)
Cooling Water Failure	Inadvertent Loss of Segregation	Abnormal Heat or Vapor Input
Coolant Failure (Other than CW)	Pressure Surge or Internal Explosion	Accumulation of Non-Condensables
Loss of Heat		Loss of Absorbent

Figure 16.6 Out of many possible scenarios with different categories, we would like to select one that will relieve our obsessive anxiety to live in a safe work environment.

Notice that we can create different scenarios for the same added valve as many as we wish but we will discuss one scenario here.

Figure 16.7 shows the "*Abnormal flow through valve*" option as the "**Scenario Type**". However, it requires further input data, namely, the required relieving flow; that explains why a yellow strip at the bottom of the form persists until the user enters the required input data; consequently, we need to enter the relieving flow via selecting the "*Reference*" option for the "**Relieving FlowMethod**" calculation, which will transform the yellow strip into green. Furthermore, selecting the orifice area from the drop-down list can be carried out here (right pane in Figure 16.7). Alternatively, it can be postponed until we reach "**Rating**" tab (see later the discussion for selection under "**Rating**" tab). There is one more selection, that is, determining the properties of the relieving phase itself as being liquid, vapor, mixture of both, or supercritical fluid. The equations used with this option ("*Direct*



Scenario Name: SCEN-1

Scenario Type: Abnormal Flow through...

Scenario Reference Stream

Reference Stream: GAS-PROD ☐ Override

Relieving Temperature: 128.7 °C Reference

Relieving Pressure: 74.73 barG Edit

Total Backpressure: 0.5000 barG Edit

Relieving Phase - Method: Vapor Direct Integration (HEM)

Viscosity Correction (Kv): 1.000

Required Relieving Flow: 4929 kg/h

Relieving Flow Method: ○ Manual ● Reference ○ Calculated

☑ Sizing Case

PSV Results	Value
Calculated Orifice [cm^2]	0.8096
Selected Orifice [cm^2]	1.264 (E)
Rated Capacity [kg/h]	7696
Capacity Used [%]	64.05
Orifice Designation	1 E 2
In/Out Flanges	600 x 150
Discharge Coefficient (Kd)	0.8500

Orifice Calculation Completed

Figure 16.7 The "*Abnormal flow through valve*" option for the "**Scenario Type**", the "**Required Relieving Flow**" value, and the "**Selected Orifice [cm^2]**" value are to be entered here.

Integration (HEM)") are based on the **H**omogeneous **E**quilibrium **M**ethod (**HEM**), which assumes the fluid mixture behaves as a pseudo-single phase fluid, with a density that is the volume-averaged density of the two phases. This method is based on the assumption that thermal and mechanical equilibrium exist as the two-phase fluid passes through the PRV. For high momentum discharges of two-phase systems in nozzles longer than 4 inches (10 cm), both thermal and mechanical equilibrium can be assumed. These assumptions correspond to the homogeneous equilibrium flow model. This method can be used for all two-phase discharge scenarios, including supercritical fluids in condensing two-phase flow. When using this method, the Aspen Plus built-in properties calculator is used in order to evaluate fluid properties along the isentropic path.

After getting the green light (i.e., the green strip) from Aspen Plus, it will do at this stage some background calculations and the results are shown both in "**Scenario Setup**" and "**Fluid Properties**" tab form. Here is a summary for terms appearing on either form.

- **Maximum Allowable BP**: Percentage of the set pressure allowed as backpressure for the valve. This value depends on the set pressure and the valve type considered (this item is shown under the "**Fluid Properties**" tab).
- **Total Backpressure**: Pressure at the outlet of the relieving device; sum of the built-up backpressure and the superimposed backpressure (constant and variable).
- **Relieving Pressure**: Pressure at the inlet of the relieving device; set pressure + allowable overpressure.
- **Relieving Temperature**: Temperature of the relieving conditions at the inlet of the relieving device.

The allowable overpressure percentage has a default value of 21% of the set pressure for **Fire** emergency scenarios and 10% for all other scenarios.

Let us take, as an example, our lovely "**GAS-PROD**" outlet stream.

The operating pressure is 1000 psia (68.947 barA (absolute) or 67.934 barG (gage)

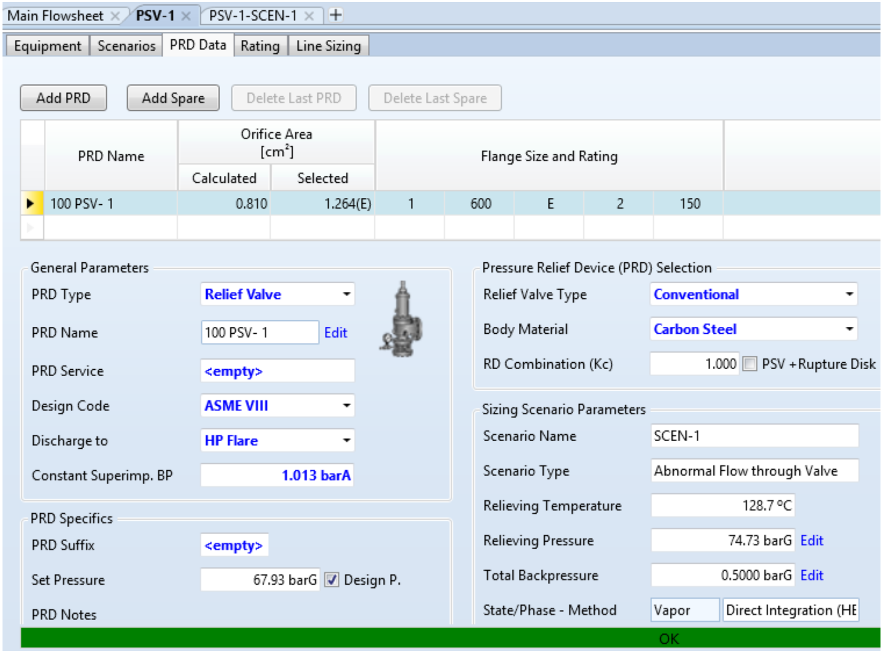
The set pressure is 67.934 barG

The allowable overpressure is 0.1 × 67.934 = 6.793 barG

The relieving pressure is 67.934 + 6.793 = 74.73 barG (shown in Figure 16.7).

For the "**Total Backpressure**" value, you may edit the value and an editbox will show up the details on how such a value is calculated by Aspen Plus. The "**Relieving Temperature**" is set to the operating temperature of "**GAS-PROD**" outlet stream.

Let us go to the third tab (see Figure 16.4), that is, "**PRD Data**" as shown in Figure 16.8. Since our gas stream leaves at a high pressure (1000 psia), we will chose "*HP Flare*" option.



PRD Name	Orifice Area [cm^2]		Flange Size and Rating				
	Calculated	Selected					
100 PSV- 1	0.810	1.264(E)	1	600	E	2	150

General Parameters

PRD Type: Relief Valve

PRD Name: 100 PSV- 1 Edit

PRD Service: <empty>

Design Code: ASME VIII

Discharge to: HP Flare

Constant Superimp. BP: 1.013 barA

PRD Specifics

PRD Suffix: <empty>

Set Pressure: 67.93 barG ☑ Design P.

PRD Notes

Pressure Relief Device (PRD) Selection

Relief Valve Type: Conventional

Body Material: Carbon Steel

RD Combination (Kc): 1.000 ☐ PSV + Rupture Disk

Sizing Scenario Parameters

Scenario Name: SCEN-1

Scenario Type: Abnormal Flow through Valve

Relieving Temperature: 128.7 °C

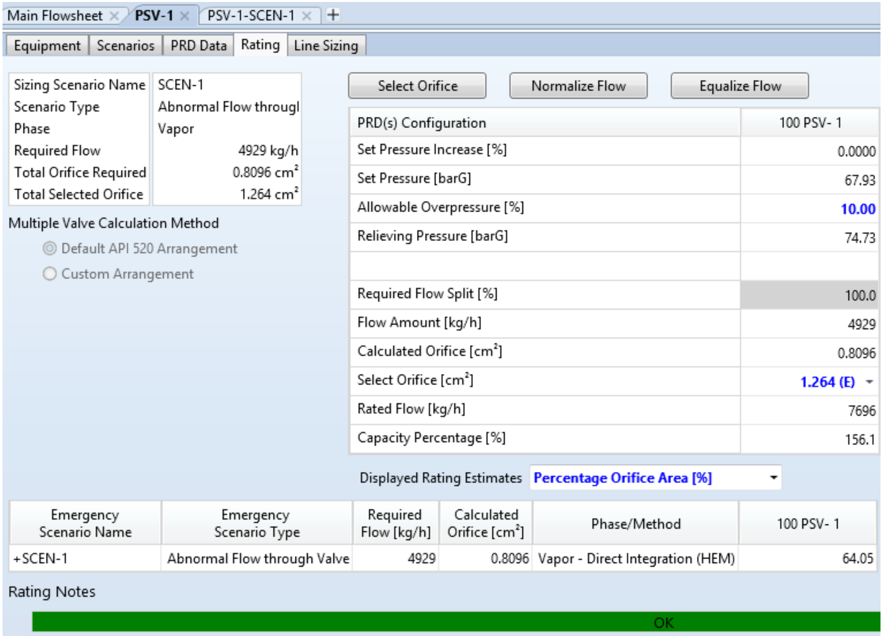
Relieving Pressure: 74.73 barG Edit

Total Backpressure: 0.5000 barG Edit

State/Phase - Method: Vapor Direct Integration (HE

Figure 16.8 Selection of "**Discharge to**" option from a drop-down list. A high-pressure (HP) flare is selected.

Under the fourth "**Rating**" tab, as shown in Figure 16.9, you may enter or adjust the orifice size specifications which will be selected from a drop-down list. Notice that if you select an orifice size larger than needed, you will end up with a yellow strip bearing the following warning message saying: "100 PSV-1: The required capacity is smaller than 60% of the PSV capacity. The selected PSV is likely to chatter. Consider selecting a smaller PSV or splitting the PSV in two or more smaller items". In principle, you can start small and grow up to the limit where you are prompted by the warning; alternatively, you may start big and shrink in size until you get the green strip. Notice that the required capacity (4929 kg/h) is bigger than 60% of the PSV capacity (7696 kg/h). Both values are shown in the right pane of Figure 16.9.



Sizing Scenario Name	SCEN-1
Scenario Type	Abnormal Flow througl
Phase	Vapor
Required Flow	4929 kg/h
Total Orifice Required	0.8096 cm^2
Total Selected Orifice	1.264 cm^2

Multiple Valve Calculation Method

◎ Default API 520 Arrangement

○ Custom Arrangement

PRD(s) Configuration	100 PSV- 1
Set Pressure Increase [%]	0.0000
Set Pressure [barG]	67.93
Allowable Overpressure [%]	10.00
Relieving Pressure [barG]	74.73
Required Flow Split [%]	100.0
Flow Amount [kg/h]	4929
Calculated Orifice [cm^2]	0.8096
Select Orifice [cm^2]	1.264 (E)
Rated Flow [kg/h]	7696
Capacity Percentage [%]	156.1

Displayed Rating Estimates: Percentage Orifice Area [%]

Emergency Scenario Name	Emergency Scenario Type	Required Flow [kg/h]	Calculated Orifice [cm^2]	Phase/Method	100 PSV- 1
+SCEN-1	Abnormal Flow through Valve	4929	0.8096	Vapor - Direct Integration (HEM)	64.05

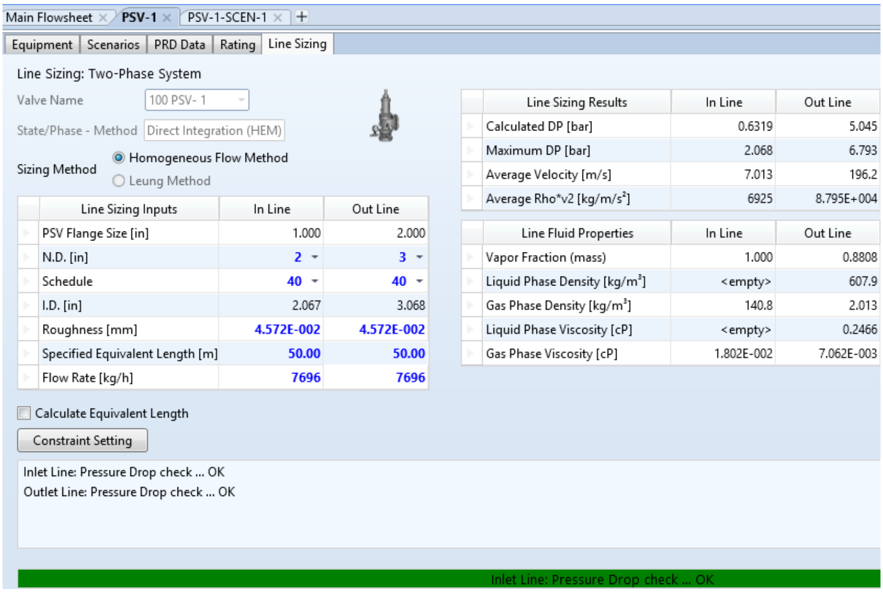
Rating Notes

OK

Figure 16.9 The orifice size specifications are checked under “**Rating**” tab.

The fifth and last “**Line Sizing**” tab pertains to the line sizing of the inlet and outlet pipe. Figure 16.10 shows that we need to specify both the nominal diameter and schedule number for both inlet and outlet pipe. Here again, we have to play tricks such that the selected nominal diameter does not end up with an undesired result. Specifically, at a very low nominal diameter value, we violate the pressure drop limitation on both inlet and outlet side of the PSV. So, start simple and grow up in size until you get the green strip.

This makes our life green and all required specifications are entered. What is next? Have a nap; it is now safe.



Line Sizing: Two-Phase System

Valve Name: 100 PSV- 1

State/Phase - Method: Direct Integration (HEM)

Sizing Method: ● Homogeneous Flow Method ○ Leung Method

Line Sizing Inputs	In Line	Out Line
PSV Flange Size [in]	1.000	2.000
N.D. [in]	2	3
Schedule	40	40
I.D. [in]	2.067	3.068
Roughness [mm]	4.572E-002	4.572E-002
Specified Equivalent Length [m]	50.00	50.00
Flow Rate [kg/h]	7696	7696

Line Sizing Results	In Line	Out Line
Calculated DP [bar]	0.6319	5.045
Maximum DP [bar]	2.068	6.793
Average Velocity [m/s]	7.013	196.2
Average Rho*v2 [kg/m/s^2]	6925	8.795E+004

Line Fluid Properties	In Line	Out Line
Vapor Fraction (mass)	1.000	0.8808
Liquid Phase Density [kg/m^3]	<empty>	607.9
Gas Phase Density [kg/m^3]	140.8	2.013
Liquid Phase Viscosity [cP]	<empty>	0.2466
Gas Phase Viscosity [cP]	1.802E-002	7.062E-003

☐ Calculate Equivalent Length

Constraint Setting

Inlet Line: Pressure Drop check ... OK
Outlet Line: Pressure Drop check ... OK

Inlet Line: Pressure Drop check ... OK

Figure 16.10 Selection of pipe sizing for the inlet and outlet pipe.

16.5 ADDING A RUPTURE DISK (RD)

In the same manner as we did with adding a PSV, we can add a rupture disk and hook it to the top liquid NGL ("**NGL-PROD**") stream as shown in Figure 16.11.

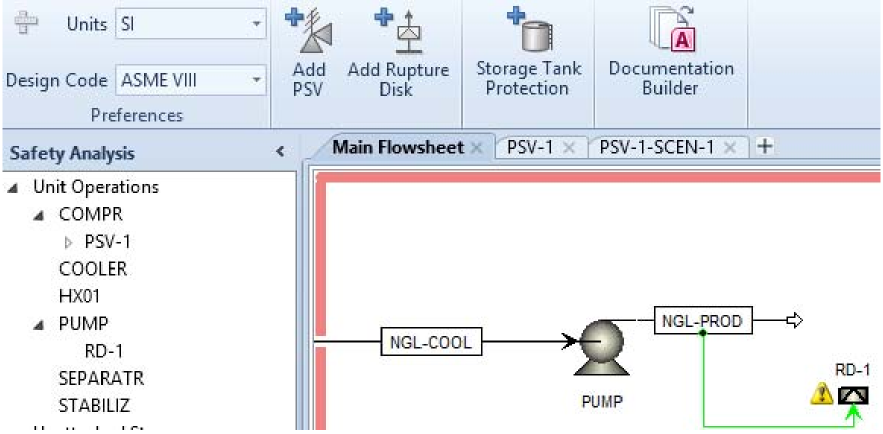
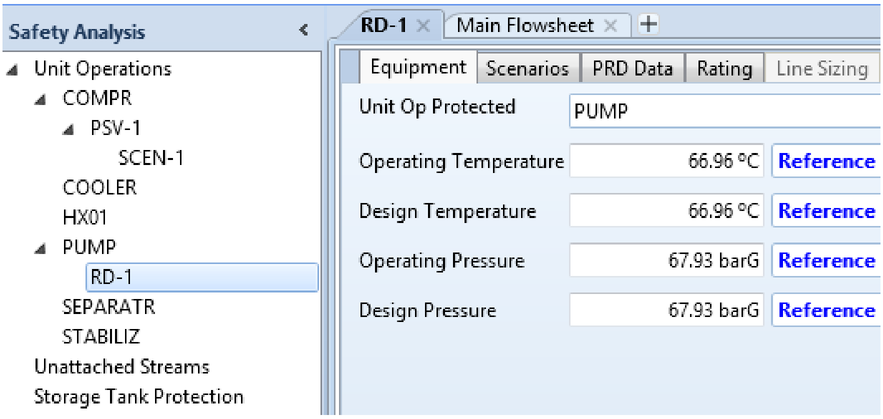


Figure 16.11 Addition of a rupture disk (RD) to the flowsheet via hooking it to "**NGL-PROD**" stream.

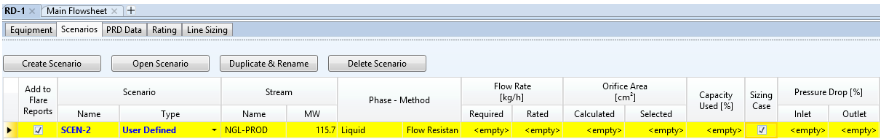
Figure 16.12 shows the "**Equipment**" tab form where the "*Reference*" option is selected versus the "*Manual*".



Unit Op Protected: PUMP
Operating Temperature: 66.96 °C Reference
Design Temperature: 66.96 °C Reference
Operating Pressure: 67.93 barG Reference
Design Pressure: 67.93 barG Reference

Figure 16.12 Selection of operating pressure and temperature using the "*Reference*" choice as opposed to "*Manual*".

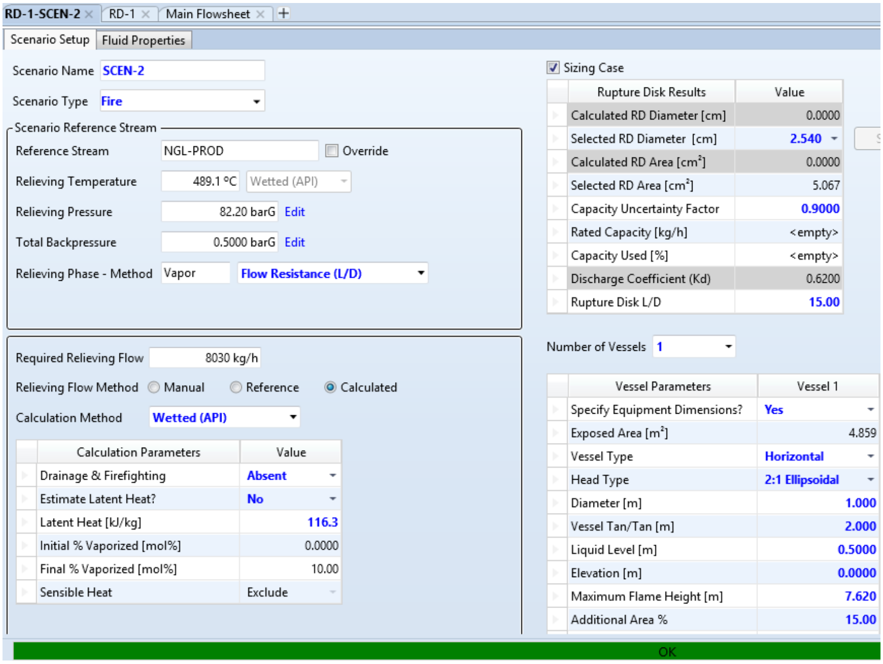
Figure 16.13 shows the creation of a scenario to be associated with "**RD-1**" disk.



Add to Flare Reports	Scenario		Stream		Phase - Method		Flow Rate [kg/h]		Orifice Area [cm²]		Capacity Used [%]	Sizing Case	Pressure Drop [%]	
	Name	Type	Name	MW			Required	Rated	Calculated	Selected			Inlet	Outlet
☑	SCEN-2	User Defined	NGL-PROD	115.7	Liquid	Flow Resistan	<empty>	<empty>	<empty>	<empty>	<empty>	☑	<empty>	<empty>

Figure 16.13 Creation of a scenario to be associated with the rupture disk "**RD-1**" disk.

Highlight the scenario ("**SCEN-2**") for "**RD-1**" disk and click on "**Open Scenario**" button to enter the scenario type and any required input data. Figure 16.14 shows the "**Scenario Setup**" tab form where we need to enter the "**Scenario Type**", the "**Relieving Phase Method**", the "**Relieving Flow Method**", and rupture disk diameter. Points worth mentioning here are as follows:



Scenario Name SCEN-2

Scenario Type Fire

Scenario Reference Stream

Reference Stream NGL-PROD ☐ Override

Relieving Temperature 489.1 °C Wetted (API)

Relieving Pressure 82.20 barG

Total Backpressure 0.5000 barG

Relieving Phase - Method Vapor Flow Resistance (L/D)

Required Relieving Flow 8030 kg/h

Relieving Flow Method ○ Manual ○ Reference ● Calculated

Calculation Method Wetted (API)

Calculation Parameters	Value
Drainage & Firefighting	Absent
Estimate Latent Heat?	No
Latent Heat [kJ/kg]	116.3
Initial % Vaporized [mol%]	0.0000
Final % Vaporized [mol%]	10.00
Sensible Heat	Exclude

☑ Sizing Case

Rupture Disk Results	Value
Calculated RD Diameter [cm]	0.0000
Selected RD Diameter [cm]	2.540
Calculated RD Area [cm^2]	0.0000
Selected RD Area [cm^2]	5.067
Capacity Uncertainty Factor	0.9000
Rated Capacity [kg/h]	<empty>
Capacity Used [%]	<empty>
Discharge Coefficient (Kd)	0.6200
Rupture Disk L/D	15.00

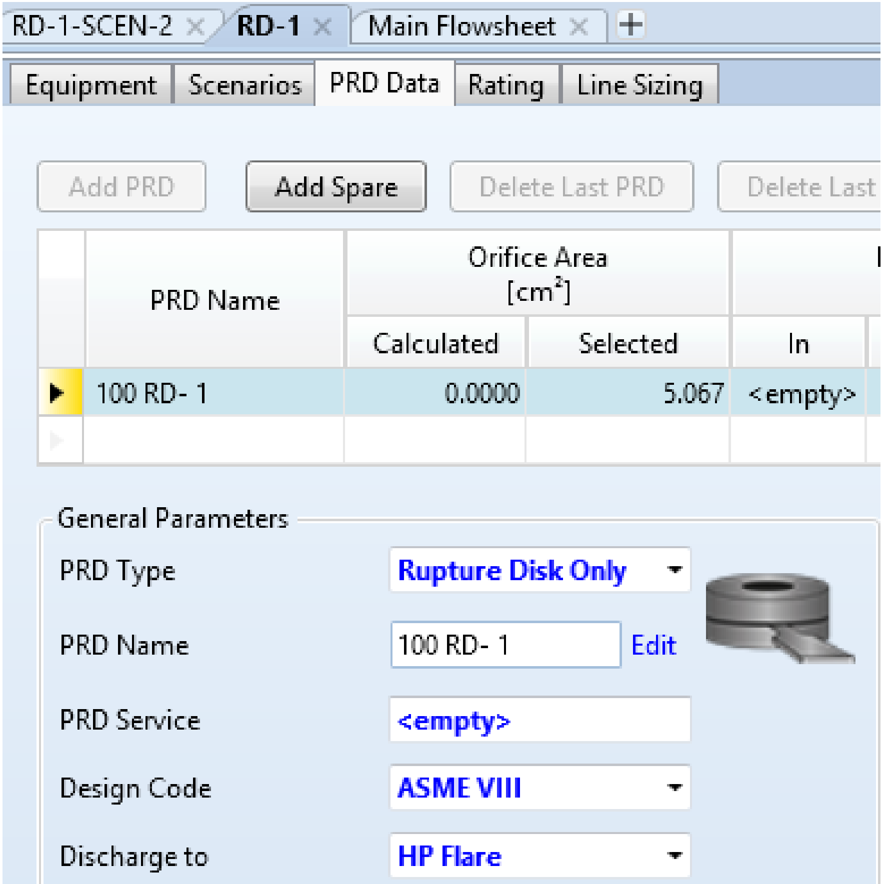
Number of Vessels 1

Vessel Parameters	Vessel 1
Specify Equipment Dimensions?	Yes
Exposed Area [m^2]	4.859
Vessel Type	Horizontal
Head Type	2:1 Ellipsoidal
Diameter [m]	1.000
Vessel Tan/Tan [m]	2.000
Liquid Level [m]	0.5000
Elevation [m]	0.0000
Maximum Flame Height [m]	7.620
Additional Area %	15.00

Figure 16.14 The “**Scenario Type**”, the “**Relieving Phase**” method, the “**Relieving Flow**” method, and RD diameter are selected in “**Scenario Setup**” tab form.

- The “**Flow Resistance L/D**” method determines the calculated size of a pressure relief system by analyzing the total system resistance to flow. This analysis takes into consideration the flow resistance of the following: The rupture disk device, piping and other piping components, entrance and exit losses, elbows, tees, reducers, and valves. You should use the “**Flow Resistance L/D**” method if: The “**8 & 5 Rule**” does not apply and the rupture disk is not installed in combination with a PSV. Refer to Aspen Plus built-in help: “**Calculation Methods for Rupture Disks**” for further information.
- For the “**Relieving Flow Method**”, the “*Wetted (API)*” or “*Semi-Dynamic Flash*” method can be used. We can use the “*Semi-Dynamic Flash*” method to rigorously calculate the relief load for a vessel that contains only liquid at relieving. This case is generally used for the analysis of a vessel that contains a multicomponent liquid with a wide boiling point range. On the other hand, using the “*Wetted (API)*” method, we can calculate the relief load for a vessel that contains some liquid at relieving conditions by estimating the latent heat of vaporization based on the duty required to vaporize a specified portion of the holdup liquid in the vessel (excluding sensible heat) on a molar or mass basis. Here, the “*Flow Resistance L/D*” and “*Wetted (API)*” method are selected.

Under “**PRD Data**” tab, we will select “*HP Flare*” from the drop-down list for “**Discharge to**” item, as shown in Figure 16.15.



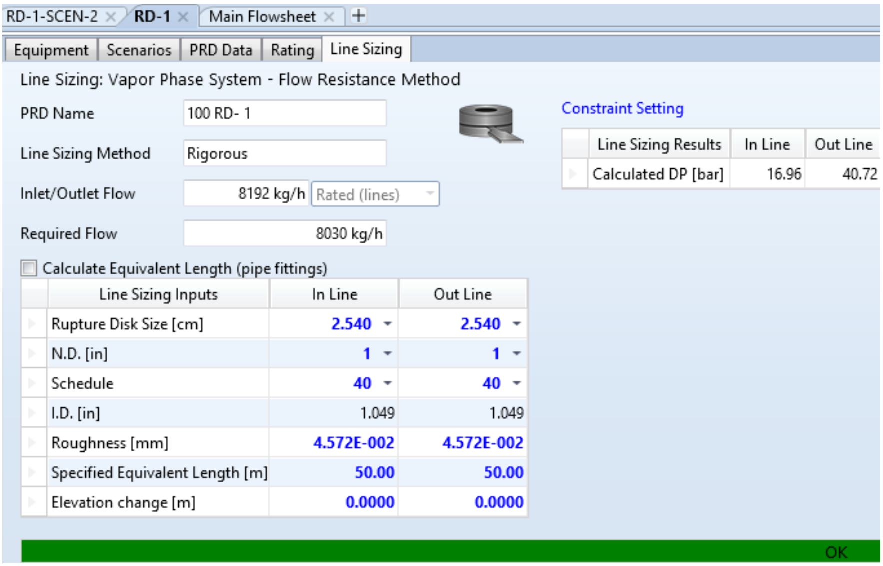
PRD Name	Orifice Area [cm^2]		
	Calculated	Selected	In
100 RD- 1	0.0000	5.067	<empty>

PRD Type: Rupture Disk Only
PRD Name: 100 RD- 1
PRD Service: <empty>
Design Code: ASME VIII
Discharge to: HP Flare

Figure 16.15 Selecting “*HP Flare*” option for “**Discharge to**” item.

Under “**Rating**” tab, we will stick to the default values.

Under “**Line Sizing**” tab, we need to enter the inline and outline pipe specifications as shown in Figure 16.16. Notice that the equivalent length for pipe fittings will be calculated and shown beneath the data presented in Figure 16.16, if the user enables calculation of the equivalent length for different pipe fittings. The user may then install additional fittings for either inlet or outlet pipeline and Aspen Plus will adjust the total equivalent length, accordingly.



Line Sizing: Vapor Phase System - Flow Resistance Method

PRD Name: 100 RD- 1

Line Sizing Method: Rigorous

Inlet/Outlet Flow: 8192 kg/h Rated (lines)

Required Flow: 8030 kg/h

☐ Calculate Equivalent Length (pipe fittings)

Line Sizing Inputs	In Line	Out Line
Rupture Disk Size [cm]	2.540	2.540
N.D. [in]	1	1
Schedule	40	40
I.D. [in]	1.049	1.049
Roughness [mm]	4.572E-002	4.572E-002
Specified Equivalent Length [m]	50.00	50.00
Elevation change [m]	0.0000	0.0000

Constraint Setting

Line Sizing Results	In Line	Out Line
Calculated DP [bar]	16.96	40.72

Figure 16.16 The inline and outline pipe specifications.

Figure 16.17 shows the "**Reports**" ribbon where the user can click on any button and generate a specifications sheet for a given safety device in the form of **PSV**, **RD**, or low-pressure storage tank protection.

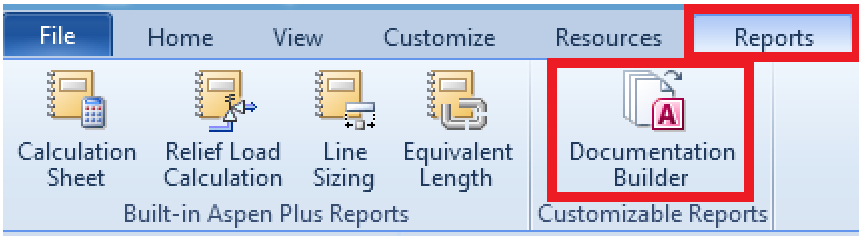
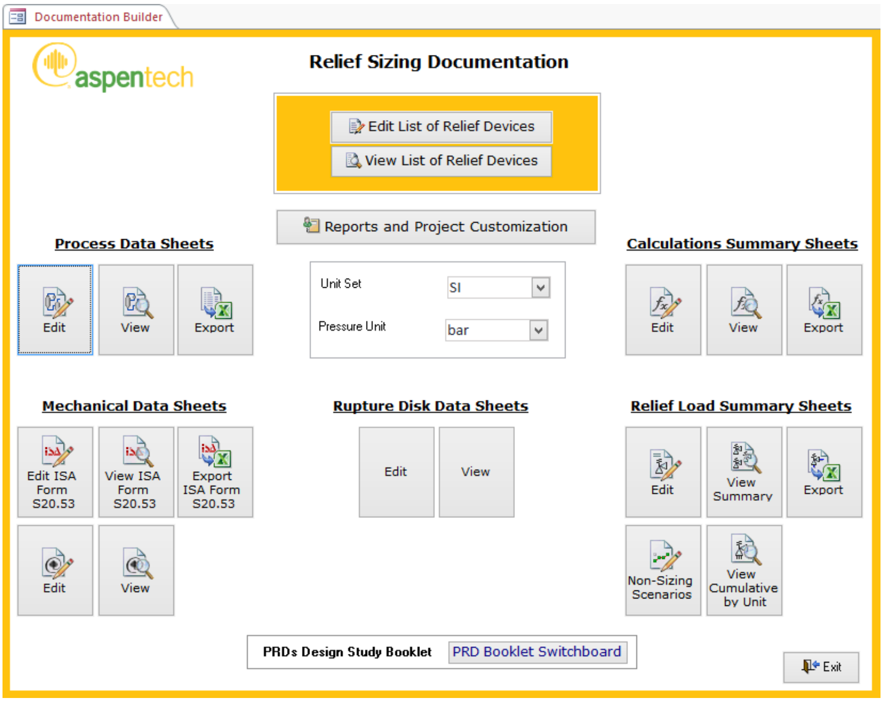


Figure 16.17 The "**Reports**" ribbon where the user can make use of generating the proper safety device sheet.

16.6 PRESENTATION OF SAFETY-RELATED DOCUMENTS

Click on "**Documentation Builder**" button in "**Reports**" ribbon and "**Documentation Builder**" window will pop up as shown in Figure 16.18, which allows the user to view a sheet for a given safety device or safety-related specifications; edit the sheet; and export to an Excel sheet for some forms. For example, to see "**RD-1**" data, click on "**View**" button under "**Rupture Disk Data Sheets**" title. On the other hand, for "**PSV-1**" results, click on "**PRD Booklet Switchboard**" button (middle bottom) and "**PRD Design Booklet - Switchboard**" tab form will show up where you may further click on "**Summary Data**" button.



Unit Set: SI
Pressure Unit: bar

Figure 16.18 The “**Documentation Builder**” window, which allows the user to manipulate safety-related documents or sheets.

16.7 PREPARATION OF FLOWSHEET FOR “ENERGY ANALYSIS” ENVIRONMENT

Before moving to the “**Energy Analysis**” environment, let us prepare the flowsheet for that purpose. We need to add blocks, with associated utility streams, to some parts of the process, which require a temperature change.

NOTE #3: *Keep in mind that Aspen Plus energy analyzer includes only utility streams in optimization, not process streams.*

Highlight the “**BOTTOMS**” stream and Under “**Modify**” ribbon, click on “**Insert**” button as shown in Figure 16.19.

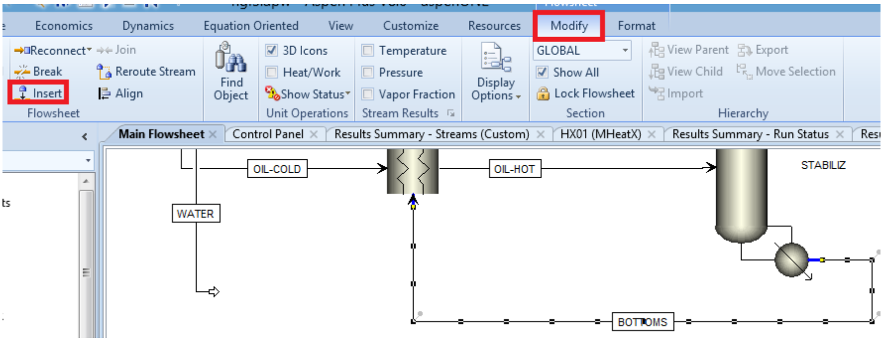
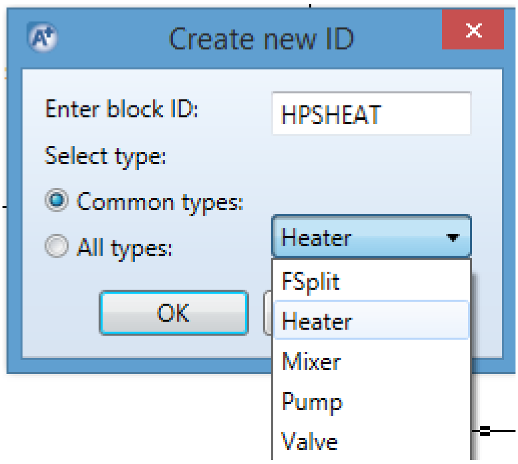


Figure 16.19 Insertion of a utility block along the "**BOTTOMS**" stream.

A pop-up window is the result as shown in Figure 16.20. It is given the name "**HPSHEAT**", to indicate the high-pressure steam heating utility.


Create new ID

Enter block ID: HPSHEAT

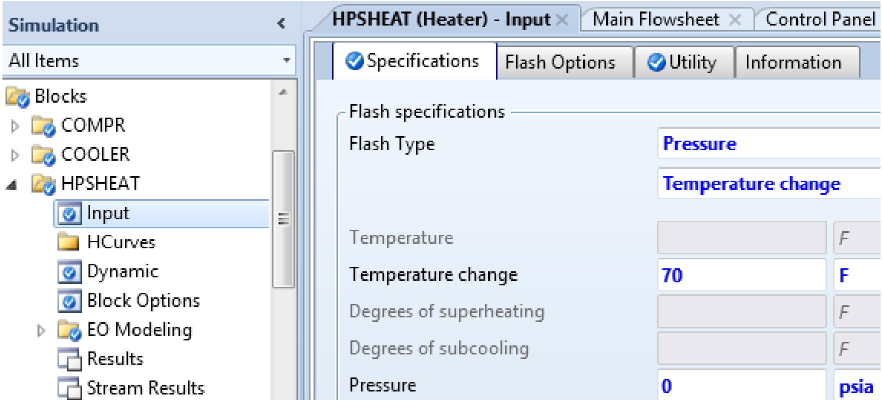
Select type:

● Common types: Heater

○ All types:

Figure 16.20 The name of the new block is entered as "**HPSHEAT**" and its type is selected as "*Heater*".

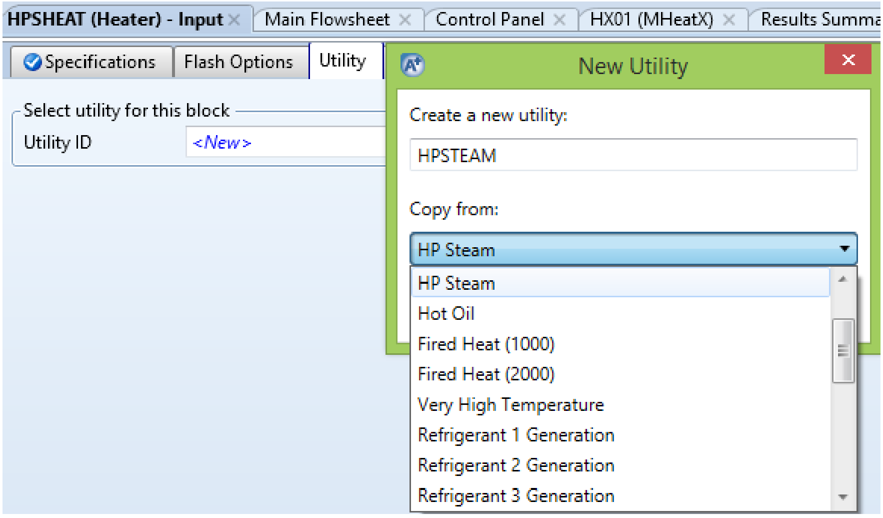
Figure 16.21 shows the "**Specifications**" tab form where we have selected the "**Flash specifications**" as "*Temperature change*" and "*Pressure*". Keep in mind that the value of 70°F is an adjustable value which can be either increased or decreased such that there is no violation for the simple heat exchange principle which requires that the temperature of steam side to be at least 18°F higher than the cold stream. The "0" pressure value means zero pressure drop between the inlet and outlet cold streams.



Flash Type: Pressure; Temperature change
Temperature: F
Temperature change: 70 F
Degrees of superheating: F
Degrees of subcooling: F
Pressure: 0 psia

Figure 16.21 The “**Specifications**” tab form for the newly added utility block.

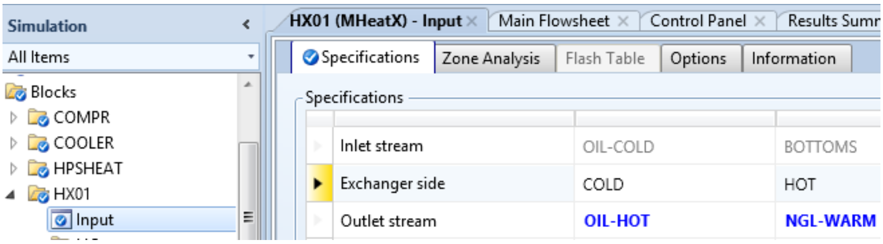
Click on “**Utility**” tab form to associate the high-pressure steam, as a utility, with “**HPSHEAT**” block. “*HP Steam*” utility is selected from the “**Copy from**” drop-down menu and is given the name “**HPSTEAM**”. as shown in Figure 16.22. Click on “**OK**” button to close the “**New Utility**” window.



Utility ID: <New>
Create a new utility: HPSTEAM
Copy from: HP Steam

Figure 16.22 The high-pressure steam utility is associated with “**HPSHEAT**” block and is given the name “**HPSTEAM**”.

Click on “**Next**” button where you need to enter the name of the outlet hot stream on the hot side of the heat exchanger as shown in Figure 16.23.



Specifications

Inlet stream	OIL-COLD	BOTTOMS
Exchanger side	COLD	HOT
Outlet stream	OIL-HOT	NGL-WARM

Figure 16.23 Entering the name of the outlet hot stream.

Figure 16.24 shows the new block, which is inserted between the outlet bottom stream of the distillation column and the inlet to the heat exchanger. The inlet and outlet stream are red-colored to draw the attention for the high-pressure steam heater.

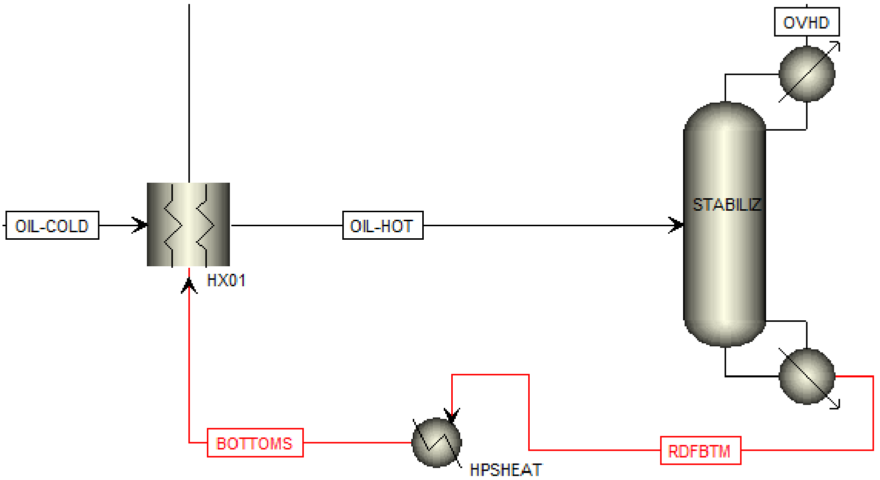
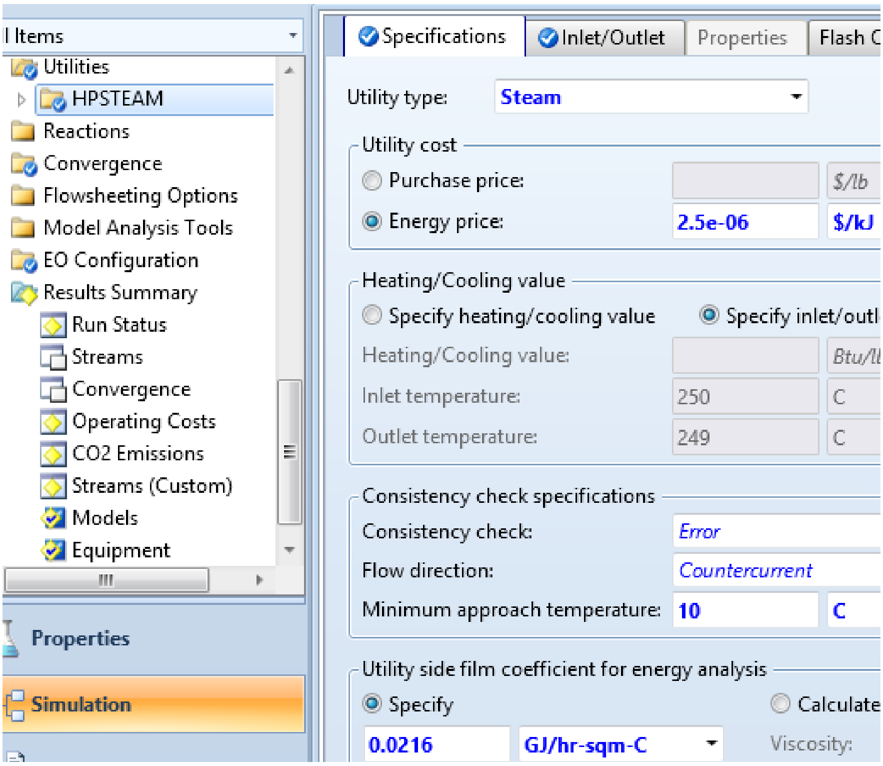


Figure 16.24 The insertion of the high-pressure steam heater to heat up the bottom stream of the stabilizer. *See Plate section for color representation of this figure*.

