RUHR-UNIVERSITÄT BOCHUM

Fakultät Maschinenbau
fortschritt studieren

RUB

Computer-Aided Process Design
Beispiele aus der simulationsgestützten Prozessentwicklung

Organization 2.0

SoSe 2024

Contact Persons

- **Dr.-Ing. Maria Polyakova**
  - E-Mail: polyakova@fluidvt.rub.de
  - Fon: 0234 32 26 470
  - Office: IC 3/121

- **Thorben Hochhaus, M.Sc.**
  - E-Mail: hochhaus@fluidvt.rub.de
  - Fon: 0234 32 26 470
  - Office: IC 3/099
- **Johannes Wloch, M.Sc.**
  - E-Mail: wloch@fluidvt.rub.de
  - Fon: 0234 32 26 470
  - Office: IC 3/099

Agenda

- **Organization of block course**
- **Presentation of example**
- **Clarification of expectations and evaluation criteria**
- **Organization of exam and exam preparation**
- **Group assignment and internal clarification of working modes**
- **Open questions and discussion**

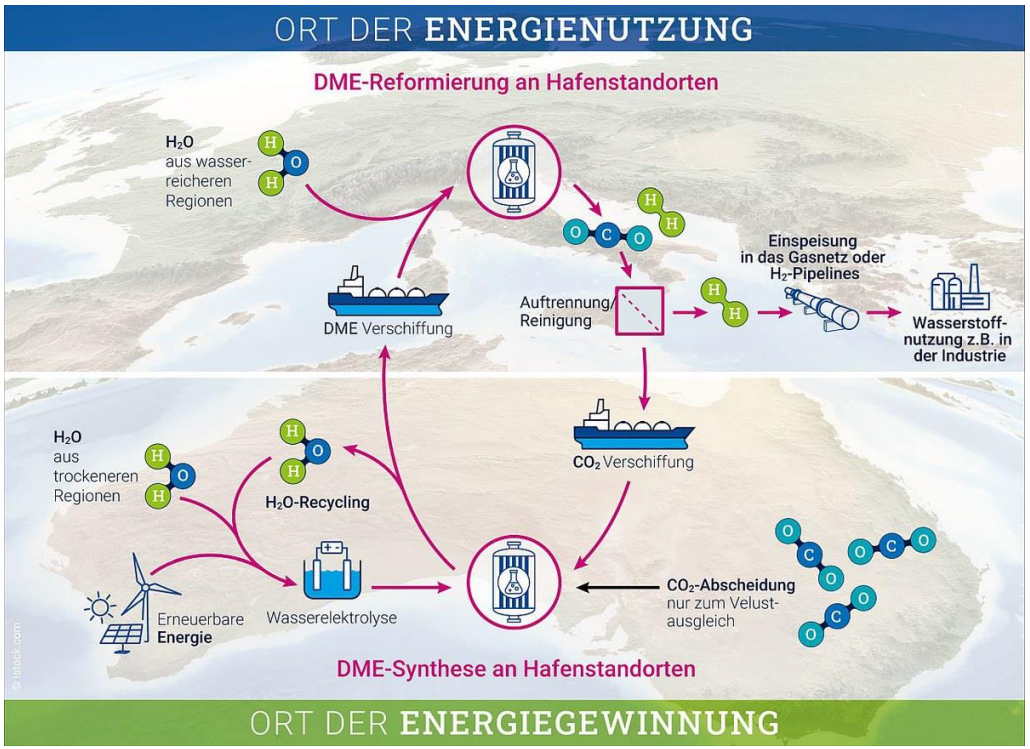
Organization of block course

- **General conditions for classroom event**
  - Course takes place in CIP Pool 3 (IC 03/452).
  - Please check that each of you can login on to the computer. Take care about it, **before** Monday, July, 22th Same for FlexNow!
  - We will share the supervision in the 10 days!

    → there is always someone there to help and answer questions (maybe one day exception in the second week)

- **Short reminder on course hours:**
  - morning 8:00 – 11:30
  - afternoon 13:00 – 17:00

This year‘s example: *DME (Dimethyl ether)*



DME includes:

- In liquid form as a solvent
- Propellant in deodorants
- Hydrogen storage

DME production: 250.000 t per year
Operating hours: 8.500 h per year

This year‘s example: *Power-to-Methanol*

Possible research questions:

- **Efficiencies (Plant, Chemical, Carbon,…)**
- **Where does the carbon come from? What does it cost?**
- **Cost calculations**
- **Where do the educts come from?**
- **GWP / Climate impact?**
- **System-wide heat integration**
- **What to use the DME for?**
- **What to use by-products / side-products for?**

Time table (for orientation only!)

