RUHR-UNIVERSITÄT BOCHUM

Fakultät Maschinenbau
fortschritt studieren

RUB

Process Engineering

Supplement to Chapter 3: Modeling of Seperation Columns

Lecture for Master-Students

Columns

Shortcut-Model

- DSTWU
- Distl
- SCFrac

Rigorous Models

- RadFrac
- MultiFrac
- PetroFrac

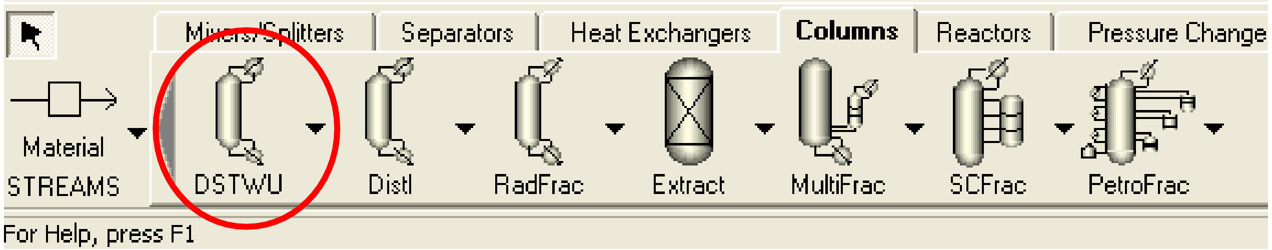
For Help, press F1

Columns

Shortcut-Model

DSTWU

- Model according to Winn, Underwood and Gilliland
- Seperation Columns with one feed and two product streams
- Determination of rr_{min} and n_{min}, as well as the current rr for a given n and vice versa
- Analogous to the McCabe-Thiele method
  - Design of the Apparatus by balancing the head (top section)
  - Residence Time in the apparatus is so long that all components are ideally mixed (equilibrium model)



Columns

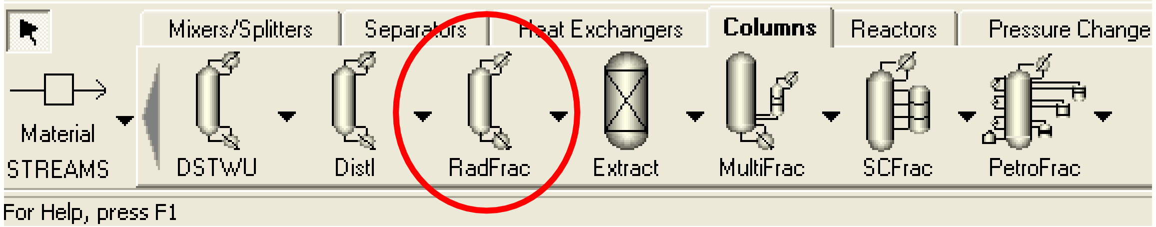
Rigorous Model

RadFrac

- Rigorous sizing and design for seperation columns
- For odinary, extractive, reactive, or azeotropic reactification, absorbers and strippers
- Balancing of <u>every stage</u> of the column
- Ideal mixing of components on every stage (equilibrium model)

RateBased

- Extension to RadFrac
- Consideration of all heat and mass transfer phenomena for balancing a stage (e.g. reaction kinetics, heat of reaction, mass transfer limitations)



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Columns

SCFrac

- Shortcut distillation model for complex petrochemical separation operations
- Determines product composition and flow rate, number of stages, and heat duty using separation factors
- e.g. crude oil fractionators or vacuum distillation for gasoline production

MultiFrac

- Rigorous design for a configuration of seperation columns of any complexity
- Heat-Integrated column, absorbers/stripper configuration, oil refinery

PetroFrac

- Oil fractionator

Classification of available methods

- **Graphical methods:**
  - McCabe-Thiele method
  - Ponchon-Merkel-Diagrams
- **Short Cut Models (DSTWU Models)**
  - Fenske /Winn
  - Underwood
  - Gilliland
- **Rigorous Models (RadFrac Models)**
  - Equilibrium Stage Model
  - Rate-Based Models