Figure 16.25 shows the utility “**Specifications**” tab form where the user may adjust two energy-related parameters: the unit cost of energy ($/unit of energy) and the utility side heat transfer film coefficient.



Utility type: Steam

Utility cost
○ Purchase price: $/lb
● Energy price: 2.5e-06 $/kJ

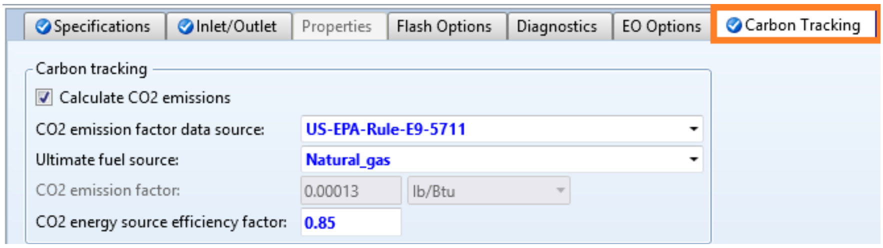
Heating/Cooling value
○ Specify heating/cooling value ● Specify inlet/outl
Heating/Cooling value: Btu/lb
Inlet temperature: 250 C
Outlet temperature: 249 C

Consistency check specifications
Consistency check: Error
Flow direction: Countercurrent
Minimum approach temperature: 10 C

Utility side film coefficient for energy analysis
● Specify ○ Calculate
0.0216 GJ/hr-sqm-C Viscosity:

Figure 16.25 Utility “**Specifications**” tab form for defining the energy unit price and film coefficient.

Finally, clicking on “**Carbon Tracking**” tab allows the user to monitor CO_2 emission rate by selecting the basis of calculation and source of fuel as shown in Figure 16.26.



Carbon tracking
☑ Calculate CO2 emissions
CO2 emission factor data source: US-EPA-Rule-E9-5711
Ultimate fuel source: Natural_gas
CO2 emission factor: 0.00013 lb/Btu
CO2 energy source efficiency factor: 0.85

Figure 16.26 The “**Carbon Tracking**” tab form for monitoring CO_2 emission rate.

Click on “**Next**” button, run the show, and watch out for any simulation or serious warning. We are ready for moving to “**Energy Analysis**” environment.

16.8 THE “ENERGY ANALYSIS” ACTIVATION

We can use the “**Energy Analysis**” environment to explore potential improvement in our plant model to reduce energy costs. Aspen Energy Analyzer examines the plant and suggests changes that can reduce our energy costs.

It is now easier to perform energy and economic analysis on Aspen Plus models. The activated analysis panel allows us running each analysis with a single click and displaying a summary of results. The analyses are automatically updated after each run. The energy analysis allows us to study possible energy-saving changes in the plant interactively in the “**Energy Analysis**” environment.

As mentioned earlier in Chapter 2, we may enable/disable activation dashboard via going to “**File**” | “**Options**” | “**Advanced**” tab and then deselecting/selecting “**Disable activation dashboard**” check button. Click on “**OK**” button to close the “**Advanced Options**” window. The “**Analysis**” dashboard will show up as in Figure 16.27.

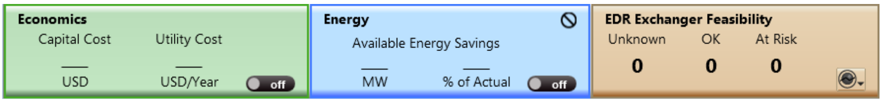
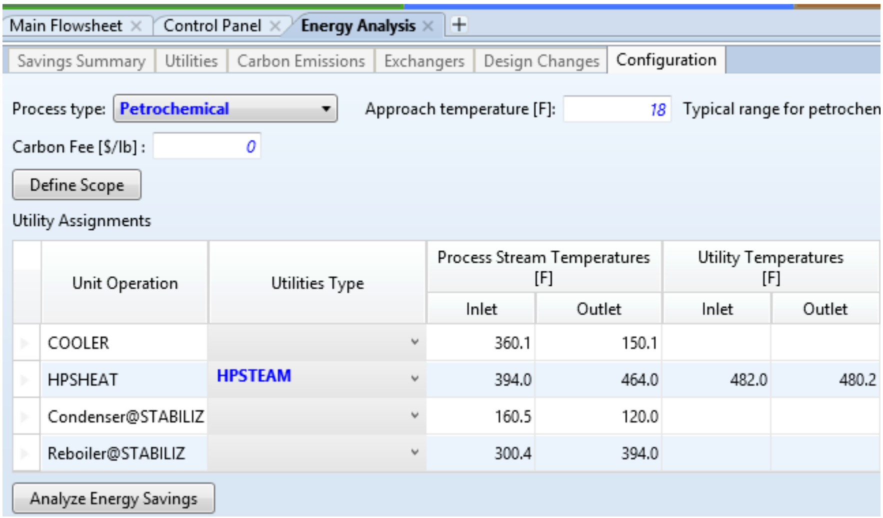


Figure 16.27 The “**Analysis**” dashboard where its shows economic, energy, and exchanger analysis.

From the dashboard, click on “**Energy**” button; this will initialize energy calculations. Figure 16.28 shows the “**Energy Analysis**” | “**Configuration**” tab window where the user may select from the drop-down menu the process type. “*Petrochemical*” type is chosen here.



Process type: Petrochemical

Approach temperature [F]: 18 Typical range for petrochen

Carbon Fee [$/lb] : 0

Utility Assignments

Unit Operation	Utilities Type	Process Stream Temperatures [F]		Utility Temperatures [F]	
		Inlet	Outlet	Inlet	Outlet
COOLER		360.1	150.1		
HPSHEAT	HPSTEAM	394.0	464.0	482.0	480.2
Condenser@STABILIZ		160.5	120.0		
Reboiler@STABILIZ		300.4	394.0		

Figure 16.28 The energy analysis configuration form for selecting the process type.

From the dashboard, click on the “On/Off” radio button, found at the bottom-right corner of the “**Energy**” button, to switch on/off the energy analysis. Figure 16.29 shows different tab windows that are augmented by numbers, chart, table, or a combination of them. For example, at the top, the number 3.33E6 Btu/h is the difference between the actual and target value of total utilities. So, 4.441E7–4.108E7 = 3.33E6 Btu/h could be a saving in total utilities, which amounts to 7.51% of the actual value of total utilities. In addition, the user may switch between “*Flow*” (Btu/h) and “*Cost*” ($/year) basis using the radio buttons shown above the chart. Other tab windows can be explored as well, such as utilities, carbon emission, and exchangers.

Basis ● Flow ○ Cost

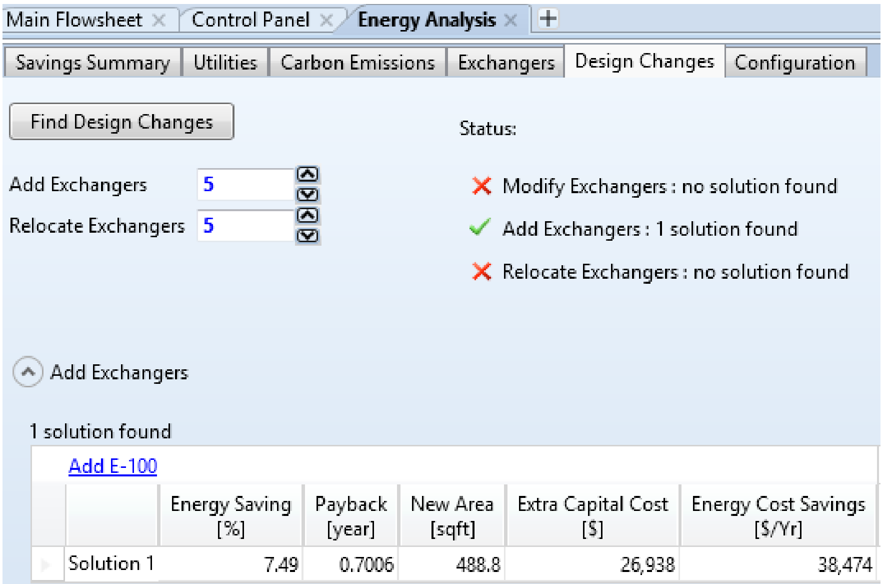
Summary Table

	Actual	Target	Available Savings	% of Actual
Total Utilities [Btu/hr]	4.441E+07	4.108E+07	3.33E+06	7.51
Heating Utilities [Btu/hr]	2.299E+07	2.133E+07	1.66E+06	7.25
Cooling Utilities [Btu/hr]	2.142E+07	1.975E+07	1.67E+06	7.78
Carbon Emissions [lb/hr]	3516	3262	254	7.22

Figure 16.29 The energy analysis results shown in different forms and the potential savings.

Furthermore, you may click on “**See Report**” button, shown at the bottom of “**Savings Summary**” tab form, and an Excel sheet will open up containing basically the same energy analysis results shown in Figure 16.29.

Now, click on “**Find Design Changes**” button, shown at the bottom of Figure 16.29. Alternatively, you may go to “**Design Changes**” tab window and click on the same button over there. Figure 16.30 shows the results of exploring new configurations that may end up with more energy cost savings.



Add Exchangers 5

Relocate Exchangers 5

Status:

✗ Modify Exchangers : no solution found

✓ Add Exchangers : 1 solution found

✗ Relocate Exchangers : no solution found

Add Exchangers

1 solution found

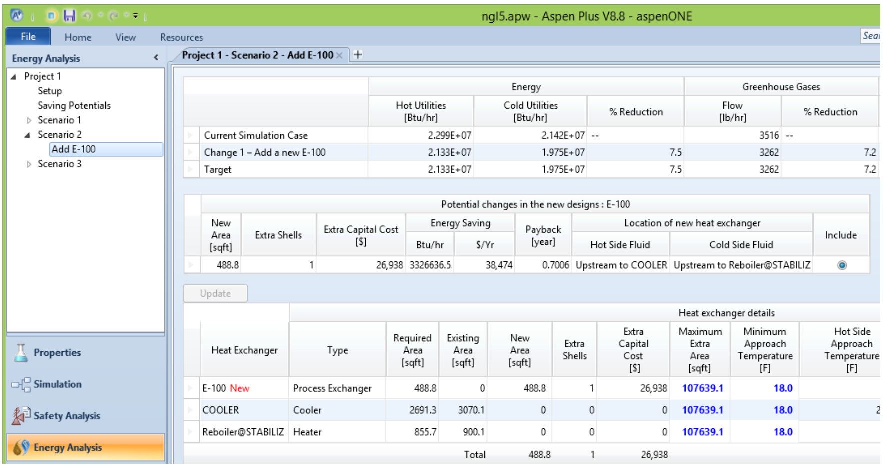
Add E-100

	Energy Saving [%]	Payback [year]	New Area [sqft]	Extra Capital Cost [$]	Energy Cost Savings [$/Yr]
Solution 1	7.49	0.7006	488.8	26,938	38,474

Figure 16.30 The potential design changes proposed by Aspen Plus energy analysis.

The energy analyzer found one solution that can save us $38,474/year but with an extra capital cost of $26,938. A comparison between the original and retrofit scenario is shown, where the latter shows a reduction in energy cost with an increase in capital cost which can be offset within 0.7 year. Notice that $\$26,938/(\$38,474/\text{year}) = 0.70$ year, which is the payback period needed to offset the extra capital cost. After 0.7 year, there will be a net energy saving at a rate of $38,474/year compared with the original configuration.

Click on "**Add E-100**" blue hyperlink to add the exchanger and "**Project 1 – Scenario 2 – Add E-100**" tab form shows up, as shown in Figure 16.31. Notice that Aspen Plus automatically switched to the fourth environment, which is, "**Energy Analysis**". The figures indicate that upon the addition of E-100 exchanger, there is at least 7% reduction in either utility costs or greenhouse gases emission rates, compared with the original scheme.



	Energy			Greenhouse Gases	
	Hot Utilities [Btu/hr]	Cold Utilities [Btu/hr]	% Reduction	Flow [lb/hr]	% Reduction
Current Simulation Case	2.299E+07	2.142E+07	--	3516	--
Change 1 – Add a new E-100	2.133E+07	1.975E+07	7.5	3262	7.2
Target	2.133E+07	1.975E+07	7.5	3262	7.2

Potential changes in the new designs : E-100

New Area [sqft]	Extra Shells	Extra Capital Cost [$]	Energy Saving		Payback [year]	Location of new heat exchanger		Include
			Btu/hr	$/Yr		Hot Side Fluid	Cold Side Fluid	
488.8	1	26,938	3326636.5	38,474	0.7006	Upstream to COOLER	Upstream to Reboiler@STABILIZ	●

	Heat exchanger details								
Heat Exchanger	Type	Required Area [sqft]	Existing Area [sqft]	New Area [sqft]	Extra Shells	Extra Capital Cost [$]	Maximum Extra Area [sqft]	Minimum Approach Temperature [F]	Hot Side Approach Temperature [F]
E-100 New	Process Exchanger	488.8	0	488.8	1	26,938	**107639.1**	**18.0**	
COOLER	Cooler	2691.3	3070.1	0	0	0	**107639.1**	**18.0**	2
Reboiler@STABILIZ	Heater	855.7	900.1	0	0	0	**107639.1**	**18.0**	
			Total	488.8	1	26,938			

Figure 16.31 The proposed energy saving scenario shows up under “**Energy Analysis**” environment.

Figure 16.32 shows “**Home**” ribbon under “**Energy Analysis**” environment.

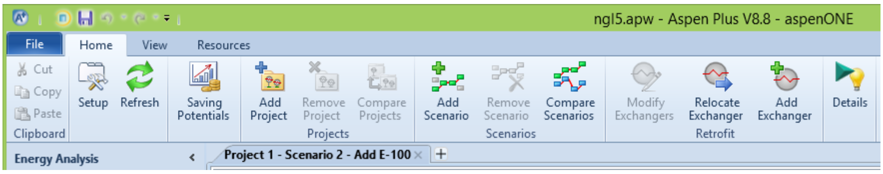
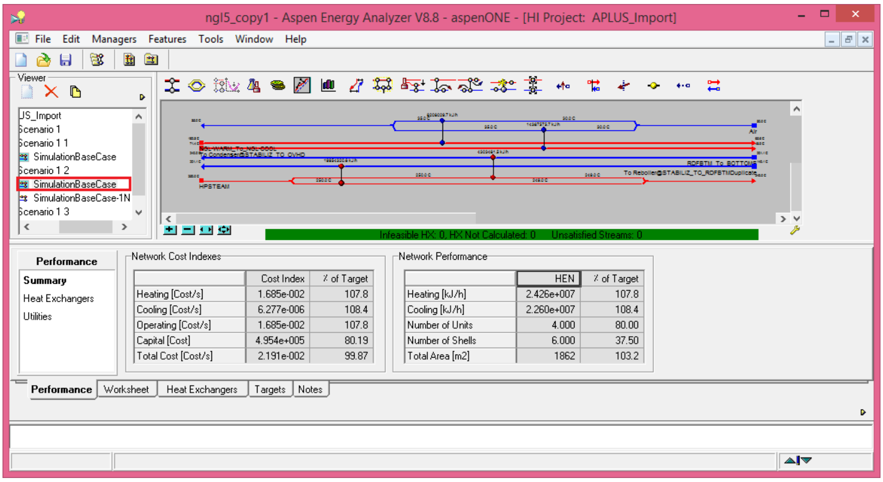


Figure 16.32 “**Home**” ribbon under “**Energy Analysis**” environment.

Clicking on “**Details**” button, found in “**Home**” ribbon, will send a copy to Aspen Energy Analyzer (AEA); however, the “**Energy Analysis**” pop-up window will tell the user that a copy of current working Aspen Energy Analyzer file will be created and loaded in a separate instance of Aspen Energy Analyzer and any changes made in the latest file will not be reflected in the table of Energy Analysis environment in the original Aspen Plus file. So if any changes are to be made by the user for Aspen Energy Analyzer file (***.hch**), then the user must save the file with a different name, because AEA-created file will be overwritten each time the “**Details**” button is clicked. Click on “**Yes**” button to close the “**Energy Analysis**” pop-up window and the proprietary Aspen Energy Analyzer main window will pop up as shown in Figure 16.33.



Infeasible HX: 0, HX Not Calculated: 0 Unsatisfied Streams: 0

Network Cost Indexes

	Cost Index	% of Target
Heating [Cost/s]	1.685e-002	107.8
Cooling [Cost/s]	6.277e-006	108.4
Operating [Cost/s]	1.685e-002	107.8
Capital [Cost]	4.954e+005	80.19
Total Cost [Cost/s]	2.191e-002	99.87

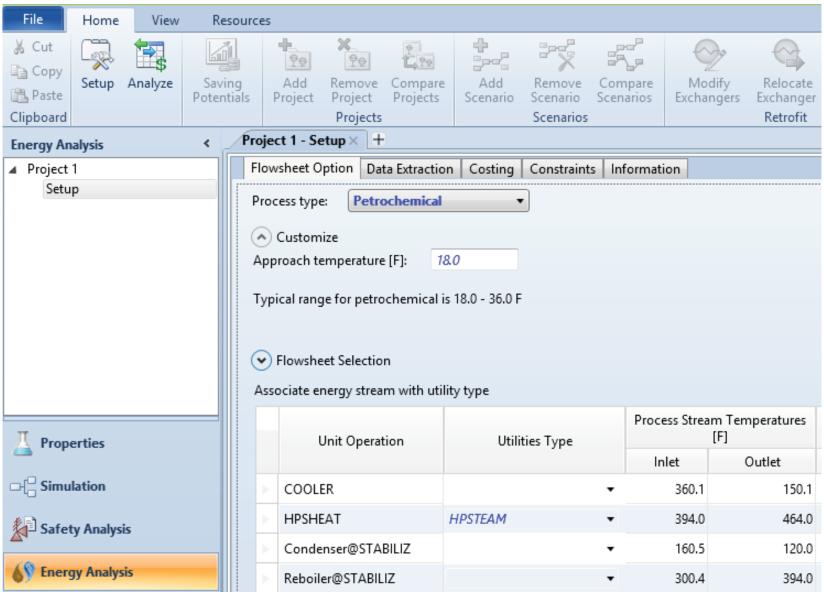
Network Performance

	HEN	% of Target
Heating [kJ/h]	2.426e+007	107.8
Cooling [kJ/h]	2.260e+007	108.4
Number of Units	4.000	80.00
Number of Shells	6.000	37.50
Total Area [m2]	1862	103.2

Figure 16.33 A copy of the energy analysis results is sent to Aspen Energy Analyzer, which can be saved as ***.hch** file.

16.9 THE “ENERGY ANALYSIS” ENVIRONMENT

Alternatively, after carrying out a successful run in Aspen Plus under steady-state condition, switch to “**Energy Analysis**” environment and Figure 16.34 will show up, which is similar to that shown in Figure 16.28. However, we will explore more features of Aspen Plus under “**Energy Analysis**” environment.



Process type: Petrochemical

Customize

Approach temperature [F]: 18.0

Typical range for petrochemical is 18.0 - 36.0 F

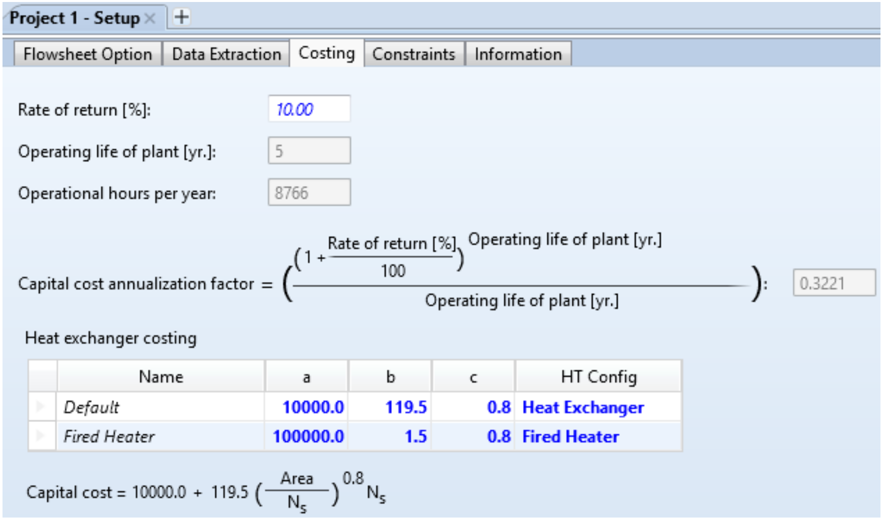
Flowsheet Selection

Associate energy stream with utility type

Unit Operation	Utilities Type	Process Stream Temperatures [F]	
		Inlet	Outlet
COOLER		360.1	150.1
HPSHEAT	HPSTEAM	394.0	464.0
Condenser@STABILIZ		160.5	120.0
Reboiler@STABILIZ		300.4	394.0

Figure 16.34 The “**Flowsheet Option**” tab window for entering process type.

Figure 16.35 shows the rate of return, the operating life of plant, and cost indices (i.e., *a*, *b*, and *c*) for different heat transfer equipment configurations. Such parameters may be adjusted to suit one’s needs.



Rate of return [%]:	10.00
Operating life of plant [yr.]:	5
Operational hours per year:	8766

$$\text{Capital cost annualization factor} = \left(\frac{\left(1+\frac{\text{Rate of return [\%]}}{100}\right)^{\text{Operating life of plant [yr.]}}}{\text{Operating life of plant [yr.]}}\right): \quad 0.3221$$

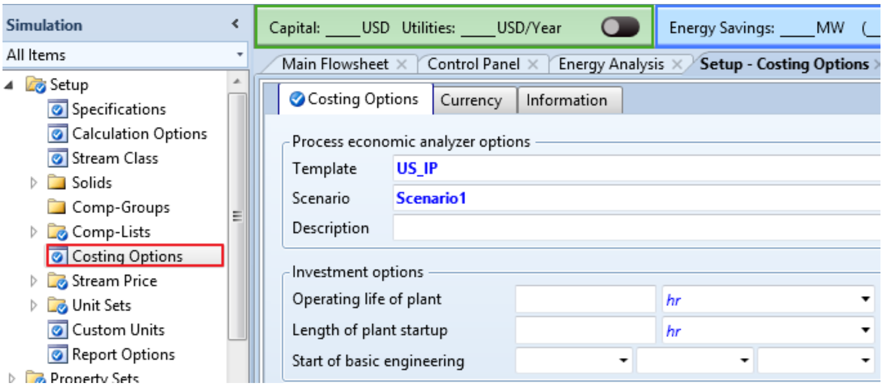
Heat exchanger costing

Name	a	b	c	HT Config
Default	10000.0	119.5	0.8	Heat Exchanger
Fired Heater	100000.0	1.5	0.8	Fired Heater

$$\text{Capital cost} = 10000.0 + 119.5\left(\frac{\text{Area}}{N_s}\right)^{0.8} N_s$$

Figure 16.35 The “**Costing**” tab form for entering cost-related parameters.

To change the shelf life of the plant, you need to switch back to “**Simulation**” environment and change it there as shown in Figure 16.36. In general, Aspen Plus watching dog is awake and asks the user to rerun the simulation once he/she switches back and forth from one to another environment. For an extra precaution, rerun under “**Simulation**” environment if any change is made.



Process economic analyzer options

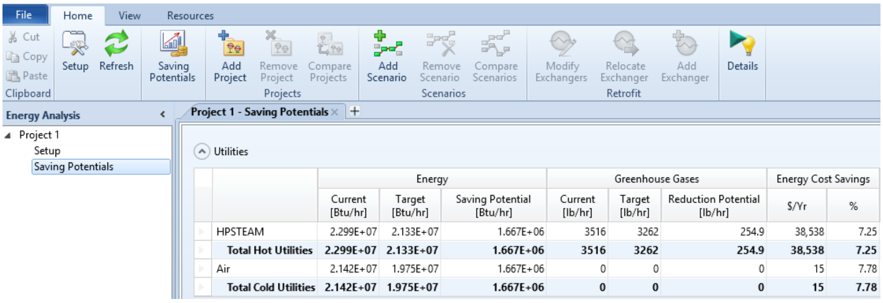
Template	US_IP
Scenario	Scenario1
Description	

Investment options

Operating life of plant		hr
Length of plant startup		hr
Start of basic engineering		

Figure 16.36 The shelf life of the plant is entered in “**Setup**” | “**Costing Options**” | “**Costing Options**” tab form.

Click on “**Analyze**” button (in the top toolbar of Figure 16.34) to initiate the energy analysis. Figure 16.37 shows a portion of the energy analysis results, which are more or



	Energy			Greenhouse Gases			Energy Cost Savings	
	Current [Btu/hr]	Target [Btu/hr]	Saving Potential [Btu/hr]	Current [lb/hr]	Target [lb/hr]	Reduction Potential [lb/hr]	$/Yr	%
HPSTEAM	2.299E+07	2.133E+07	1.667E+06	3516	3262	254.9	38,538	7.25
Total Hot Utilities	**2.299E+07**	**2.133E+07**	**1.667E+06**	**3516**	**3262**	**254.9**	**38,538**	**7.25**
Air	2.142E+07	1.975E+07	1.667E+06	0	0	0	15	7.78
Total Cold Utilities	**2.142E+07**	**1.975E+07**	**1.667E+06**	**0**	**0**	**0**	**15**	**7.78**

Figure 16.37 A portion of the energy analysis results.

less similar to those shown earlier in Figure 16.29. To modify, relocate, or add exchangers, first we create a scenario to represent the process changes. If we make changes in the base process, we can click on "**Refresh**" to update the analyses.

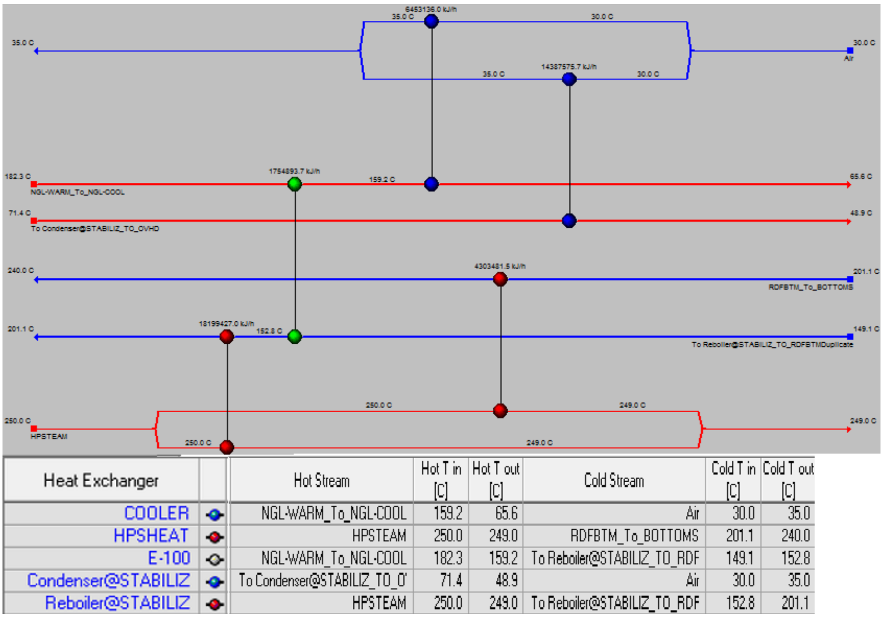
Clicking on "**Details**" button will bring the main window of Aspen Energy Analyzer exactly as that shown earlier in Figure 16.33. Notice that to find new potential improvement in existing plant layout, then you need to go back to "**Simulation**" environment where you will find the energy activation dashboard is on and you can proceed starting from Figure 16.29.

16.10 THE ASPEN ENERGY ANALYZER

I will not elaborate on Aspen Energy Analyzer (formerly known as Aspen HXNet) as it is beyond the scope of this textbook. In brief, it is designed for analyzing and improving the performance of heat exchanger networks (HENs). Aspen Energy Analyzer's focus is on analyzing the networks from an operations' as well as a design's point of view. HEN operations features are designed to provide the user with an understanding of current plant operation and related issues such as fouling. Furthermore, fouling mitigation strategies can be studied and simulated in Aspen Energy Analyzer. The designer can use Aspen Energy Analyzer to identify and compare options to improve the performance and reduce the gap between current and thermodynamic optimum operations. To perform any heat integration study from a design or operations perspective, Aspen Energy Analyzer needs the process requirements and the HEN that achieves the process requirements. The terminology that is used in Aspen Energy Analyzer is "scenario" for process requirements and "design" for the HEN. Let us relax for a while and look what Aspen Energy Analyzer tells us.

Figure 16.38 shows the heat exchanger network in the form of a box with arrows, line, and dumbbell. The blue color (e.g., the top box-and-whisker plot) indicates a cooling medium and red color (e.g., the bottom box-and-whisker plot) heating medium. If you cannot read temperature values shown on the heat exchanger network plot, then you would better look at the table just below the plot itself. If you cannot see numbers in that table, then you would better see an optician.

The box with arrows represents the heat exchange process; for example, a cold air stream utility enters at 30°C while it is in exchange with "**NGL-WARM**" stream at 159.2°C and the air leaves at 35°C, whereas "**NGL-WARM**" is cooled down to "**NGL-COOL**" stream at 65.6°C. Have a look at the attached table shown below HEN image. The same story for air stream is said with respect to “**STABILIZ**” condenser where the temperature is reduced from the dew-point 71.4 down to the bubble-point 48.9°C (with a phase change for the process fluid). The two blue dumbbells shown in Figure 16.38 thus indicate the utilization of cold utility, such as air, in cooling down hot streams. On the contrary, the two red dumbbells indicate the utilization of hot utility, such as the high-pressure steam, in heating up cold streams. Finally, the green dumbbell indicates the recommended modification (retrofit) E-100 exchanger, which exchanges heat between “**NGL-WARM**” stream at 182.3°C being cooled down to 159.2°C; in return, the “**STABILIZ**” reboiler stream is partly heated from 149.1 to 152.8°C. Then, the “**STABILIZ**” reboiler stream is continued to be heated from 152.8 up to 201.1°C using HP-steam utility.



Heat Exchanger		Hot Stream	Hot T in [C]	Hot T out [C]	Cold Stream	Cold T in [C]	Cold T out [C]
COOLER	●	NGL-WARM_To_NGL-COOL	159.2	65.6	Air	30.0	35.0
HPSHEAT	●	HPSTEAM	250.0	249.0	RDFBTM_To_BOTTOMS	201.1	240.0
E-100	●	NGL-WARM_To_NGL-COOL	182.3	159.2	To Reboiler@STABILIZ_TO_RDF	149.1	152.8
Condenser@STABILIZ	●	To Condenser@STABILIZ_TO_O'	71.4	48.9	Air	30.0	35.0
Reboiler@STABILIZ	●	HPSTEAM	250.0	249.0	To Reboiler@STABILIZ_TO_RDF	152.8	201.1

Figure 16.38 Aspen Energy Analyzer demonstrates the heat exchanger network with the recommended energy-saving retrofit layout. *See Plate section for color representation of this figure*.

In a similar fashion, “**NGL-WARM**” stream is cooled down to “**NGL_COOL**” via two successive cooling steps: the first step is achieved by E-100 exchanger followed by the second step, which is, utilizing cold air.

HOMEWORK/CLASSWORK 16.1 (ADDING A STORAGE TANK PROTECTION)

Let us concentrate a 50 wt% water–acetone feed mixture into 90+ wt% acetone via a single-flash drum followed by storing the product at 45°C and 1 bar, as shown in Figure 16.39. Acetone can be used as nail polish remover (10 parts acetone and 1 part H_2O; amounts to 90.9 wt% acetone) in addition to an emollient and preservative, such

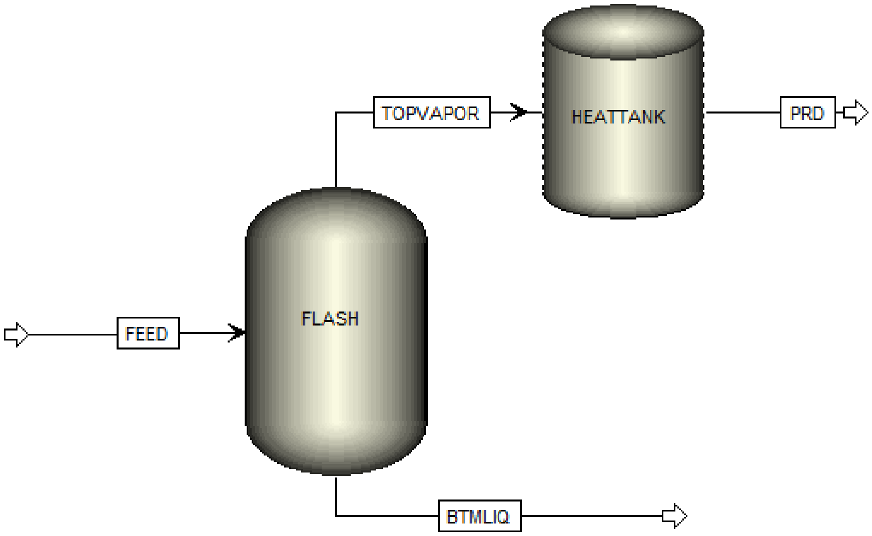


Figure 16.39 The flowsheet for concentrating 50 wt% water–acetone mixture.

as olive oil and vitamin E (http://www.nailcarehq.com/is-acetone-a-safe-nail-polish-remover/).

The 50/50 wt% feed stream enters at 25°C and 1 atm with 1000 kg/h total flow rate. The "**FLASH**" block is operated at 1 atm and a vapor fraction of 0.2. To achieve the flashing condition, the low-pressure steam utility will be used to account for both sensible and latent heat requirement. The vapor stream with 90+ wt% of acetone will enter "**HEATTANK**" block, which is maintained at 45°C and 1 atm via a cooling process where air utility is used to achieve that.

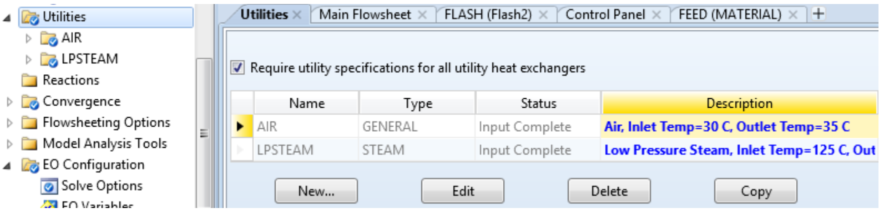
Complete the following tasks:

a) Using "*Specialty Chemicals with Metric Units*" template, create an Aspen Plus project. Under "**Properties**" environment, add the following components: acetone and water. The default property method is "**NRTL**". Assure that the option: "**Estimate missing parameters by UNIFAC**" is selected under "**Methods**" | "**Parameters**" | "**Binary Interaction**" | "**NRTL-1**" sheet. Click on "**Reset**" followed by "**Next**" button to run the simulation under "**Properties**" environment and watch out for messages of "**Control Panel**" for any error or serious warning.

b) Switch to "**Simulation**" environment and add "**FLASH**" as "**V-DRUM1**" block from "**Model Palette**" | "**Separators**" tab | "**Flash2**" group. Add "**HEATTANK**" as "**TANK**" block from "**Model Palette**" | "**Exchangers**" tab | "**Heater**" group. Add the required input and output stream for each block, as shown in Figure 16.39.

c) Enter the feed stream properties as mentioned above.

d) Under “**Utilities**” folder create two utilities: one for air and another for the low-pressure steam. If you select “**Require utility specifications for all utility heat exchangers**” option, then Aspen Plus will require you to associate each of the two blocks with a given utility, as shown in Figure 16.40. Subsequently, associate “**FLASH**” block with “**LPSTEAM**” heating utility and “**HEATTANK**” with “**AIR**” cooling utility using the “**Utility**” tab form for each block.



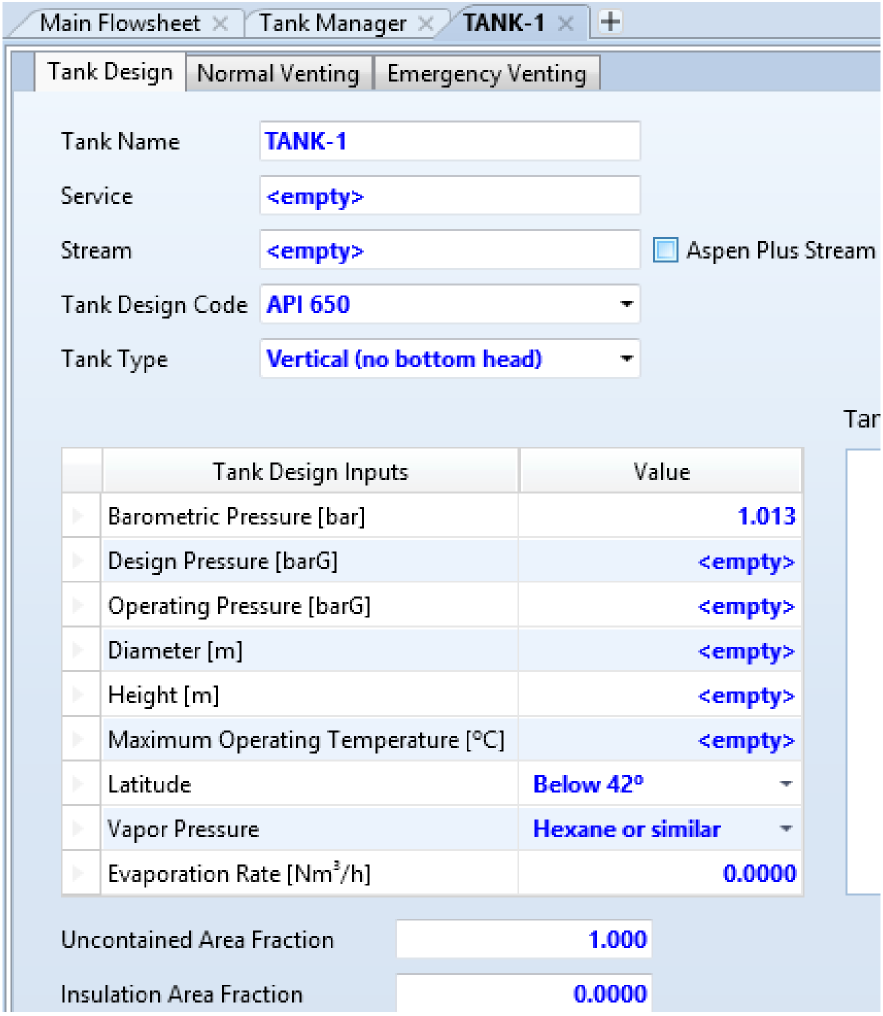
☑ Require utility specifications for all utility heat exchangers

Name	Type	Status	Description
AIR	GENERAL	Input Complete	Air, Inlet Temp=30 C, Outlet Temp=35 C
LPSTEAM	STEAM	Input Complete	Low Pressure Steam, Inlet Temp=125 C, Out

Figure 16.40 Creation of two utilities to be associated with the two blocks.

e) Run the show; watch out for any error or serious warning. Monitor the stream results, in particular, the phase of each stream whether it is liquid or vapor.

f) Upon obtaining successful results, switch to “**Safety Analysis**” environment. In “**Home**” ribbon click on “**Storage Tank Protection**” button and the “**Tank Manager**” form shows up. Click on “**Add**” button to add a tank with the default name “**TANK-1**”. Notice that a yellow strip shows up indicating missing information to be filled in by the user. Highlight the row that bears the name of the tank and click on “**Edit**” button to enter the required input data. The first “**Tank Design**” tab will show up as given in Figure 16.41. Here, your duty is to enter different parameters and settings. For the sake of learning, I will let the user try different Aspen Plus flowsheet streams to associate the storage tank with. That simply means that there is one possible process flowsheet stream, which upon selection will give estimates for the liquid movement, thermal movement, and preliminary device area for inbreathing and outbreathing case. Select “**Aspen Plus Stream**” checkbox shown in Figure 16.41 and the “**Stream Selection**” form will show up as in Figure 16.42. Moreover, for the “**Tank Design Code**” option it can be one of two choices: “*API 650*” or “*API 620*”. These are standard safety rules and measures set by **A**merican **P**etroleum **I**nstitute and Aspen Plus will recommend either one based on the specifications you supply as input parameters.



Tank Name	TANK-1
Service	<empty>
Stream	<empty> ☐ Aspen Plus Stream
Tank Design Code	API 650
Tank Type	Vertical (no bottom head)

Tank Design Inputs	Value
Barometric Pressure [bar]	1.013
Design Pressure [barG]	<empty>
Operating Pressure [barG]	<empty>
Diameter [m]	<empty>
Height [m]	<empty>
Maximum Operating Temperature [°C]	<empty>
Latitude	Below 42°
Vapor Pressure	Hexane or similar
Evaporation Rate [Nm^3/h]	0.0000

Uncontained Area Fraction	1.000
Insulation Area Fraction	0.0000

Figure 16.41 The “**Tank Design**” tab form where the user is required to enter more input parameters and settings.