Tag	Datum	Inhalt
	15.07.2024	Announcement of the process example, clarification of expectations, division into groups and start of literature research
1	22.07.2024	**Short presentations of the groups on literature research (~ 15 min per group)** Aspen Plus® 101 → Clarification of need
2	23.07.2023	Definition of the boundary conditions for modelling the process example. Simulation studies for the reaction
3	24.07.2023	Reaction simulation studies: Reaction kinetics Determining the reaction conditions
4	25.07.2023	Development and design of the necessary separation sequence Sequential implementation of the separation sequence
5	26.07.2023	Sequential implementation of the separation sequence Rigorous modelling of the separation sequence
6	29.07.2023	Detailed analysis and optimization of the separation sequence
7	30.07.2023	Recirculation and closing of material cycles Optimisation calculations for the overall process
8	31.07.2023	Analysis of overall flowsheet / process, heat integration, system optimization

Expectations for processing the assignment (impulse!)

- **Literature review DME production (until July, 22th)**
  - General information, …
    - Advantages, disadvantages, application scenarios, relelvant boundary conditions,…
  - Input materials and their properties, prices and availability
  - Reaction products and their properties, use, prices and quantities produced
  - Common reactant qualitiesReaction pathways / reaction networks
  - Process alternatives
  - Reactor systems / catalysts / operating conditions
  - Material data of the reaction mixture and estimation of the separation effort
- **Overall goal:** Do not only search for values and pictures, do also evaluate critically and look for reasonable sources for the validation of your simulation!
- **First estimation of mass and energy balances based on simple KPIs!**

Expectations for processing the assignment (impulse!)

- **Investigation of reaction system:**
- **Equilibrium analysis taking into account the influence on conversion/yield/selectivity:**
  - Reactant composition
  - Temperature
  - Pressure
- **Selection of a suitable reactor-catalyst system and kinetics to describe the reaction**
- **Investigation of the kinetic reactor, taking into account the influence on conversion/yield/selectivity through**
  - Composition
  - Temperature
  - Pressure
  - Geometry parameters →Residence time
  - Conversion / selectivity diagrams

Expectations for processing the assignment (impulse!)

- **Development of the separation sequence**:
  - Detailed definition of the separation task and research of the required substance data / substance properties
  - Develop a suitable separation sequence using the known heuristic rules
    - Customise the separation sequence
    - Plan recirculation
    - Determine operating parameters
    - Consider the possibilities of heat integration
  - Rough calculation of initial values using simple balances (rectification, absorption)
  - Successive implementation of the separation sequence in Aspen Plus
  - Detailed design of the rectification columns using the following tools: Design Specs, sensitivity analyses, optimization

- **Goal: Optimised separation with low operating and investment cost**

Expectations for processing the assignment (impulse!)

- **Heat integration:**
- Estimation of the integration potential using the pinch point method
  - If necessary with Aspen Energy Analyser
- Calculation of possible interconnection of heat exchanger networks
  - If necessary with Aspen Energy Analyser
- Heat Pumps appliacation …

Evaluation criteria for the presenation and the exam / discussion

- **Expertise / content elaboration**
- **Critical reflection of the results achieved for each process step / sub-process**
- **Transparent presentation of assumptions and other relevant parameters**
- **Transparent presentation of data used for model validation**
- **Clear design of slides and illustrations / figures**
- **Clear visualization of the results**
- **Cooperation during the course**
- **Presentation style and confidence**

Short presentations on literature review:
Feedback on the preparation and the presentation of results

Organization of exam

- **Examination procedure:**
  - Exam is performed as a group exam (with individual evaluations!)
  - **Procedure:** 30 minutes presentation per group
    5 minutes break
    ~45 minutes oral exam per group
    (= Discussion of the process example and the results based on your slides.)
  - **Dates:** Exams are possible in these periods: 12.08-16.08 and 02.09-10.09; 20.09
    As a group, please name a preferred date on Monday, July 22st

Example for a structure of the presentation:

- Assignment – Litertaure Review – Reaction – Separation – Analysis – Process Integration – System Evaluation

Organization on exam preparation & helpful hints

- **Take the opportunity to get feedback in the short presentations!**
- **Use the time we are available for questions as intensively as possible!**
- **Use the opportunity to prepare for future tasks and situations in industry!**
- **Do not postpone questions or ambiguities!**
- **Consultation hours for last questions and discussions for exam preparation:**
  - by arragement

Group division and organization

- **If needed: short introduction**

- **How will you organize your work?**
  - Sharing and securing data
  - Meeting before and after the block seminar
  - …

- **Do you need anything else from us?**
  - …

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Open questions?