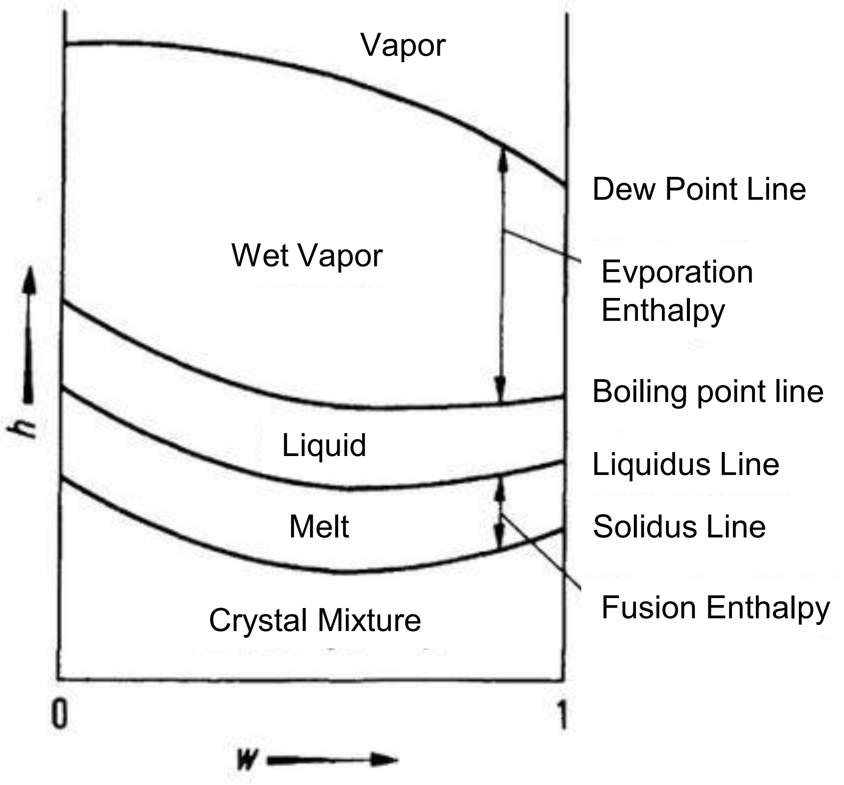
McCabe-Thiele method

- **Assumptions:**
  - Valid exclusively for binary mixtures
  - Constant molar overflow (constant volume flows) in the rectifying and stripping sections of the column
  - Within the considered temperature and pressure range, the enthalpies of vaporization have constant values
  - Enthalpies of mixing and heat losses are neglected

  → Energy for condensing 1 mole of vapor = Energy for evaporating 1 mole of liquid
- **Calculation of the operatingline for the rectifying section from a balance around the column head**
- **Important limiting cases:**
  - Reflux Ratio → ∞ → Operating line lies on the 45°-Line
  - Number of stages → ∞ → Operating line intersects the y-axis as a function of the minimum reflux ratio $(1/v_{min}+1)$

Ponchon-Merkel-Diagram

- **Prerequisite: Known pure-component and mixture enthalpies across the entire concentration range**



Short-Cut Models

- **Assumptions:**
  - Multi-component systems are reduced to a binary separation problem
  - Assumption of constant separation factors on every stage
  - Assumption of constant volume flows in the rectifying and stripping sections