Of course, the storage tank protection calculations can be made without referring to any process flowsheet stream. However, selecting the proper stream will minimize the required input data. For example, tank vapor molecular weight, relieving gas temperature, and relieving gas molecular weight data will be calculated for naming a specific flowsheet stream. Upon selecting one stream and continue filling in the required input data for the three tab forms, you will eventually notice that if the selected stream is not the proper choice, then Aspen Plus will show a colored strip saying that “**The flash indicates there is no vapor present under emergency venting conditions**”. You should realize now which stream to associate the storage tank with, out of the four possible streams.

g) Fill in the missing information under “**Tank Design**” tab. Notice that the design pressure value lies between 0 and 1 barG. It represents the maximum pressure the tank wall and

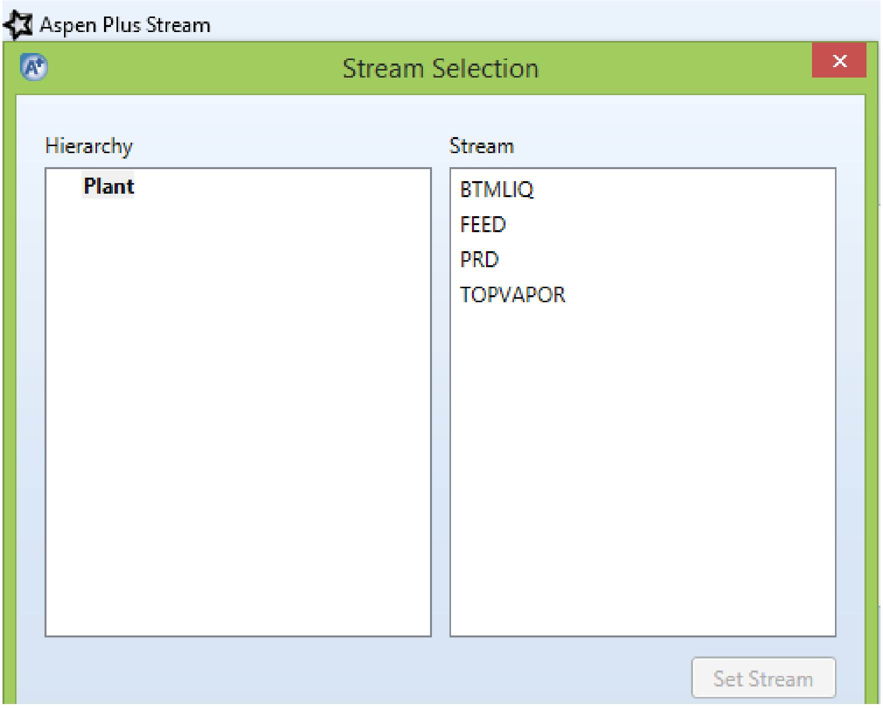


Figure 16.42 If "**Aspen Plus Stream**" checkbox is activated, then the user will be required to select a process flowsheet stream to associate the storage tank with.

structure can handle. The operating pressure also lies between 0 and 1 barG. However, in our case, all process flowsheet streams are run at 1 atm absolute (or, 0 barG). For the tank diameter and height, the value is left to the user to choose from. Notice that according to API specifications for shop-welded flat bottom tanks (API SPEC. 12 F), the approximate working capacity divided by the nominal (total) capacity varies between 0.8 for a small capacity tank (volume 14.7 m^3, ID = 2.5 m, height = 3.0 m) to 0.96 for a large capacity tank (volume = 81.5 m^3, ID = 4.7, height = 4.7 m). The evaporation rate (N m^3/h) can be assumed zero, although I calculated the value based on the diffusivity of acetone in air under unimolecular diffusion (UMD) case to be around 0.03 m^3/h for a mass transfer area of 12.5 m^2.

h) Fill in the missing information under "**Normal Venting**" tab. Notice that the set pressure can be set to 0 mbarG, which is the pressure at the inlet of the device at which the relief device starts opening under service conditions. It varies between 0 and 1000 mbarG (i.e., 1 barG). For the vacuum set pressure, the value varies between 0 and −1000 mbarG. This represents the pressure at the inlet of the relieving device protecting for vacuum conditions, and it has to be below the operating pressure of the tank. The maximum liquid inflow and outflow value can be entered in light of the volumetric flow rate (m^3/h) of the liquid "**PRD**" stream.

i) Fill in the missing information under "**Emergency Venting**" tab. Notice that the set pressure can be set to 0 mbarG, which is the pressure at which the relieving device starts to open upon service conditions. It varies between 0 and 1000 mbarG (i.e., 1 barG). For the bottom tan above grade, it can be a value between 0 and definitely less than the flame height and it is used to calculate the wetted exposed surface area of a storage tank. See Aspen Plus built-in help titled: "**Storage Tank Exposed Area Calculations**".

j) Report the results by clicking on "**Calculation Sheet**" button in "**Reports**" ribbon. Alternatively, the results are also shown in the right pane of both "**Normal Venting**" tab and "**Emergency Venting**" tab form.

HOMEWORK/CLASSWORK 16.2 (SEPARATION OF C2/C3/C4 HYDROCARBON MIXTURE)

Let us consider the feed to be made of three components which are: Ethane, propane, and *n*-butane. However, water will be added as it is required when we have water or steam as utility.

Complete the following tasks:

a) Using "*Gas Processing with Metric Units*" template, create an Aspen Plus project. Under "**Properties**" environment, add the following components: ethane, propane, *n*-butane, and water. The default property method is "**PENG-ROB**". Click on "**Reset**" followed by "**Next**" button to run the simulation under "**Properties**" environment and watch out messages of "**Control Panel**" for any error or serious warning.

b) Switch to "**Simulation**" environment and add twice the "**FRACT1**" block from "**Model Palette**" | "**Columns**" tab | "**RadFrac**" group. Add the required input and output stream for each block, as shown in Figure 16.43.

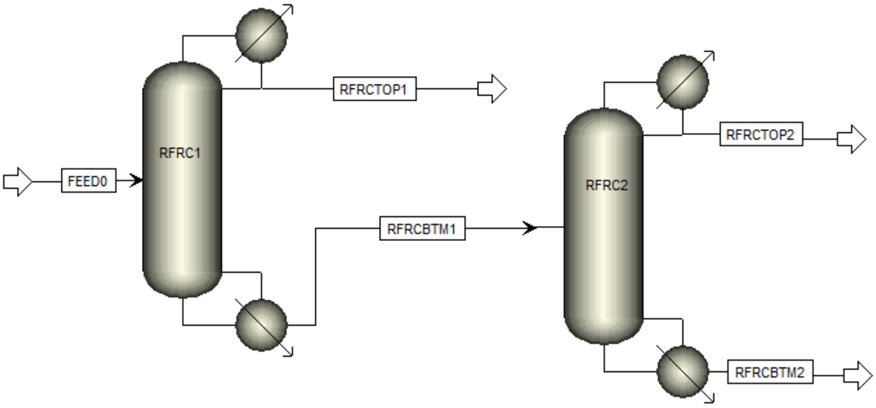
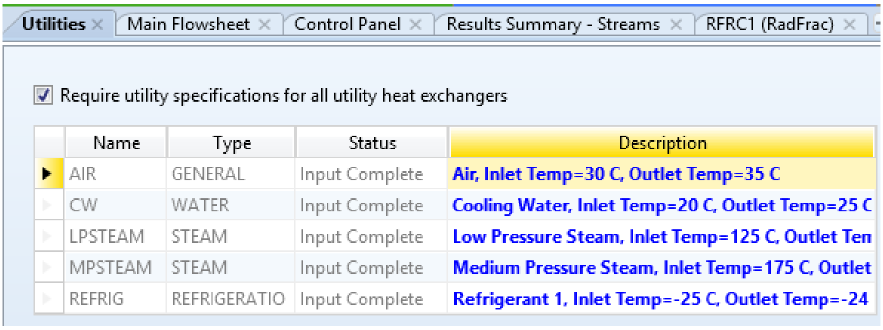


Figure 16.43 The process flowsheet for C2/C3/C4 separation.

c) Under "**Utilities**" folder, create the following utilities, which will be used for cooling and heating purpose, as shown in Figure 16.44. If you select "**Require utility specifications for all utility heat exchangers**" option, then Aspen Plus will require you to associate both reboiler and condenser for each distillation tower with a given utility. Subsequently, associate "**RFRC1**" condenser with "**REFRIG**" cooling utility, "**RFRC1**" reboiler with "**MPSTEAM**" heating utility, "**RFRC2**" condenser with "**CW**" cooling utility, and "**RFRC2**" reboiler with "**MPSTEAM**" heating utility, using the "**Condenser**" and "**Reboiler**" tab form for each distillation column. "**LPSTEAM**" and "**AIR**" utility will be utilized later at energy analysis stage.



☑ Require utility specifications for all utility heat exchangers

	Name	Type	Status	Description
▶	AIR	GENERAL	Input Complete	Air, Inlet Temp=30 C, Outlet Temp=35 C
	CW	WATER	Input Complete	Cooling Water, Inlet Temp=20 C, Outlet Temp=25 C
	LPSTEAM	STEAM	Input Complete	Low Pressure Steam, Inlet Temp=125 C, Outlet Ten
	MPSTEAM	STEAM	Input Complete	Medium Pressure Steam, Inlet Temp=175 C, Outlet
	REFRIG	REFRIGERATIO	Input Complete	Refrigerant 1, Inlet Temp=-25 C, Outlet Temp=-24

Figure 16.44 Creation of utilities for cooling and heating purpose.

d) Enter the feed stream properties: The total flow rate is 1 kmol/s, $P = 30$ bar, $T = 25°C$, and one-third mole fraction each for the three hydrocarbon components. No water is present in the feed stream.

e) For "**RFRC1**" block input data: # of stages = 30, total condenser, reflux ratio = 5, the molar distillate to feed ratio is 0.99999 based on ethane, the feed stage enters at stage #10 from top, and the condenser pressure = 25 bar.

f) For "**RFRC2**" block input data: # of stages = 20, total condenser, reflux ratio = 5, the molar distillate to feed ratio is 0.9999 based on propane, the feed stage enters at stage #10 from top, and the condenser pressure = 18 bar.

g) Run the show, watch out any error or serious warning. Monitor the stream results, in particular, the mass fraction is at least *0.99* for each of the three components in three product streams: "**RFRCTOP1**", "**RFRCTOP2**", and "**RFRCBTM2**".

h) Upon obtaining successful results, switch to "**Safety Analysis**" environment. Add one pressure safety valve ("**PSV-1**") and one rupture disk ("**RD-1**") and associate each with a process stream as shown in Figure 16.45.

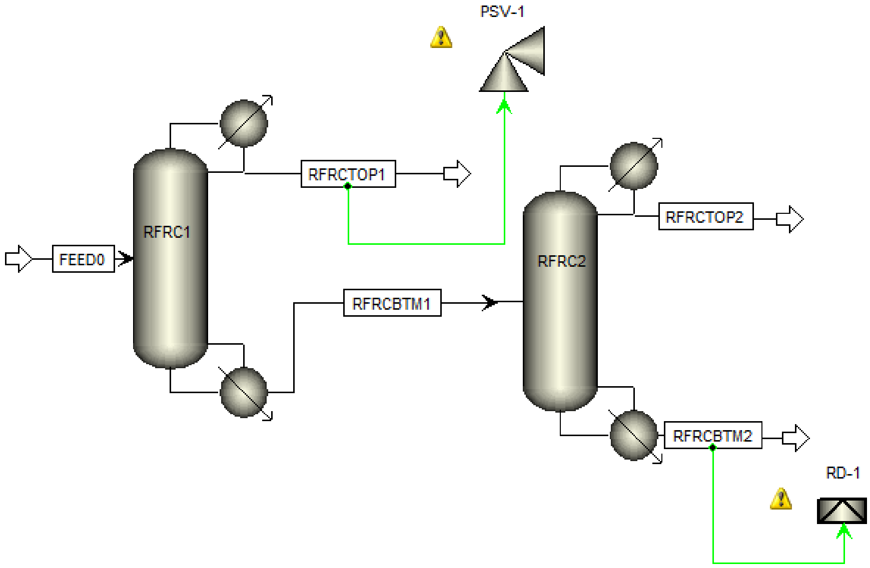


Figure 16.45 Adding one PSV and one RD for the process flowsheet.

i) For "**PSV-1**" input data: Set the "**Scenario Type**" as "*Reflux Failure*" and set "**Discharge to**" option to "*HP Flare*". Complete missing design specifications such that you do not end up with any design violation. In addition, you have to enter both the nominal diameter and schedule # for both inline and outline pipe such that you do not violate the pressure drop restriction imposed on both sides of the valve.

j) For "**RD-1**" input data: Set the "**Scenario Type**" as "*Abnormal Heat or Vapor Input*" and set "**Discharge to**" option to "*HP Flare*". Complete missing design specifications such that you do not end up with any design violation. In addition, you have to enter both the nominal diameter and schedule # for both inline and outline pipe such that you do not violate the minimum flow requirement.

k) Report the results by clicking on "**Documentation Builder**" button in "**Reports**" ribbon.

l) Switch back to "**Simulation**" environment and activate the energy analysis. Report the utility cost ($/year) and rate (Gcal/h) for heating and cooling. Also, report the carbon emission flow (tonne/h).

m) Click on the "**Find Design Changes**" button to see if there exists any recommended retrofit.

n) Can we replace the refrigeration "**REFRIG**" utility of "**RFRC1**" condenser by either "**CW**" or "**AIR**"? Why not? Try either one and see what Aspen Plus tells you.

o) Let us see if we can improve the process heat exchangers network (HEN) by introducing the following three heater-type blocks, as shown in Figure 16.46. Such blocks can be added from "**Model Palette**" | "**Exchangers**" tab | "**Heater**" group. For "**HEATER1**" block, use it to heat the condenser ("**S-1**") stream from 1.7 up to 25°C. The "**COOLER1**" and "**COOLER2**" block will be used to cool down "**RFRC2**" two product streams down to 25°C. Heating and cooling process will be isobaric (i.e., zero pressure drop between the inlet and outlet steam).

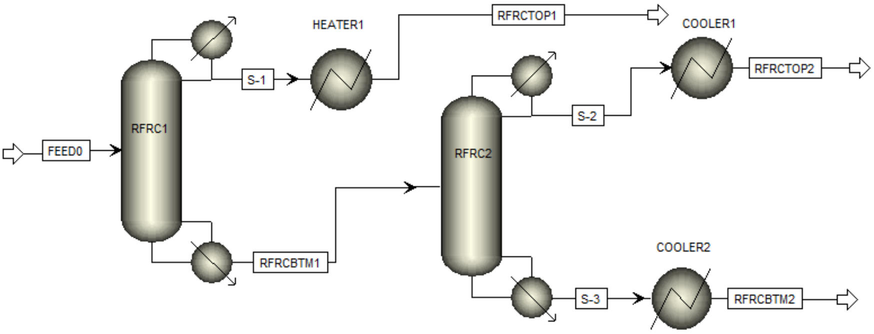


Figure 16.46 Inclusion of three heater-type blocks: one heater and two coolers.

p) Click on "**Reset**" followed by "**Run**" button. After obtaining the green light from Aspen Plus, activate the energy analysis. Report the utility cost ($/year) and rate (Gcal/h). Also, report the carbon emission rate (tonne/h). Is there any potential saving in energy cost?

q) Click on the "**Find Design Changes**" button to see if there exists any recommended retrofit.

r) Apply the recommended retrofit by clicking on "**Add E-100**" blue hyperlink.

s) Based on the given figures, show how Aspen Plus estimates the payback period of the recommended scheme.

t) Delete scenarios that contribute nothing by clicking on "**Compare Scenarios**" button, which shows a table of scenarios comparison.

u) Click on "**Details**" button, to send a copy to Aspen Energy Analyzer and show a plot similar to that shown in Figure 16.38.

v) In brief, write down what the recommended "**E-100**" retrofit is all about.

17

ASPEN PROCESS ECONOMIC ANALYZER (APEA)

17.1 OPTIMIZED PROCESS FLOWSHEET FOR ACETIC ANHYDRIDE PRODUCTION

To demonstrate how to evaluate the economic attributes of a chemical process, we use the production of acetic anhydride from acetone, as explained in Chapter 6. We focus here on how to evaluate the total annual cost, which is made of operating and fixed cost, in addition to cost indices that indicate the profitability of the process.

Figure 17.1 shows the optimized process flowsheet for acetic anhydride production. The process flowsheet for acetic anhydride production is made of PFR with a recycle for the unreacted acetone, followed by two downstream separation units:

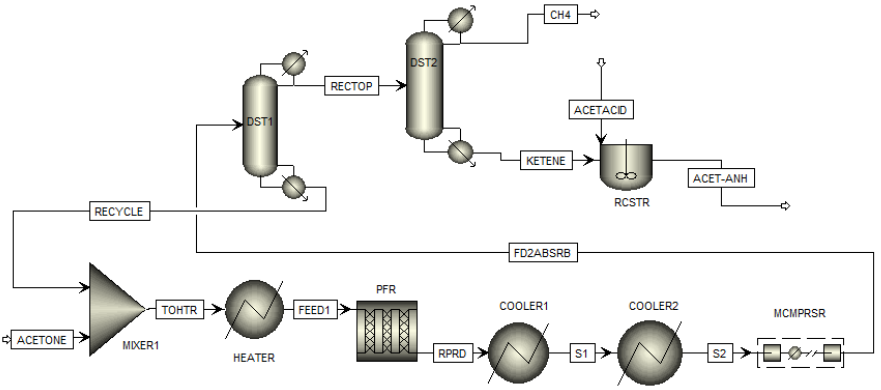


Figure 17.1 The process flowsheet for acetic anhydride production with recycling of the unreacted acetone.

Aspen Plus®: Chemical Engineering Applications, First Edition. Kamal I.M. Al-Malah.

Companion Website: www.wiley.com/go/Al-Malah/AspenPlusApplications

rectifying and distillation column and finally the conversion of ketene and acetic acid into acetic anhydride using CSTR. However, the difference from that in Chapter 6 lies in recycling of the bottom stream out of the rectifier, adding one heater and two coolers, a multistage compressor, and the application of high pressure conditions throughout the downstream processing steps. The idea here is to explore different alternatives in design configuration when it comes to APEA-mapped objects.

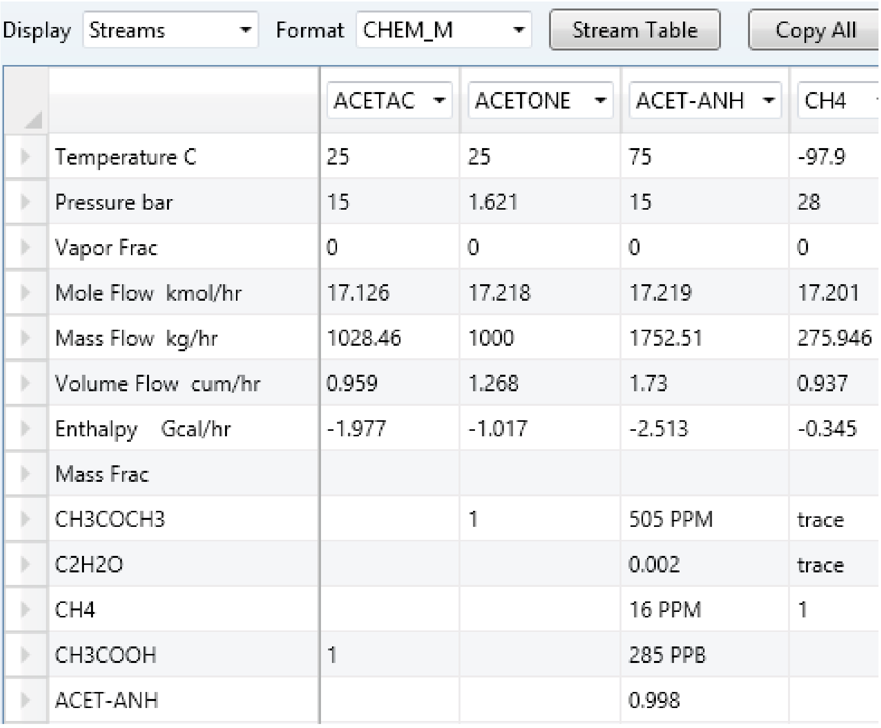
Figure 17.2 shows a portion of the Aspen-generated "**Input File**" for acetic anhydride production. See Chapter 6 for further information about the reaction kinetics and chemical equilibrium.

```
COMPONENTS: CH3COCH3/C2H2O/CH4/CH3COOH/ACET-ANH/WATER.
PROPERTIES: WILS-NTH, TRUE-COMPS=YES, ESTIMATE ALL.
STREAM ACETACID: TEMP=25°C, PRES=15 bar, MOLE-FLOW CH3COOH
   17.126 kmol/hr.
STREAM ACETONE: TEMP=25°C. PRES=1.6 <atm> MASS-FLOW=1000 kg/hr of pure
  CH3COCH
BLOCK MIXER1 MIXER: PARAM
BLOCK COOLER1 HEATER: Outlet TEMP=140°C. PRES=0 (i.e., ΔP=0).
   UTILITY-ID=GLPSTEAM.
BLOCK COOLER2 HEATER: PARAM TEMP=90°C. PRES=0 (i.e., ΔP=0).
   UTILITY-ID=AIR
BLOCK HEATER HEATER: PARAM TEMP=1035 K, PRES=1.6 <atm>, MAXIT=40.
  UTILITY-ID=FH1000.
BLOCK DST1 RADFRAC: PARAM NSTAGE=14, ALGORITHM=STANDARD MAXOL=25,
  DAMPING=NONE, COL-CONFIG CONDENSER=TOTAL, REBOILER=KETTLE, FEEDS
  FD2ABSRB #7 ABOVE-STAGE, PRODUCTS: RECYCLE #14 Liquid / RECTOP #1
  Liquid, P-SPEC: Stage #1 @ 29 bar, COL-SPECS: Bottom/Feed Ratio=1.0,
  MOLE-RR=6. Bottom/Feed PARAMS: Feed Stream=FD2ABSRB Component
   Basis=CH3COCH3. COND-UTIL=REFRIG4, and REB-UTIL=HPSTEAM.
BLOCK DST2 RADFRAC: PARAM NSTAGE=14 ALGORITHM=STANDARD MAXOL=75
   LL-METH=HYBRID & DAMPING=MEDIUM, PARAM2 SALTS=IGNORE-CHECK, COL-CONFIG
   CONDENSER=TOTAL, REBOILER=KETTLE, FEEDS RECTOP #7 ABOVE-STAGE, PROD-
  UCTS: KETENE #14 Liquid / CH4 #1 Liquid, P-SPEC: Stage #1 @ 28 bar,
   COL-SPECS: Distillate/Feed=0.9999, MOLE-RR=4, Distil-
  late/Feed PARAMS:
   Feed Stream=RECTOP Component Basis =CH4. COND-UTIL=REFRIG4
   REB-UTIL=LPSTEAM
BLOCK RCSTR RCSTR: PARAM TEMP=75°C. PRES=15 bar. NPHASE=1 PHASE=L,
  RES TIME=1.5 <hr> BLOCK-OPTION FREE-WATER=NO REACTIONS RXN-IDS=R-2.
  UTILITY UTILITY-ID=CWATER.
BLOCK PFR RPLUG: PARAM TYPE=ADIABATIC LENGTH=3. <meter> DIAM=1.
  <meter> & PRES=1.6 <atm> REACTIONS RXN-IDS=R-1.
BLOCK MCMPRSR COMPR: PARAM NSTAGE=4 TYPE=ASME-ISENTROPIC PRES=29 bar.
  COOLER-NPHAS=1 & SB-MAXIT=30 SB-TOL=0.0001, FEEDS: S2 at stage
  #1, PRODUCTS: FD2ABSRB at stage #4, COOLER-SPECS: #1 DUTY=0 / #2
  TEMP=150°C
   / #3 TEMP=150°C / #4 DUTY=0, BLOCK-OPTION FREE-WATER=NO, COOLER-UTL=AIR,
   and SPECS-UTL=ELECTRIC.
REACTIONS R-1: POWERLAW, REAC-DATA 1 PHASE=V, RATE-CON 1 PRE-EXP=
   8.19733E+014 ACT-ENERGY=284521.7 <kJ/kmol> STOIC 1 MIXED CH3COCH3 –1. /
   C2H2O 1. / CH4 1. POWLAW-EXP 1 MIXED CH3COCH3 1.
REACTIONS R-2: POWERLAW, REAC-DATA 1 EQUIL, STOIC 1 MIXED C2H2O –1. /
   CH3COOH –1. / ACET-ANH 1.
```

Figure 17.2 A portion of the Aspen Plus-generated "**Input File**" pertaining to process flowsheet shown in Figure 17.1.

Moreover, for “**Methods**” | “**Parameters**” | “**Binary Interaction**” | “**WILSON-1**” | “**Input**” tab sheet, the “**Estimate missing parameters by UNIFAC**” option is selected.

Figure 17.3 shows the simulation results where only the input and output streams are shown.



	ACETAC	ACETONE	ACET-ANH	CH4
Temperature C	25	25	75	-97.9
Pressure bar	15	1.621	15	28
Vapor Frac	0	0	0	0
Mole Flow kmol/hr	17.126	17.218	17.219	17.201
Mass Flow kg/hr	1028.46	1000	1752.51	275.946
Volume Flow cum/hr	0.959	1.268	1.73	0.937
Enthalpy Gcal/hr	-1.977	-1.017	-2.513	-0.345
Mass Frac				
CH3COCH3		1	505 PPM	trace
C2H2O			0.002	trace
CH4			16 PPM	1
CH3COOH	1		285 PPB	
ACET-ANH			0.998	

Figure 17.3 Production of an extra pure acetic anhydride and of the side product pure methane.

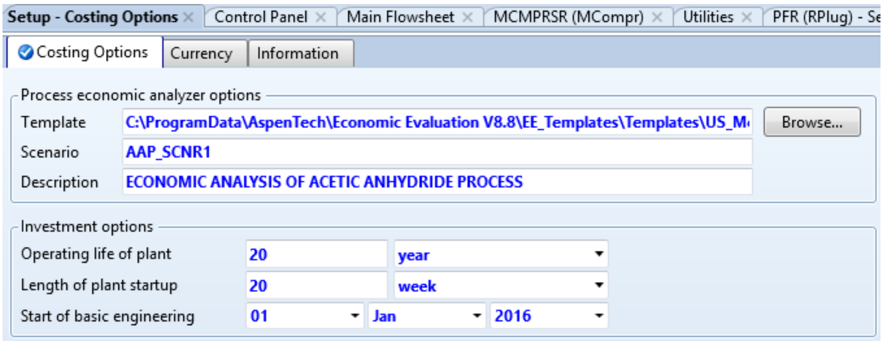
17.2 COSTING OPTIONS IN ASPEN PLUS

The costing options include the selection of the basis for cost estimation, defining feed and product stream prices, and defining utilities in terms of pricing and associating them with pieces of equipment, such as a pump, compressor, condenser, reboiler, and heater.

17.2.1 Aspen Process Economic Analyzer (APEA) Estimation Template

In “**Navigation**” panel, let us go to “**Setup**” | “**Costing Options**” | “**Costing options**” tab form. We use this form to specify the template and options for performing costing analysis on the given process using APEA, as shown in Figure 17.4.

The different options, appearing in Figure 17.4, are explained in the following:



Template: C:\ProgramData\AspenTech\Economic Evaluation V8.8\EE_Templates\Templates\US_M

Scenario: AAP_SCNR1

Description: ECONOMIC ANALYSIS OF ACETIC ANHYDRIDE PROCESS

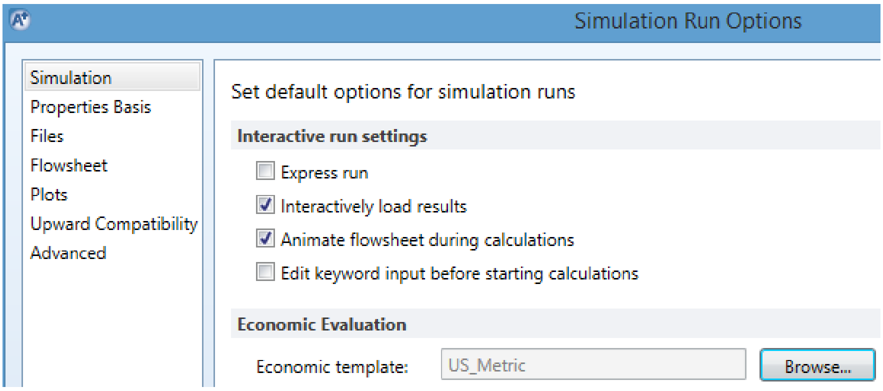
Operating life of plant: 20 year

Length of plant startup: 20 week

Start of basic engineering: 01 Jan 2016

Figure 17.4 The "**Costing Options**" tab form where we customize APEA and investment options.

- **Template:** Click on "**Browse**" button to select one of the provided APEA templates or alternatively one of your own. These templates correspond to different locations around the world and different unit sets for the cost reports (IP = Inch-Pound units, or Metric). The default costing template can be specified in the "**File**" | "**Options**" | "**Simulation Run Options**" dialog box, specifically the "**Simulation**" tab, as shown in Figure 17.5.
- **Scenario:** Specify a name here to identify the scenario. The APEA files are stored in a subfolder with this name. You can use different scenario names to generate different costing reports for variations in a model.
- **Description:** Text specified here appears in the header of APEA reports.
- **Operating life of plant, Length of plant startup, Start of basic engineering:** These values are used by APEA in its costing calculations. If these are not specified, default values will be taken from the costing template.



☐ Express run

☑ Interactively load results

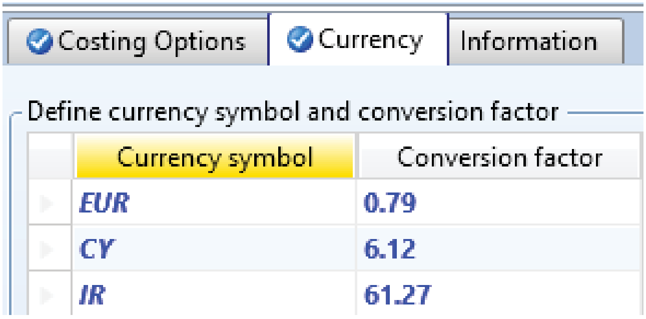
☑ Animate flowsheet during calculations

☐ Edit keyword input before starting calculations

Economic template: US_Metric

Figure 17.5 Selection of the economic template to be associated with APEA.

Click on the "**Currency**" tab (shown in Figure 17.4) if you wish to use your own local currency. Use this sheet to define currency symbols and conversion factors. For each symbol, the conversion factor is the number of units of that currency equal to US$1. We will use US$ here; however, for the sake of demonstrating how to use a currency other than US$, Figure 17.6 shows the conversion factor between Euro (€), Chinese Yuan (CY), and Indian Rupee (IR) on one side versus US$1.0 for each entry. The conversion factor is thus equal to currency per US$1.0.



Define currency symbol and conversion factor

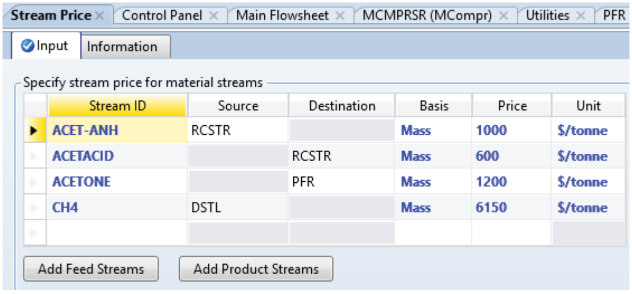
Currency symbol	Conversion factor
EUR	0.79
CY	6.12
IR	61.27

Figure 17.6 Currency conversion factor between Euro (€), Chinese Yuan (CY), and Indian Rupee (IR) on one side versus US$1.0 for each entry.

Keep in mind that when you define a currency symbol here, all the other units, based on the selected currency (cost per length, cost per area, cost per time, etc.), are automatically defined using the new currency unit. To prevent the unit lists from getting too long, you may define a maximum of three currency symbols. Moreover, you may not use this "**Currency**" tab sheet if you have defined currency symbols on the other "**Setup**" | "**Custom Units**" | "**Setup**" tab sheet. If you want to make use of this "**Currency**" tab sheet instead of that one, go to that sheet and delete all the currency-related custom units first.

17.2.2 Feed and Product Stream Prices

Next, move to "**Setup**" | "**Stream Price**" | "**Input**" form. We will enter the basis, price, and unit for each feed or product stream. Click on "**Add Feed Streams**" button to enter the price-related parameter for each feed stream. After handling feed streams prices, click on "**Add Product Streams**" button to enter the price-related parameter for each product stream. Figure 17.7 shows the entered numbers for all input and output streams of acetic anhydride production (see Figure 17.3). Notice the following points:



Specify stream price for material streams

Stream ID	Source	Destination	Basis	Price	Unit
ACET-ANH	RCSTR		Mass	1000	$/tonne
ACETACID		RCSTR	Mass	600	$/tonne
ACETONE		PFR	Mass	1200	$/tonne
CH4	DSTL		Mass	6150	$/tonne

Figure 17.7 The price-related parameters for feed and product streams.

- The prices are quoted (November 2014) from two Chinese sites: www.made-in-china.com and www.alibaba.com.
- The last (**Unit**) column has many options, one of them is \$/tonne and another \$/ton. One tonne is the metric ton that is equal to 1000 kg and the ton is the imperial ton (2240 lb), or 1016.047 kg.
- The price of an extra pure CH_4 (not liquefied natural gas LNG) is reported as 1 \$/l, and it is stored in a pressurized cylinder at room temperature and critical/super critical pressure. Thus, the critical density (0.1627 kg/l) is used to convert the unit price based on mass, because liquid methane will be incompressible as is the case with liquids above their critical temperatures, in general. If there is a price for CH_4 as a bulk rate or whole sale, then it will be better to adopt it here, instead of the estimated price.

17.2.3 Utility Association with a Flowsheet Block

For a given utility, you can either use the built-in defined utility, such as electricity, or define your own. In previous versions of Aspen, the unit price was not supplied but now with Aspen Plus® latest versions, you have the luxury to make use of the unit price for a given utility, in addition to other parameters, such as the utility side film heat transfer coefficient for most utilities.

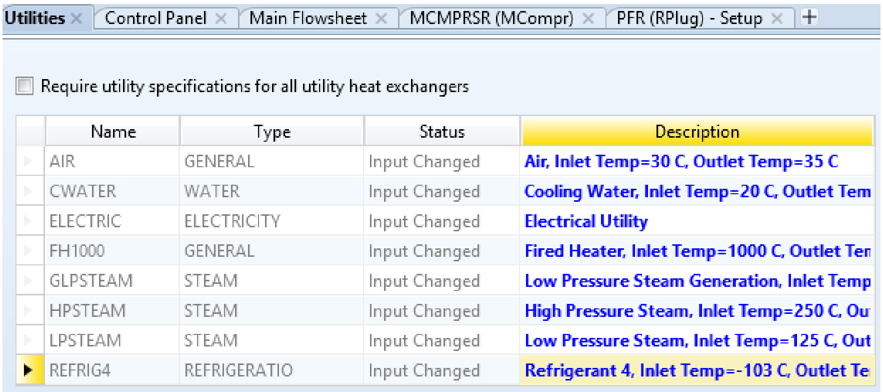
NOTE #1: *To save the user's head from an extra headache, it is strongly recommended to run the simulator and converge to successful results before making any association between a utility type and a given block, which requires a form of energy input or output.*

Under "**Utilities**" folder, you may add as many as it takes of utility types to later associate each with one or more of the flowsheet blocks. As a rule of thumb, before you associate a utility type with a given block, you have to be aware of the following issues:

- Does the block require heating, cooling, or a form of energy like electricity?
- If heating or cooling is required, then you need to check for the proper utility type based on the temperature difference approach between the cooling and heating medium. Keep in mind that the heating medium has to be at least 10°C (or 18°F) higher than the cooling medium. This is called the minimum temperature approach. If the user violates this requirement, Aspen Plus will inform the user about the temperature cross condition while getting a violation ticket from Aspen Plus police officer. On the other hand, for a refrigerator utility, the minimum temperature approach is set to 2°C, by default.
- If a choice is to be made between air and cooling water, air is cheaper than cooling water.
- It is a good practice to look at the temperature of the inlet and outlet stream associated with a given block. This will help the user decide on the proper utility type. Moreover, the outlet stream temperature from a condenser (or reboiler) will also help in this regard.
- Watch out the heat duty associated with a reactor or any other unit operation (i.e., flash unit) to decide if heating or cooling is needed.
- For a process flowsheet with recycle as in our case here, it is a good strategy to associate one utility type at a time, run the simulation, assure that the solution converges to

reasonable results, and consecutively continue associating a utility type with a given block until you are completely done with the utility association procedure. In fact, upon the addition of either water or steam as a utility, Aspen Plus will require the addition of water to the list of components, under "**Properties**" environment. After doing this marginal (off-shore) step, Aspen Plus will not converge until I make some mild modifications to the second distillation tower. Of course, this behavior is justifiable with recycled processes as the set of algebraic/differential equations, describing the physical picture, becomes highly intermingled and entangled.

Figure 17.8 shows a list of some defined utilities borrowed from Aspen Plus database.



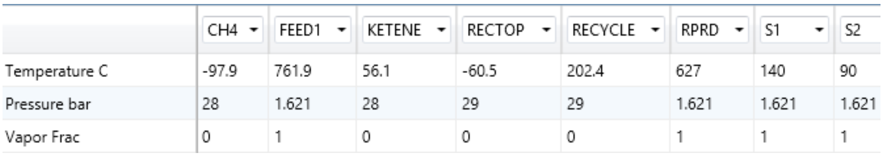
☐ Require utility specifications for all utility heat exchangers

Name	Type	Status	Description
AIR	GENERAL	Input Changed	Air, Inlet Temp=30 C, Outlet Temp=35 C
CWATER	WATER	Input Changed	Cooling Water, Inlet Temp=20 C, Outlet Tem
ELECTRIC	ELECTRICITY	Input Changed	Electrical Utility
FH1000	GENERAL	Input Changed	Fired Heater, Inlet Temp=1000 C, Outlet Ter
GLPSTEAM	STEAM	Input Changed	Low Pressure Steam Generation, Inlet Temp
HPSTEAM	STEAM	Input Changed	High Pressure Steam, Inlet Temp=250 C, Ou
LPSTEAM	STEAM	Input Changed	Low Pressure Steam, Inlet Temp=125 C, Out
REFRIG4	REFRIGERATIO	Input Changed	Refrigerant 4, Inlet Temp=-103 C, Outlet Te

Figure 17.8 A list of some defined utilities taken from Aspen Plus database.

<u>**NOTE #2:**</u> *The difference between "**GLPSTEAM**" and "**LPSTEAM**" utility is a matter of how water enters the utility setup as either saturated liquid or saturated vapor, respectively. Moreover, the checkbox: "**Require utility specifications for all utility heat exchangers**" is not enforced at the beginning; however, it will be enforced at the end just to assure that we did not miss any block requiring some sort of energy to be added or be taken off. See point #10 in the following text.*

Figure 17.9 shows the stream results in terms of pressure, temperature, and phase state. Let us start from left and go right along the list of streams.



	CH4	FEED1	KETENE	RECTOP	RECYCLE	RPRD	S1	S2
Temperature C	-97.9	761.9	56.1	-60.5	202.4	627	140	90
Pressure bar	28	1.621	28	29	29	1.621	1.621	1.621
Vapor Frac	0	1	0	0	0	1	1	1

Figure 17.9 The stream results in terms of P, T, and phase state.

1. Methane gas leaves the *condenser* of “**DST2**” column at $T = -97.9$°C and $P = 28$ bar; hence, we need a refrigeration utility to do the job, which is condensation at such a very low T value. Thus, “*REFRIG4*” utility can do the job; hence, we associate it with this condenser.
2. “**FEED1**” stream leaves the *heater* at $T = 761.9$°C, where both “**RECYCLE**” and “**ACETONE**” stream enter the same heater but at temperatures lower than 761.9°C. Hence, heating is required to account for the sensible heat. Consequently, we will associate “*FH1000*” utility with the heater.
3. At the same time, “**FEED1**” stream enters the *PFR* at $T = 761.9$°C; however, the PFR is run under *adiabatic* condition; hence, there is no need to worry about heat effects.
4. “**KETENE**” stream leaves the *reboiler* of “**DST2**” column at $T = 56.1$°C. Hence, we need to heat up the falling down liquid to partially vaporize it. “*LPSTEAM*” utility will be used in this regard.
5. “**RECTOP**” stream leaves the *condenser* of “**DST1**” column at $T = -60.5$°C. Hence, we need to cool down the rising up vapor to liquefy it for refluxing purpose. “*REFRIG4*” utility will be used in this regard. I have to admit here that refrigerant 3 (phase change at −64°C) will do the job here but I am reluctant to stick to what I have here simply because time is running out on my side to make such a modification and ask a permission from AspenTech, Inc. for licensing any modification I make within this textbook as far as snapshots, taken for any of their software platforms, are concerned.
6. “**RECYCLE**” stream leaves the *reboiler* of “**DST1**” at $T = 202.4$°C. Hence, we need to heat up the falling down liquid to partially vaporize it. “*HPSTEAM*” utility will be used in this regard.
7. “**RPRD**” stream leaves the PFR reactor at $T = 627$°C and at the same time we need to introduce it to the first distillation tower but at a high pressure value; hence, we need a multistage compressor to achieve this task. However, compression is more efficient when the inlet feed to compressor exists at a low temperature. Consequently, we will carry out two successive cooling steps. The first “**COOLER1**” *cooler* will reduce the temperature of “**RPRD**” stream down to 140°C (i.e., T of “**S1**” stream) while at the same time “*GLPSTEAM*” utility will be generated. The second “**COOLER2**” *cooler* will complete the job by further reducing the temperature down to 90°C (i.e., T of “**S2**” stream), utilizing “*AIR*” utility.
8. “*AIR*” utility is used under “**MCMPRSR**” | “**Setup**” | “**Cooler**” tab sheet. See also point #10 in the following text.
9. The last block will be “**RCSTR**”. Looking at “**RCSTR**” | “**Results**” | “**Summary**” tab sheet will reveal that it has a heat duty of −0.297618 Gcal/h. This means that to maintain “**RCSTR**” isothermally (at $T = 75$°C) running, we need to take off such an amount of heat. “*CWATER*” utility will be used in this regard. Notice that if “*AIR*” is used instead, then the following message will show up in “**Control Panel**”: “Block: RCSTR Model: RCSTR

```
*  WARNING
    MINIMUM APPROACH TEMPERATURE VIOLATED IN UTILITY AIR
    IN RCSTR        BLOCK RCSTR
    BLOCK TEMPERATURES       3.109851D+02 K AND     3.481500D+02 K
```

```
UTILITY TEMPERATURES      3.081500D+02  K AND      3.031500D+02  K
MINIMUM APPROACH TEMPERATURE      1.000000D+01  K"
```

In fact, I tried "*AIR*" as the first choice as opposed to "*CWATER*" utility, because air is cheaper than cooling water.

10. Now, enforce the option: "***Require utility specifications for all utility heat exchangers*** *" found in* "***Utilities***" folder. You will notice that "**MCMPRSSR**" block shows a half-filled red circle, indicating the status of missing information. Go to "**MCMPRSR**" | "**Setup**" | "**Specs**" tab sheet and enter "*ELECTRIC*" utility for the "**Utility**" entry. At the same time, "*AIR*" utility is already entered under "**Cooler**" tab sheet for the same multi-stage compressor.

Reinitialize, run the show, and check if there is any error or serious warning.

NOTE #3: *Before moving to costing steps for a chemical process, one has to assure that the simulator ends up with a converging and reasonable solution that is free of errors or serious warnings.*

17.3 THE FIRST ROUTE FOR CHEMICAL PROCESS COSTING

The *first* route is via economic activation mode within Aspen Plus environment itself. This is straightforward and requires a less intervention by the user. However, if there are serious design errors/warnings then the second route will be the choice. Figure 17.10 (*top*) shows "**Economic**" ribbon where only "**Send to APEA**" button is active. This will be

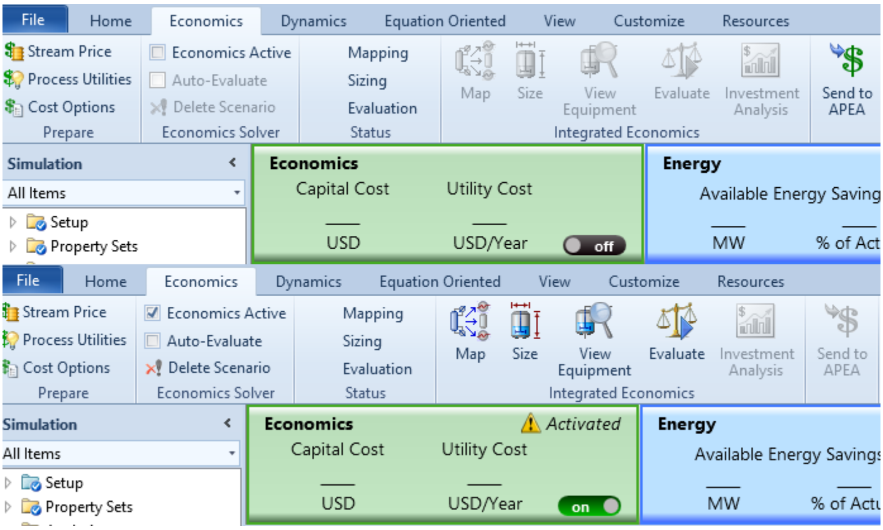


Figure 17.10 The "**Economics**" ribbon allows the user to carry out further costing and economic analysis step, using the stand-alone APEA (*top*) or Aspen Plus assisted by the economic analyzer (*bottom*).

covered in the upcoming section regarding using the dedicated stand-alone Aspen Plus Economic Analyzer (APEA). For now, select “**Economics Active**” checkbox, and you will notice that economics-related buttons will become active as shown in Figure 17.10 (*bottom*). It shows the different costing-related buttons, starting from left to right: “**Map**”, “**Size**”, “**View Equipment**”, “**Evaluate**”, and “**Investment Analysis**”.

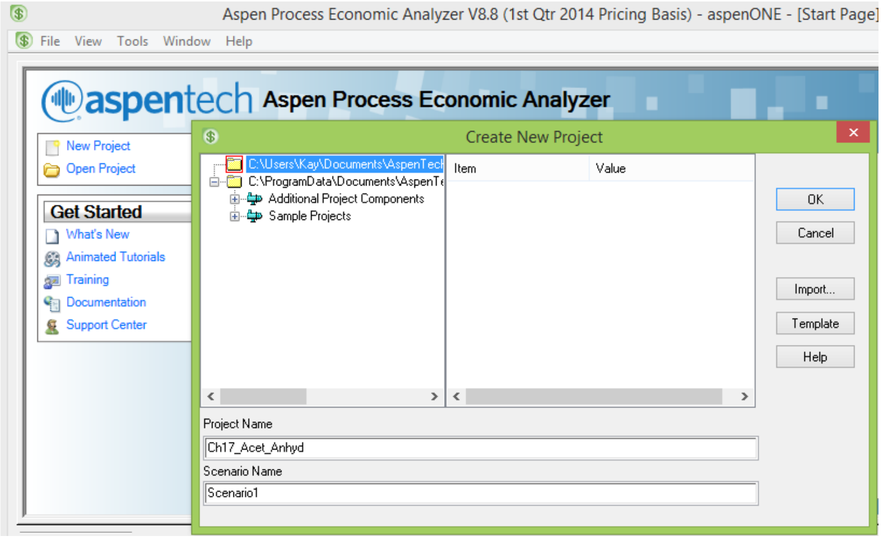
Once you activate the economics algorithm, the following message is shown in “**Control Panel**”:

```
->Created costing scenario C:\Kamal\ASPEN\Aspen Plus
  V8.8\ch17\Ch17_Acet_AnhydCost\AAP_SCNR1
```

We will not travel on the first route, because the second route is a more comprehensive in terms of allowing the user to manipulate different properties of APEA-mapped objects and recheck (i.e., reevaluate) to assure that the project design scenario is error-free. After the user gets acquainted by the second route, he/she may go through the first route all the way until the end and will find out that all steps are fully covered in the second route in depth using APEA. APEA is an exclusive dedicated environment, which allows the user to go down to the granular level in terms of geometrical design considerations.

17.4 THE SECOND ROUND FOR CHEMICAL PROCESS COSTING

After clicking on “**Send to Economics**” button, the main document interface (MDI) window of a separate Aspen Plus piece of software called <u>*Aspen Process Economic Analyzer (APEA)*</u> will open up together with the <u>*first*</u> “**Create New Project**” child window, as shown in Figure 17.11. Fill in any missing information and click on “**OK**” button to close the <u>*first*</u> child window. Moreover, the left pane shows some useful links where the user can benefit from to get acquainted by the economic aspects.



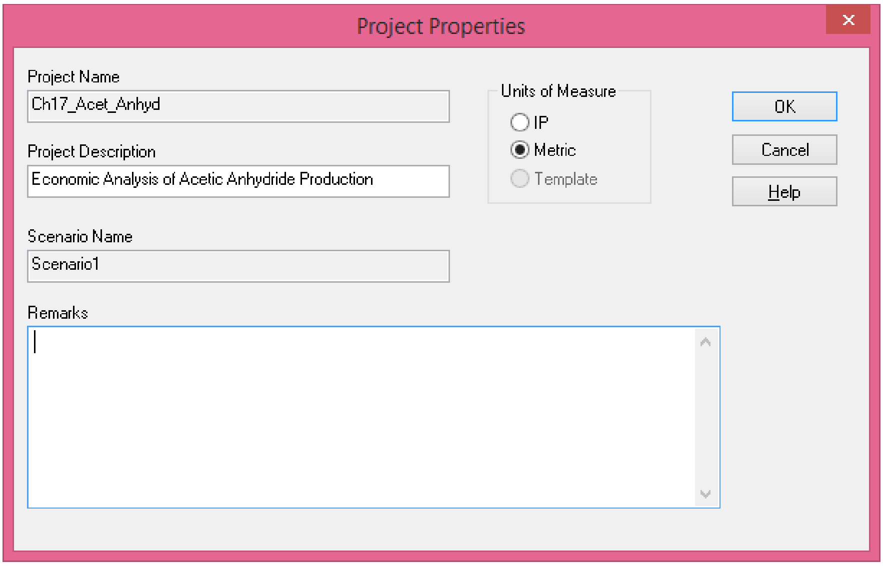
Project Name: Ch17_Acet_Anhyd

Scenario Name: Scenario1

Figure 17.11 The <u>first</u> “**Create New Project**” child window of APEA.

17.4.1 Project Properties

Upon clicking on "**OK**" button in Figure 17.11, the *second* "**Project Properties**" child window will show up as in Figure 17.12. Give a description for the project, select the "**Units of Measure**" option, and click on "**OK**" button to close the *second* child window and proceed to the *third* child window (Figure 17.13).



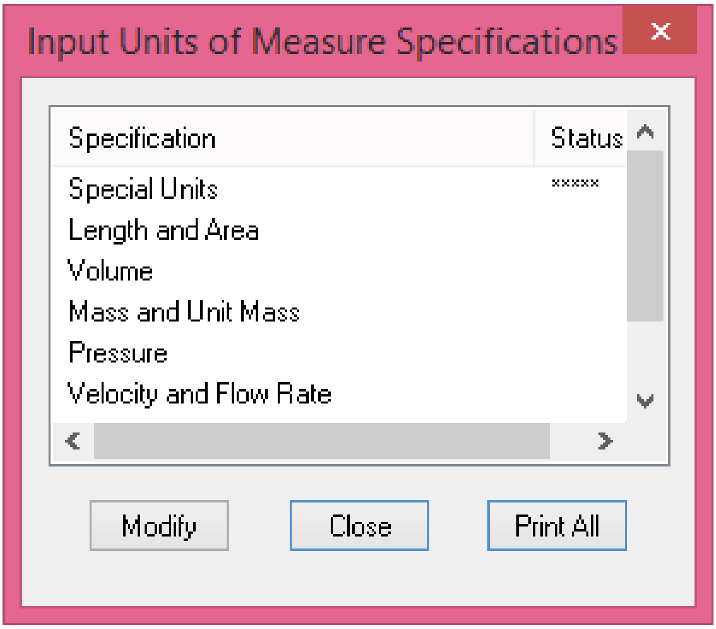
Project Name
Ch17_Acet_Anhyd

Project Description
Economic Analysis of Acetic Anhydride Production

Scenario Name
Scenario1

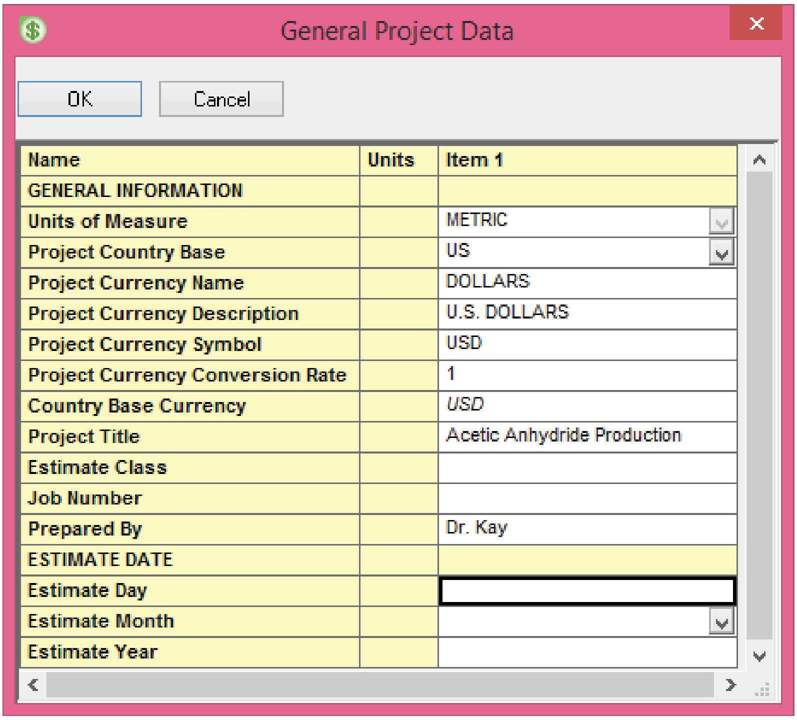
Figure 17.12 The second "**Project Properties**" child window of APEA.

The *third* "**Input Units of Measure Specifications**" child window will pop up as in Figure 17.13. You can modify here the unit of measure associated with any physical quantity or leave it as is and modify it later from within APEA main window using the pertinent form. Click on "**Close**" button to proceed to the *fourth* child window (Figure 17.14).



Specification	Status
Special Units	xxxxx
Length and Area	
Volume	
Mass and Unit Mass	
Pressure	
Velocity and Flow Rate	

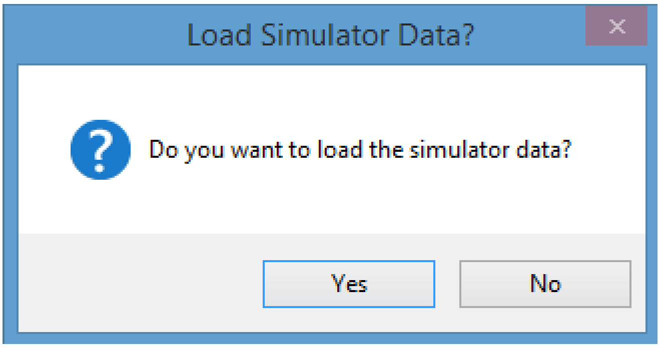
Figure 17.13 The <u>third</u> "**Input Units of Measure Specifications**" child window.



Name	Units	Item 1
GENERAL INFORMATION		
Units of Measure		METRIC
Project Country Base		US
Project Currency Name		DOLLARS
Project Currency Description		U.S. DOLLARS
Project Currency Symbol		USD
Project Currency Conversion Rate		1
Country Base Currency		*USD*
Project Title		Acetic Anhydride Production
Estimate Class		
Job Number		
Prepared By		Dr. Kay
ESTIMATE DATE		
Estimate Day		
Estimate Month		
Estimate Year		

Figure 17.14 The <u>fourth</u> "**General Project Data**" child window of APEA.

The *fourth* “**General Project Data**” child window will pop up as in Figure 17.14. For example, you may enter the project title, your name, and estimate date in the dedicated records. Click on “**OK**” button to proceed to the *fifth* child window (Figure 17.15).

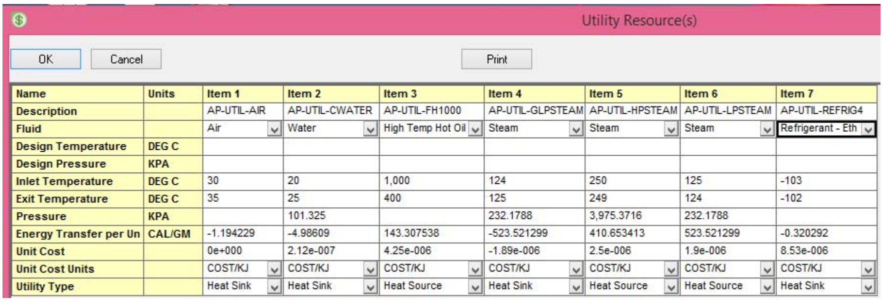


Do you want to load the simulator data?

Figure 17.15 The fifth (“**Load Simulator Data?**”) child window.

17.4.2 Loading Simulator Data

The *fifth* (“**Load Simulator Data?**”) child window will pop up as in Figure 17.15. Click on “**Yes**” button to proceed to the *sixth* child window (Figure 17.16).



Name	Units	Item 1	Item 2	Item 3	Item 4	Item 5	Item 6	Item 7
Description		AP-UTIL-AIR	AP-UTIL-CWATER	AP-UTIL-FH1000	AP-UTIL-GLPSTEAM	AP-UTIL-HPSTEAM	AP-UTIL-LPSTEAM	AP-UTIL-REFRIG4
Fluid		Air	Water	High Temp Hot Oil	Steam	Steam	Steam	Refrigerant - Eth
Design Temperature	DEG C							
Design Pressure	KPA							
Inlet Temperature	DEG C	30	20	1,000	124	250	125	-103
Exit Temperature	DEG C	35	25	400	125	249	124	-102
Pressure	KPA		101.325		232.1788	3,975.3716	232.1788	
Energy Transfer per Un	CAL/GM	-1.194229	-4.98609	143.307538	-523.521299	410.653413	523.521299	-0.320292
Unit Cost		0e+000	2.12e-007	4.25e-006	-1.89e-006	2.5e-006	1.9e-006	8.53e-006
Unit Cost Units		COST/KJ	COST/KJ	COST/KJ	COST/KJ	COST/KJ	COST/KJ	COST/KJ
Utility Type		Heat Sink	Heat Sink	Heat Source	Heat Sink	Heat Source	Heat Source	Heat Sink

Figure 17.16 The sixth “**Utility Resource(s)**” child window for changing fluid type associated with a given utility.

The *sixth* “**Utility Resource(s)**” child window will pop up as in Figure 17.16. Pay attention to match the right “**Fluid**” type with each utility. Use the bottom scroll bar to proceed to other hidden utilities. In particular, pay attention that “*AIR*” utility is associated with air fluid, “*FH100*” utility with high-temperature hot oil, and “*REFRIG4*” with refrigerant ethane. Click on “**OK**” button to proceed to the main window (Figure 17.17).

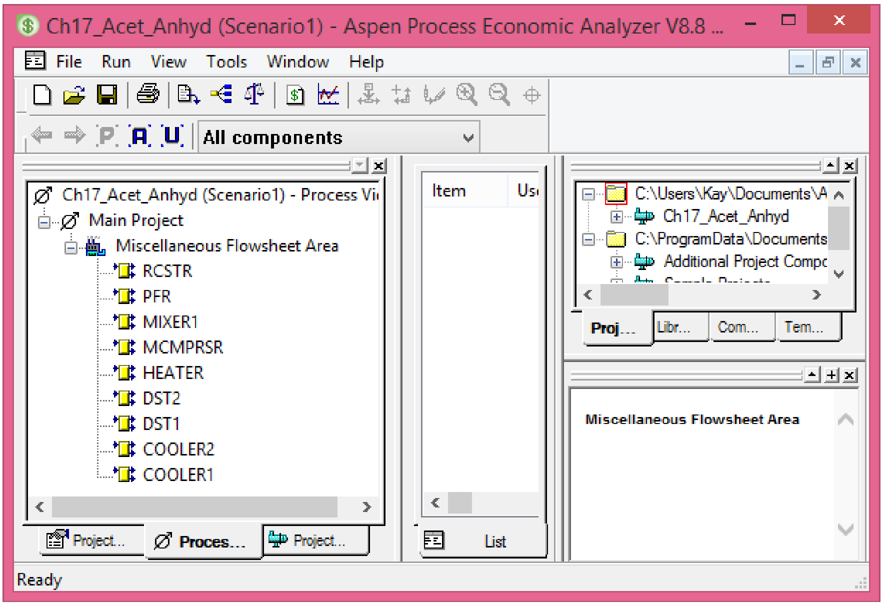


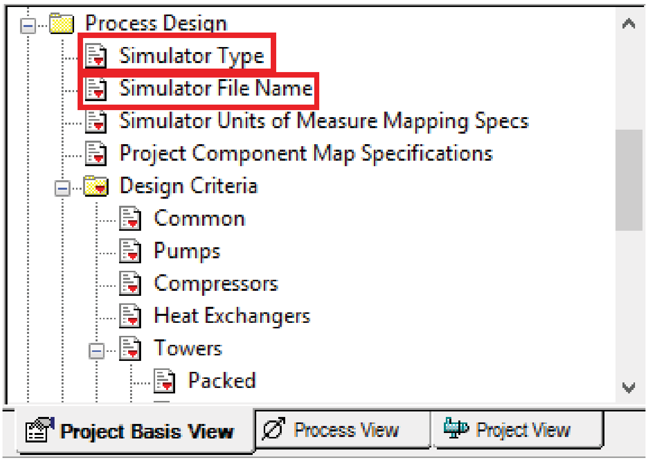
Figure 17.17 The main (parent) window of APEA with three view tabs to help manage the project and modify any project entity.

The main (parent) window of APEA will show up as in Figure 17.17. It has three view tabs by which one can look at the project content, carry out editing/modification steps, and rerun so that new changes take into effect. We will show the features that pertain to the costing issue.

Just next to the printer icon, shown at the top toolbar of the main window, there are different icons that represent the "**Load Data**", "**Map**", "**Evaluate**", "**Capital Costs**", and "**Investment Analysis**" button, respectively.

Notice that we have already loaded the simulator data as indicated by Figure 17.15 and also as shown in Figure 17.17 under "**Process View**" tab that we have imported flowsheet blocks of acetic anhydride production. If we have not done so (as is the case when the user opens a new APEA project from scratch), then we need to specify the simulator type and data file using the proper forms as shown in Figure 17.18. Under "**Project Basis View**" tab, right-click on "**Simulator Type**" form, to tell APEA what the simulator type is, whereby you can select from a list and, after closing the first form, repeat the same thing for "**Simulator File Name**" form where you guide APEA to the location of ***.apw** file, which pertains to the successful steady-state solution of the process flowsheet project. After carrying out these two form modifications, then the user must click on "**Load Data**" ( ) button to import the flowsheet blocks into the newly created, from scratch, APEA project.

Notice that other shown forms can be edited and modified as well.

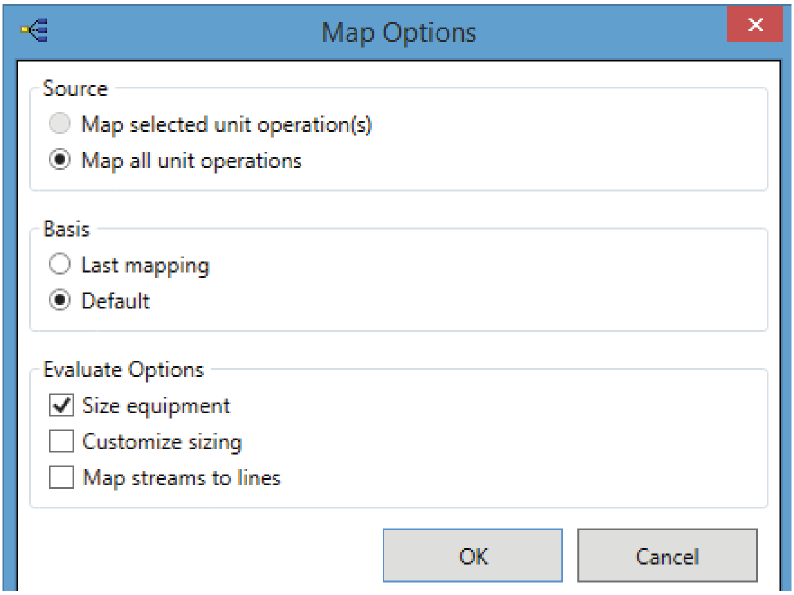


- Process Design
  - Simulator Type
  - Simulator File Name
  - Simulator Units of Measure Mapping Specs
  - Project Component Map Specifications
  - Design Criteria
    - Common
    - Pumps
    - Compressors
    - Heat Exchangers
    - Towers
      - Packed

Figure 17.18 The location of the forms to change or define the simulator type and read data from ***.apw** file.

17.4.3 Mapping and Sizing

Click on the "**Map Simulator Items**" ( ) button and you will get "**Map Options**" window. Check "*Size equipment*" option from "**Evaluate Options**" box. "*Customize sizing*" option is selected only if you would like to interfere with the details of equipment sizing. I prefer to leave it unselected. See Figure 17.19. Click on "**OK**" button to proceed.



Map Options

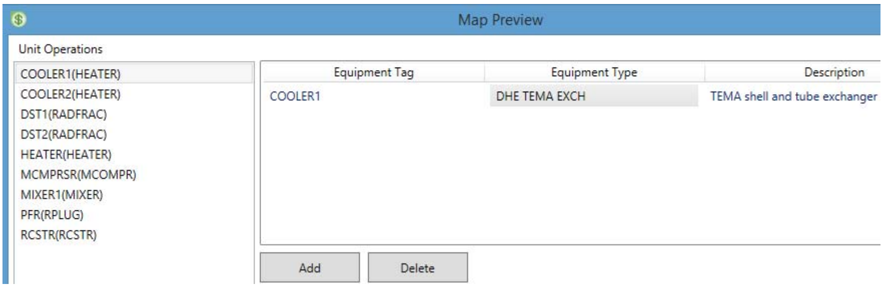
Source
○ Map selected unit operation(s)
● Map all unit operations

Basis
○ Last mapping
● Default

Evaluate Options
☑ Size equipment
☐ Customize sizing
☐ Map streams to lines

Figure 17.19 "**Map Options**" windows for mapping flowsheet objects with APEA built-in objects.

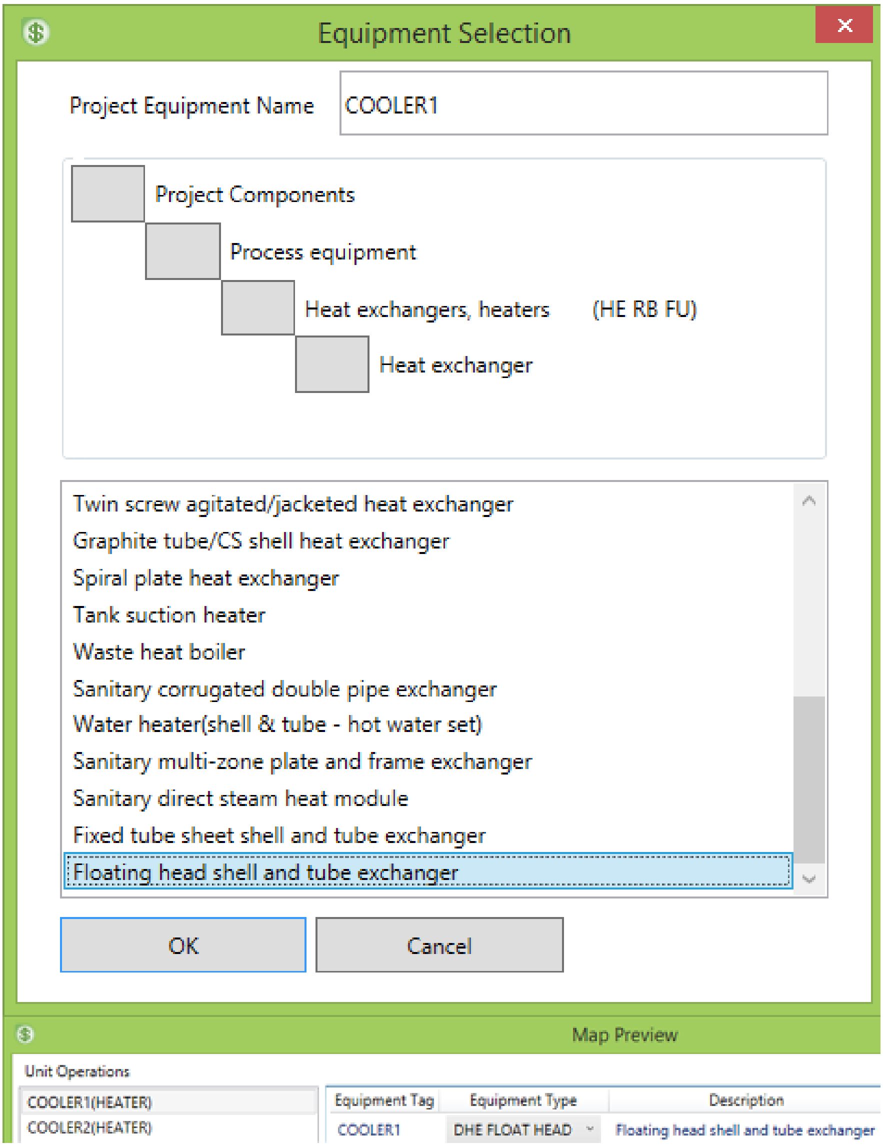
Figure 17.20 shows the selection of APEA-mapped object with “**COOLER1**” block. Notice that you can stick with what is selected by APEA, modify the recommended APEA project component via clicking on the corresponding item found under the second column titled: “**Equipment Type**”, or highlight it and then use “**Delete**” button to remove from the list. On the left pane, you will see the simulator items (i.e., blocks), which are already matched with APEA project items (middle pane) labeled by equipment tag and type. The description gives a very short summary about each mapped object.



Equipment Tag	Equipment Type	Description
COOLER1	DHE TEMA EXCH	TEMA shell and tube exchanger

Figure 17.20 The APEA-mapped object with “**COOLER1**” block.

Since we have a significant temperature difference between the hot and cold stream, click on “*DHE TEMA EXCH*” record (or row) and “**Equipment Selection**” window will show up. Go to “**Heat exchangers, heater**” menu item followed by “**Heat exchanger**” submenu item to select “*Floating head shell and tube exchanger*” option as shown in Figure 17.21 (*top*). Click on “**OK**” button to close the equipment selection window. The newly mapped heat exchanger type is now shown in the map preview window (*bottom*).



Project Equipment Name: COOLER1

- Project Components
  - Process equipment
    - Heat exchangers, heaters (HE RB FU)
      - Heat exchanger

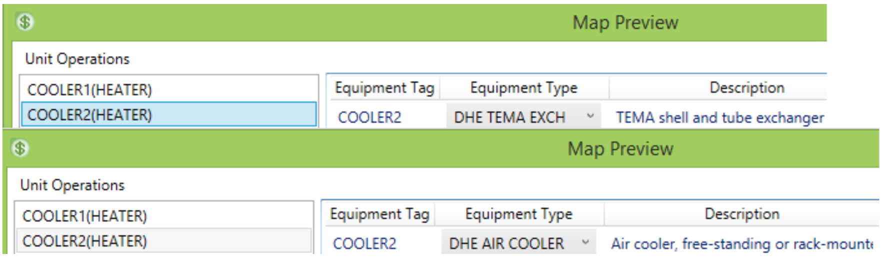
Twin screw agitated/jacketed heat exchanger
Graphite tube/CS shell heat exchanger
Spiral plate heat exchanger
Tank suction heater
Waste heat boiler
Sanitary corrugated double pipe exchanger
Water heater(shell & tube - hot water set)
Sanitary multi-zone plate and frame exchanger
Sanitary direct steam heat module
Fixed tube sheet shell and tube exchanger
Floating head shell and tube exchanger

Unit Operations
COOLER1(HEATER)
COOLER2(HEATER)

Equipment Tag	Equipment Type	Description
COOLER1	DHE FLOAT HEAD	Floating head shell and tube exchanger

Figure 17.21 The “**Equipment Selection**” window whereby to modify the old mapped heat exchanger type (*top*) and the updated map preview after selecting the newly mapped exchanger (*bottom*).

Figure 17.22 shows the old and new mapped heat exchanger type with flowsheet “**COOLER2**” object. The change is made to reflect the fact that “*AIR*” utility is associated with “**COOLER2**” block. To make the replacement of the old by the new exchanger type, simply click on “*DHE TEMA EXCH*” record under the second (“**Equipment Type**”) column and follow the procedure, outlined earlier in the previous step pertaining to “**COOLER1**” block.

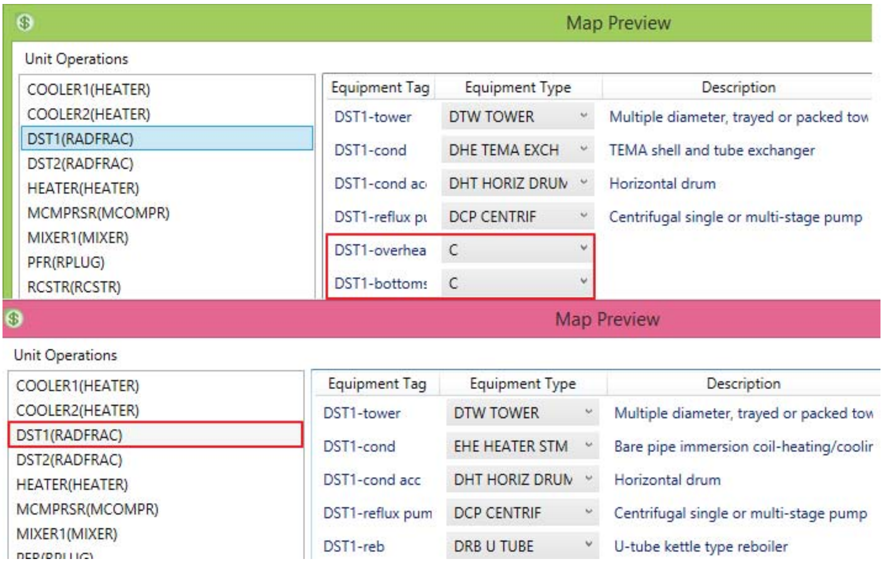


Equipment Tag	Equipment Type	Description
COOLER2	DHE TEMA EXCH	TEMA shell and tube exchanger

Equipment Tag	Equipment Type	Description
COOLER2	DHE AIR COOLER	Air cooler, free-standing or rack-mount

Figure 17.22 The old (*top*) and new (*bottom*) APEA-mapped object with "**COOLER2**" block.

For both "*DST1(RADFRAC)*" and "DST2*(RADFRAC)*" simulator item shown on the left pane, you will notice that there are more than one mapped APEA project item. This is simply because the distillation column will be made of the multitray column itself plus what is called the column accessories, such as reboiler, condenser, drum, and the pump. We will delete both "*DST1-overhead split*" and "*DST1-bottoms split*" mapped object. This is simply because "*C*" objects from the "**Equipment Type**" list (middle column) produce nothing (i.e., not mapped to a physical object that has a cost). Thus, highlight the corresponding "**Equipment Tag**" record one at a time and click on "**Delete**" button. Repeat the same procedure for the second "**Equipment Tag**" item and then delete. Moreover, the column condenser was remapped from "*DHE TEMA EXCH*" to "*EHE HEATER STM*" (i.e., bare pipe immersion coil), as shown in Figure 17.23.



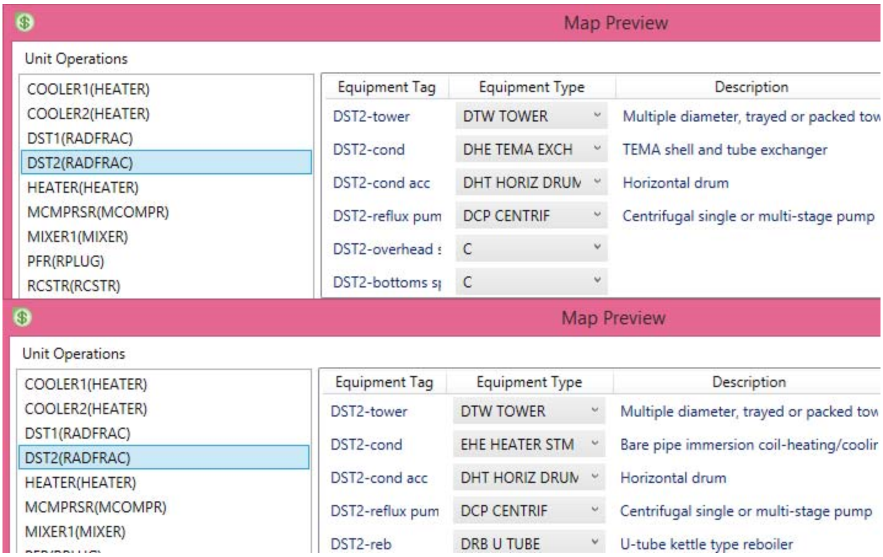
Equipment Tag	Equipment Type	Description
DST1-tower	DTW TOWER	Multiple diameter, trayed or packed tow
DST1-cond	DHE TEMA EXCH	TEMA shell and tube exchanger
DST1-cond ac	DHT HORIZ DRUM	Horizontal drum
DST1-reflux pu	DCP CENTRIF	Centrifugal single or multi-stage pump
DST1-overhea	C	
DST1-bottom	C	

Equipment Tag	Equipment Type	Description
DST1-tower	DTW TOWER	Multiple diameter, trayed or packed tow
DST1-cond	EHE HEATER STM	Bare pipe immersion coil-heating/coolir
DST1-cond acc	DHT HORIZ DRUM	Horizontal drum
DST1-reflux pum	DCP CENTRIF	Centrifugal single or multi-stage pump
DST1-reb	DRB U TUBE	U-tube kettle type reboiler

Figure 17.23 The unmapped "**C**" equipment type are deleted (top). The old (*top*) and new (*bottom*) APEA-mapped objects with "**DST1(RADFRAC)**" block.

NOTE #4: In “***Map Preview***” window under “**Add**” and “**Delete**” button, *there exists “**Configuration**” drop-down list, for* *both distillation columns*, *which the user can select from. Each option will view the column in a different configuration. You may click on the image, shown on the right side of the configuration menu, to zoom it in. For example, the difference between “Standard – Single” and “Standard – Total” option lies in the fact that in the former case the reflux pump takes care only of the reflux stream, whereas in the latter it handles both the reflux and distillate (overhead liquid product) stream. You may explore other options as well.*

For “**DST2(RADFRAC)**” block, again, we will delete both “*DST2-overhead split*” and “*DST2-bottoms split*” mapped object as we explained that in the “**DST1**” column case. Moreover, the column condenser is remapped from “*DHE TEMA EXCH*” to “*EHE HEATER STM*” (i.e., bare pipe immersion coil), as shown in Figure 17.24.

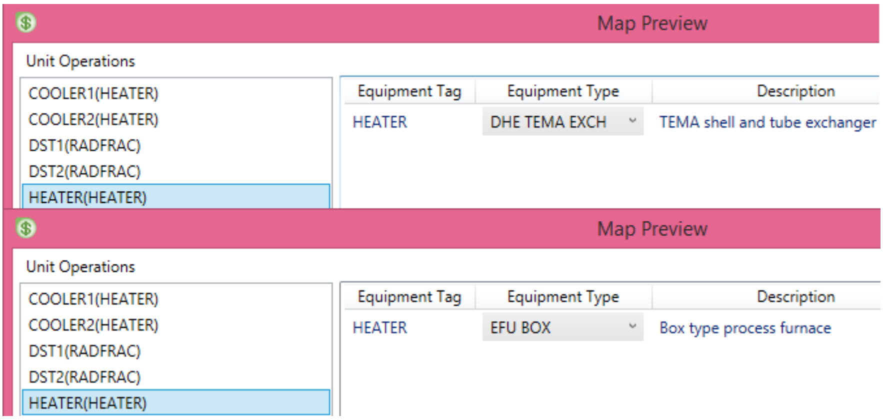


Equipment Tag	Equipment Type	Description
DST2-tower	DTW TOWER	Multiple diameter, trayed or packed tow
DST2-cond	DHE TEMA EXCH	TEMA shell and tube exchanger
DST2-cond acc	DHT HORIZ DRUM	Horizontal drum
DST2-reflux pum	DCP CENTRIF	Centrifugal single or multi-stage pump
DST2-overhead s	C	
DST2-bottoms s	C	

Equipment Tag	Equipment Type	Description
DST2-tower	DTW TOWER	Multiple diameter, trayed or packed tow
DST2-cond	EHE HEATER STM	Bare pipe immersion coil-heating/coolir
DST2-cond acc	DHT HORIZ DRUM	Horizontal drum
DST2-reflux pum	DCP CENTRIF	Centrifugal single or multi-stage pump
DST2-reb	DRB U TUBE	U-tube kettle type reboiler

Figure 17.24 The old (*top*) and new (*bottom*) APEA-mapped objects with “**DST2(RADFRAC)**” block.

For “**HEATER**” block, we will remap the old “*DHE TEMA EXCH*” type to “*EFU BOX*” type (i.e., box type process furnace) which will reflect the “*FH1000*” utility associated with “**HEATER**” block, as shown in Figure 17.25.



COOLER1(HEATER)
COOLER2(HEATER)
DST1(RADFRAC)
DST2(RADFRAC)
HEATER(HEATER)

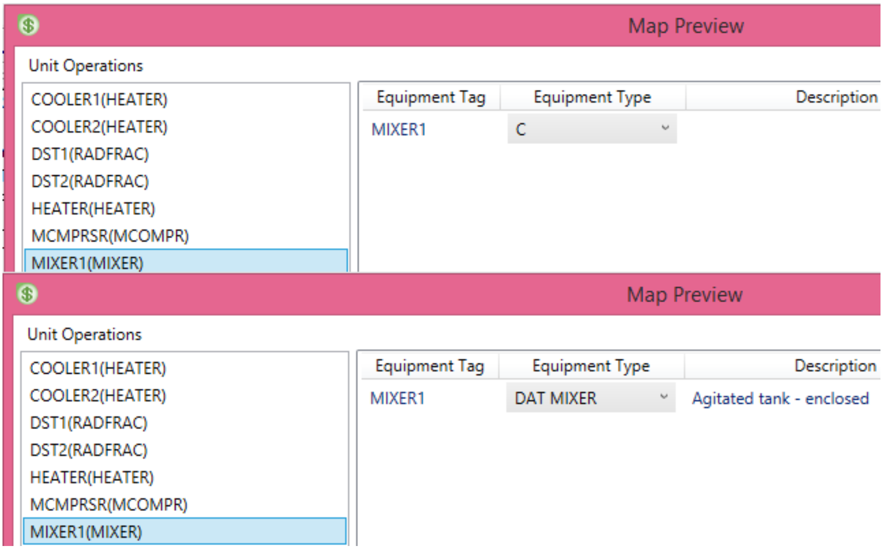
Equipment Tag	Equipment Type	Description
HEATER	DHE TEMA EXCH	TEMA shell and tube exchanger

COOLER1(HEATER)
COOLER2(HEATER)
DST1(RADFRAC)
DST2(RADFRAC)
HEATER(HEATER)

Equipment Tag	Equipment Type	Description
HEATER	EFU BOX	Box type process furnace

Figure 17.25 The old (*top*) and new (*bottom*) APEA-mapped object with “**HEATER**” block.

For “**MIXER1**” block, we will remap the old “*C*” type to “*DAT MIXER*” type (i.e., agitated tank—enclosed), which will reflect a typical agitation tank, as shown in Figure 17.26.



COOLER1(HEATER)
COOLER2(HEATER)
DST1(RADFRAC)
DST2(RADFRAC)
HEATER(HEATER)
MCMPRSR(MCOMPR)
MIXER1(MIXER)

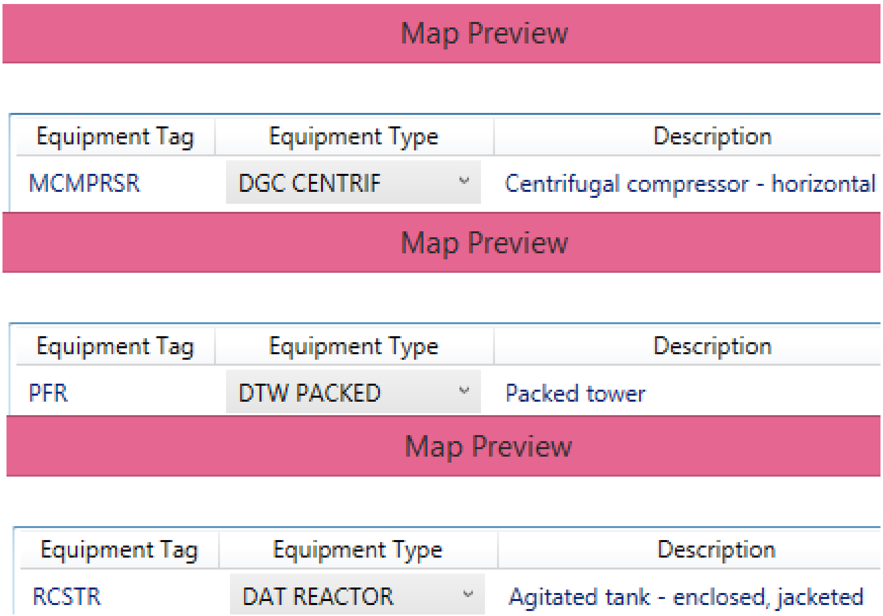
Equipment Tag	Equipment Type	Description
MIXER1	C	

COOLER1(HEATER)
COOLER2(HEATER)
DST1(RADFRAC)
DST2(RADFRAC)
HEATER(HEATER)
MCMPRSR(MCOMPR)
MIXER1(MIXER)

Equipment Tag	Equipment Type	Description
MIXER1	DAT MIXER	Agitated tank - enclosed

Figure 17.26 The old (*top*) and new (*bottom*) APEA-mapped object with “**MIXER1**” block.

Finally, for the three blocks “**MCMPRSR**”, “**PFR**”, and “**RCSTR**”, their default APEA-mapped objects will remain intact as shown in Figure 17.27.



Map Preview

Equipment Tag	Equipment Type	Description
MCMPRSR	DGC CENTRIF	Centrifugal compressor - horizontal

Map Preview

Equipment Tag	Equipment Type	Description
PFR	DTW PACKED	Packed tower

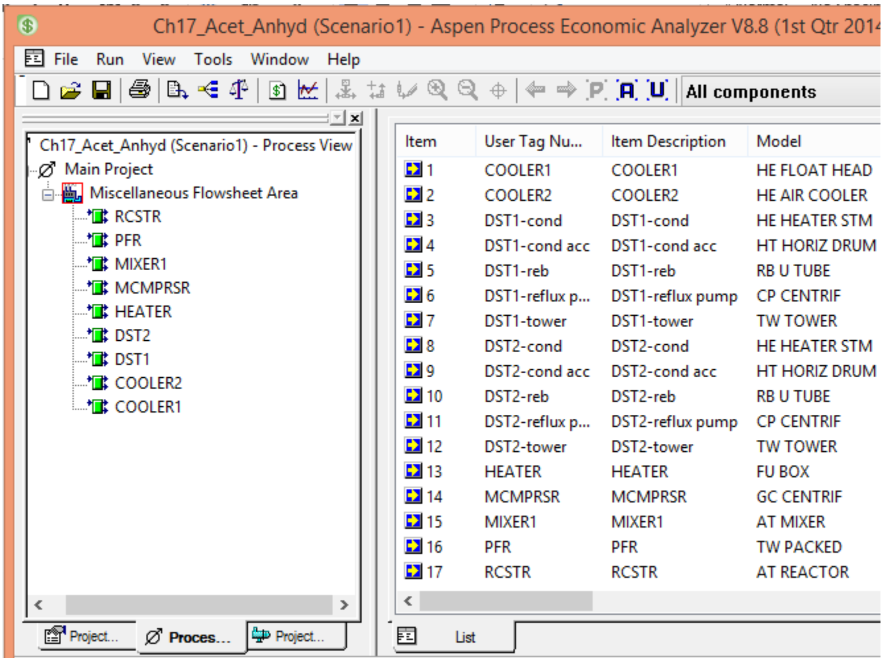
Map Preview

Equipment Tag	Equipment Type	Description
RCSTR	DAT REACTOR	Agitated tank - enclosed, jacketed

Figure 17.27 The default APEA-mapped objects with “**MCMPRSR**”, “**PFR**”, and “**RCSTR**” block.

After carrying out all modification and deletion steps, click on “**OK**” button to close “**Map Preview**” window and proceed to the next step.

Figure 17.28 shows the main window of APEA where all flowsheet blocks are now mapped to APEA built-in pieces of equipment with configurations. Of course such known configurations, however, can be further modified by the user more than once such that the new changes are free of design errors (according to APEA engineering standards and codes) and meet the user’s needs. We will show the tune-up process shortly.



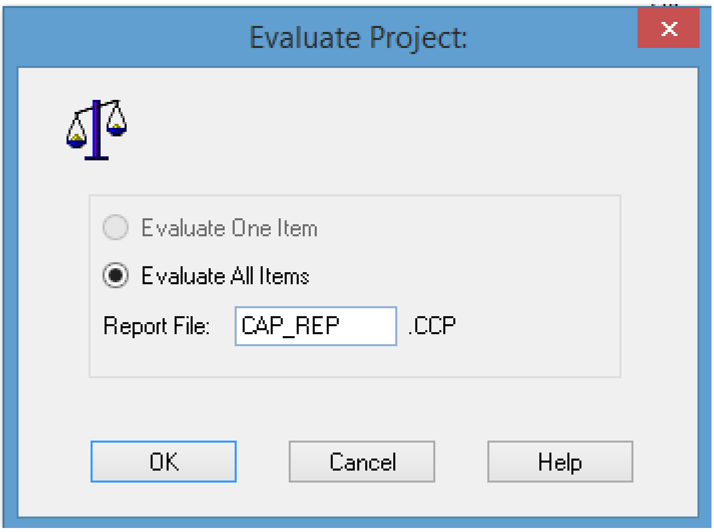
Ch17_Acet_Anhyd (Scenario1) - Process View
- Main Project
  - Miscellaneous Flowsheet Area
    - RCSTR
    - PFR
    - MIXER1
    - MCMPRSR
    - HEATER
    - DST2
    - DST1
    - COOLER2
    - COOLER1

Item	User Tag Nu...	Item Description	Model
1	COOLER1	COOLER1	HE FLOAT HEAD
2	COOLER2	COOLER2	HE AIR COOLER
3	DST1-cond	DST1-cond	HE HEATER STM
4	DST1-cond acc	DST1-cond acc	HT HORIZ DRUM
5	DST1-reb	DST1-reb	RB U TUBE
6	DST1-reflux p...	DST1-reflux pump	CP CENTRIF
7	DST1-tower	DST1-tower	TW TOWER
8	DST2-cond	DST2-cond	HE HEATER STM
9	DST2-cond acc	DST2-cond acc	HT HORIZ DRUM
10	DST2-reb	DST2-reb	RB U TUBE
11	DST2-reflux p...	DST2-reflux pump	CP CENTRIF
12	DST2-tower	DST2-tower	TW TOWER
13	HEATER	HEATER	FU BOX
14	MCMPRSR	MCMPRSR	GC CENTRIF
15	MIXER1	MIXER1	AT MIXER
16	PFR	PFR	TW PACKED
17	RCSTR	RCSTR	AT REACTOR

Figure 17.28 After a complete mapping, APEA is ready for the next step, which is evaluation.