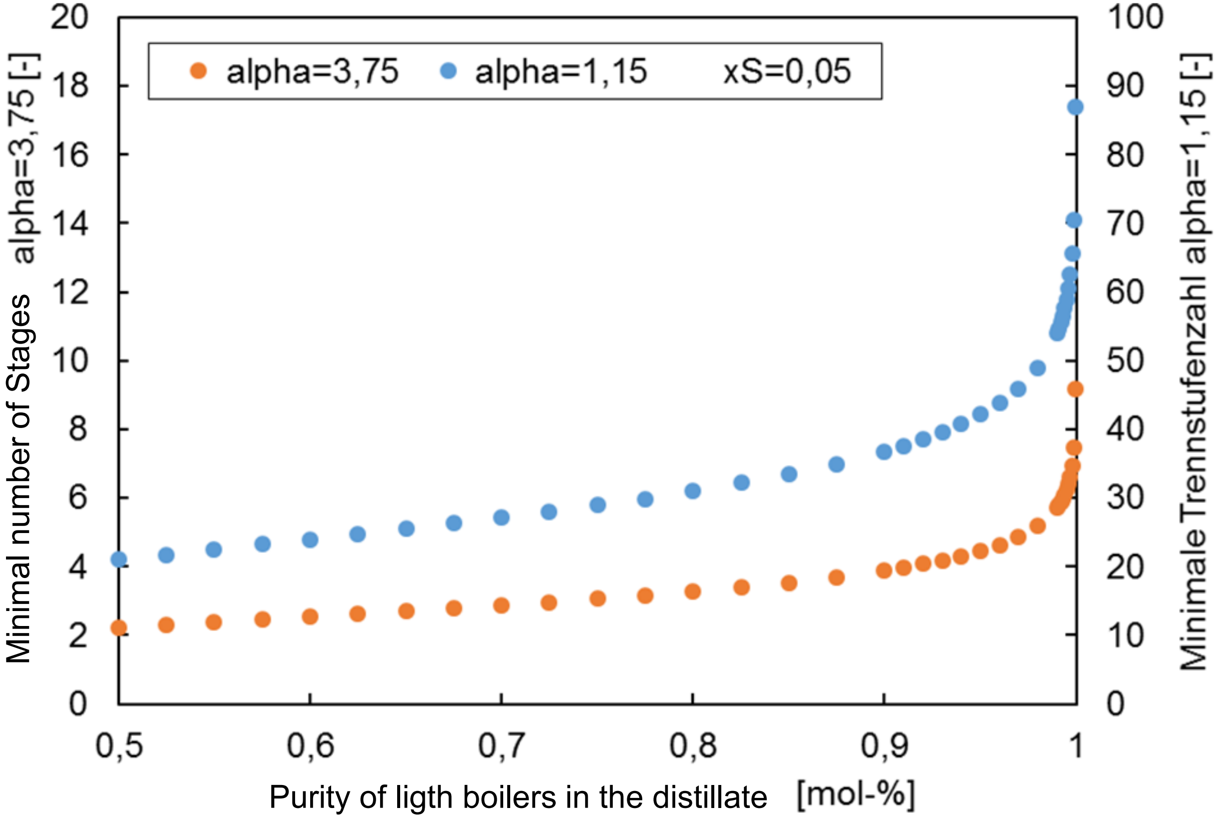
- **Enables the determination of:**
  - N_{min}, N, v_{min}, v, $\dot{V}_L$, $\dot{V}_D$, $\dot{Q}_{cond}$, $\dot{Q}_{reb}$

- ***Minimum number of separation stages according to Fenske or Winn***
- ***Minimum reflux ratio according to Underwood***
- ***Number of stages and reflux ratio according to Gilliland***

Minimum number of separation stages according to Fenske or Winn

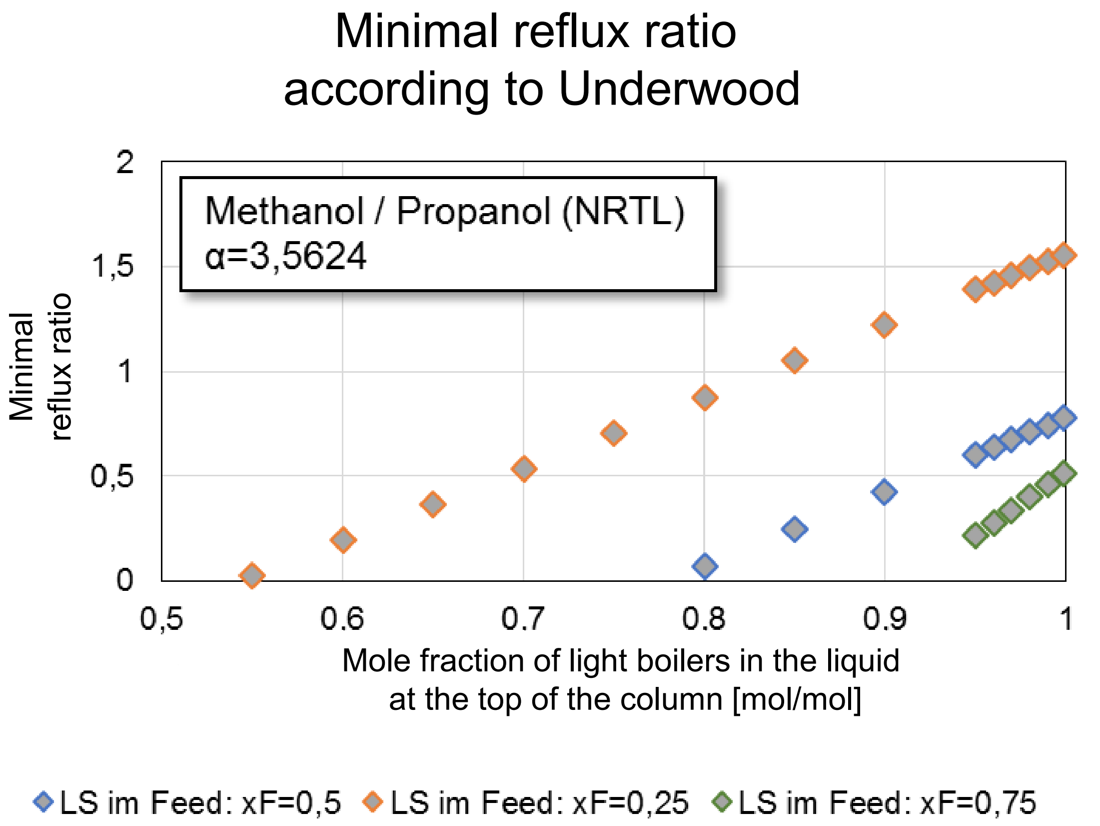
- **For the minimum number of stages, the reflux ratio goes → ∞**

$$N_{t,min} = \frac{\lg \dfrac{x_S \cdot (1 - x_D)}{x_D \cdot (1 - x_S)}}{\lg \alpha_{12}}$$



Minimum reflux ratio according to Underwood

- **For the minium reflux ratio, the number of stages goes → ∞**
- $rr_{min} = \frac{1}{\alpha_{12}-1} \cdot \left(\frac{x_{Kopf,LS}}{x_{Feed,LS}} - \alpha_{12} \cdot \frac{1-x_{Kopf,LS}}{1-x_{Feed,LS}} \right)$