17.4.4 Project Evaluation

Click on "**Evaluate Project**" ( ) button and "**Evaluate Project:**" window will show up as in Figure 17.29. Enter the name of the "**Report File**" with extension .**CCP**. Click on "**OK**" button to proceed.



○ Evaluate One Item

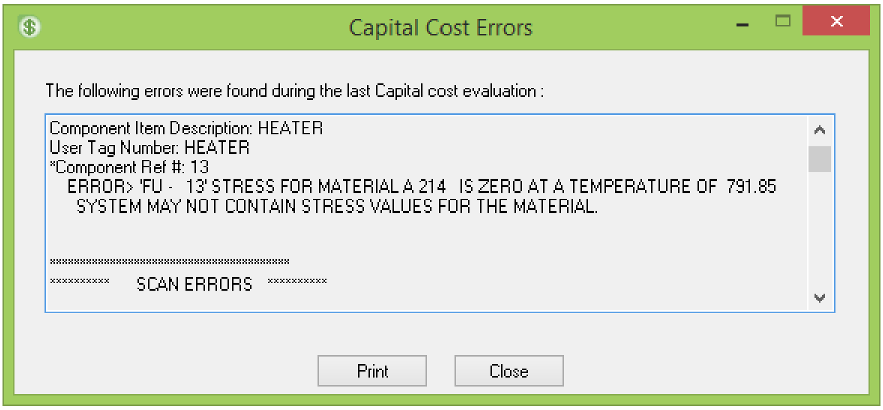
● Evaluate All Items

Report File: CAP_REP .CCP

Figure 17.29 The "**Evaluate Project:**" window whereby the user enters the name of the report file.

If things go smooth then you will reach the final executive summary for costs without hassles. However, you may get warning or error messages during the evaluation step regarding sizing or missing input data of some pieces of equipment. Click on "**OK**" button for each warning (or error) message window, which may appear in order to proceed. We will show how to fix such size- or geometry-related errors.

Toward the end, you will get the following pop-up "**Capital Cost Errors**" window, as shown in Figure 17.30, which is basically a summary report of either geometrical design-related errors or warnings. Click on "**Print**" button to have the report in the form of a hardcopy or softcopy (i.e., PDF file) so that you can keep track on the source of error associated with one or more pieces of equipment found in the project under economic analysis.



The following errors were found during the last Capital cost evaluation :

```
Component Item Description: HEATER
User Tag Number: HEATER
*Component Ref #: 13
   ERROR> 'FU -   13' STRESS FOR MATERIAL A 214   IS ZERO AT A TEMPERATURE OF  791.85
    SYSTEM MAY NOT CONTAIN STRESS VALUES FOR THE MATERIAL.


****************************************
**********     SCAN ERRORS    **********
```

Figure 17.30 The "**Capital Cost Errors**" window, which summarizes geometrical design-related errors.

Notice that even with such errors, APEA will give you an executive summary (see Section 17.4.6) for the project. However, we need to work on such errors and fix them before looking at the final executive summary of the project.

17.4.5 Fixing Geometrical Design-Related Errors

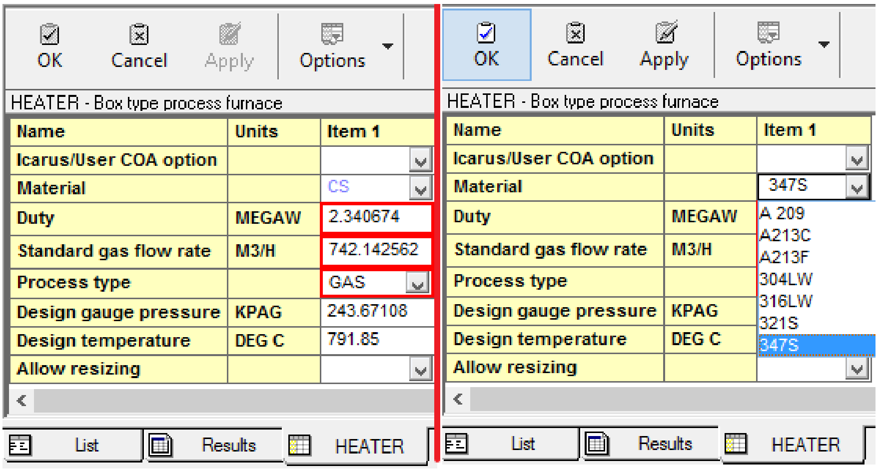
If you look at the generated report, you will find that APEA reports an error, which is due to improper entry, such as the type of material of construction or a property value that is out of range. On the other hand, the warning message alarms the user that there might be an error incurred in the user's selected mapped object specifications.

Let us start with one error at a time and try to fix the error and please APEA at the same time.

The first error says

```
"Component Item Description: HEATER
User Tag Number: HEATER
*Component Ref #: 13
ERROR> 'FU - 13' STRESS FOR MATERIAL A 214 IS ZERO AT A TEMPERATURE
  OF 791.85
SYSTEM MAY NOT CONTAIN STRESS VALUES FOR THE MATERIAL".
```

This means that material of construction A214 (Carbon Steel) is not suitable for a high-temperature heater. Under "**Project View**" tab, right-click on "**HEATER**" icon and select "**Modify Item**" submenu. Let us replace A214 by SS347. From the "**Material**" drop-down list, select 347S. Click on "**Apply**" followed by the inner "**Evaluate**" button, so that the change takes into effect, as shown in Figure 17.31. The inner "**Evaluate**" button appears two buttons after "**Options**" button shown in Figure 17.31. Of course, the user may click on the outer "**Evaluate**" button (shown in the top toolbar) but in the latter case the entire project will be reevaluated.



HEATER - Box type process furnace

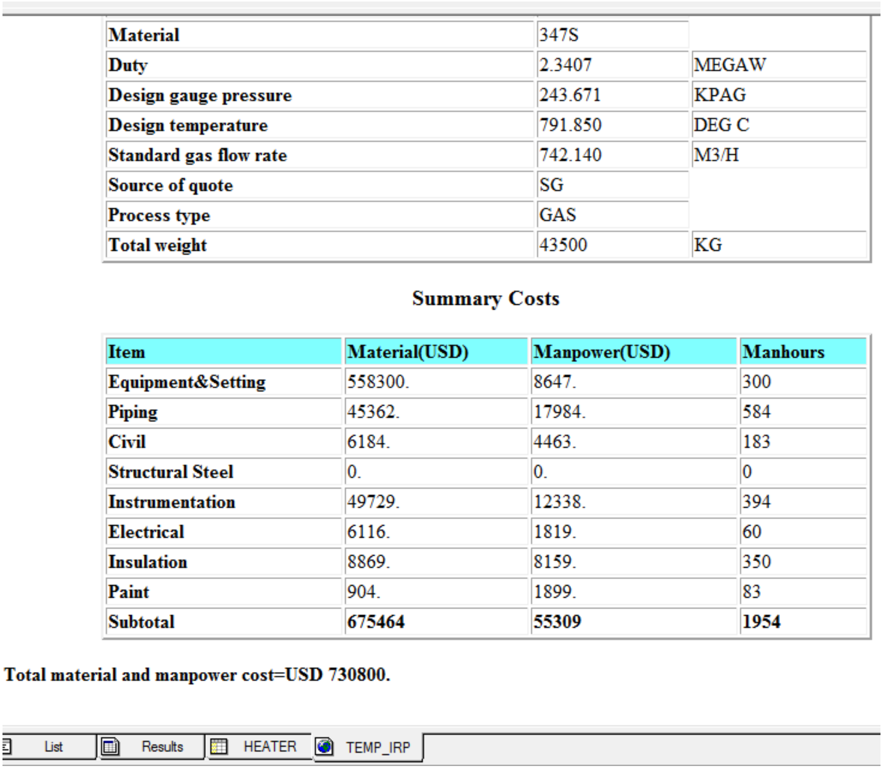
Name	Units	Item 1
Icarus/User COA option		
Material		CS
Duty	MEGAW	2.340674
Standard gas flow rate	M3/H	742.142562
Process type		GAS
Design gauge pressure	KPAG	243.67108
Design temperature	DEG C	791.85
Allow resizing		

HEATER - Box type process furnace

Name	Units	Item 1
Icarus/User COA option		
Material		347S
Duty	MEGAW	A 209
Standard gas flow rate	M3/H	A213C A213F
Process type		304LW
Design gauge pressure	KPAG	316LW
Design temperature	DEG C	321S 347S
Allow resizing		

Figure 17.31 Replacing "**CS**" (*left*) by "**347S**" (*right*) to suit the high-temperature heating operation.

Figure 17.32 shows that APEA is now happy with the new value and gives a new item report plus the capital cost for the item under concern. If the outer “**Evaluate**” button is clicked on, we will notice that the error appearing in Figure 17.30 will disappear.



Material	347S	
Duty	2.3407	MEGAW
Design gauge pressure	243.671	KPAG
Design temperature	791.850	DEG C
Standard gas flow rate	742.140	M3/H
Source of quote	SG	
Process type	GAS	
Total weight	43500	KG

Summary Costs

Item	**Material(USD)**	**Manpower(USD)**	**Manhours**
Equipment&Setting	558300.	8647.	300
Piping	45362.	17984.	584
Civil	6184.	4463.	183
Structural Steel	0.	0.	0
Instrumentation	49729.	12338.	394
Electrical	6116.	1819.	60
Insulation	8869.	8159.	350
Paint	904.	1899.	83
Subtotal	**675464**	**55309**	**1954**

Total material and manpower cost=USD 730800.

Figure 17.32 The reevaluation of “**HEATER**” object after modification of material of construction.

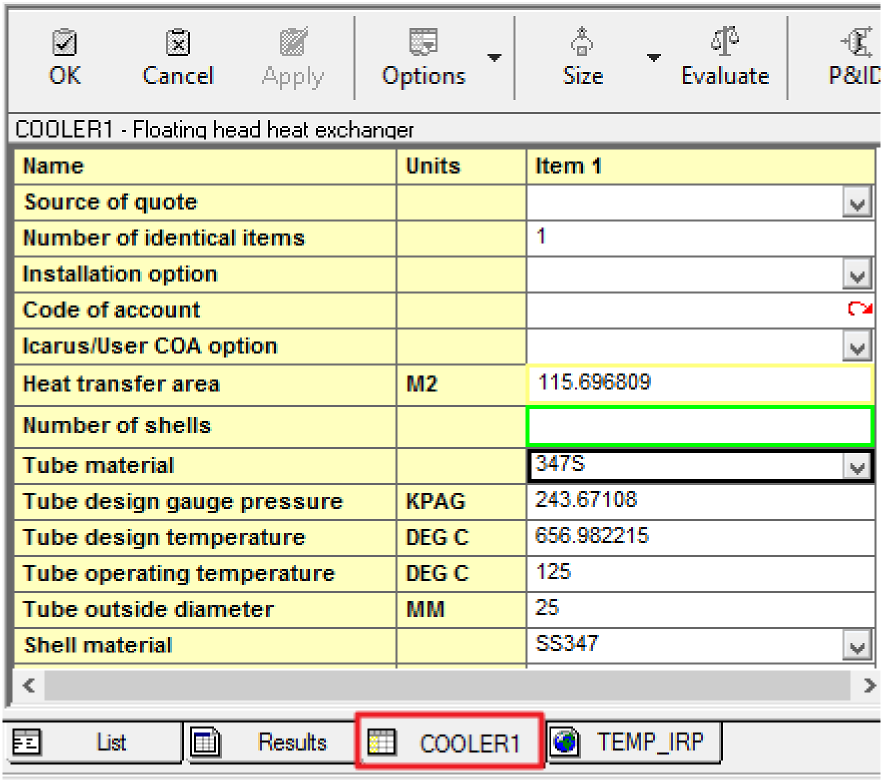
On the other hand, the warnings are not serious as in the following two warnings:
The first warning says

```
“Component Item Description: COOLER1
User Tag Number: COOLER1
*Component Ref #: 1
WARN > ’HE - 1’ DESIGN TEMPERATURE TOO HIGH FOR VACUUM OR EXTERNAL
  PRESSURE DESIGN”.
```

If we use “**347S**” and “**SS347**” as material of construction for both tube and shell as in Figure 17.33, then the warning will disappear. Again, do not forget to click on “**Apply**” followed by the inner “**Evaluate**” button to update the economic analyzer.

The second warning says

```
“Component Item Description: PFR
User Tag Number: PFR
*Component Ref #: 16
WARN > ’TW - 16’ PACKING TYPE “AND/OR VOLUME INCORRECT”.
```

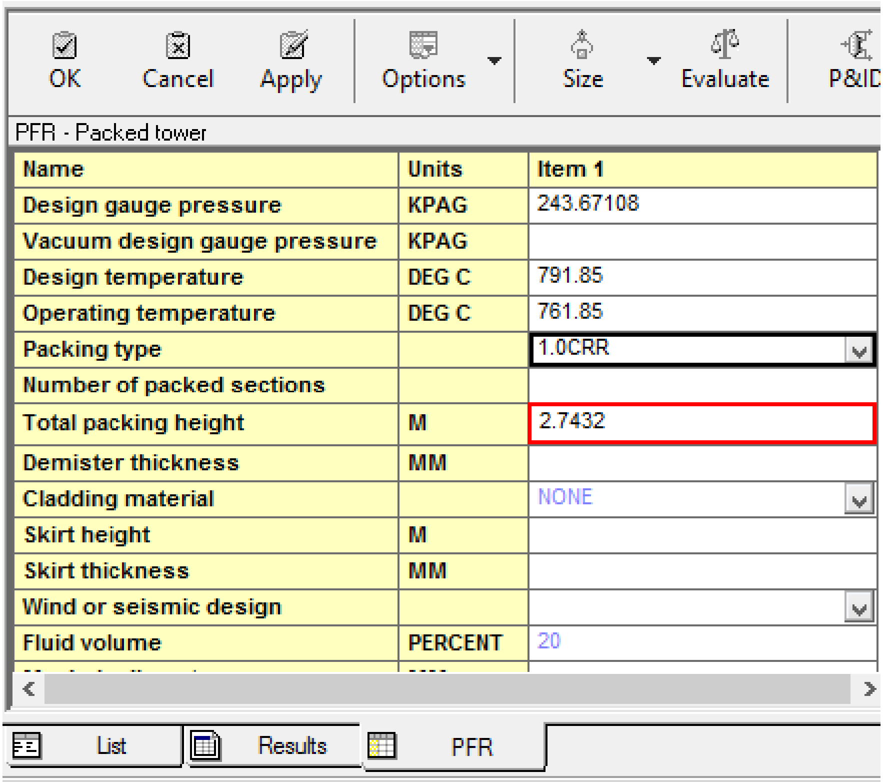


COOLER1 - Floating head heat exchanger

Name	Units	Item 1
Source of quote		
Number of identical items		1
Installation option		
Code of account		
Icarus/User COA option		
Heat transfer area	M2	115.696809
Number of shells		
Tube material		347S
Tube design gauge pressure	KPAG	243.67108
Tube design temperature	DEG C	656.982215
Tube operating temperature	DEG C	125
Tube outside diameter	MM	25
Shell material		SS347

Figure 17.33 Assigning the material of construction for both tube and shell of “**COOLER1**” exchanger.

If we use “*1.0 CRR Ceramic raschig ring*” as the “**Packing type**” as in Figure 17.34, it will do the job.



PFR - Packed tower

Name	Units	Item 1
Design gauge pressure	KPAG	243.67108
Vacuum design gauge pressure	KPAG	
Design temperature	DEG C	791.85
Operating temperature	DEG C	761.85
Packing type		1.0CRR
Number of packed sections		
Total packing height	M	2.7432
Demister thickness	MM	
Cladding material		NONE
Skirt height	M	
Skirt thickness	MM	
Wind or seismic design		
Fluid volume	PERCENT	20

Figure 17.34 Selection of “**Packing type**” of “**PFR**” as “*1.0 CRR Ceramic raschig ring*”.

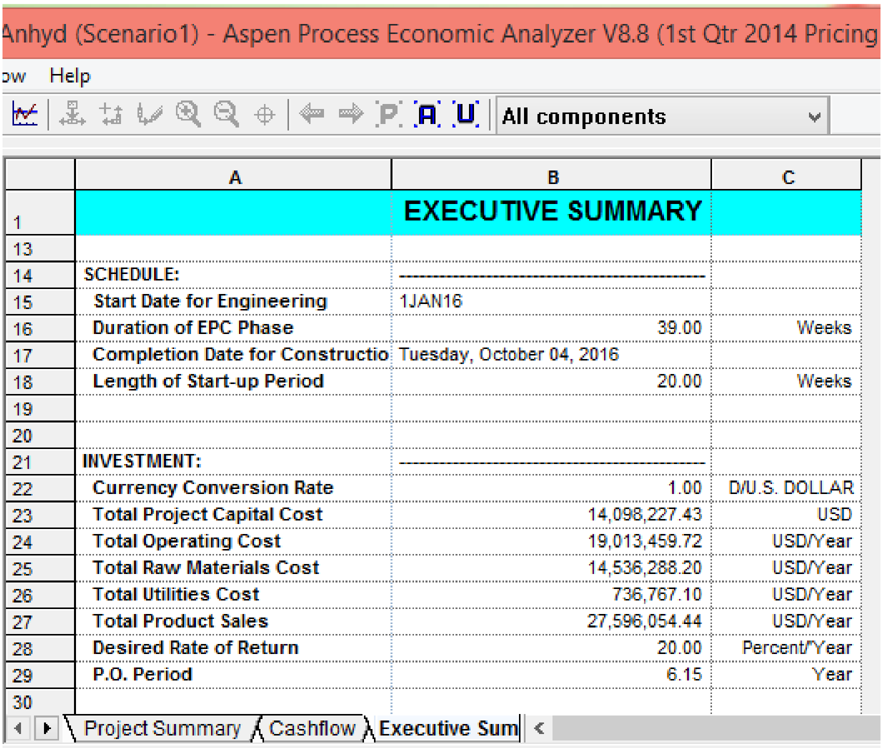
After carrying out all the aforementioned changes, reevaluate the project using “**Evaluate Project**” (⚖) button. To double check, watch out again the pop-up windows to assure that the project evaluation step is <u>*error-free*</u> although it may <u>*contain unserious warnings*</u>. Notice that the overall cost will be definitely affected by the modification steps that we have already carried out.

<u>**NOTE #5:**</u> *with APEA environment, the user may modify any form within the project itself simply by viewing the project under “**Project Basis View**” tab where you can highlight any form icon, right-click, and select “**Edit …** ” submenu to open its corresponding form. Depending on what you modify, it may require you to carry out further steps, such as mapping and/or evaluation, so that changes take into effect.*

17.4.6 Executive Summary

Upon clicking on the “**Evaluate Project**” (⚖) button, the “**Executive Summary**” tab form will show up as in Figure 17.35. You may click on other shown tabs as well.

More on profitability indices are detailed in Section 17.4.8.

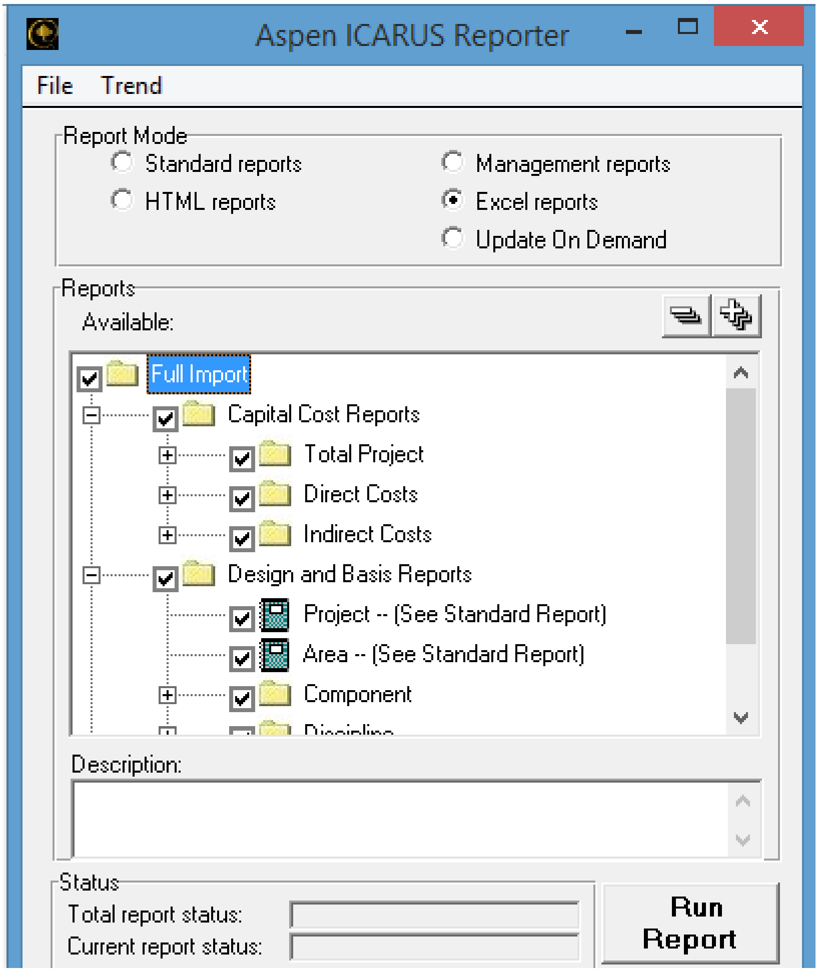


	A	B	C
1		EXECUTIVE SUMMARY	
13			
14	SCHEDULE:	--	
15	Start Date for Engineering	1JAN16	
16	Duration of EPC Phase	39.00	Weeks
17	Completion Date for Constructio	Tuesday, October 04, 2016	
18	Length of Start-up Period	20.00	Weeks
19			
20			
21	INVESTMENT:	--	
22	Currency Conversion Rate	1.00	D/U.S. DOLLAR
23	Total Project Capital Cost	14,098,227.43	USD
24	Total Operating Cost	19,013,459.72	USD/Year
25	Total Raw Materials Cost	14,536,288.20	USD/Year
26	Total Utilities Cost	736,767.10	USD/Year
27	Total Product Sales	27,596,054.44	USD/Year
28	Desired Rate of Return	20.00	Percent/Year
29	P.O. Period	6.15	Year
30			

Figure 17.35 The "**Executive Summary**" tab form where it shows overall costs without details.

17.4.7 Capital Costs Report

Clicking on "**Capital Costs**" ($) button (top toolbar) will allow the user to generate a *full-fledge* report, as shown in Figure 17.36, in the form of spreadsheets that include all cost-based technical project details, including design, equipment, civil, structural, piping, mechanical, steel, instrumental, electrical, insulation, paint, labor, management, and the project metrics, such as Independent Project Analysis (IPA) metrics and Project Evaluation System (PES) summary and cost check. The report can be presented in two forms: "*Interactive*" (On-Screen, *.html, *.xls) and "*Evaluation*" (*.ccp/prp, *.irp/cci, *.srp/*.scn).



Report Mode
○ Standard reports
○ HTML reports
○ Management reports
● Excel reports
○ Update On Demand

Reports
Available:
☑ Full Import
  ☑ Capital Cost Reports
    ☑ Total Project
    ☑ Direct Costs
    ☑ Indirect Costs
  ☑ Design and Basis Reports
    ☑ Project -- (See Standard Report)
    ☑ Area -- (See Standard Report)
    ☑ Component
    ☐ Discipline

Description:

Status
Total report status:
Current report status:

Figure 17.36 The full-fledge report that can be generated upon clicking on "**Capital Costs**" button found in the top toolbar.

17.4.8 Investment Analysis

NOTE #6: *To present the results in Excel sheets, while APEA main window is active, go to "**Tools**" | "**Options**" and select "**View Spreadsheets in Excel**" option.* Then, clicking on "**Investment Analysis**" (📈) button will open up an Excel file where again it has many worksheets, which view the project from different perspectives.

The *Total Operating Cost*, shown in Figure 17.35, must be definitely smaller than the *Total Product Sales, in order for a project to be profitable*. Notice that the total operating cost includes the following subcosts ($/year), as shown in Table 17.1 with figures borrowed from the Excel "**Project Summary**" sheet. *Notice that the figures ($/year) may slightly*

TABLE 17.1 Items to Be Included in Evaluating the Total Operating Cost, Expressed in $/year.

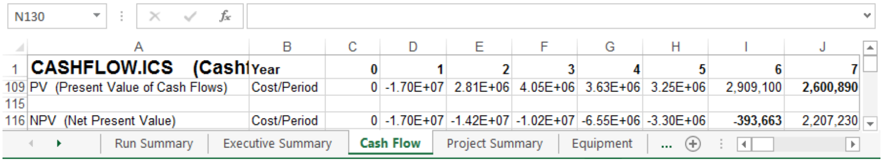
	Total Operating Cost	($/year)
1.	Total raw materials cost	14,536,300
2.	Total utilities cost	736,767
3.	Operating labor cost	1,240,000
4.	Maintenance cost	108,000
5.	Operating charges	310,000
6.	Plant overhead	674,000
	Subtotal operating cost	17,605,100
7.	General and admin cost	1,408,400
	Total operating cost = Subtotal op. cost + G and A cost	17,605,100 + 1,408,400 = 19,013,500

change from one project evaluation run to another. For example, the total operating cost is reported as 19,013,460 $/year in Figure 17.35, whereas it is reported in Excel sheet as 19,013,500 $/year.

There are different investment project indicators that are used by engineers and financers to tell how profitable the given project is. Notice that the investment analysis parameters are based on the *economic life of the project being set to 10 years by default*, which is different from the number of periods for analysis where the latter is set to 20 years by default. To change the investment analysis parameters, in "**Project Basis View**" tab, under "**Investment Analysis**" folder right-click on "**Investment Parameters**" form and select "**Edit** … " submenu item. Make the required change, click on "**Apply**" followed by "**OK**" button, and finally reevaluate the project using "**Evaluate Project**" button.

The first indicator is the net present value (NPV) of the project.

Figure 17.37 shows a portion of "**Cash Flow**" Excel sheet where it shows that NPV is negative for the first 6 years and becomes positive after that, which means that the project appears to be profitable, from year seven onward. See Section 17.A.1.



	A	B	C	D	E	F	G	H	I	J
1	**CASHFLOW.ICS (Cash**	**Year**	**0**	**1**	**2**	**3**	**4**	**5**	**6**	**7**
109	PV (Present Value of Cash Flows)	Cost/Period	0	-1.70E+07	2.81E+06	4.05E+06	3.63E+06	3.25E+06	2,909,100	**2,600,890**
115										
116	NPV (Net Present Value)	Cost/Period	0	-1.70E+07	-1.42E+07	-1.02E+07	-6.55E+06	-3.30E+06	**-393,663**	2,207,230

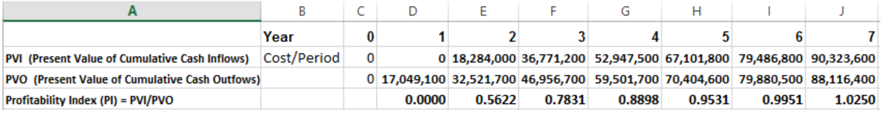
Figure 17.37 A portion of Aspen-generated Excel sheet (under **Cash Flow** tab) where it shows **PV** and **NPV** values over the 20 years (i.e., the number of periods for analysis).

The second indicator is the discounted payout period (DPP). See Section 17.A.2. DPP represents the length of time required to recover the cost of an investment. The payout (or, payback) period of a given investment project is an important determinant of whether to undertake the project, as longer payback periods are typically not desirable for investment projects. In light of Figure 17.37, the discounted payout period of the investment project is calculated as

$$\text{DPP} = \text{Years with negative NPV} + \frac{|\text{NPV}|}{\text{PV}} = 6 + \frac{|393,663|}{2,600,890} = 6.15136\,\text{years} \qquad (17.1)$$

Notice that the payout period indicator ignores any benefits that occur after the payback period and, therefore, does not measure profitability. In addition, it ignores the time value of money. Hence, other indicators should be looked upon as well.

The third indicator is the profitability index (*PI*). See Section 17.A.3. According to Aspen Plus built-in help, the profitability index shows the relative profitability of any project; it shows the present value of the benefits relative to the present value of the costs. *For each period, this number is computed by dividing the Present Value of the Cumulative Cash Inflows (PVI) by the Present Value of the Cumulative Cash Outflows (PVO)*. If the profitability index is greater than one, then the project appears to be profitable. If this index is less than one, then the project appears not to be profitable. If this number equals one then the project incurs no losses or gains (break-even point). Figure 17.38 shows that PI becomes greater than one by the end of the seventh year and reaches maximum by the end of the proposed life-time of the plant (*PI* = *1.079 at t* = *10 years*).

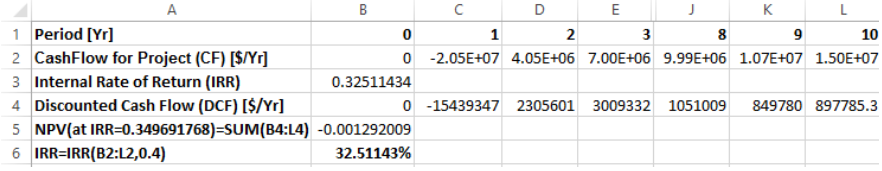


A	B	C	D	E	F	G	H	I	J
	Year	0	1	2	3	4	5	6	7
PVI (Present Value of Cumulative Cash Inflows)	Cost/Period	0	0	18,284,000	36,771,200	52,947,500	67,101,800	79,486,800	90,323,600
PVO (Present Value of Cumulative Cash Outfows)		0	17,049,100	32,521,700	46,956,700	59,501,700	70,404,600	79,880,500	88,116,400
Profitability Index (PI) = PVI/PVO			0.0000	0.5622	0.7831	0.8898	0.9531	0.9951	1.0250

Figure 17.38 The profitability index for each period is equal to **PVI/PVO** ratio.

The fourth indicator is the internal rate of return (IRR). See also Section 17.A.4. IRR indicator is also used for judging the investment project profitability. It is the rate at which the present value of all cash flows is zero. It is also known as the Discounted Cash-Flow Rate of Return. Aspen Plus calculates the value at the "End Period for Economic Life of Project" (i.e., **EPELP** = 10 years). At the "End Period for Economic Life of Project", it is assumed the *salvage value of the plant and the working capital are recovered*. *IRR is the after-tax interest rate at which the organization can borrow funds and break even at the end of the project life*. The higher the IRR value is, the more profitable the investment project will be.

Referring to Section 17.A.4, Figure 17.39 shows that at IRR = 0.32511434, NPV ≈ 0. Notice that it is a matter of "trial-and-error" attempt to find the root of NPV equation as a function of r (i.e., $r = IRR$). See Section 17.A.4. Notice that the discounted cash flow (DCF) for each entry (i.e., year) is given by $\mathrm{DCF} = \mathrm{CF}/((1 + \mathrm{IRR})^n)$. For example, using excel sheet notation, $\mathrm{C4} = \mathrm{C2}/((1 + \$\mathrm{B3})\hat{}\mathrm{C1}) = -20{,}458{,}900/(1 + 0.32511434)^1 = -15{,}439{,}347$.



	A	B	C	D	E	J	K	L
1	Period [Yr]	0	1	2	3	8	9	10
2	CashFlow for Project (CF) [$/Yr]	0	-2.05E+07	4.05E+06	7.00E+06	9.99E+06	1.07E+07	1.50E+07
3	Internal Rate of Return (IRR)	0.32511434						
4	Discounted Cash Flow (DCF) [$/Yr]	0	-15439347	2305601	3009332	1051009	849780	897785.3
5	NPV(at IRR=0.349691768)=SUM(B4:L4)	-0.001292009						
6	IRR=IRR(B2:L2,0.4)	32.51143%						

Figure 17.39 NPV is very close to zero at IRR = 0.32511434.

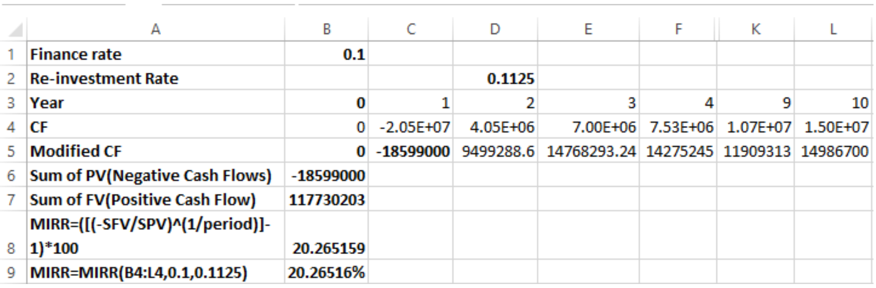
Alternatively, we can use the Microsoft Excel built-in IRR formula:

$$\boldsymbol{IRR = IRR(B2 : L2, 0.4) = 32.51143\,\%}$$

where B2:L2 are the entered cash flow (CF) values borrowed from Aspen-generated Excel sheet under "**Cash Flow**" tab, and 0.4 is the initial guess for IRR.

The fifth indicator is the modified internal rate of return (MIRR). See Section 17.A.5. Two criteria are critical in evaluating the modified internal rate of return. First, if the sign of the rate of return is negative, the project appears not to be profitable. If the sign is positive, then the project appears to be profitable. If the rate of return equals zero then the project incurs no losses or gains (break-even point). In addition, if the rate of return is greater than the rate obtained from other opportunities (i.e., investing in a bank), then the project probably shall be undertaken.

The estimation of MIRR for given finance (10%) and reinvestment (11.25%) rate is shown in Figure 17.40 for our acetic anhydride investment project. *The estimation of MIRR is carried out by multiplying the negative* ***CF*** *by* $1/(1 \pm 0.1)^n$ *for* $n = 0,1$ *and the positive* ***CF*** *by* $(1 \pm 0.1125)^{10-n}$ *for* $n = 2,3, \ldots, 10$. Notice that MIRR is equal 20.265%, which is a function of finance and reinvestment rate being plugged in MIRR formula. SPV stands for sum of *present value* (at $t = 0$ year), which represents the sum of negative cash flow. On the other hand, SFV stands for sum of *future value* (at $t = 10$ years), which represents the sum of positive cash flow.



	A	B	C	D	E	F	K	L
1	**Finance rate**	**0.1**						
2	**Re-investment Rate**			**0.1125**				
3	**Year**	**0**	1	2	3	4	9	10
4	**CF**	0	-2.05E+07	4.05E+06	7.00E+06	7.53E+06	1.07E+07	1.50E+07
5	**Modified CF**	**0**	**-18599000**	9499288.6	14768293.24	14275245	11909313	14986700
6	**Sum of PV(Negative Cash Flows)**	**-18599000**						
7	**Sum of FV(Positive Cash Flow)**	**117730203**						
8	**MIRR=([(-SFV/SPV)^(1/period)]-1)*100**	**20.265159**						
9	**MIRR=MIRR(B4:L4,0.1,0.1125)**	**20.26516%**						

Figure 17.40 The estimation of *MIRR* while multiplying the negative CF by $1/(1 + 0.10)^n$ and the positive CF by $(1 + 0.1125)^{10-n}$.

CF values were taken from Aspen-generated Excel sheet under "**Cash Flow**" tab with entry called: "**CF (CashFlow for Project)**".

Alternatively, we can use the Microsoft Excel built-in MIRR formula:

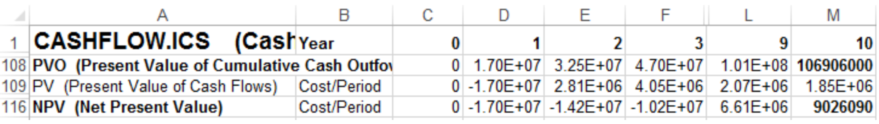
$$\boldsymbol{MIRR = MIRR(}B4 : L4, 0.1, 0.1125)$$

where B4:L4 are the entered cash flow values borrowed from Aspen-generated Excel sheet under "**Cash Flow**" tab, 0.1 and 0.1125 stand for the finance and reinvestment rate, respectively.

Notice that MIRR = 20.265% is more conservative than the liberal IRR = 32.511% in terms of estimating the rate of return on a given project.

The sixth indicator is the net rate of return (NRR): The net rate of return for the *last period* is calculated by dividing the NPV by the present value of cumulative outflows (as shown in Figure 17.41) and then multiplying the result by 100%.

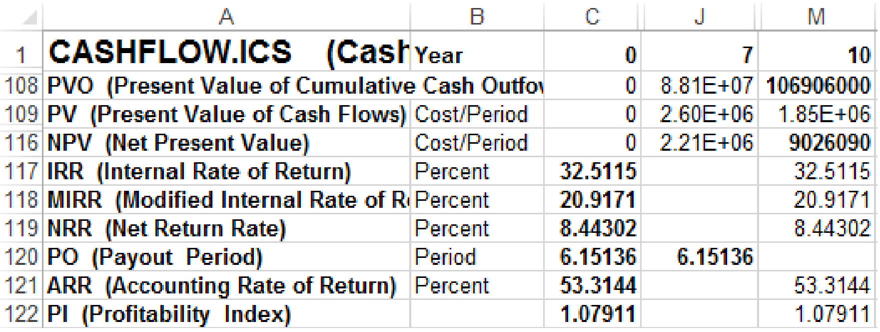
$$\begin{aligned}\text{NRR} &= \frac{\text{NPV (net present value)}}{\text{PVO (present value of cumulative cash outfows)}} \times 100\% \\ &= \frac{9,026,090}{106,906,000} \times 100\% = 8.44\% \qquad (17.2)\end{aligned}$$



	A	B	C	D	E	F	L	M
1	**CASHFLOW.ICS (Cash**	**Year**	**0**	**1**	**2**	**3**	**9**	**10**
108	**PVO (Present Value of Cumulative Cash Outfo**		0	1.70E+07	3.25E+07	4.70E+07	1.01E+08	**106906000**
109	PV (Present Value of Cash Flows)	Cost/Period	0	-1.70E+07	2.81E+06	4.05E+06	2.07E+06	1.85E+06
116	**NPV (Net Present Value)**	Cost/Period	0	-1.70E+07	-1.42E+07	-1.02E+07	6.61E+06	**9026090**

Figure 17.41 NPV and PVO value both at $t = 10$ years.

Finally, Figure 17.42 shows the list of all economic indices for the current investment project.



	A	B	C	J	M
1	**CASHFLOW.ICS (Cash**	**Year**	**0**	**7**	**10**
108	**PVO (Present Value of Cumulative Cash Outfo**		0	8.81E+07	**106906000**
109	**PV (Present Value of Cash Flows)**	Cost/Period	0	2.60E+06	1.85E+06
116	**NPV (Net Present Value)**	Cost/Period	0	2.21E+06	**9026090**
117	**IRR (Internal Rate of Return)**	Percent	**32.5115**		32.5115
118	**MIRR (Modified Internal Rate of R**	Percent	**20.9171**		20.9171
119	**NRR (Net Return Rate)**	Percent	**8.44302**		8.44302
120	**PO (Payout Period)**	Period	**6.15136**	**6.15136**	
121	**ARR (Accounting Rate of Return)**	Percent	**53.3144**		53.3144
122	**PI (Profitability Index)**		**1.07911**		1.07911

Figure 17.42 The cost indices for the acetic anhydride production investment project.

NOTE #7: *Net present value analysis and rate of return analysis may yield conflicting results. When this occurs, the results from the net present value analysis should be followed.*

More detailed problems that involve costing are discussed in Chapter 18.

HOMEWORK/CLASSWORK 17.1 (FEED/PRODUCT UNIT PRICE EFFECT ON PROCESS PROFITABILITY)

Study the effect of increasing the unit price of acetic anhydride and CH_4 (product streams) on the economic indices for project. Rerun the economic analysis for acetic anhydride production via adjusting the unit price of product/feed streams.

HOMEWORK/CLASSWORK 17.2 (USING EUROPEAN ECONOMIC TEMPLATE)

Rerun the economic analysis for acetic anhydride production via selecting the European metric template (EU_METRIC.izt), as shown in Figure 17.4. Do not forget to also change the economic template in "**File**" | "**Options**" | "**Simulation Run Options**" dialog box| "**Simulation**" tab (see Figure 17.5).

HOMEWORK/CLASSWORK 17.3 (PROCESS PROFITABILITY OF ACETONE RECOVERY FROM SPENT SOLVENT)

A company XYZ has a spent water–acetone solvent as a byproduct stream. The company will investigate the potential of recovering acetone from the spent solvent using MIBK, as shown in Figure 17.43. Water will be knocked down from the bottom of the extractor, whereas the top stream will be sent to "**RadFrac**"-type distillation tower such that pure acetone will be withdrawn as the top stream and the bottom stream will be further sent to a decanter where it will be mainly separated into two liquid streams: the first liquid will be pure MIBK and the second will be pure water. MIBK stream can then be recycled to the inlet of the extraction unit but for the purpose of avoiding simulation stability/convergence problems in the presence of a recycle stream, we will be satisfied with the flowsheet as is, with the understanding that the net consumption of MIBK will be the difference in mass flow rate between "**MIBK**" and "**1LIQMIBK**" stream. Of course, the difference will be MIBK gone with the wind (i.e., goes with "**EXTRCBTM**" stream).

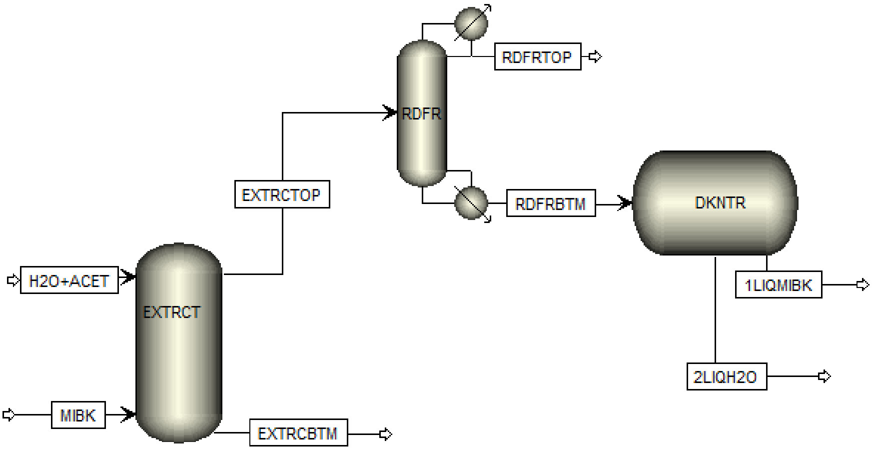


Figure 17.43 Separation of acetone from water using MIBK.

Figure 17.44 shows the annotated "**Input File**" file, generated by Aspen Plus, to decipher input data by the user.

```
DESCRIPTION: Specialty Chemicals Simulation with Metric Units, Prop-
  erty Method: NRTL.
COMPONENTS: ACETONE C3H6O-1 /WATER H2O /MIBK C6H12O-2.
PROPERTIES: NRTL FREE-WATER=STEAMNBS.
ESTIMATE: ALL, NRTL ALL ALL UNIFAC.
STREAM H2O+ACET: SUBSTREAM MIXED, TEMP=25C, PRES=1 atm, MASS-FLOW
  ACETONE 500 kg/hr / WATER 500 kg/hr.
STREAM MIBK: SUBSTREAM MIXED, TEMP=25C, PRES=1 atm, MASS-FLOW MIBK 800
  kg/hr.
BLOCK DKNTR: DECANTER, PARAM TEMP=30C. PRES=1 atm, L2-COMPS=WATER,
  MAXIT=60, UTILITY: UTILITY-ID=CWATER.
BLOCK RDFR: RADFRAC, PARAM NSTAGE=30 ALGORITHM=STANDARD MAXOL=60
  & GAMMA-MODEL=COMBINED LL-METH=HYBRID DAMPING=NONE, PARAM2
  SALTS=IGNORE-CHECK, COL-CONFIG CONDENSER=TOTAL REBOILER=KETTLE, FEEDS
  EXTRCTOP 15, PRODUCTS RDFRBTM 30 L / RDFRTOP 1 L, Pressure-Spec:
  Stage #1 P=0.7 atm, COL-SPECS MASS Distillate: Feed Ratio=1.
  MOLE-RR=10, Feed Basis: Feed Stream: EXTRCTOP, COMPS=ACETONE,
  BLOCK-OPTION FLASH-METHOD=INSIDE-OUT, UTILITIES: COND-UTIL=AIR
  REB-UTIL=LPSTEAM.
BLOCK CEXTRC1: EXTRACT, PARAM NSTAGE=40 MAXOL=60 MAXIL=30,
  OLMETH=WEGSTEIN, FEEDS: H2O+ACET Stage #1 / MIBK: Stage #40, PROD-
  UCTS: EXTRCBTM Stage #40 L1 / EXTRCTOP Stage #1 L2, Pressure-Spec
  Stage #1 P=1 atm, T-SPEC Stage #1 T=25C. L1-COMPS WATER, L2-COMPS
  MIBK.
```

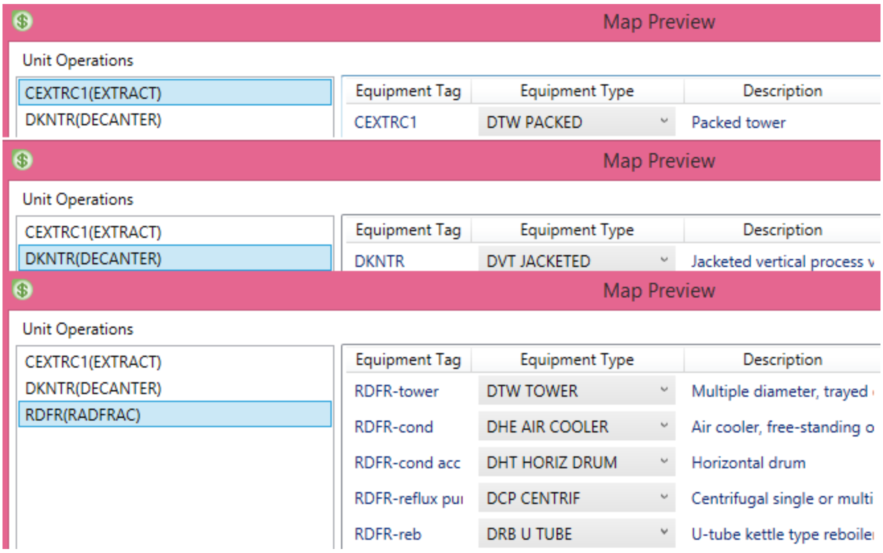
Figure 17.44 Aspen Plus generated "**Input File**" deciphering user's input data.

Carry out the following tasks:

1. In light of the given process flowsheet and input file, you have to reach at a successful steady-state solution.
2. Do not forget to associate the three utilities: cooling water, air, and low-pressure steam, respectively, with "**DKNTR**" block, "**RadFrac**" type column condenser, and the column reboiler, as indicated in Figure 17.44. The decanter is found in "**Model Palette**" | "**Separators**" | "**Decanters**" group. Rerun the show and assure that you end up with successful results.
3. Assign a unit price for each feed and product stream. Keep in mind that "**MIBK**" and "**1LIQMIBK**" stream will have the same unit price of pure MIBK. "**H2O+ACET**" feed stream will be a spent solvent process stream, which can be assigned a very low unit price value. "**2LIQH2O**" and "**EXTRCBTM**" stream will be essentially water streams, which can be used as a cooling water utility stream. Finally, "**RDFRTOP**" stream will be pure acetone stream. Basically, we say that we want to recover the precious acetone (about 50 kg/h) from the spent-solvent stream while consuming the net difference between inlet and outlet MIBK flow rate (about 0.873 kg/h). This lost amount will go into "**EXTRCBTM**" stream. It is worth investigating the potential profitability of this project. Rerun the show and assure that you end up with successful results.
4. In "**Economics**" ribbon, click on "**Send to Economics**" button. APEA main document interface (MDI parent) window with the *first* "**Create New Project**" child window will show up. Fill in any missing information and click on "**OK**" button to close the *first*

child window. The *second* (“**Project Properties**”) child window will show up. Give a description for the project, select the units of measure option, and click on “**OK**” button to close the second child window.

5. The *third* (“**Input Units of Measure Specifications**”) child window will pop up. Click on “**Close**” button to proceed.
6. The *fourth* (“**General Project Data**”) child window will pop up. You may enter the project title and your name under “**Project Title**” and “**Prepared by**” record. Click on “**OK**” button to proceed.
7. The *fifth* (“**Load Simulator Data?**”) child window will pop up. Click on “**Yes**” button to proceed.
8. The *sixth* (“**Utility Resource(s)**”) child window will pop up. Change the “**Fluid**” type for each utility as it fits. Click on “**OK**” button to proceed.
9. The main (parent) window of APEA will show up and it should contain the three blocks.
10. Click on the “**Map Simulator Items**” ( ) button and you will get “**Map Options**” window. Select “*Map all unit operations*”, “Default”, and “*Size equipment*” options. Click on “**OK**” button to proceed.
11. Figure 17.45 shows the selection of mapped APEA items for the three flowsheet objects. Click on “**OK**” button to proceed.



Map Preview

Unit Operations

CEXTRC1(EXTRACT)
DKNTR(DECANTER)

Equipment Tag	Equipment Type	Description
CEXTRC1	DTW PACKED	Packed tower

Map Preview

Unit Operations

CEXTRC1(EXTRACT)
DKNTR(DECANTER)

Equipment Tag	Equipment Type	Description
DKNTR	DVT JACKETED	Jacketed vertical process v

Map Preview

Unit Operations

CEXTRC1(EXTRACT)
DKNTR(DECANTER)
RDFR(RADFRAC)

Equipment Tag	Equipment Type	Description
RDFR-tower	DTW TOWER	Multiple diameter, trayed
RDFR-cond	DHE AIR COOLER	Air cooler, free-standing o
RDFR-cond acc	DHT HORIZ DRUM	Horizontal drum
RDFR-reflux pu	DCP CENTRIF	Centrifugal single or multi
RDFR-reb	DRB U TUBE	U-tube kettle type reboile

Figure 17.45 The APEA-mapped objects with flowsheet objects.

12. Click on “**Evaluate Project**” button and “**Evaluate Project:**” window will show up. Enter the name of the “**Report File**” with extension .**CCP**. Click on “**OK**” button to proceed.
13. You may get warning or error messages during the evaluation step regarding sizing or missing input data of some pieces of equipment. Click on “**OK**” button for each warning (or error) message window which may appear in order to proceed. I will show you later how to fix such size- or geometry-related errors.

14. For the specifications I have selected, I got two messages: one regarding the specification of the bare (or naked) area of the tubes for the air-cooled “**RDFR**” condenser and another message regarding the specification of the extraction column in terms of diameter and height. To fix the first problem, under “**Project View**” tab, highlight or right-click on “**RDFR-cond**” item, select “**Modify Item**” submenu, enter the value of “**Bare tube area 1st service**” equal to 30 m^2, and click on “**Apply**”, followed by “**Evaluate**” button. Once you get a successful evaluation result, click on “**OK**” button to close the form. Notice that such a figure is calculated based on the heat duty of the condenser, the film heat transfer coefficient of air taken from “**AIR**” utility properties, and the mean temperature difference between the cold and hot stream temperature. With a bare tube area of 30 m^2, the extended surface area will be about 600 m^2, which is sufficiently enough to meet the heat transfer area requirement.
15. Repeat the same procedure but this time for the extraction column regarding the column diameter, its height, and the height of the packing bed. Enter the vessel diameter as 3.048 m, vessel tangent to tangent height as 4 m, total packing height as 3 m, and the packing type as alumina. Click on “**Apply**”, followed by “**Evaluate**” button. Once you get a successful evaluation result, click on “**OK**” button to close the form.
16. After fixing the indicated problems, *reevaluate* the entire project by clicking on “**Evaluate Project**” button so that the new changes take into effect.
17. Report the executive summary for the project indicating different profitability indices. Is it profitable? If it is not profitable, what do you recommend to make it profitable?

APPENDIX 17.A

APPENDIX 17.A.1 NET PRESENT VALUE (NPV) FOR A CHEMICAL PROCESS PLANT

C_{TCI} (\$)	Total Capital Investment Cost, $C_{TCI} = C_{Land} + C_{TDC}$
C_{Land} (\$)	Cost of Land
AC_{Land} (\$/year)	Annual Cost of Land = C_{Land}/Loan period. The annual installment to be paid for bank
C_{TDC} (\$)	Total Depreciable Capital = factor × $(C_{IBLI} + C_{Site} + C_{Buildings} + C_{Offsite\ facilities})$; factor = 1.2
C_{IBLI} (\$)	Inside Battery Limits Investment Cost (i.e., installed cost of all pieces of equipment)
C_{Start} (\$/year)	Startup Cost (To keep your business running smoothly in its startup phase, you will need enough capital to cover all expenses until you reach the break-even point)
C_{WC} (\$/year)	Working Capital (NOTE: In UK, Water Closet) = Current Assets − Current Liabilities
GSR (\$/year)	Gross Sales Revenue
$C_{M\text{-}ND}$ (\$/year)	Cost of Manufacturing (No Depreciation)
GE (\$/year)	General Expenses

DC (\$/year)	Depreciation Cost (5-year Modified Accelerated Cost Recovery System (MACRS). Under this system, the capitalized cost of tangible property is recovered over a specified life by annual deductions for depreciation) $= 0.20 \times \mathrm{C}_{\mathrm{TDC}}$
TAX (\$/year)	Income Tax $= r \times$ Taxable Income $= r \times (\mathrm{GSR} - \mathrm{C}_{\mathrm{Start}} - \mathrm{C}_{\mathrm{M\text{-}ND}} - \mathrm{GE} - \mathrm{DC})$
r	Tax Rate (If tax is 40%, then $r = 0.4$)
CF (\$/year)	Cash Flow $= (\mathrm{GSR} - \mathrm{AC}_{\mathrm{Land}} - \mathrm{C}_{\mathrm{Start}} - \mathrm{C}_{\mathrm{M\text{-}ND}} - \mathrm{C}_{\mathrm{WC}} - \mathrm{GE} - \mathrm{TAX})$
DCF_n (\$/year)	Discounted Cash Flow $= \mathrm{CF}_n/(1 + \mathrm{ROR})^n$. Also called *PV (Present Value of CF)*
n	Years of Operation, $n = 0,1,2,3, \ldots, \mathrm{EPELP}$
EPELP	End Period for Economic Life of Project
ROR	Rate of Return or Interest Rate (Aspen Terminology). For example, $\mathrm{ROR} = 0.20$
NPV (\$/year)	The Sum of DCF up to J^{th} year $= \sum_{j=0}^{\mathrm{J^{th}\ year}} \mathrm{DCF}_j = \sum_{j=0}^{\mathrm{J^{th}\ year}} (\mathrm{CF}_j)/(1 + \mathrm{ROR})^j$

APPENDIX 17.A.2 DISCOUNTED PAYOUT (PAYBACK) PERIOD (DPP)

The discounted payout period (DPP) is the time in which the initial cash outflow of an investment is expected to be recovered from the cash inflows generated by the investment. It is one of the simplest investment appraisal techniques.

Formula:

The formula to calculate discounted payout period of a project depends on whether the cash flow per period from the project is even or uneven. In case they are even, the formula to calculate payout period is

$$\mathrm{DPP} = \frac{\text{Initial investment}}{\text{Cash inflow per period}}$$

When cash inflows are uneven, we need to calculate the cumulative net cash flow for each period and then use the following formula for payback period:

$$\mathrm{DPP} = A + \frac{B}{C}$$

where

A	The last period with a negative cumulative cash flow
B	The absolute value of cumulative cash flow at the end of the period A
C	The cash flow during the period after A

EXAMPLE 17.1 (UNIFORM CASH FLOW)

Company Z is planning to undertake a project requiring initial investment of \$120 million. The project is expected to generate \$30 million per year for 7 years. Calculate the discounted payout period of the project.

Solution:

$$\text{DPP} = \text{Initial Investment} \div \text{Annual Cash Flow} = \$120\text{M} \div \$30\text{M/Year} = 4.0\ \text{Year}$$

EXAMPLE 17.2 (NON-UNIFORM CASH FLOW)

Company Z is planning to undertake another project requiring initial investment of \$60 million and is expected to generate \$10 million in Year 1, \$15 million in Year 2, \$18 million in Year 3, \$25 million in Year 4, and \$30 million in Year 5. Calculate the discounted payback value of the project.

Year	Cash Flow in Millions	Cumulative Cash Flow in Millions
0	−60	−60
1	10	−50
2	15	−35
3	18	−17
4	25	8
5	30	38

$$\text{DPP} = 3 + |-17| \div 25 = 3.68\ \text{years}$$

APPENDIX 17.A.3 PROFITABILITY INDEX

Profitability index, also known as profit investment ratio (PIR) and value investment ratio (VIR), is an investment appraisal technique, which represents the ratio of payoff to investment of a proposed project. It is a useful tool for ranking projects because it allows you to quantify the amount of value created per unit of investment. The ratio is calculated as

$$\text{Profitability index} = \frac{\text{Present value of future cash flow}}{\text{Initial investment required}}$$

$$\text{Profitability index} = 1 + \frac{\text{Net present value}}{\text{Initial investment required}}$$

Profitability index is actually a modification of the net present value method. While present value is an absolute measure (i.e., it gives as the total dollar figure for a project), the profitability index is a relative measure (i.e., it gives the figure as a ratio).

Decision Rule:

Accept a project if the profitability index is greater than 1 and reject if less than 1.

EXAMPLE 17.3

Company X is undertaking a project at a cost of $80 million, which is expected to generate future net cash flows with a present value of $100 million. Calculate the profitability index.

Solution: Profitability Index = PV of Future Net Cash Flows/Initial Investment Required

Profitability Index = $100M/$80M = 1.25

Alternatively, the information about NPV and initial investment can be used to calculate profitability index as follows:

Net present value = PV of net future cash flows − initial investment required

Net present value = $100M − $80M = $20M.

Profitability index = 1 + (Net present value/initial investment required)

Profitability index = 1 + $20M/$80M = 1.25

APPENDIX 17.A.4 INTERNAL RATE OF RETURN (IRR)

Internal rate of return (IRR) is the discount rate at which the net present value of an investment becomes zero. In more specific terms, the IRR of an investment is the discount rate at which the net present value of costs (negative cash flows) of the investment equals the net present value of the benefits (positive cash flows) of the investment.

Decision Rule:

A project should only be accepted if its IRR is NOT less than the target internal rate of return. When comparing two or more mutually exclusive projects, the project with the highest value of IRR should be considered.

IRR Calculation:

At IRR, net present value (NPV) is zero:

$$\text{NPV}(r) = \sum_{i=0}^{N=10} \frac{\text{CF}_i}{(1+r)^i} = 0$$

where,

r is the internal rate of return (IRR); i stands for years of operation; and CF_i is the net cash inflow evaluated at the end of year i.

Notice that NPV will be a function of r, and we need to find r such that NPV is set to zero. This is a non-linear algebraic equation where we need to find the root r of NPV equation by the "trial and error" procedure such that NPV approaches zero. The variable r lies in the denominator of the positive term of NPV equation. Consequently, increasing r will make NPV less positive and vice versa decreasing r will make NPV more positive. You can guess a value of r and based on the estimated value of NPV (positive/negative), you will increase/decrease r such that NPV eventually approaches zero.

Notice that a spreadsheet application, such as Microsoft Excel, has built-in functions to calculate IRR. In Microsoft Excel, this function is "=IRR(*values*, initial guess)", where *values* can be in the form of Excel absolute/reference cells or be bracketed in two curly braces as in {a,b,c,d, … } to indicate an array of data.

APPENDIX 17.A.5 MODIFIED INTERNAL RATE OF RETURN (MIRR)

MIRR is an improved version of the IRR calculation. IRR assumes that positive cash flows are reinvested at the same rate of return as that of the investment (i.e., the project which generates them). This assumption is questionable as funds are reinvested at a rate that reflects the organization's cost of capital or return on cash. Consequently, if we stick with the assumption of equal rate for both negative and positive cash flow, then IRR gives an optimistic (i.e., overestimated) rate of return for the cash flows. In addition, for projects with alternating positive and negative cash flows, more than one IRR may be found, which may lead to confusion.

To use MIRR, two interest rates are needed:

1. The reinvestment rate for the positive cash flow
2. The finance rate for the negative cash flow.

MIRR Calculation:

$$\mathrm{MIRR}\,(\%) = \left[\left[\frac{\mathrm{FV(postive\ cash\ flow,\ reinvestment\ rate)}}{-\mathrm{PV(negative\ cash\ flow,\ finance\ rate)}}\right]^{\frac{1}{\mathrm{EPELP}}} - 1\right] \times 100\%$$

where EPELP is the "**E**nd **P**eriod for **E**conomic **L**ife of **P**roject" (i.e., **EPELP** = 10 years, by default), PV is the sum of cash flows (brought to the beginning of the first period), and FV is the sum of positive cash flows (brought to the end of the last period). Notice that the minus sign, preceding PV, can climb from the denominator to the numerator and the result will be the same. Figure 17.40 shows that the minus sign is in the numerator, instead of the denominator.

Notice that a spreadsheet application, such as Microsoft Excel, has built-in functions to calculate MIRR. In Microsoft Excel, this function is "=MIRR(*values*, finance_rate, reinvest_rate)", where *values* can be in the form of Excel absolute/reference cells or be bracketed in two curly braces as in {a,b,c,d, … } to indicate an array of data.

In principle, MIRR sums the discounted negative cash flows to the starting time taking into account the finance rate and sums the positive cash flows to the final period taking into account the reinvestment rate.

EXAMPLE 17.4

If an investment project has the following cash flows:

Year (Yr)	0	1	2	3
Cash flow (CF) ($/year)	−1000	−2000	3000	4000

Using Microsoft Excel built-in function IRR = IRR({−1000,−2000,3000,4000},0.4) = 56%

0.4 is a guess value for IRR.

To calculate the MIRR, let us assume a finance rate of 10% and a reinvestment rate of 15%.

$$\text{PV} = \frac{-1000}{(1+0.1)^{0-0}} + \frac{-2000}{(1+0.1)^{1-0}} = \text{-}1000 - 1818.2 = \text{-}2818.2$$

$$\text{FV} = 3000 \times (1+0.15)^{3-2} + 4000 \times (1+0.15)^{3-3} = 3450 + 4000 = 7450$$

$$\text{MIRR}\,(\%) = \left[\left[\frac{7450}{-(-2818.2)}\right]^{\frac{1}{3}} - 1\right] \times 100\% = 38.3\%$$

Using Microsoft Excel built-in function MIRR = MIRR({−1000,−2000,3000,4000}, 0.1,0.15) = 38.3%

Notice that MIRR < IRR.

18

TERM PROJECTS (TP)

NOTE #0: *In the previous chapters, I elaborated on the design aspects pertaining to each assigned problem, as the student (or reader) is supposed to be a beginner and has to grab the premises of Aspen Plus® technology. Now, the fact that you are reading this statement means you have thoroughly gone through each tutorial of previous chapters and you are now ready to accept the challenge and tackle new design problems with a minimum supervision or intervention by the instructor. I will minimize deciphering the design aspects unless otherwise I find that deciphering some serves as prerequisite for succeeding steps as in control and dynamics, for example.*

Are you ready?

If the answer is absolutely yes, then you are welcome to continue;

Else if the answer is semi-yes, then you may continue but from time to time you need to refer to the pertinent running tutorial/topic before you attempt to tackle a specific task;

Else if the answer is no, then you ought to go back and do your homework;

Else if no answer at all, then you are here by mistake. Abort and exit;

End if.

18.1 TP #1: PRODUCTION OF ACETONE VIA THE DEHYDRATION OF ISOPROPANOL

It is desired to produce about 100,000 tons/year (1 year = 8,000 operating hours) of pharmaceutical-grade acetone (99.9 wt%) via the gas-phase dehydration of isopropanol

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Aspen Plus®: Chemical Engineering Applications, First Edition. Kamal I.M. Al-Malah.

Companion Website: www.wiley.com/go/Al-Malah/AspenPlusApplications

(IP-OH) using a catalyst. The reaction is first order with respect to the concentration of *IP-OH*, and occurs in the vapor phase over a catalyst. This catalyst is available in the form of cylindrical pellets 12 mm in length and 6 mm in diameter, suitable for use in packed-bed reactors. Since Ergun's equation will be used on the Pressure sheet for calculating the pressure drop, specify the particle diameter of each bed particle to be Sauter mean diameter, $D_{\mathrm{Eq}} = 6V/A = 7.2$ mm, where V is the particle volume and A its area and the shape factor will be 1 for a spherical particle having an equivalent diameter = 7.2 mm.

Reaction pathways, kinetics, and physical characteristics for this catalyst are as follows. The main reaction for producing acetone is

$$(\mathrm{CH_3})_2\mathrm{CHOH} \rightarrow (\mathrm{CH_3})_2\mathrm{CHO} + \mathrm{H_2}$$

The kinetics for this reaction is given (Kellogg, R., Luck, P., and Harper, A. (1998). *The Production of Acetone*, http://www.owlnet.rice.edu/~ceng403/gr11298/acetone.html (accessed April 15, 2016).) as

$$-r_{\mathrm{IP-OH}} = kC_{\mathrm{IP-OH}} \quad \left(\frac{\mathrm{kmol\,IP-OH}}{\mathrm{m^3 reactor \cdot s}}\right) \quad \text{Rate basis under “}\textbf{Kinetic}\text{” tab: Reac (vol)}$$

$$k = 3.51 \times 10^5 \exp\left(-\frac{72\,380}{\mathrm{RT}}\right), \; k \text{ has units of } \left(\frac{\mathrm{m^3 gas}}{\mathrm{m^3 reactor \cdot s}}\right) \text{ and } C_{\mathrm{IP-OH}}$$

$$\text{has units of } \left(\frac{\mathrm{kmol\,IP-OH}}{\mathrm{m^3 gas}}\right) \tag{18.1}$$

Alternatively, the reaction rate can be expressed (http://www.che.cemr.wvu.edu/publications/projects/acetone/acetone1.PDF) as

$$-r_{\mathrm{IP-OH}} = kC_{\mathrm{IP-OH}} \quad \left(\frac{\mathrm{kmol\,IP-OH}}{\mathrm{kg\,catalyst \cdot s}}\right) \quad \text{Rate basis under “}\textbf{Kinetic}\text{” tab: Cat (wt)}$$

$$k = 2.9167 \times 10^2 \exp\left(-\frac{72\,380}{\mathrm{RT}}\right), \; k \text{ has units of } \left(\frac{\mathrm{m^3 gas}}{\mathrm{kg\,cat \cdot s}}\right) \text{ and } C_{\mathrm{IP-OH}}$$

$$\text{has units of } \left(\frac{\mathrm{kmol\,IP-OH}}{\mathrm{m^3 gas}}\right) \tag{18.2}$$

The activation energy in the kinetic expression here has units of *J/mol* (or *kJ/kmol*). The density of the solid catalyst, $\rho_s = 2{,}500\ \mathrm{kg/m^3}$ and the packed bed voidage of the cylindrical pellets = 0.5. The packed-bed reactor has a tube diameter = 1.5 inch, length of catalyst filled tubes = 10 ft (3.05 m), number of tubes = 200, and an overall heat transfer coefficient from tubes to heating medium = 50 W/($\mathrm{m^2 \cdot {}^\circ C}$). In addition, several side reactions occur to a small extent, but these reactions are ignored due to their insignificance at temperatures below 400°C. Note that the reaction rate is increased by an increase in pressure, as this increases the concentration of the reactant. The catalyst used is zinc oxide and zirconium oxide combination (6–12% ZrO), which works very well over reaction temperatures from 300 to 400°C with minimal degradation (D. F. Othmer, R. E. Kirk, J. I. Kroschwitz. (1976).

M. Howe-Grant (Editor). "*Encyclopaedia of Chemical Technology*", 3rd edn, vol. 1, John Wiley and Sons, New York, USA, pp. 182–194; D. F. Othmer, R. E. Kirk, J. I. Kroschwitz. (1991). M. Howe-Grant (Editor). "*Encyclopaedia of Chemical Technology*", 4th edn, vol. 1, John Wiley and Sons, New York, USA, pp. 92–100).

NOTE #1: *Both Equations* 18.1 *and* 18.2 *can be used to describe the kinetics of the gas-phase dehydration of isopropanol (IP-OH) using zinc/zirconium oxide catalyst. I tried both of them and both give the same results, given that the user properly enters the kinetic parameters and the rate basis as Reac(vol) for Equation* 18.1 *and Cat (wt) for Equation* 18.2*, under "****Kinetic****" tab of the power law reaction type. Moreover, Aspen Plus does not provide the essence on how to account for catalyst deactivation with time; thus, both reactions will give 100% conversion once we hit the required residence time (i.e., required tube length) and thus there is no need for further downstream separation processes. You can verify this by extending the tube length to higher values and see how the conversion will be affected by increasing the length. However, since the real life has always some miserable episodes, catalyst deactivation is inevitable and thus will reduce the overall conversion below 1.0. Consequently, the reactor geometric specifications are chosen such that to mimic the real life of having a conversion less than unity and thus requiring downstream separation processes to recycle the unreacted IP-OH to the inlet of the reactor while getting the pure acetone "****2ACTNTNK****" stream and the by-product hydrogen–acetone "****H2–ACTN****" stream.*

NOTE #2: *To have a flowsheet that contains a recycle stream will cause a headache for Aspen Plus simulator itself and thus for the user as well. As a remedy or rule of thumb, first run the entire process without recycling the stream from the bottom of the distillation tower and adjust the operating conditions within each block, in addition to geometrical specifications of "****DSTL****" block, until you almost reach a pure IP-OH stream. At this stage, reconnect the destination of this leaving stream back to the inlet of the first mixer. Alternatively, you may purge out a small fraction of the bottom liquid stream and recycle the rest of it to the inlet of the reactor. See Section 18.10 in this regard.*

Figure 18.1 shows the process flowsheet for the gas-phase dehydration of IP-OH using zinc/zirconium oxide catalyst, followed by a cooling, flashing, distillation, and mixing step. Notice that "**HEATEX1**" is used to heat up the coming cold feed while at the same time cooling the hot product stream prior to sending the latter to downstream separation. The flowsheet also shows both temperature and pressure for each inlet and outlet stream. By this, I will help the student come up with the final design specifications needed to accomplish the mission. Keep in mind that there may be more than one route to end up with pure acetone and by-product stream other than the one shown here.

Notice that water must be added to the list of components if it is defined as a utility, either as cooling water or steam, but not a process fluid.

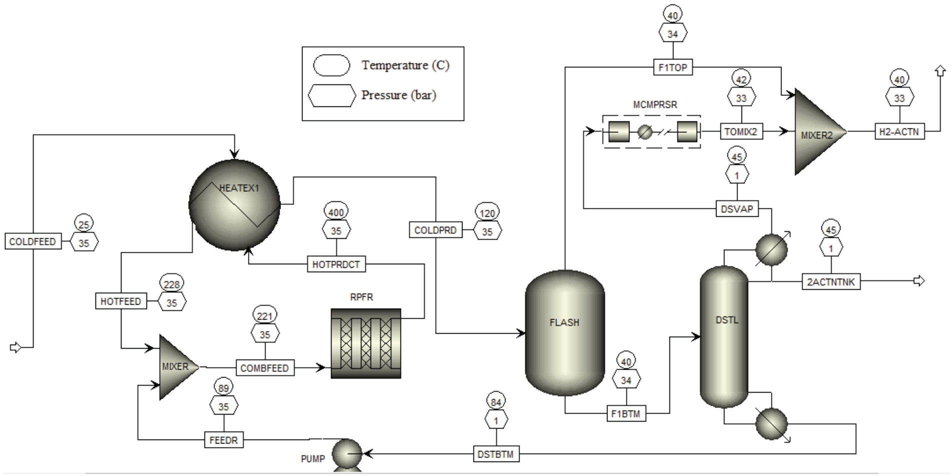
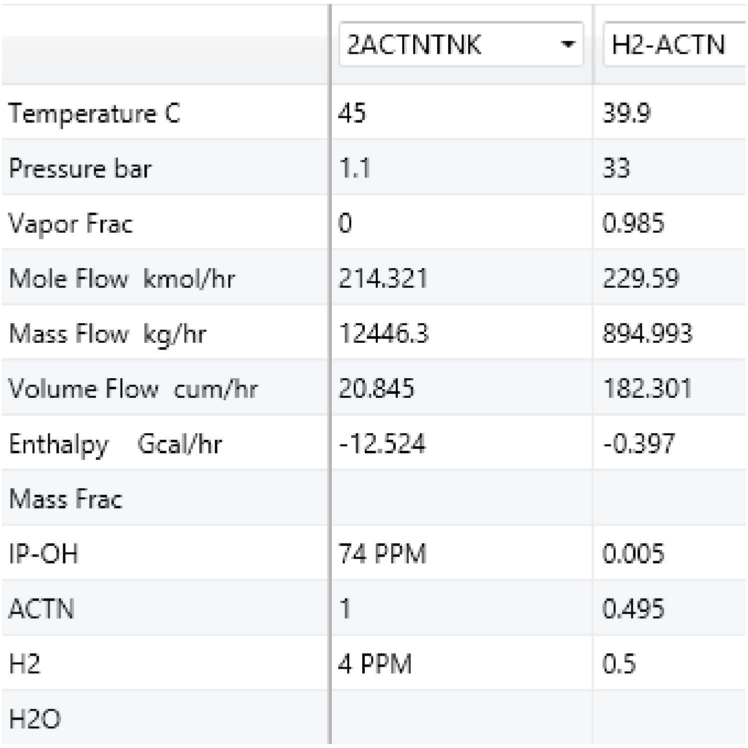


Figure 18.1 The process flowsheet for the gas-phase dehydration of IP-OH using zinc/zirconium oxide catalyst, followed by a cooling, flashing, distillation, and mixing step.

Figure 18.2 shows the properties of product streams.



	2ACTNTNK	H2-ACTN
Temperature C	45	39.9
Pressure bar	1.1	33
Vapor Frac	0	0.985
Mole Flow kmol/hr	214.321	229.59
Mass Flow kg/hr	12446.3	894.993
Volume Flow cum/hr	20.845	182.301
Enthalpy Gcal/hr	-12.524	-0.397
Mass Frac		
IP-OH	74 PPM	0.005
ACTN	1	0.495
H2	4 PPM	0.5
H2O		

Figure 18.2 Properties of product streams.

The outlet “**H2-ACTN**” stream, out of “**MIXER2**” block, is mainly 50 : 50 (mass %) H_2:acetone mixture with trace amounts of IP-OH. This stream can be marketed as such, because it can be used in the formation of diamond layer and microcrystallites, where the microwave plasma reactor with an operating frequency amounting to 2.45 GHz and maximum input microwave power of 5 kW at a self-sustaining temperature of the substrate is used. Hydrogen–acetone mixture is used in growth of diamond film. The unit price is mass-weighted between price of acetone and that of hydrogen.

For further information on application of H_2–acetone mixture in carbon nanotube (CNT) technology see

- The 7th Russian-French Workshop on Nanosciences and Nanotechnologies, 3–6 June 2013, Novosibirsk, Russia.
- Sun, Z., Shi, X., Wang, X., and Sun, Y. (1997) Synthesis of diamond via low pressure polymer precursor using microwave plasma-two dimensional growth phenomena. *Materials Science and Engineering*, **B47**, 167–170.

Your task is to decide on the property method and come up with the proper design to end up with at least 99.9 wt% pure acetone at the indicated annual production rate. Define the unit price for each feed and product stream. Associate a utility with a block where it is required. Carry out energy analysis to see if there exists any recommended retrofit. Using APEA, carry out process economic analysis and report the economic profitability indices for the investment project.

18.2 TP #2: PRODUCTION OF FORMALDEHYDE FROM METHANOL (SENSITIVITY ANALYSIS)

It is desired to produce about 120,000 tons/year (1 year = 8,000 operating hours) of formaldehyde (99.1 wt%) and the by-product pure nitrogen which originally onsets from the inlet air. Consider the solid-catalyzed gas-phase conversion of methanol to formaldehyde according to the following reaction:

$$CH_3OH + \frac{1}{2}O_2 \rightarrow HCHO + H_2O \tag{18.3}$$

$$-r_{CH_3OH} = 4.762 \times 10^{-5} \times \exp\left[-17,630 \times \left(\frac{1}{T} - \frac{1}{485}\right)\right] P^{0.5}_{CH_3OH} P^{0.1}_{O_2} \tag{18.4}$$

Nevertheless, formaldehyde may undergo complete oxidation:

$$HCHO + \frac{1}{2}O_2 \rightarrow CO + H_2O \tag{18.5}$$

$$-r_{HCHO} = \frac{2.8246 \times 10^{-10} \times \exp\left[-8,710 \times \left(\frac{1}{T} - \frac{1}{485}\right)\right] P_{O_2} P_{HCHO}}{\left[1 + \left[212,818.09 \times \exp\left[-5,290 \times \left(\frac{1}{T}\right)\right]\right] P_{HCHO}\right]^2} \tag{18.6}$$

The catalyst is present in the multitube plug-flow reactor with a bed voidage of 0.5 and a particle density of 2 g/cm^3. Figure 18.3 shows the process flowsheet for the solid-catalyzed gas-phase formaldehyde synthesis from methanol where it is made of the mixer, plug-flow reactor, flash unit #1 for knocking down water, flash unit #2 for substantially striping off N_2, and flash unit #3 for further separation of HCHO from N_2.

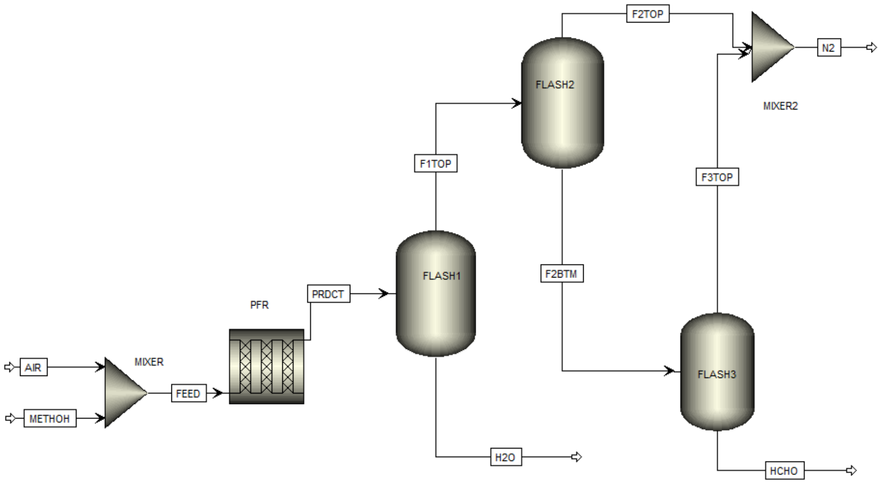


Figure 18.3 The flowsheet for the solid-catalyzed gas-phase formaldehyde synthesis from methanol, where it is made of the mixer, PFR, flash unit #1 for knocking down water; flash unit #2 for substantially striping off N_2, and flash unit #3 for further separation of HCHO from N_2.

Your tasks are as follows:

- **Decide on the property method and come up with the proper design to end up with at least 99.1 wt% pure formaldehyde and 99.1 wt% pure nitrogen at the indicated annual production rate.**
- **Carry out four sensitivity analyses one for each block, starting from "PFR" down to "FLASH3" block to see the effect of both operating pressure and temperature inside each unit on the mole fraction ratio HCHO/CO (i.e., selectivity) in "PRDCT" stream, the mass fraction of HCHO in "F1TOP" stream, the mass-fraction of N_2 in "F2TOP" stream, and the mass-fraction of HCHO in "HCHO" stream, respectively.**
- **Define the unit price for each feed and product stream. Associate a utility with a block where it is required.**
- **Using APEA, carry out process economic analysis and report the economic profitability indices for the investment project.**

18.3 TP #3: PRODUCTION OF DIMETHYL ETHER (PROCESS ECONOMICS AND CONTROL)

18.3.1 Economic Analysis

A feasibility study on the production of 99.5 wt% dimethyl ether (DME) is to be performed. The plant is capable of producing 50,000 metric tons (1 year = 8,000 operating hours) of DME per year via the catalytic dehydration of methanol over an acid zeolite catalyst. The goal is to design a grass-roots facility, which safely and efficiently produces DME. DME is used primarily as a propellant. DME is miscible with most organic solvents and it has a high solubility in water (DuPont Talks About its DME Propellant. *Aerosol Age*, May and

June, 1982). The production of DME is via the catalytic dehydration of methanol over an amorphous alumina catalyst treated with 10.2% silica. DME is produced by the following reaction:

$$2CH_3OH \rightarrow CH_3OCH_3 + H_2O \tag{18.7}$$

In the temperature range of normal operation (250–400°C), there are no significant side reactions. Therefore, the reactor is kinetically controlled in the given temperature range. Above 250°C, the rate equation is given by (Bondiera, J., and Naccache, C. (1991) Kinetics of methanol dehydration in dealuminated H-mordenite: model with acid and base active centers. *Applied Catalysis*, **69**, 139–148) as:

$$-r_{\text{methanol}} = k_o \exp\left(-\frac{E}{RT}\right) p_{\text{methanol}} \tag{18.8}$$

where $k_o = 0.336111\ \text{kmol/(m}^3\ \text{reactor} \cdot \text{s} \cdot \text{Pa)}$, $E = 80.48\ \text{kJ/mol}$, and p_{methanol} = partial pressure of methanol (Pa). Catalyst is significantly deactivated at temperatures above 400°C, and the reactor should be designed so that this temperature should not be exceeded anywhere in the reactor. Since the DME reaction is not highly exothermic, the proper temperatures can be maintained by preheating the feed to no more than 250°C and running the reactor adiabatically. The catalyst particle density is about 4 g/cm^3 with a voidage of 0.5. A single-tube packed bed plug-flow reactor will be used to carry out the conversion process followed by an absorption process to separate water from DME. Based on the given homogeneous gas-phase kinetics, it is found that the conversion is 100 complete for the given feed pressure and temperature running under adiabatic condition. Figure 18.4 shows a schematic for the catalytic dehydration of methanol over the acid zeolite catalyst. The flowsheet is configured to be fully pressure-driven for carrying out process control-related tasks.

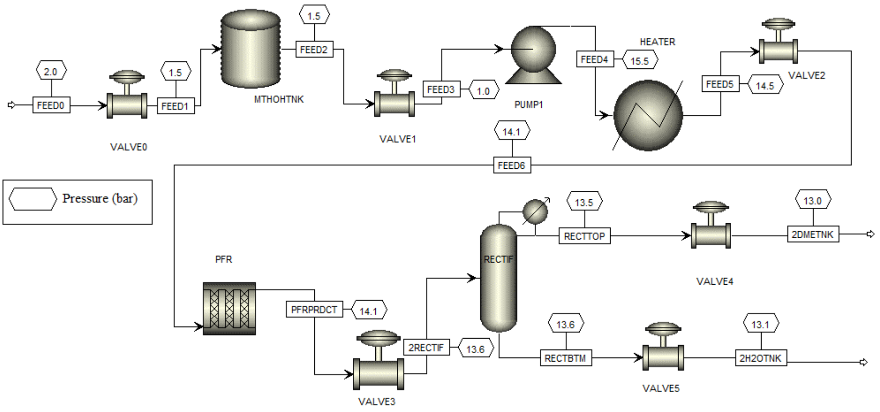


Figure 18.4 A schematic for the catalytic dehydration of methanol. The flowsheet is configured to be fully pressure-driven for carrying out process control-related tasks.

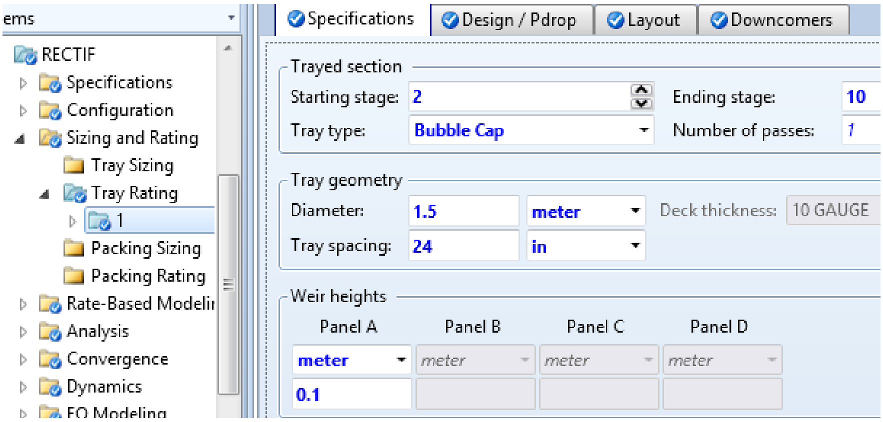
Your initial tasks are as follows:

- **Decide on the property method and come up with the proper design to end up with a purity level, which is at least 99.9 wt% for DME and 99.8 wt% for water at the indicated annual production rate.**

- **Define the unit price for each feed and product stream. Associate a utility with a block where it is required.**
- **Using APEA, carry out process economic analysis and report the economic profitability indices for the investment project.**

18.3.2 Process Dynamics and Control

Since the specifications, while the dynamic option is on for the distillation tower (Click on "**Dynamics**" ribbon **|** "**Dynamics Mode**" button), are quite many, some snapshots are shown in Figures 18.5 and 18.6:



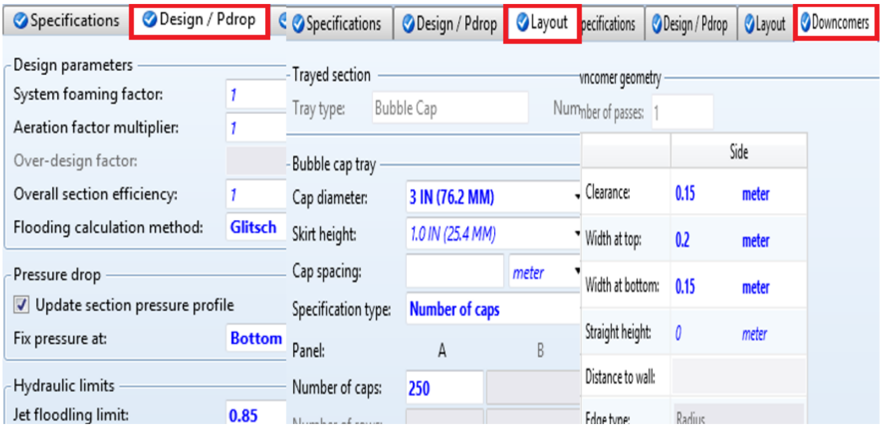
Trayed section
Starting stage: 2
Ending stage: 10
Tray type: Bubble Cap
Number of passes: 1

Tray geometry
Diameter: 1.5 meter
Deck thickness: 10 GAUGE
Tray spacing: 24 in

Weir heights

Panel A	Panel B	Panel C	Panel D
meter	meter	meter	meter
0.1			

Figure 18.5 Tray rating specifications needed for a rigorous hydraulics modeling.



Design parameters
System foaming factor: 1
Aeration factor multiplier: 1
Over-design factor:
Overall section efficiency: 1
Flooding calculation method: Glitsch

Pressure drop
☑ Update section pressure profile
Fix pressure at: Bottom

Hydraulic limits
Jet floodling limit: 0.85

Trayed section
Tray type: Bubble Cap

Bubble cap tray
Cap diameter: 3 IN (76.2 MM)
Skirt height: 1.0 IN (25.4 MM)
Cap spacing: meter
Specification type: Number of caps

Panel:	A	B
Number of caps:	250	

vncomer geometry
Number of passes: 1

	Side	
Clearance:	0.15	meter
Width at top:	0.2	meter
Width at bottom:	0.15	meter
Straight height:	0	meter
Distance to wall:		
Edge type:	Radius	

Figure 18.6 Further specifications for tray rating, needed for a rigorous hydraulics modeling.