Number of stages and reflux ratio according to Gilliland

- **Empirical Correlations**

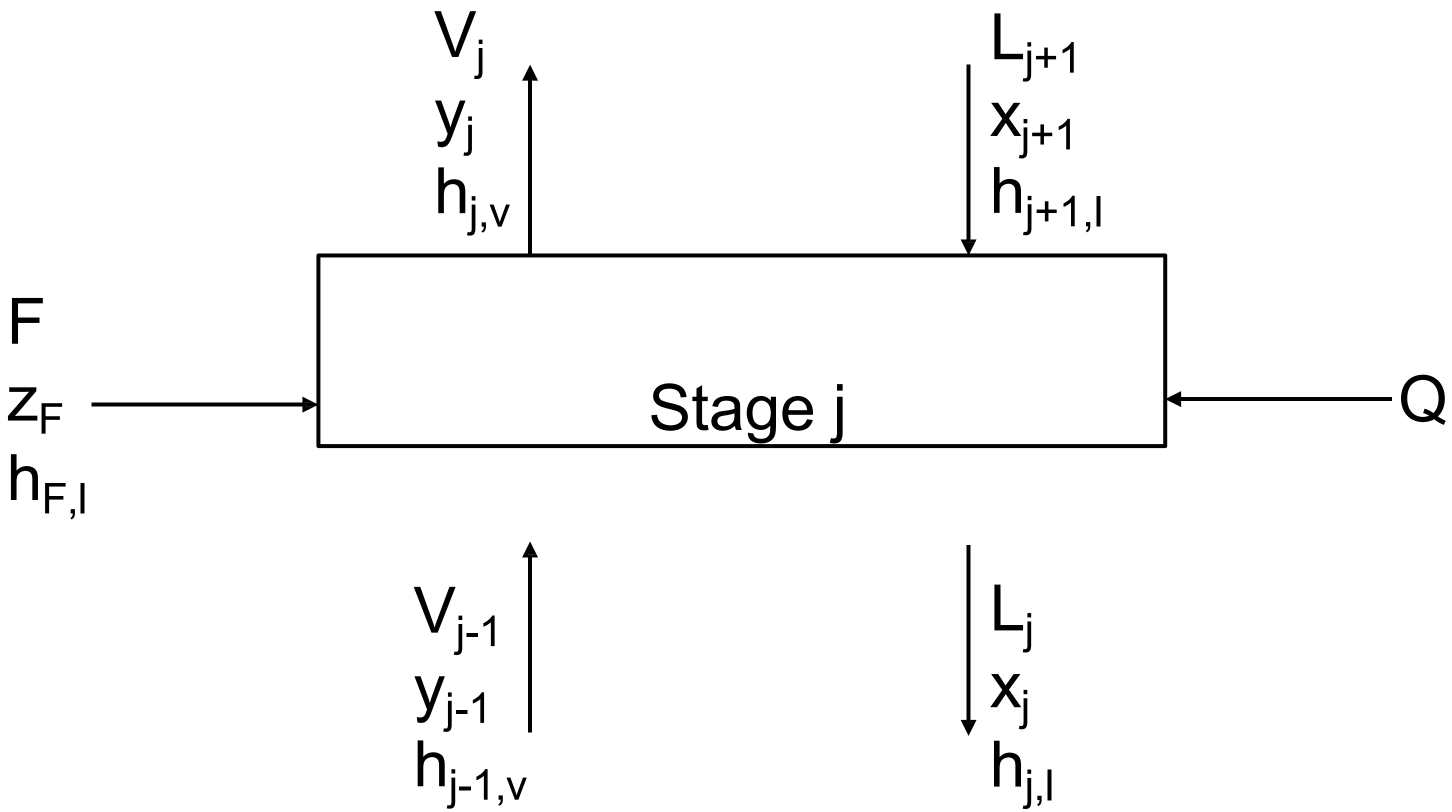
- **Reflux Ratio:** $\boldsymbol{v = 1{,}05 \ldots 1{,}3} \quad \boldsymbol{\cdot\, v_{min}}$

- **Number of stages:**

$$\frac{N - N_{min}}{N + 1} = 1 - \exp\left[\frac{(1 + 54 \cdot X)(X - 1)}{(11 + 117 \cdot X)\, X^{0{,}5}}\right]$$

With $X = \frac{v - v_{min}}{v + 1}$

Equilibrium stage model (I)



Assumptions:

- Balancing of two separate phases
- No reaction
- Steady State Operation

Equilibrium stage model (II)

- **Material Balance**
  - $L_{j+1} \cdot x_{i,j+1} - L_j \cdot x_{i,j} + V_{j-1} \cdot y_{i,j-1} - V_{j+1} \cdot y_{i,j} + F_j \cdot z_{i,F} = 0$
- **Equilibrium Balance**
  - $y_{i,j} - K_{i,j} \cdot x_{i,j} = 0 \quad mit \;\; K_i = y_i / x_i \quad K = f(T, p, x_i, y_i)$
- **Summation Condition**
  - $\sigma \, y_{i,j} - 1 = \sigma \, x_{i,j} - 1 = 0$
- **Heat Balance**
  - $L_{j+1} \cdot h_{j+1,l} - L_j \cdot h_{j,l} + V_{j-1} \cdot y_{j-1,v} - V_{j+1} \cdot y_{j,v} + F_j \cdot h_{F,j} + Q = 0$

j: Theoretical Stage
i: Component

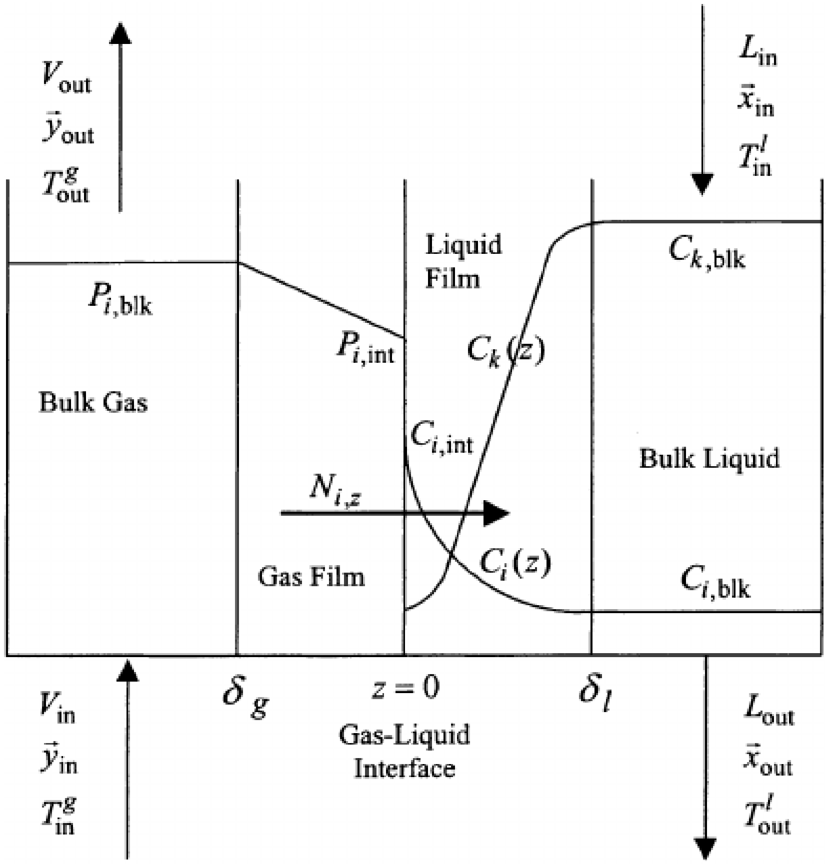
Equilibrium stage model (III)

- **Material Balance:**
  One equation per theoretical stage **(N)** and component **(n)**
  → ∑**N·n** equations
- **Equilibrium Condition:**
  Must be satisfied on every stage N and for every component n
  → ∑**N·n** Equations
- **Summation Condition:**
  Applies to gas phase and liquid on every stage
  →∑**2·N** Equations
- **Heat Balance:**
  Must be satisfied on every theoretical stage
  → **N** Equations

In total, this results in **(2n+3)** equations per stage and consequently a total of **N·(2n+3)** Equations per Column.

Example: Binary mixture with 10 theoretical stages: 70 Equations

Rate-Based Models



MERSHQ-Equations:

<u>M</u>aterial Balance

<u>E</u>nergy Balance

Mass- and Heat Transfer <u>R</u>ate Equations

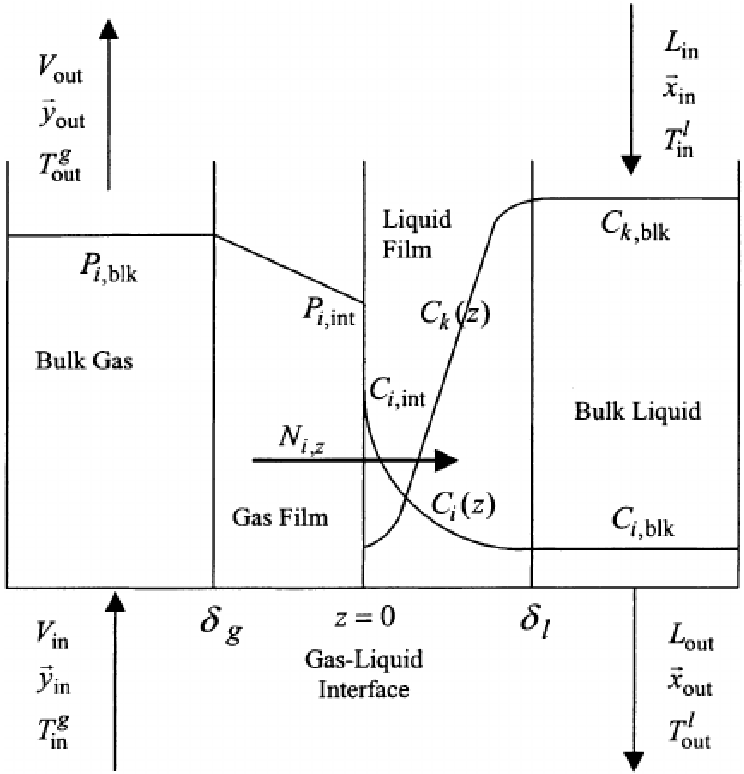
<u>S</u>ummation Equations

<u>H</u>ydraulic Equation for Pressure Drop

E<u>q</u>uilibrium Equations

Mass transfer models: two-film theory

- **Assumptions:**
  - Mass transfer from a stagnant liquid surface to a flowing fluid.
  - Mass transfer occurs only within the boundary layer.
  - The film thickness is assumed to be known and constant.
  - Steady State operation.



Mass transfer models: Penetration theory

- **Concept:**
  - Flow turbulence in the bulk phase of the media reaches the phase interface as so called „turbulent eddies“
  - The fluid elements transported to the boundary layer remain there for a certain amount of time and are subsequently displaced by following elements
    → The assumption of a stationary boundary layer no longer exists here
  - The boundary layer experience constant displacement and renewal
  - During the mean contact time of the fluid elements at the phase interface, mass transfer occurs via unsteady state diffusion

Mass transfer models: Surface renewal theory

- **Extension of penetration theory**
- **Assumptions:**
  - No constant mean contact time of the fluid elements at the phase interface between gas and liquid
  - In this case, the residence time of the elements in the boundary layer is described by a residence time distribution function
  - Surface renewal occurs by means of recurring, non uniform flow fields

Example of correlation for mass transport (tray columns)

- **AIChE Correlation for Bubble Tray Design (1958)**
  - Based on equimolar counter diffusion of binary mixtures through a film (two film theory according to Danckwerts et al.)
  - 3 boundary conditions
    - Mass transport of a component in the phase is proportional to the difference in concentration or partial pressure at the phase interface
    - Equilibrium at the phase interface
    - Hold-Up of the transferred component in the boundary layer is negligible
  - Calculation of mass transport using geometric, fluid dynamic and thermodynamic variables
- **Gerster et. al correlation (1958)**
  - Extension of fluid dynamics through eddy diffusion coefficents
- **Hughmark correlation (1971)**
  - Extension using surface renewal theory and penetration theory

Example of correlations for heat transport (tray columns)

- **Chilton und Colburn Analogie**
  - Heat transport is analogous to mass transport (calculatedusing the Prandtl number and the Schmidt number
  - Mostly used in process design and rarely yields large deviations, as it is an empirical approximation of turbulent, eddy-driven diffusion models

Example of correlations for the phase interface (tray columns)

- **Scheffe und Weiland**
  - Empirical equation developed through experiments using standardized trays and material mixtures
  - Phase Interface a = f(Re_L, Re_G, geometry)