For the dynamic option of methanol tank, PFR, and distillation column, choose the following specifications:

"**MTHOHTNK**" tank: Under "**Vessel**" tab, "**Vessel type**": "*Vertical*", "**Head type**": "*Flat*", "**Length**": "*5 m*", "**Diameter**": "*5 m*". Under "**Initial Condition**" tab, "**Initial condition for liquid volume fraction**": "*0.5*", and select "*Include overall liquid level controller*" for "**Options**" under "**Controllers**" tab.

"**PFR**" reactor: Under "**Catalyst Specification**" tab, select "*No heat-transfer*" for "**Catalyst heat transfer option**", because "**PFR**" is run adiabatically.

"**RECTIF**" column: Under "**Condenser**" tab, select "*Constant duty*". Under "**Reboiler**" tab, select "*Constant duty*". Under "**Reflux Drum**" tab, select "**Vessel type**": "*Vertical*", "**Head type**": "*Elliptical*", "**Length**": "*3 m*", and "**Diameter**": "*3 m*". Under "**Sump**" tab, select "**Head type**": "*Elliptical*", "**Height**": "*3 m*", and "**Diameter**": "*3 m*". Under "**Hydraulics**" tab, select "**Hydraulics**": "*Rigorous*". Finally under "**Controllers**" tab, select "**Temperature (top stage)**" controller with "*Reflux flow rate*" as the manipulated variable.

Hint: To lessen the headache that you may encounter upon running the simulation, first carry out the steady-state version without dynamics option and assure that there are no serious warnings or any severe error. After that, enter the dynamic specifications shown earlier, reinitialize, and run the simulator with dynamics option on. See Chapter 15 for more information on Aspen Plus Dynamics. After clicking on "**Pressure Driven**" button, found in "**Dynamics**" ribbon of Aspen Plus, the flowsheet as it appears in APD environment is supposed to be similar to that shown in Figure 18.7. Take a notice that a dead-time element was inserted for each control loop and control units (i.e., nodes) were renamed, flipped left/right, or flipped up/down.

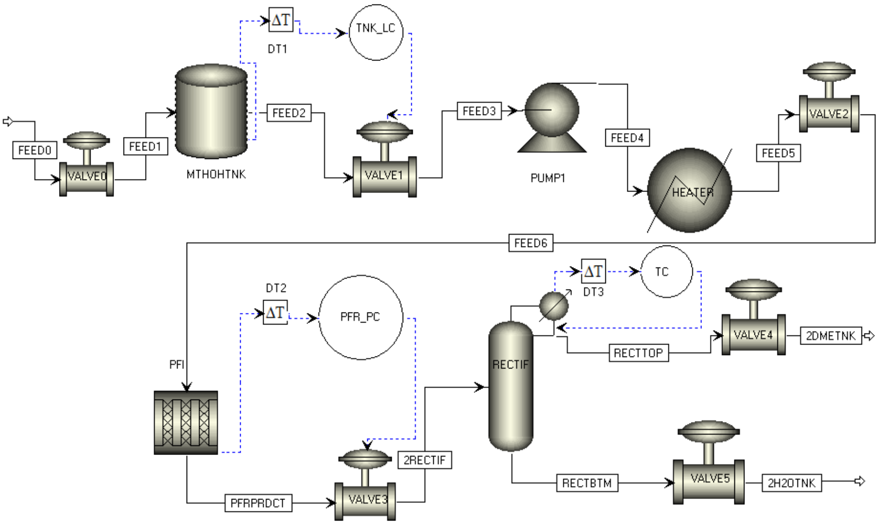


Figure 18.7 The controlled process of "Production of DME via catalytic dehydrogenation of methanol" with three control loops being installed: The first is for liquid-level "**TNK_LC**" control; the second is for pressure "**PFR_PC**" control; and the third is for temperature "**TC**" control. A dead-time element was inserted for each control loop.

Your control-related tasks are as follows:

- **Carry out the Closed-Loop Auto-Tune Variation (ATV) Test for three controllers and in the following recommended order: Start with temperature controller, followed by the pressure controller, and finally ending with liquid level controller. Notice that the liquid-level controller is simply proportional-only controller.**
- **Finally, for each of the three controllers, carry out a positive and negative step change both in set-point and load disturbance. So, you will have four case studies for each of the three controller. Report the results.** ***To have a reasonable controlled dynamic response, do not exceed the limit of ±5% of the initial set-point or load point.***

18.4 TP #4: PRODUCTION OF ACETIC ACID VIA PARTIAL OXIDATION OF ETHYLENE GAS

It is desired to produce about 60,000 tons/year (1 year = 8,000 operating hours) of acetic acid (99.9 wt%) and the by-product pure CO_2. In addition, an air liquefaction process will be installed to utilize pure oxygen in acetic acid synthesis and have pure N_2 as the by-product. The kinetic data and catalyst properties were quoted from: (Yap, F.T. (1996) One-step oxidation of ethylene to acetic acid using hydrophobic catalysts. MS thesis. University of Alberta, Canada). Polystyrene di-vinyl-benzene (PSDVB), a copolymer of styrene and di-vinylbenzene, is used as a high purity polymeric catalyst support. Palladium catalyst is mounted on PSDVB support by the impregnation method, where the support is impregnated by methanol solution, followed by dissolved $PdCl_2$ ($PdCl_2$ in 20 wt% HCl) solution, subject to evaporation, drying, and reduction step, using H_2 gas.

Consider the palladium-catalyzed gas-phase conversion of ethylene to acetic acid according to the following reaction:

$$C_2H_4 + O_2 \rightarrow CH_3COOH \tag{18.9}$$

$$-r_{C_2H_4}\left(\frac{\text{kmol}}{\text{kg catalyst}\cdot\text{s}}\right) = 1.762\times10^{-6}\times\exp\left[-23,720\times\left(\frac{1}{T}-\frac{1}{300}\right)\right]P_{O_2}^{0.5}P_{C_2H_4}^{1.0} \tag{18.10}$$

Nevertheless, ethylene may undergo complete oxidation:

$$C_2H_4 + 3O_2 \rightarrow 2\ CO_2 + 2H_2O \tag{18.11}$$

$$-r_{C_2H_4}\left(\frac{\text{kmol}}{\text{kg catalyst}\cdot\text{s}}\right) = 2.1597\times10^{-10}\times\exp\left[-74,050\times\left(\frac{1}{T}-\frac{1}{300}\right)\right]P_{O_2}^{1.5}P_{C_2H_4}^{1.0} \tag{18.12}$$

The activation energy has units of J/mol (kJ/kmol). The catalyst is present in the CSTR with a bed voidage of 0.5 and catalyst loading of 5 kg.

Your job is to design a process flowsheet made of an air liquefaction process to utilize pure O_2 as a feed to the reactor while making use of N_2, the liquid nitrogen, which can be later used as a utility stream or blanket/inert atmosphere. In addition to the proper design of CSTR, you should carry out downstream treatment steps needed to assure the separation of acetic acid from other constituents and have CO_2 as a pure stream. Carry out process economic analysis to see the profitability of the project.

18.5 TP #5: PYROLYSIS OF BENZENE

Diphenyl ($C_{12}H_{10}$) is an important industrial intermediate substance. One production scheme involves the pyrolytic dehydrogenation of benzene (C_6H_6) (Fogler, H.S. (1999) *Elements of Chemical Reaction Engineering*, 3rd edn, Prentice Hall, Upper Saddle River, pp. 77–79). During the process, triphenyl ($C_{18}H_{14}$) is also formed by a secondary reaction. The kinetic data were modified in line with Aspen Plus standard notation for a homogeneous reaction.

The gas-phase reactions are as follows:

$$2C_6H_6 \rightleftharpoons C_{12}H_{10} + H_2 \tag{18.13}$$

$$C_6H_6 + C_{12}H_{10} \rightleftharpoons C_{18}H_{14} + H_2 \tag{18.14}$$

Rate laws:

$$-r_{C_6H_6} = (k_1 \times p^2_{C_6H_6} - k_2 \times p_{C_{12}H_{10}} \times p_{H_2}) \tag{18.15}$$

$$k_1\left(\frac{\text{kmol}}{\text{s}\cdot\text{m}^3\cdot\text{Pa}^2}\right) = 3.2353726 \times 10^{-6} \exp\left(-\frac{15,203.2716}{T}\right) \tag{18.16}$$

$$k_2\left(\frac{\text{kmol}}{\text{s}\cdot\text{m}^3\cdot\text{Pa}^2}\right) = 1.234762 \times 10^{3} \exp\left(-\frac{13,501.76}{T}\right) \times T^{-3.13} \times \exp^{(0.00163\times T)} \tag{18.17}$$

$$-r_{C_{12}H_{10}} = (k_3 \times p_{C_6H_6} \times p_{C_{12}H_{10}} - k_4 \times p_{C_{18}H_{14}} \times p_{H_2}) \tag{18.18}$$

$$k_3\left(\frac{\text{kmol}}{\text{s}\cdot\text{m}^3\cdot\text{Pa}^2}\right) = 3.7544919 \times 10^{-6} \exp\left(-\frac{15,203.2716}{T}\right) \tag{18.19}$$

$$k_4\left(\frac{\text{kmol}}{\text{s}\cdot\text{m}^3\cdot\text{Pa}^2}\right) = 1.13808 \times 10^{7} \exp\left(-\frac{15,935.76}{T}\right) \times T^{-4.32} \times \exp^{(0.00315\times T)} \tag{18.20}$$

Your job is to design a process flowsheet made of the main reactor and downstream pieces of equipment needed to assure the separation of each constituent, namely the unreacted benzene, di- and triphenyl. Hydrogen and a small fraction of benzene can be flared off, sent to a storage vessel to be used as a precursor or feedstock for other benzene-based chemical processes, or to a flash drum to separate them into pure benzene and pure hydrogen as well. Carry out economic analysis and show profitability indices.

18.6 TP #6: REUSE OF SPENT SOLVENTS

A pharmaceutical company XXX ends up with a solvent mixture that is made of acetone, methanol, and water. Unfortunately, acetone and methanol form an azeotrope. You may examine this azeotropic condition using Aspen Plus itself via "**Analysis**" group found in "**Home**" ribbon under both "**Properties**" and "**Simulation**" environment. A close inspection for the residue curves map for this ternary mixture will reveal that one way to get around this hectic problem is simply by adding water to an existing acetone–methanol azeotrope, which will be broken or shifted to non-azeotropic conditions, depending on the added amount (i.e., final equilibrium composition). Given the flow rate of the solvent mixture as 1500 kg/h at 37°C and 1.05 atm with a mass fraction of 0.7, 0.25, and 0.05 for acetone, methanol, and water, respectively, your goal is to design the flowsheet made of the proper pieces of equipment such that you end up with pure stream for each of the three constituents. Also, carry out a sensitivity study to examine the effect of flow rate of added water on the performance of the solvent recovery system. Assume that the spent solvent mixture is free of charge as it represents the by-product of pharmaceutical operations.

Carry out a profitability study for XXX company telling them when they will be able to recover what they pay for the solvent recovery system via selling, of course, the pure solvents generated by the proposed solvent recovery plant.

18.7 TP #7: SOLIDS HANDLING: PRODUCTION OF POTASSIUM SULFATE FROM SODIUM SULFATE

Refer to Chapter 14 appendices regarding Aspen Plus nomenclature about expressing a solid material in different forms. The production of potassium sulfate will be tackled using two different expressions for solid material form.

The first solid form is conventional inert solid (CISOLID) as shown in the following two reactions:

In the first reactor, the formation of glaserite ($Na_2SO_4 \cdot 3K_2SO_4$) solid material will be based on the reaction between saturated potassium chloride solution and sodium sulfate as a solid material, according to the following reaction:

$$6KCl(MIXED) + 4Na_2SO_4(CISOLID) \rightarrow Na_2K_6(SO_4)_4(CISOLID) + 6NaCl(MIXED) \tag{18.21}$$

In the second reactor, the formation of potassium sulfate (K_2SO_4) solid material will be based on the reaction between saturated potassium chloride solution and glaserite as a solid material, according to the following reaction:

$$2KCl(MIXED) + Na_2K_6(SO_4)4(CISOLID) \rightarrow 4K_2SO_4(CISOLID) + 2NaCl(MIXED) \tag{18.22}$$

The second solid form is conventional inert with particle size distribution (CIPSD) as shown in the following two reactions:

In the first reactor, the formation of glaserite ($Na_2SO_4 \cdot 3K_2SO_4$) solid material will be based on the reaction between saturated potassium chloride solution and sodium sulfate as a solid material, according to the following reaction:

$$6KCl(MIXED) + 4Na_2SO_4(CIPSD) \rightarrow Na_2K_6(SO_4)_4(CIPSD) + 6NaCl(MIXED) \tag{18.23}$$

In the second reactor, the formation of potassium sulfate (K_2SO_4) solid material will be based on the reaction between saturated potassium chloride solution and glaserite as a solid material, according to the following reaction:

$$2KCl(MIXED) + Na_2K_6(SO_4)4(CIPSD) \rightarrow 4K_2SO_4(CIPSD) + 2NaCl(MIXED) \tag{18.24}$$

Your task is to design the proper flowsheet in terms of carrying out these two consecutive reactions in two reactors in series separated by the proper pieces of equipment needed to separate the solid material from the remaining mother liquor. Use both approaches with or without a particle size distribution (PSD). For the second case, you must assign PSD for the simulation and at least once for the first inlet solid feed stream. The kinetic data are missing; hence, you should know how to tackle such a case based on selecting the right reactor model found under "Reactors" tab in "Model Palette" and assuming a fractional conversion for the limiting reactant for each reaction.

Select the proper annual production capacity, expressed in tons per year. Assign a stream cost for feed and product streams as well as utilities associated with the heat duty accompanying each reactor. Report the overall net cost flow under "Results Summary" | "Operating Costs" expressed as ($/h).

18.8 TP #8: SOLIDS HANDLING: PRODUCTION OF $CaCO_3$-BASED AGGLOMERATE AS A GENERAL ADDITIVE

Refer to Chapter 14 appendices regarding Aspen Plus nomenclature about expressing a solid material in different forms. In your analysis here, use the main stream class of type MIXCIPSD, which includes both conventional inert with particle size distribution (CIPSD) and mixed (MIXED) substream. Hence, you need to decide on the proper particle size distribution for solid streams before and after leaving the grinder and agglomerator as well.

It is desired to produce calcium carbonate-based powder that can be used as an additive (e.g., thickener or filler) in different formulations, including, but not limited to, pharmaceutical, food, and detergent applications. Calcium carbonate will be prepared (i.e., ground) and then mixed with the solid calcium sulfate in a mixer. The output stream from the mixer will be sent to the fluidized bed unit, which will act as agglomerator where the combined solid powder is thoroughly mixed with the binding material, which is introduced as tiny droplets via the spray/sprinkler system. The binding material is an aqueous solution of glycine (5 wt%). Hot and dry air will be introduced from the bottom of the fluidized bed so that it helps remove the excess amount of moisture after being used in the binding/agglomeration step. The exhaust air will be humid and the solid product will be dry with at least 97.5 wt% solid material.

Your task is to come up with the design of a steady-state flowsheet that will handle the production of the dry solid powder of $CaCO_3$-based agglomerate, while selecting the proper annual production capacity, expressed in tons per year.

18.9 TP #9: SOLIDS HANDLING: FORMULATION OF DI-AMMONIUM PHOSPHATE AND POTASSIUM NITRATE BLEND FERTILIZER

Refer to Chapter 14 appendices regarding Aspen Plus nomenclature about expressing a solid material in different forms. In your analysis here, use the main stream class of type MIXCIPSD, which includes both conventional inert with particle size distribution (CIPSD) and mixed (MIXED) substream. Hence, you need to decide on the proper particle size distribution for the simulation and for solid stream leaving the dryer as well.

It is desired to formulate an inorganic fertilizer that is mainly made of the three essential ingredients: nitrogen (N), phosphate (P_2O_5), and potash (K_2O). The label of a fertilizer package or bag indicates the product percentages of nitrogen (N), phosphate (P_2O_5), and potash (K_2O), respectively. For example, a 20–24–12 fertilizer contains 20 wt% nitrogen, 24 wt% phosphate, and 12 wt% potash. What else is present in the fertilizer? Notice that the sum does not add up to 100% simply because the fertilizer may contain other elements, such as carbon, hydrogen, oxygen, sulfur, iron, and zinc. For example, ammonium nitrate (NH_4^+ NO_3^-) has a grade of 35–0–0 with 35% of the content from nitrogen (0 phosphate and 0 potash) and 65% from hydrogen and oxygen. N Fraction $= (14 + 14)/(14 + 4 + 14 + 48) = 28\,g/80\,g = 0.35$. The four numbers, in the denominator, indicate the molecular mass of each species found in the chemical formula.

It is desired to produce a pelletized fertilizer blend made of potassium nitrate (KNO_3) and di-ammonium phosphate ($(NH_4)_2HPO_4$). The feed stream will be made of an aqueous solution of these two types of fertilizers. The feed will be pumped to the top of the spray dryer where it will meet a hot and low-humidity air introduced to the bottom of the dryer. Two streams will leave the dryer: the first is the dry solid product and the second is humid air. These two exit streams will be mixed or merged into one combined stream where the latter will be sent to a gas cyclone, which will act as a dust collector. At the cyclone, the bottom leaving stream will be the main solid product stream. The top stream, leaving the gas cyclone, mainly air containing very small-size carried (suspended) solid particles, will be sent to a fabric filter that will knock down the solid material. The knocked-down solid material will be mixed with the main solid product stream leaving the bottom of the gas cyclone. The combined solid product stream will be our final finished product (the pelletized fertilizer).

On the other hand, the “pass-through fabric filter” stream will be sent to a gas blower to slightly increase its pressure before it is dumped into the environment.

Your task is to come up with the design of a steady-state flowsheet that will handle the formulation of the dry solid powder made of the two fertilizers. Select the proper annual production capacity, expressed in tons per year.

18.10 TP #10: “FLOWSHEETING OPTIONS” | “CALCULATOR”: GAS DE-SOURING AND SWEETENING PROCESS

A sour gas is like natural gas, or any other gas, containing considerable amounts of hydrogen sulfide (H_2S). Natural gas is usually considered sour if H_2S concentration is higher than a threshold (say 100 ppm by volume under standard temperature and pressure). However, this threshold may vary from one country to another or even from one application to another within the same country. A natural gas that has H_2S content below the agreed-upon threshold is denoted as “sweet gas”.

Although the terms acid gas and sour gas may interchangeably be used, in fact, a sour gas is any gas that contains hydrogen sulfide content higher than the threshold, whereas an acid gas is any gas that contains chemical species giving rise to the formation of an acidic gas medium (i.e., lowering pH) in the presence of moisture, such as carbon dioxide (CO_2). Keep in mind that hydrogen sulfide itself also gives rise to an acidic gas medium as well. Thus, carbon dioxide itself is an acid gas, not a sour gas. In addition to being toxic, hydrogen sulfide, in the presence of moisture, has detrimental effects on many metal structures, causing sulfide stress corrosion cracking. Natural gas typically contains several ppm of volatile sulfur compounds, but depending on the oil well location, the sulfur content may run higher up to several orders of magnitude.

In "**Properties**" environment, add the required components, namely, water, N_2, CO_2, H_2S, and KOH.

Using the electronic wizard, select the unsymmetric reference state for ionic components, include all chemical species present into the electrolytic portray, select water dissociation, deselect both salt and ice formation, express hydrogen ion type as H^+, and select the "**True component approach**", which I call it the chemist's approach, as the simulation approach to decide on the number and type of chemistry reactions as well as Henry's components.

It is worth mentioning here that Aspen Plus provides built-in examples (see, e.g., "**C:\Program Files (x86)\AspenTech\Aspen Plus V8.8\GUI\Examples\Amines_ELECNRTL**") regarding the modeling aspects of an absorber and stripper using different absorbing/stripping agents and operating conditions. Both "**ELECNRTL**" and "**ENRTL-RK**" rate-based methods are used. Here, we combined the absorption and stripping processes in addition to allowing a recycle stream from stripper back to the inlet of the absorber. Moreover, a make-up liquid feed will compensate the lost absorbent in purge stream. The purge stream will purge other chemical species, which will otherwise accumulate within the internal loop of the combined process. Typically, the purge is used to control the solvent recirculation rate and the makeup is used to control the solvent strength.

Finally, the top product stream from stripper will be cooled to knock out water prior to sending the stream as a feed for Claus process for sulfur recovery. See Figure 18.8.

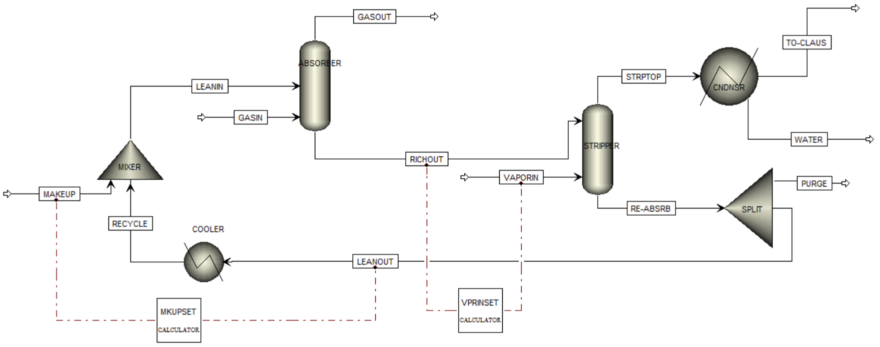
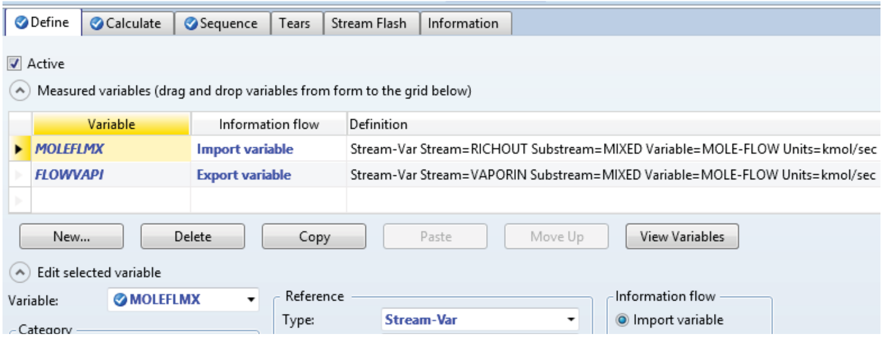


Figure 18.8 The flowsheet for gas desouring and sweetening with recycling stream.

On the one hand, your job is to assure that both undesired species CO_2 and H_2S will be almost completely removed from the inlet gas ("**GASIN**") stream and will leave with the spent liquid ("**RICHOUT**") stream while ending up with desoured and sweetened pure (99.8 wt%) nitrogen ("**GASOUT**") gas stream. On the other hand, the "**RICHOUT**" stream will enter the stripping unit where a vapor stream will strip the already absorbed CO_2 and H_2S compounds and dump them into the outlet gas ("**STRPTOP**") stream. A condenser at room temperature and pressure can be installed prior to introducing the "dirty guys" to Claus process.

As a result of recycling stream, we need to install a "**Calculator**" loop that will assure a smooth run and eventually end up with a converging solution. Remember that we use “**Calculator**” blocks to insert our own FORTRAN statements or Excel spreadsheet calculations into the flowsheet computations. For instance, we can calculate and set input variables before they are used (i.e., a feed forward control).

Since this is the first time, I introduce the “**Calculator**” option found under “**Flowsheeting Options**” while in “**Simulation**” environment, I will elaborate on its details. The “**Calculator**” loop allows the user to calculate (i.e., adjust), for example, a stream property (the export variable) as a function of a monitored (import) variable, where the latter may change its value from one run (i.e., loop) to another especially when it comes to the presence of an internal loop (i.e., recycling stream) as in our case. Figure 18.9 shows “**Define**” tab window for the first “**Calculator**” loop, shown in Figure 18.8 as a dashed-line loop, called “**VPRINSET**”, where we define one “**Import**” variable called “**MOLEFLMX**” which stands for the molar flow rate of “**RICHOUT**” stream and “**FLOWVAPI**”, as an “**Export**” variable, which stands for the molar flow rate of “**VAPORIN**” stream.



☑ Active

Measured variables (drag and drop variables from form to the grid below)

Variable	Information flow	Definition
MOLEFLMX	Import variable	Stream-Var Stream=RICHOUT Substream=MIXED Variable=MOLE-FLOW Units=kmol/sec
FLOWVAPI	Export variable	Stream-Var Stream=VAPORIN Substream=MIXED Variable=MOLE-FLOW Units=kmol/sec

Edit selected variable

Variable: MOLEFLMX

Reference

Type: Stream-Var

Information flow

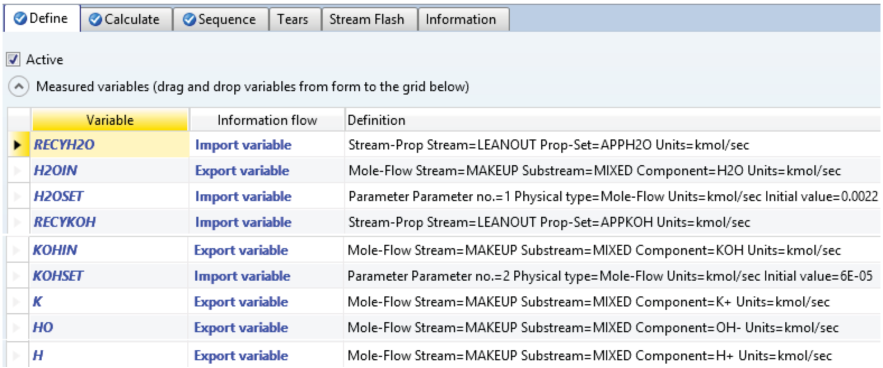
● Import variable

Category

Figure 18.9 The “**Define**” tab window for defining an “**Import**” and “**Export**” variable, which can be used in “**Calculate**” tab window, as part of a “**Calculator**” case study, as part of “**Flowsheeting Options**”.

In “**Calculate**” tab window, define the following FORTRAN statement: **FLOWVAPI = 0.25* MOLEFLMX**. This statement simply says that the inlet vapor molar flow rate (the export variable) is set to 0.25 of that of the spent absorber (the import variable). In “**Sequence**” tab window, select “*Use import/export variables*” option from the drop-down menu to “**Execute**” and be sure that the import/export variables are properly defined underneath.

The second “**Calculator**” loop, shown in Figure 18.8 as a dashed-line loop, called “**MKUPSET**”, which has to deal with the make-up feed-forward control. Figure 18.10 shows the list of either import or export variable being defined under “**Define**” tab. Starting from top, “**RECYH2O**” stands for the apparent component flow rate of water in “**LEANOUT**” stream; “**H2OIN**” the molar flow rate of water in the make-up feed; “**H2OSET**” a prescribed/set-point value for inlet water molar flow rate (see the FORTRAN code under “**Calculate**” tab); “**RECYKOH**” the apparent component flow rate of KOH in “**LEANOUT**” stream; “**KOHIN**” the molar flow rate of KOH in the make-up feed; “**KOHSET**” a prescribed/setpoint value for inlet KOH molar flow rate (see the FORTRAN code under “**Calculate**” tab); and “**K**”, “**HO**”, and “**H**” stand for the molar flow rate of K^+, OH^-, and H^+ ion in the make-up feed, respectively. Notice that you need to create or



☑ Active

Measured variables (drag and drop variables from form to the grid below)

Variable	Information flow	Definition
RECYH2O	Import variable	Stream-Prop Stream=LEANOUT Prop-Set=APPH2O Units=kmol/sec
H2OIN	Export variable	Mole-Flow Stream=MAKEUP Substream=MIXED Component=H2O Units=kmol/sec
H2OSET	Import variable	Parameter Parameter no.=1 Physical type=Mole-Flow Units=kmol/sec Initial value=0.0022
RECYKOH	Import variable	Stream-Prop Stream=LEANOUT Prop-Set=APPKOH Units=kmol/sec
KOHIN	Export variable	Mole-Flow Stream=MAKEUP Substream=MIXED Component=KOH Units=kmol/sec
KOHSET	Import variable	Parameter Parameter no.=2 Physical type=Mole-Flow Units=kmol/sec Initial value=6E-05
K	Export variable	Mole-Flow Stream=MAKEUP Substream=MIXED Component=K+ Units=kmol/sec
HO	Export variable	Mole-Flow Stream=MAKEUP Substream=MIXED Component=OH- Units=kmol/sec
H	Export variable	Mole-Flow Stream=MAKEUP Substream=MIXED Component=H+ Units=kmol/sec

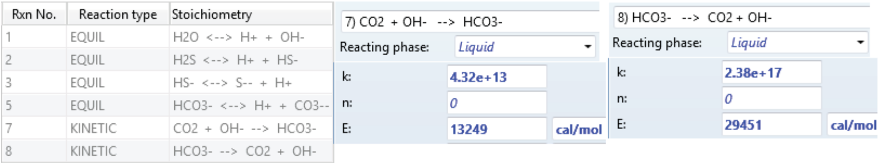
Figure 18.10 The list of import/export variables to be used in “**MKUPSET**” calculator loop.

define two property sets: the first accounts for the apparent component molar flow rate of water and the second for the apparent component molar flow rate of KOH. Such properties are denoted as FAPP in Aspen Plus terminology.

In “**Calculate**” tab window, enter the following FORTRAN code:

```
K=0
HO=0
H=0
H2OIN = H2OSET
IF(RECYH2O.LT. 1D35)
H2OIN = H2OSET - RECYH2O
IF(H2OIN .LT. 0D0) H2OIN = 0
KOHIN =KOHSET
IF(RECYKOH .LT. 1D35)
KOHIN = KOHSET - RECYKOH
IF(KOHIN .LT. 0D0) KOHIN = 0
```

The inlet gas (“**GASIN**”) stream has a flow rate of 166.667 l/min and has the following molar/volumetric composition: H_2O 0.04, CO_2 0.02, H_2S 0.01, and N_2 0.93. The inlet make-up liquid flow rate can be initially assumed as 100 kg/h of 4 wt% NaOH solution; however, its value and composition will be adjusted by the calculator loop. The following reactions will take place in liquid phase at each packed stage of the absorption tower as given by Figure 18.11.



Rxn No.	Reaction type	Stoichiometry
1	EQUIL	H2O <--> H+ + OH-
2	EQUIL	H2S <--> H+ + HS-
3	EQUIL	HS- <--> S-- + H+
5	EQUIL	HCO3- <--> H+ + CO3--
7	KINETIC	CO2 + OH- --> HCO3-
8	KINETIC	HCO3- --> CO2 + OH-

7) CO2 + OH- --> HCO3-

Reacting phase: Liquid

k: 4.32e+13

n: 0

E: 13249 cal/mol

8) HCO3- --> CO2 + OH-

Reacting phase: Liquid

k: 2.38e+17

n: 0

E: 29451 cal/mol

Figure 18.11 The equilibrium- and rate-based reactions which take place in the liquid phase at each packed stage of the absorption column.

> **NOTE #3:** *To display (or hide) the calculator block and/or its connections, on the flowsheet, while the flowsheet window is active, go to “**Top**” toolbar | “**Modify**” tab and click on “**Display Options**” button.*

Notice that you need to create a reaction set while selecting “**REAC-DIST**” (i.e., reactive distillation) from the drop-down list. Define the aforementioned six reactions, where four of them are of equilibrium type and the last two are of kinetic type. For the absorption column, in “**Specifications**” | “**Reactions**” | “**Specifications**” tab sheet, define the starting and ending stage where the reaction will take place, associate the created reaction set with the selected range of packed stages, and assign the residence time (under “**Residence Times**” tab) for liquid (e.g., 2 s) for the selected range of packed stages. Repeat the same procedure for the stripper using the same reaction set mentioned earlier.

Decide on the proper operating conditions for each block, the fraction to be recycled out of (“SPLIT”) block, the packing material in terms of its packing characteristics, section diameter, and section packed height for both absorber and stripper such that gas desouring and sweetening process is achieved.

18.11 TP #11: USING MORE THAN ONE PROPERTY METHOD AND STREAM CLASS: SOLID CATALYZED DIRECT HYDRATION OF PROPYLENE TO ISOPROPYL ALCOHOL (IPA)

Isopropyl alcohol (IPA) is an intermediate petrochemical, which can be used as a solvent in different home, hospital, and industry applications. Moreover, it can be used as a feedstock for the production of acetone and other compounds.

The acid-catalyzed direct hydration of propylene is given by

$$CH_3CH = CH_2 + H_2O \overset{k_1,k_2}{\Longleftrightarrow} (CH_3)_2CHOH \qquad (18.25)$$

Di-isopropyl ether (DIPE) is the main by-product. The side-product formation can be expressed as:

$$CH_3CH = CH_2 + (CH_3)_2CHOH \overset{k_3,k_4}{\Longleftrightarrow} ((CH_3)_2CH)_2O \qquad (18.26)$$

It is worth mentioning here that there are two types of propylene hydration processes: direct and indirect. The direct technology has an advantage of cost savings in terms of capital investment, processing, and maintenance relative to that of the indirect process, where the latter requires handling the reconcentration of sulfuric acid, in addition to corrosion and pollution nagging problems. Nevertheless, the direct process requires a high-energy usage and the need for a highly concentrated propylene.

One of the direct hydration processes is to use catalytic (i.e., reactive) distillation. Nevertheless, this process usually ends up with water–IPA azeotrope. One way to tackle such a problem, as in politics, is to live with it (i.e., the azeotrope is sold as such). On other hand, prevention/remedy measures such as shift in azeotrope composition and dehydration of IPA can be implemented to end up with anhydrous IPA product. Here, we will use calcium oxide to react with water and the product will precipitate as calcium hydroxide, which will be separated from the liquid anhydrous solid-free IPA (99.9 wt%) using the filtering process. Such a reaction is real fast and exothermic and goes to completion.

Reactive distillation represents the simultaneous processes of catalytic reaction and multistage distillation in a single reactive distillation column. A reactive distillation column thus combines the reactor and a series of distillation columns, hence, yields to an overall cost effective process by reducing the number of process vessels, materials transport, and required control devices.

So, in our case, we will have a packed distillation tower, where the catalyst will be placed on two separate packed trays. The catalyst packing will function as both a promoting and an L/V mass transfer medium. The heterogeneous catalyst-based reactive distillation is denoted as catalytic distillation (CD), as opposed to the homogeneous reactive distillation.

Equilibrium-limited reactions are recommended candidates for catalytic distillation; the equilibrium reaction can be shifted toward the desired product side simply by continuously separating products from reactants while the reaction is in progress. Ion-exchanged resins, such as tungsten oxide and zeolite, have been reported to have a high activity for liquid-phase hydration of propylene to IPA (Petrus, L., De Roo, R.W., Stamhuis, E.J., and Joosten, G.E.H. (1984) Kinetics and equilibria of the hydration of propene over a strong acid ion exchange resin as catalyst. *Chemical Engineering Science*, **39** (3), 433–446). For example, Amberlyst, an acid ion-exchange resin, can be used if the reaction temperature lies between 320 and 450 K. If the thermal stability of an acid ion-exchange catalyst is of concern, then alternative catalysts having a high thermal stability can be used, such as acidic inorganic catalysts.

In “**Properties**” environment, add the following compounds: propylene, water, IPA, DIPE, propane, calcium oxide as solid, and calcium hydroxide as both solid and conventional. Select a property method for the aforementioned chemicals while taking into account that the applied pressure can be as high as 12 bar. Assure that you have successfully characterized the system. Switch to “**Simulation**” environment and add the flowsheet blocks and material streams as shown in Figure 18.12.

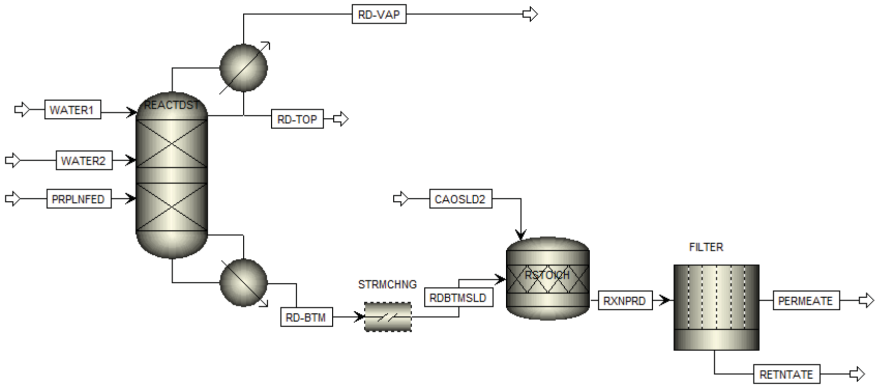
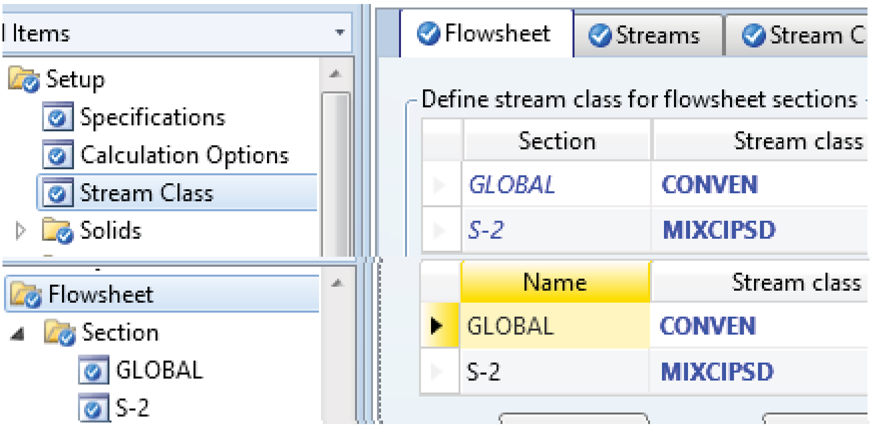


Figure 18.12 The flowsheet for IPA production using the solid-catalyzed direct hydration of propylene.

Figure 18.12 shows the flowsheet for the production of IPA using the solid catalyzed direct hydration of propylene. Starting from left, we have the solid-catalyst packed distillation column, where the catalyst is situated at two packed stages at the location where water feed is introduced and the rest of stages will be packed but without a catalyst loading. The second block, that is, “**STRMCHNG**” is simply installed for assuring a smooth transition between two flowsheet sections (i.e., zones): On the one hand, the first section consists of the catalytic distillation tower plus its input and output streams. On the other hand, the second section consists of the last two blocks: the reactor and filter. Notice that the “**STRMCHNG**” block itself can be allocated on either side of the two sections. What is really import here at this stage is that “**RD-BTM**” stream is defined as that of the first section; that is, the stream class is “**CONVEN**”. On the other hand, “**RDBTMSLD**” stream has a stream class of type “**MIXCIPSD**”. This explains why “**STRMCHNG**” block acts as mediator between two different flowsheet sections, where each section is characterized by a different stream class and property method as well.

To create a new section, highlight one block, for example, “**RSTOICH**”, and select “**Change Section** … ” item from the shortcut context menu. If this is the first time, then select “**Create new section:**” option and give it a name, say, “**S2**”. Repeat the same procedure for “**FILTER**” block but in the last step select “**Move to section:**” option and select “**S2**” from the dropdown menu. Repeat the last procedure for “**STRMCHNG**” block. You can see the default and newly created flowsheet section in “**Flowsheet**” | “**Section**” window. The stream class type associated with each section can be seen in “**Setup**” | “**Stream Class**” | “**Flowsheet**” tab window. See Figure 18.13. It is left to the user to decide on the stream class type for the newly created flowsheet section. Here, we have chosen its type to be “**MIXCIPSD**”, which stands for mixed conventional inert solid with a particle size distribution. Notice that “**MIXCIPSD**” stream class includes both “**MIXED**” and “**CIPSD**” substreams. The reason for such a selection is simply to account for solid handling of both solids calcium oxide and hydroxide. One may also account for solid handling using “**MIXCISLD**” stream class, instead of “**MIXCIPSD**”, for “**S2**” flowsheet section, without assigning a particle size distribution for some or all of the inlet and outlet streams of “**RSTOICH**” and “**FILTER**” blocks.



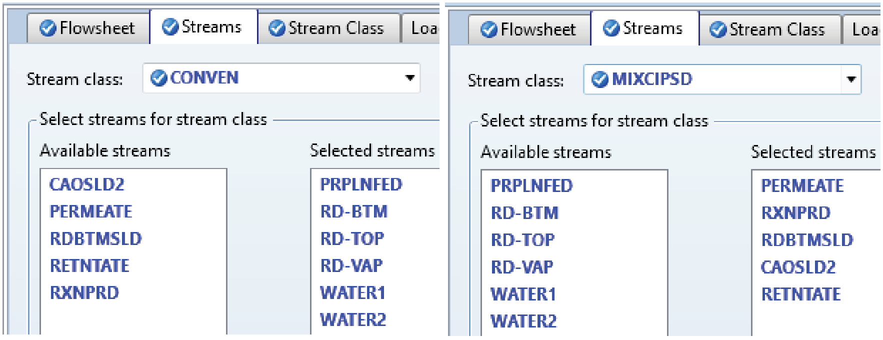
Define stream class for flowsheet sections

Section	Stream class
GLOBAL	CONVEN
S-2	MIXCIPSD

Name	Stream class
GLOBAL	CONVEN
S-2	MIXCIPSD

Figure 18.13 The flowsheet section and their associated stream class types.

Figure 18.14 shows how the given material streams are classified as either “**CONVEN**”, as in the “**GLOBAL**” section or “**MIXCIPSD**”, as in “**S2**” section. Notice here that “**RD-BTM**” stream appears as “**CONVEN**” type, whereas “**RDBTMSLD**” stream appears as “**MIXCIPSD**” type. Here comes the smooth transition between one section and another as “**STRMCHNG**” block does.



Stream class: CONVEN

Select streams for stream class

Available streams	Selected streams
CAOSLD2	PRPLNFED
PERMEATE	RD-BTM
RDBTMSLD	RD-TOP
RETNTATE	RD-VAP
RXNPRD	WATER1
	WATER2

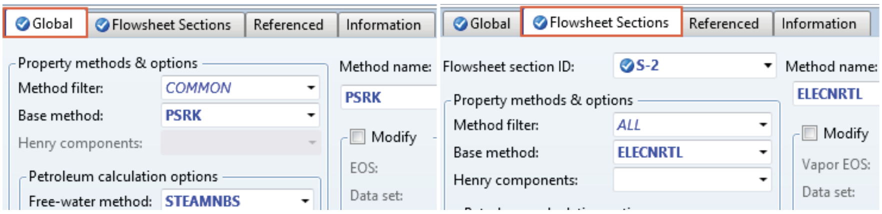
Stream class: MIXCIPSD

Select streams for stream class

Available streams	Selected streams
PRPLNFED	PERMEATE
RD-BTM	RXNPRD
RD-TOP	RDBTMSLD
RD-VAP	CAOSLD2
WATER1	RETNTATE
WATER2	

Figure 18.14 Classification of all material streams based on their location within a flowsheet section.

Once we have defined two sections we can go back to “**Properties**” environment and associate a new property method for the newly created section, as shown in Figure 18.15. Do not forget to successfully run the simulator under “**Properties**” environment before moving to “**Simulation**” environment.



Property methods & options

Method filter: COMMON

Base method: PSRK

Henry components:

Petroleum calculation options

Free-water method: STEAMNBS

Method name: PSRK

☐ Modify

EOS:

Data set:

Flowsheet section ID: S-2

Method name: ELECNRTL

Property methods & options

Method filter: ALL

Base method: ELECNRTL

Henry components:

☐ Modify

Vapor EOS:

Data set:

Figure 18.15 Assigning a property method for “**S-2**” section, which is different from the “**Global**” section.

Select the proper basis for the production capacity. You need to decide on the proper operating conditions for the catalytic distillation columns as far as the inlet and outlet flow rates are concerned, operating temperature and pressure, the location of the two reaction zones, and the feed tray location. Moreover, you need to decide on the proper packing material in terms of its packing characteristics, section diameter, and section packed height. You need to define a reaction set of type “REAC-DIST” (i.e., reactive distillation) from the drop-down list. Define the aforementioned two equilibrium reactions (Eqs. 18.25 **and** 18.26**). For the second part, that is, solids handling, you need to associate a reaction set with “STOICH” reactor based on the extent of conversion (i.e., fractional conversion) for either reactant, the operating pressure and temperature, and the outlet PSD. Finally, you need to specify the solid–liquid separation parameters for the filtering medium. Keep in mind that other solids separation devices, shown in the model palette, can be implemented in replacement of the aforementioned cascade. Finally, carry out feasibility study or profitability analysis for the proposed project.**

18.12 TP #12: POLYMERIZATION: PRODUCTION OF POLYVINYL ACETATE (PVAC)

Polyvinyl acetate (PVAC), referred to as wood glue, is a white glue and has different brand names in the market: carpenter's glue, school glue, Elmer's glue (in the United States), or PVA glue. It is a rubbery synthetic polymer that belongs to the polyvinyl esters family and is of thermoplastic polymer type. As a result of heating, a thermoplastic polymer passes from the solid state through the semi-liquid (alternatively semi-solid) state or transition temperature region until it finally melts and becomes (liquid-like) structure with a pronounced reduction in viscosity upon moving from the glass-transition to the liquid-like rubbery region. In the glass transition zone, it is usually described as viscoelastic material, and WLF-kinetic better describes the viscosity as a function of temperature. The degree of polymerization of PVAC varies from 100 up to 5000. The ester groups of PVAC is vulnerable to base hydrolysis and will slowly convert PVAC into polyvinyl alcohol and acetic acid. Moreover, PVAC is susceptible to polymer biodegradation by a number of microorganisms such as filamentous fungi, algae, yeasts, lichens, and bacteria.

In cited literature, there exist different routes for the production of PVAC from its monomer vinyl acetate (VNLACET). For example, Theis *et al*. (Theis, A., Davis, T.P., Stenzel, M.H., and Barner-Kowollik, C. (2006) Probing the reaction kinetics of vinyl acetate free radical polymerization via living free radical polymerization (MADIX). *Polymer*, **47**, 999–1010) examined the kinetic parameters of PVAC production from VNLACET at 80°C using 2,2′-azobisisobutyronitrile (AIBN) as an initiator and 2-ethoxythiocarbonylsulfanyl-propionic acid methyl ester (EPAME) as a mediator (i.e., chain transfer agent), which is a reversible addition-fragmentation transfer (RAFT) chain length-dependent termination (CLD-T) step.

Select the proper "**Polymers**" sub-template. Add the following components: vinyl-acetate (VNLACET), ethyl-acetate (ETHACET), AIBN, poly vinyl-acetate (PVAC) as polymer, and finally vinyl-acetate-R (VAC-R) as segment. Do not forget to characterize polymer and its repeating unit under "**Polymers**" | "**Characterization**" tab sheets. Also, let Aspen Plus perform GPC distribution calculation. Refer to "**Polymer**" | "**Distributions**" sheet.

After successfully carrying out properties analysis step, switch to "**Simulation**" environment and add the following flowsheet blocks as well as the associated input and output streams. See Figure 18.16.

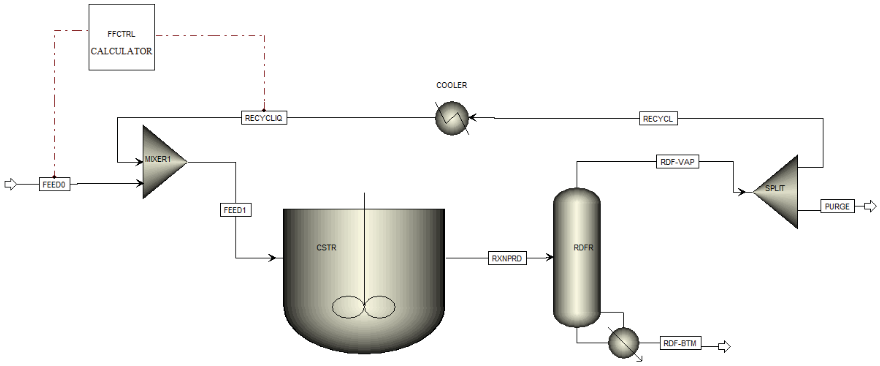


Figure 18.16 Production of poly vinyl acetate with recycle of solvent and unreacted vinyl acetate monomer.

Notice that the "**FFCTRL**" calculator acts as a feed forward control to adjust feed flow parameters in terms of individual amounts for each of the monomer, solvent, and initiator. The split fraction for "**SPLIT**" block can be as low as 0.0005 for "**PURGE**" stream, which practically means a complete recycle of the unreacted monomer and solvent.

In addition, you need to specify a free radical ("**FREE-RAD**") type of reaction and associate it with CSTR. Use PVAC as polymer; VNLACET as monomer; VAC-R as repeating unit; AIBAN as initiator; and ETHACET as solvent. Use the following pre-exponential constants as borrowed from Theis *et al*. (citation mentioned earlier), as shown in Table 18.1.

TABLE 18.1 Kinetic Parameters for Decomposition, Initiation, Propagation, and Termination Steps for Production of Polyvinyl Acetate (PVAC).

Type	Comp1	Comp2	Pre-Exp (1/s)
INIT-DEC	AIBAN		1.1e−4
CHAIN-INI	VNLACET		2,306.7
PROPAGATION	VNLACET	VNLACET	142,560
TERM-COMB	VNLACET	VNLACET	9.9e+8

The gel effect can be accounted for via using gel effect parameters with correlation number 2 specified in "**Gel Effect**" tab form. Alternatively, the gel effect parameters, shown in Chapter 12, can be reused.

At the top, do not forget to carry out the outlined steps shown in Chapter 12: Improving Convergence to facilitate the solver convergence. Work on selecting the proper flow and operating conditions for feed stream as well as those for each block. Associate a utility with a block whenever necessary.

Report the polymer properties found in the bottom stream of the absorption tower. Assign a unit price for inlet and outlet streams. Carry out profitability analysis for the proposed plant.

In the last part of this problem, save your simulation file under a separate name and define the chain transfer agent: 2-ethoxythiocarbonylsulfanyl-propionic acid methyl ester (EPAME) as part of components by utilizing the molecular structure of EPAME as shown in Figure 18.17. This can be defined using the built-in molecular editor which can be found

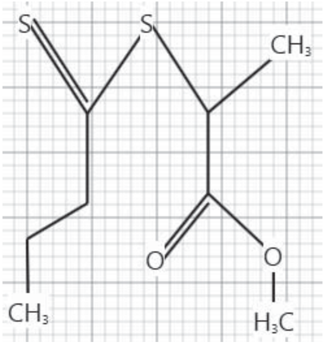


Figure 18.17 The molecular structure of EPAME as it should appear in molecular editor.

under "**Molecular Structure**" | "**EPAME**" | "**Structure**" tab while being in "**Properties**" environment.

Modify the free radical reaction to include EPAME as transfer agent while other species remain the same as in the first part. For the following free radical substep:

CHAT-AGENT with VNLACET and EPAME as Comp1 and Comp2, respectively.

Assign a value of 1927.2 1/s as pre-exponent kinetic parameter.

Adjust the feed to include EPAME in addition to other species as well.

See how the inclusion of a chain transfer agent, such as EPAME, affects the polymer characteristics of PVAC.

18.13 TP #13: POLYMERIZATION: EMULSION COPOLYMERIZATION OF STYRENE AND BUTADIENE TO PRODUCE SBR

Emulsion copolymerization of styrene-butadiene to produce rubber is one of the most widely used polymers in the world today. The process has some advantages. It can be used under mild reaction conditions that are tolerant to water and requires only the absence of oxygen. The process is relatively less sensitive to impurities and flexible enough to using a range of functionalized and non-functionalized monomers. Moreover, emulsion copolymerization gives high solids contents with low reaction viscosity and is thus a cost-effective process. The physical state of the emulsion (colloidal) system makes it easy to control the process. Thermal and viscosity problems are much less severe than those of bulk polymerization.

It is worth mentioning here that Aspen Plus provides built-in examples (see, "**C:\Program Files (x86)\AspenTech\Aspen Plus V8.8\GUI\Examples\Polymers**") regarding the modeling aspects of some common polymerization processes. The kinetic and component data will be borrowed from the built-in example for a batch process of emulsion copolymerization of styrene and butadiene. However, the flowsheet will be modified for a flow not a batch process.

Select the proper "**Polymers**" subtemplate. Add the following components: water (H_2O) as dispersant, styrene (STY) as one monomer, 1,3-butadiene (BD) as another monomer, generic-polymer-component (POLYMER) as polymer, styrene-R (STY-SEG) as one segment, butadiene-R-1 (BD-SEG) as another segment, *tert*-dodecyl-mercaptan (TDM) as chain transfer agent, ammonium-per-sulfate, $(NH_4)_2S_2O_8$, (APS) as initiator, and finally sorbitan-monooleate (SORBITAN) as emulsifier. Remember that the type of emulsifier does not interfere with the polymerization substeps. In fact, I have run this emulsion copolymerization process using different emulsifiers. Instead of sorbitan-monooleate, I used sorbitan-laurate as an emulsifier. The critical micelle concentration (CMC) for such emulsifiers is about 0.002 wt% in water. The surface coverage for such emulsifiers can be assumed to be 5×10^6 m^2/kmol.

Both emulsifiers work fine. It is worth mentioning here that in such a hybrid medium, our goal is to emulsify oil-based materials, such as styrene and butadiene in an aqueous medium (i.e., water), thus we need a non-ionic surfactant, such as sorbitan monooleate or laurate, to do the emulsification of oil in water. In addition to POLYNRTL, POLYSRK property method was also successfully tested.

Do not forget to characterize polymer and its repeating unit under “**Polymers**” | “**Characterization**” tab sheets. Also, let Aspen Plus perform GPC distribution calculation. Refer to “**Polymer**” | “**Distributions**” sheet.

After successfully carrying out properties analysis step, switch to “**Simulation**” environment and add the following flowsheet blocks as well as the associated input and output streams, as shown in Figure 18.18.

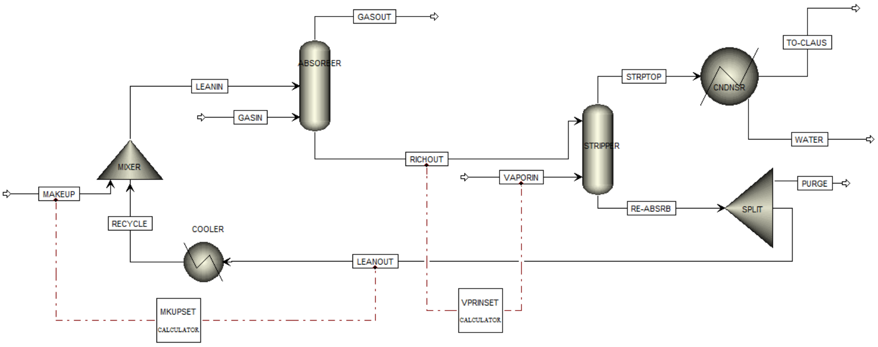
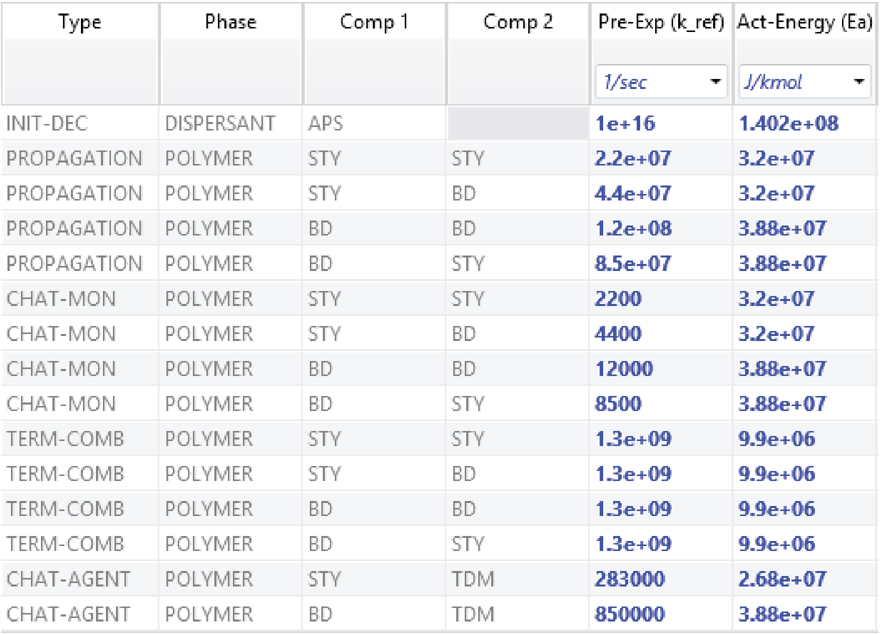


Figure 18.18 The process flowsheet for emulsion copolymerization of styrene butadiene to produce SBR.

In addition, you need to specify a free radical (“**EMULSION**”) type of reaction and associate it with PFR. Use POLYMER as polymer; H_2O as dispersant; both STY and BD as monomers; STY-SEG and BD-SEG as repeating units; APS as initiator; and TDM as transfer agent. Use the following pre-exponential constants as borrowed from the built-in example, as shown in Figure 18.19. Watch out for the order of emulsion copolymerization



Type	Phase	Comp 1	Comp 2	Pre-Exp (k_ref)	Act-Energy (Ea)
				1/sec	J/kmol
INIT-DEC	DISPERSANT	APS		1e+16	1.402e+08
PROPAGATION	POLYMER	STY	STY	2.2e+07	3.2e+07
PROPAGATION	POLYMER	STY	BD	4.4e+07	3.2e+07
PROPAGATION	POLYMER	BD	BD	1.2e+08	3.88e+07
PROPAGATION	POLYMER	BD	STY	8.5e+07	3.88e+07
CHAT-MON	POLYMER	STY	STY	2200	3.2e+07
CHAT-MON	POLYMER	STY	BD	4400	3.2e+07
CHAT-MON	POLYMER	BD	BD	12000	3.88e+07
CHAT-MON	POLYMER	BD	STY	8500	3.88e+07
TERM-COMB	POLYMER	STY	STY	1.3e+09	9.9e+06
TERM-COMB	POLYMER	STY	BD	1.3e+09	9.9e+06
TERM-COMB	POLYMER	BD	BD	1.3e+09	9.9e+06
TERM-COMB	POLYMER	BD	STY	1.3e+09	9.9e+06
CHAT-AGENT	POLYMER	STY	TDM	283000	2.68e+07
CHAT-AGENT	POLYMER	BD	TDM	850000	3.88e+07

Figure 18.19 The kinetic parameters associated with emulsion copolymerization substeps.

substeps as generated by Aspen Plus. If the sequence of such substeps is not the same as that shown here, then under “**Reactions**” tab, for the created reaction set, you may highlight one substep, right-click, and then select “**Reorder**” submenu item to put the substeps in the same fashion as shown here.

Moreover, under “**PFR**” | “**Convergence**” | “**Integration Loop**” tab, choose the “**Error scaling method**” to be “*Hybrid*”.

Your task is to select the proper feed and operating conditions of each block. Assign unit price for inlet and outlet streams, associate a utility with a block whenever necessary. Report the polymer properties. Carry out an economic analysis. Repeat the flowsheet using the second emulsifier, that is, sorbitan laurate. Test both property methods mentioned earlier.

18.14 TP #14: POLYMERIZATION: FREE RADICAL POLYMERIZATION OF METHYL METHACRYLATE TO PRODUCE POLY(METHYL METHACRYLATE)

Poly(methyl methacrylate) (PMMA) is a transparent thermoplastic, used in sheet form as a lightweight or shatterproof alternative to soda-lime glass. It is also used as a casting resin, in inks and coatings, and in lubricating oils and hydraulic fluids to avoid formation of a highly viscous fluid at severely very cold weather.

It is worth mentioning here that Aspen Plus provides built-in examples (see, “**C:\Program Files (x86)\AspenTech\Aspen Plus V8.8\GUI\Examples\Polymers**”) regarding the modeling aspects of some common polymerization processes. The kinetic and component data will be borrowed from the built-in example for a batch process of free radical polymerization of methyl methacrylate. However, the flowsheet will be modified for a flow not a batch process.

Select the proper “**Polymers**” sub-template. Add the following components: water (H_2O) to be used later as cooling/heating medium, methyl methacrylate (MMA) as monomer, ethyl-acetate (EA) as solvent, poly(methyl methacrylate) (PMMA) as polymer, methyl methacrylate-R (MMA-R) as segment, and finally AIBN, $C_8H_{12}N_4$ (AIBN) as initiator.

Do not forget to characterize polymer and its repeating unit under “**Polymers**” | “**Characterization**” tab sheets. Also, let Aspen Plus perform GPC distribution calculation. Refer to “**Polymer**” | “**Distributions**” sheet.

Allow calculation of pairwise interaction parameters.

After successfully carrying out properties analysis step, switch to “**Simulation**” environment and add the following flowsheet blocks as well as the associated input and output streams. See Figure 18.20.

In addition, you need to specify a free radical (“**FREE-RAD**”) type of reaction and associate it with CSTR. Use PMMA as polymer; MMA as monomer; MMA-R as repeating unit; AIBAN as initiator; and EA as solvent. Use the following pre-exponential constants

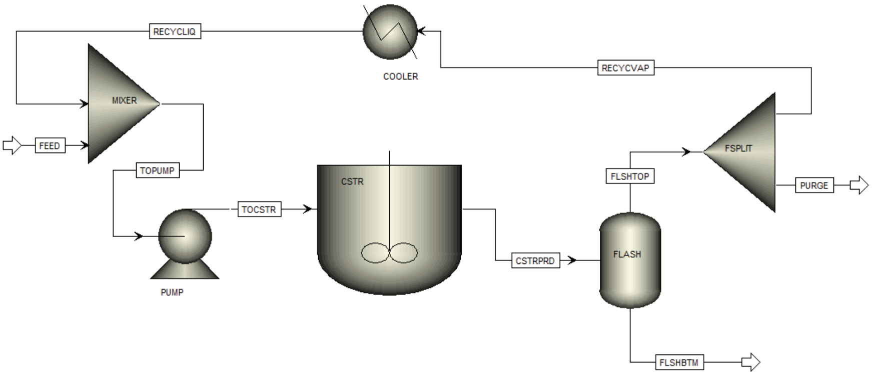


Figure 18.20 A flowsheet for production of poly(methyl methacrylate) with a recycle of solvent and unreacted methyl methacrylate monomer.

and activation energy values as borrowed from the built-in example, as shown in Table 18.2. Watch out for the order of free radical polymerization substeps as generated by Aspen Plus. If the sequence of such substeps is not the same as that shown here, then under "**Reactions**" tab, for the created reaction set, you may highlight one substep, right-click, and then select "**Reorder**" submenu item to put the substeps in the same fashion as shown here. Use an efficiency value of *0.5* for the "**CHAIN-INI**" substep with the default number of radians to be *2*.

TABLE 18.2 Kinetic Parameters for Decomposition, Initiation, Propagation, and Termination Steps for Production of Poly(Methyl Methacrylate).

Type	Comp1	Comp2	Pre-Exp (1/h)	Act-Energy (cal/mol)
INIT-DEC	AIBAN		4.509e+17	29,330.3
CHAIN-INI	MMA		1.7712e+9	4,356.55
PROPAGATION	MMA	MMA	1.7712e+9	4,356.55
CHAT-MON	MMA	MMA	2.58372e+13	17,944.5
CHAT-SOL	MMA	EA	1.68228e+12	15,692.2
TERM-DIS	MMA	MMA	3.528e+11	701.49

At the top, do not forget to carry out the outlined steps shown in Chapter 12: Improving Convergence to facilitate the solver convergence.

Work on selecting the proper flow and operating conditions for feed stream as well as those for each block. Associate a utility with a block whenever necessary. Report the polymer properties of the product stream. Assign a unit price for inlet and outlet streams. Carry out profitability analysis for the proposed plant.

18.15 TP #15: LHHW KINETICS: PRODUCTION OF CYCLOHEXANONE-OXIME (CYCHXOXM) VIA CYCLOHEXANONE AMMOXIMATION USING CLAY-BASED TITANIUM SILICALITE (TS) CATALYST

The liquid-phase ammoximation of ketone over titanium zeolites is utilized to synthesize oxime, a key intermediate in the manufacture of caprolactam. Unlike other commercial processes, liquid-phase ammoximation of cyclohexanone over titanium-containing zeolites can be carried out in one step, without use of hazardous chemicals, and no generation of by-products.

Select the proper "**Chemicals**" sub-template. Add the following components: water (H_2O) both as reaction medium and by-product, ammonia (NH_3) as the first reacting species, hydrogen-peroxide (H_2O_2) as the second reaction species, cyclohexanone (CYCHEX) as the third reacting species, cyclohexanone-oxime (CYCHXOXM) as the main product, and finally *tert*-butyl-alcohol (BUTANOL) as a cosolvent.

Allow calculation of pairwise interaction parameters. After successfully carrying out properties analysis step, switch to "**Simulation**" environment and add the following flowsheet blocks as well as the associated input and output streams. See Figure 18.21. The purge stream can be as low as 0.1 fraction of the entering feed stream to "**SPLIT**" block which is found under "**Mixers/Splitter**" tab in "**Model Palette**".

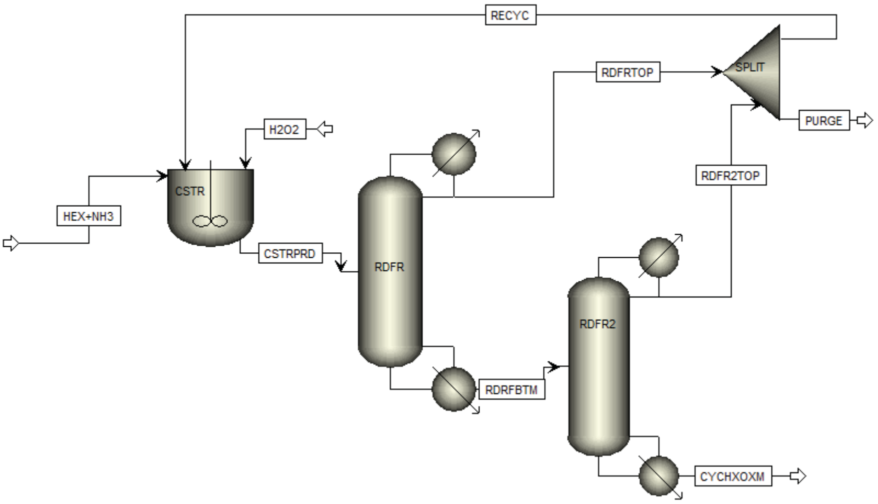


Figure 18.21 A Flowsheet for production of cyclohexanone-oxime (CYCHXOXM) via cyclohexanone ammoximation using the clay-based titanium silicalite (TS) catalyst.

In addition, you need to specify LHHW ("**LHHW**") type of reaction and associate it with CSTR. The following reaction occurs as TS-catalyzed liquid-phase reaction at 353 K.

$$\text{CYCHEX} + \text{NH}_3 + \text{H}_2\text{O}_2 \rightarrow \text{CYCHXOXM} + 2\text{H}_2\text{O}$$

$$\text{Reaction rate} = \text{A}e^{\left(-\frac{E}{RT}\right)} \frac{[\text{NH}_3][\text{H}_2\text{O}_2]}{K_\text{S} + [\text{H}_2\text{O}_2]}$$

where

Reaction rate: $\frac{\text{kmol}}{\text{kg cat}\cdot\text{s}}$
A: $1.8333 \times 10^{10}\ \frac{\text{m}^3}{\text{kg cat}\cdot\text{s}}$
E: 93.2 kJ/mol
K_S: 0.05 kmol/m^3 at $T = 353$ K

The above-listed kinetic data were taken from (Dong, C., Wang, K., Zhang, J.S., and Luo, G.S. (2015) Reaction kinetics of cyclohexanone ammoximation over TS-1 catalyst in a microreactor. *Chemical Engineering Science*, **126**, 633–640) and were converted into the proper basis, in line with Aspen Plus standard basis for reaction kinetics. Refer to Chapter 7 of this textbook on how to properly enter both driving force and adsorption term for LHHW type reaction. Moreover, the catalyst loading is 10 kg per 10 m^3 reactor volume and the solid particle density is 3093 kg/m^3.

Work on selecting the proper flow and operating conditions for feed streams and those for each block. Associate a utility with a block whenever necessary. Assign a unit price for inlet and outlet streams. Carry out profitability analysis for the proposed plant.

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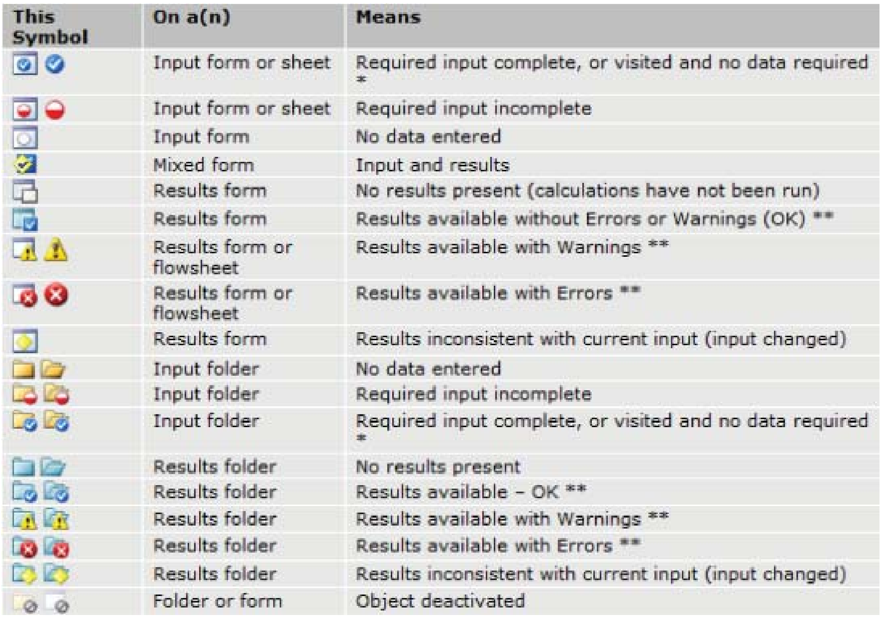

This Symbol	On a(n)	Means
✓ ✓	Input form or sheet	Required input complete, or visited and no data required *
⊖ ⊖	Input form or sheet	Required input incomplete
○	Input form	No data entered
✓	Mixed form	Input and results
☐	Results form	No results present (calculations have not been run)
✓	Results form	Results available without Errors or Warnings (OK) **
⚠ ⚠	Results form or flowsheet	Results available with Warnings **
✗ ✗	Results form or flowsheet	Results available with Errors **
◆	Results form	Results inconsistent with current input (input changed)
📁 📂	Input folder	No data entered
📁⊖ 📂⊖	Input folder	Required input incomplete
📁✓ 📂✓	Input folder	Required input complete, or visited and no data required *
📁 📂	Results folder	No results present
📁✓ 📂✓	Results folder	Results available – OK **
📁⚠ 📂⚠	Results folder	Results available with Warnings **
📁✗ 📂✗	Results folder	Results available with Errors **
📁◆ 📂◆	Results folder	Results inconsistent with current input (input changed)
⊘ ⊘	Folder or form	Object deactivated

Figure 1.15 Different color-coded symbols used by Aspen Plus to help the user better understand the status of the solver.

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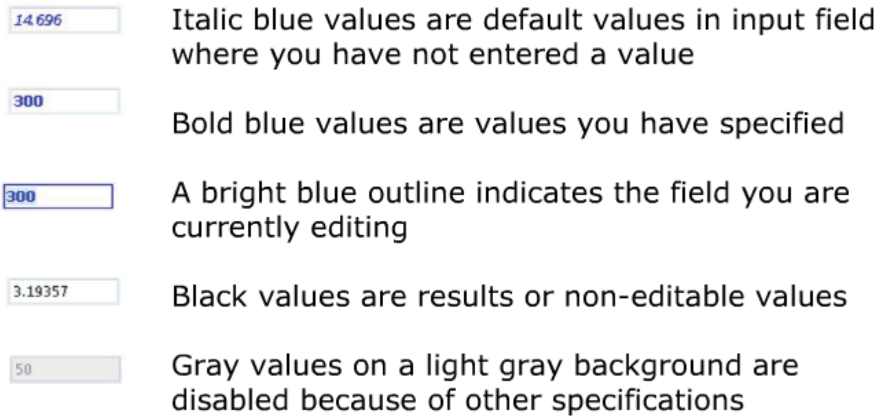


Italic blue values are default values in input field where you have not entered a value

Bold blue values are values you have specified

A bright blue outline indicates the field you are currently editing

Black values are results or non-editable values

Gray values on a light gray background are disabled because of other specifications

Figure 1.16 The field color coding adopted by Aspen Plus for the text of an input form, which is either editable or noneditable by the user.

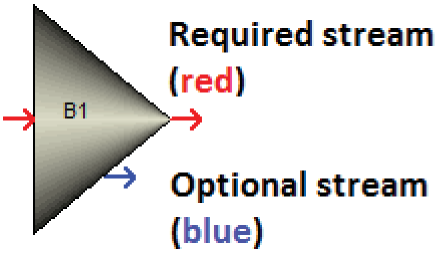


Figure 2.6 Upon selecting the stream type and moving the mouse to the workspace of the process flowsheet, the required and optional stream will show up in the red and blue color, respectively.

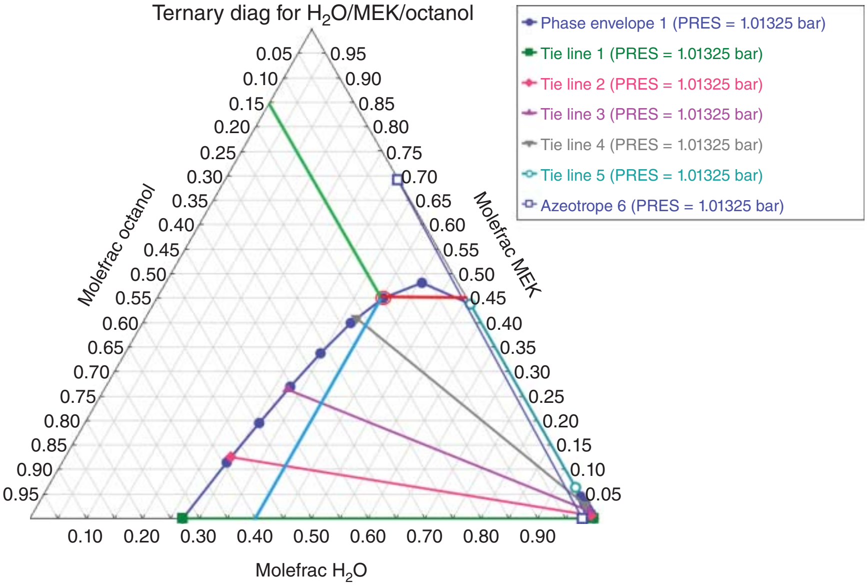
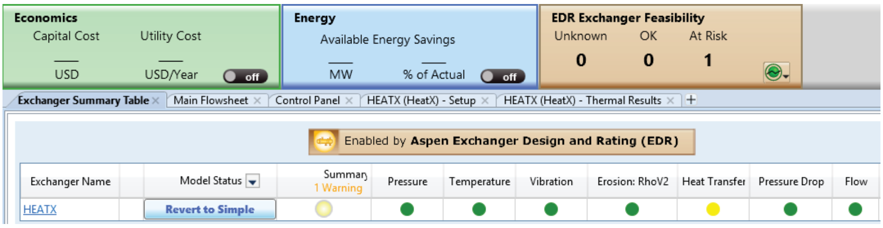


Figure 5.25 The triangle diagram showing the location of the operable region for extraction processes. The blue standalone square on the right side represents an azeotropic condition for the binary mixture of MEK and water.

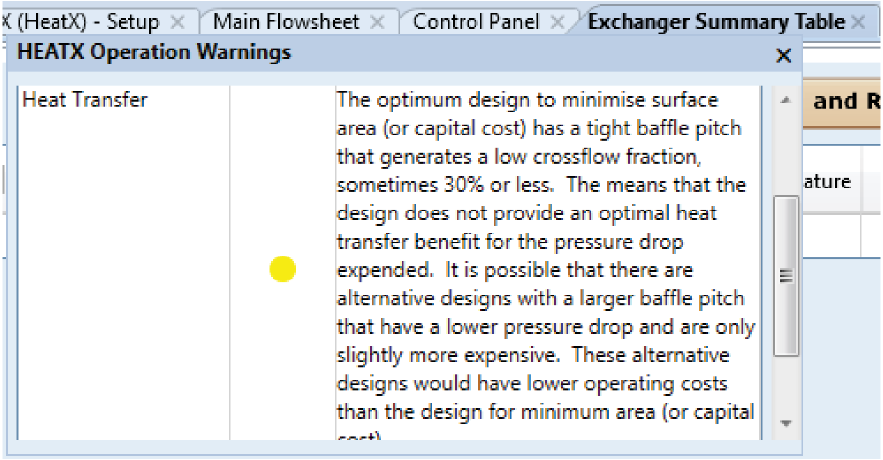


EDR Exchanger Feasibility

Unknown	OK	At Risk
0	0	1

Exchanger Name	Model Status	Summary 1 Warning	Pressure	Temperature	Vibration	Erosion: RhoV2	Heat Transfer	Pressure Drop	Flow
HEATX	Revert to Simple	○	●	●	●	●	●	●	●

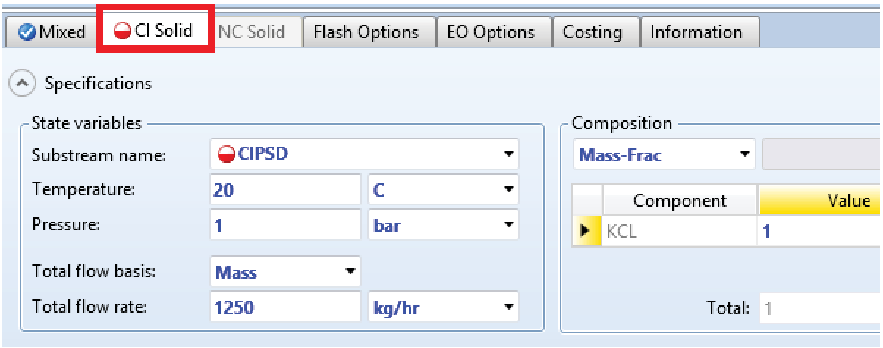
Figure 10.29 The technical judgment by Aspen Plus EDR exchanger on the entered geometrical specifications. All issues are labeled as green except one issue (yellow) with warning.



HEATX Operation Warnings

Heat Transfer ● The optimum design to minimise surface area (or capital cost) has a tight baffle pitch that generates a low crossflow fraction, sometimes 30% or less. The means that the design does not provide an optimal heat transfer benefit for the pressure drop expended. It is possible that there are alternative designs with a larger baffle pitch that have a lower pressure drop and are only slightly more expensive. These alternative designs would have lower operating costs than the design for minimum area (or capital

Figure 10.30 Aspen Plus EDR suggests other alternatives, geometrical configurations that may result in further lowering of pressure drop and are potentially slightly more expensive.



State variables

Substream name: CIPSD

Temperature: 20 C

Pressure: 1 bar

Total flow basis: Mass

Total flow rate: 1250 kg/hr

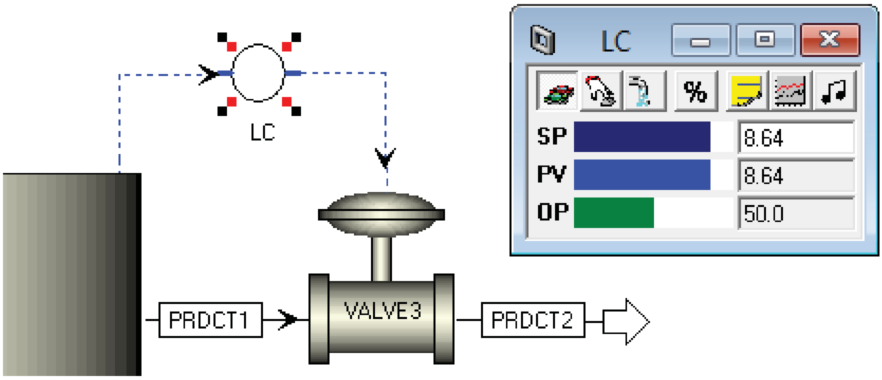
Composition

Mass-Frac

Component	Value
KCL	1

Total: 1

Figure 14.3 Entering *P*, *T*, flow rate, and composition of the feed stream, which is treated as **C**onventional **I**nert solid with **P**article **S**ize **D**istribution ("**CIPSD**").



SP 8.64

PV 8.64

OP 50.0

Figure 15.32 The controller faceplate where the set point (“**SP**”), process variable (“**PV**”), and controller output (“**OP**”) signals are displayed at the bottom left part as three horizontal bars, with numerical values given in the boxes.

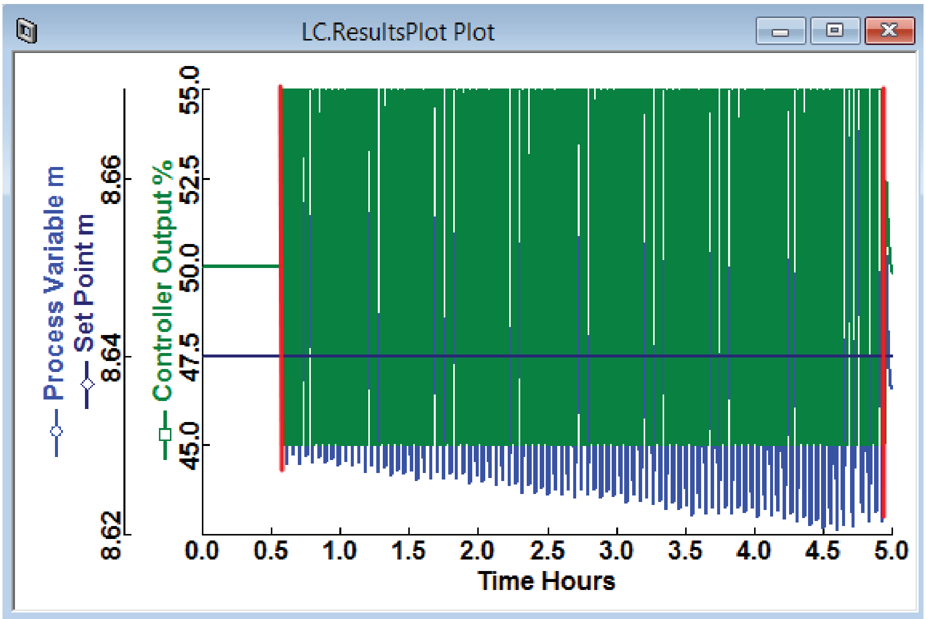
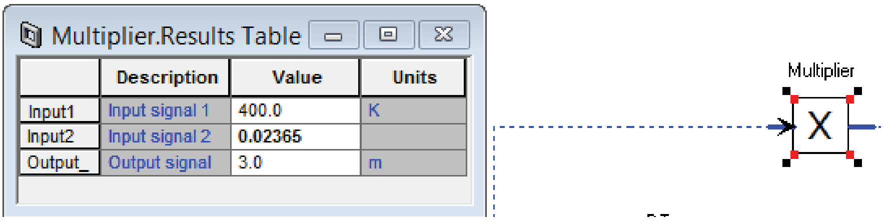


Figure 15.46 The closed-loop ATV test for tuning-up "**LC**" controller, where the test period lies between the two red lines.



	Description	Value	Units
Input1	Input signal 1	400.0	K
Input2	Input signal 2	0.02365	
Output_	Output signal	3.0	m

Figure 15.97 The "**Multiplier.Results Table**" form where the signal from "**TC**" loop is multiplied by an adjustable parameter, that is, "**Input2**", and the "**Output_**" signal will be calculated and transmitted to "**LC**" loop as a set point.

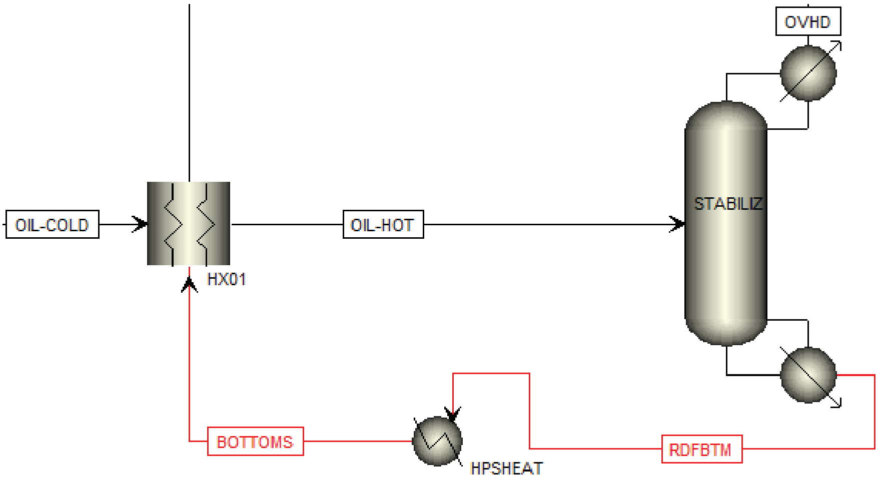
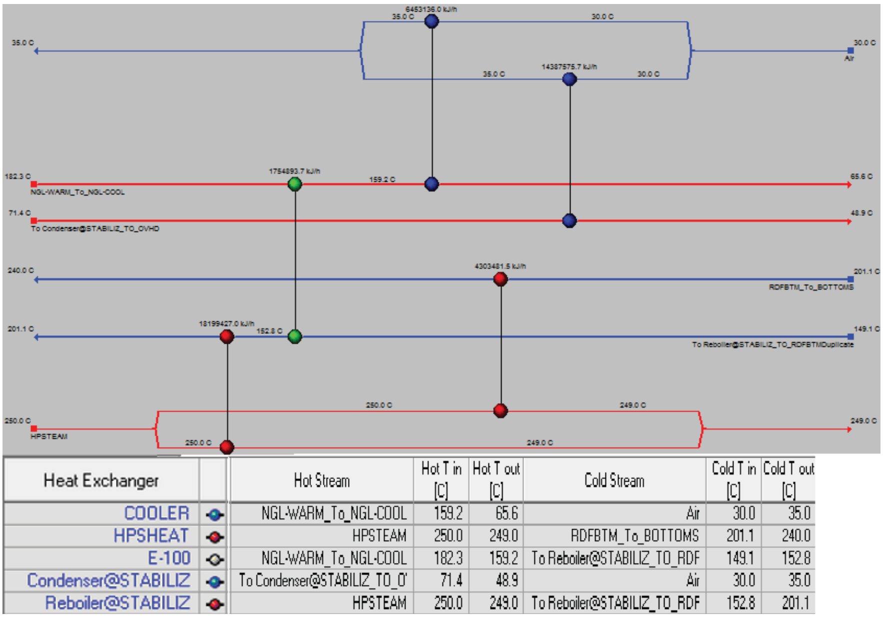


Figure 16.24 The insertion of the high-pressure steam heater to heat up the bottom stream of the stabilizer.



Heat Exchanger		Hot Stream	Hot T in [C]	Hot T out [C]	Cold Stream	Cold T in [C]	Cold T out [C]
COOLER	●	NGL-WARM_To_NGL-COOL	159.2	65.6	Air	30.0	35.0
HPSHEAT	●	HPSTEAM	250.0	249.0	RDFBTM_To_BOTTOMS	201.1	240.0
E-100	○	NGL-WARM_To_NGL-COOL	182.3	159.2	To Reboiler@STABILIZ_TO_RDF	149.1	152.8
Condenser@STABILIZ	●	To Condenser@STABILIZ_TO_O'	71.4	48.9	Air	30.0	35.0
Reboiler@STABILIZ	●	HPSTEAM	250.0	249.0	To Reboiler@STABILIZ_TO_RDF	152.8	201.1

Figure 16.38 Aspen Energy Analyzer demonstrates the heat exchanger network with the recommended energy-saving retrofit layout.

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