$$a = 0{,}270 Re_G^{0{,}375} Re_L^{0{,}247} W'^{0{,}515}$$

$$Sh_G = 9{,}93 Re_G^{0{,}865} Re_L^{0{,}130} W'^{0{,}369} Sc_G^{0{,}5}$$

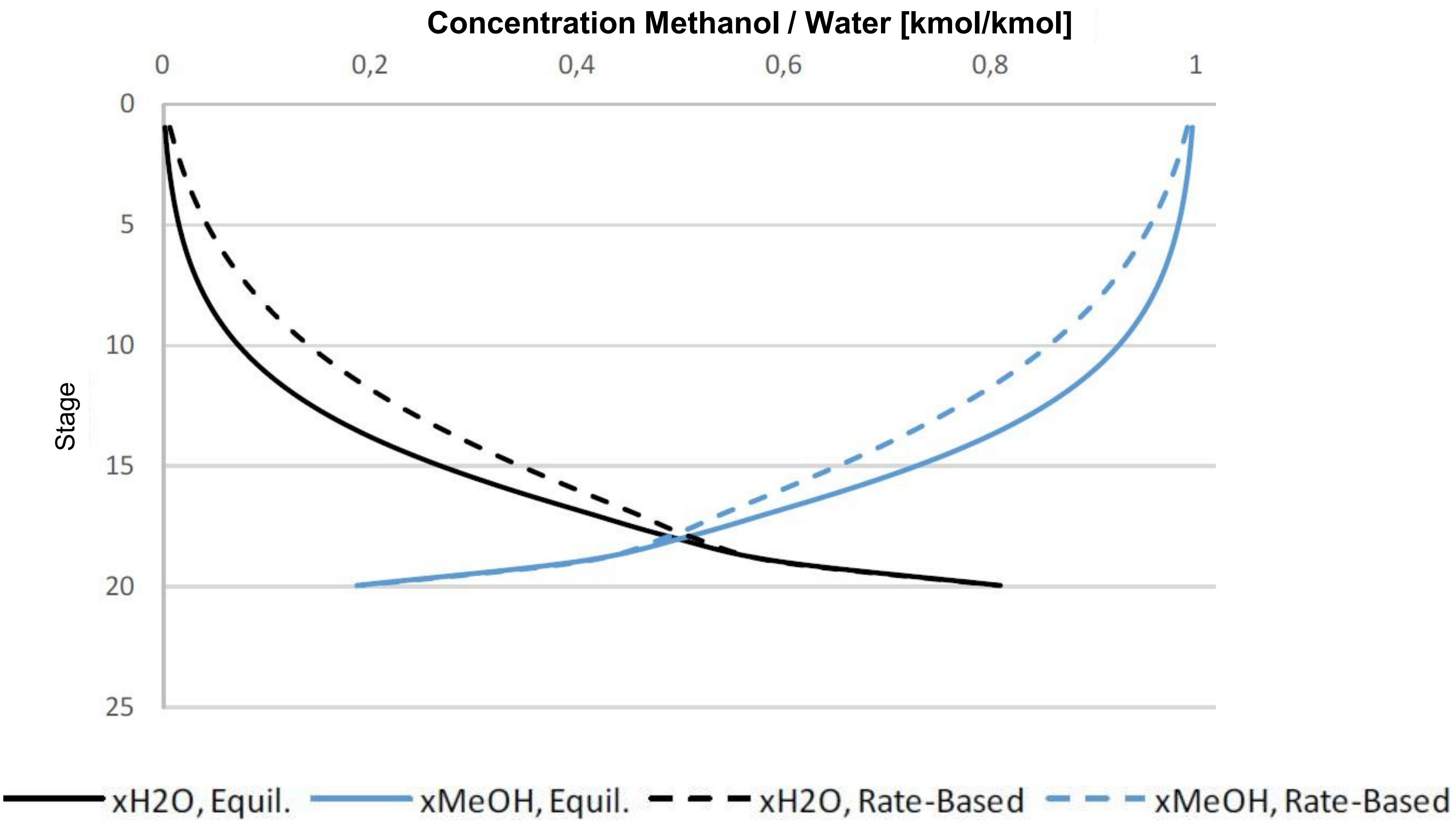
$$Sh_L = 125 Re_G^{0{,}684} Re_L^{0{,}087} W'^{0{,}051} Sc_L^{0{,}5}$$

Required thermodynamic material properties

Equilibrium Stage Models	**Rate-Based Models**
Activity coefficients	Activity coefficients
Vapor pressures	Vapor pressures
Fugacity coefficients	Fugacity coefficients
Densities	Densities
Enthalpies	Enthalpies
	Diffusion coefficients
	Viscosities
	Surface tension
	Thermal conductivities
	Mass transfer coefficients
	Heat transfer coefficients
	Phase interfaces

Difference between equilibrium and non-equilibrium models

- **Mixture Methanol / Water (α=3,75)**



Rigorous Solution Methods (RadFrac Family)

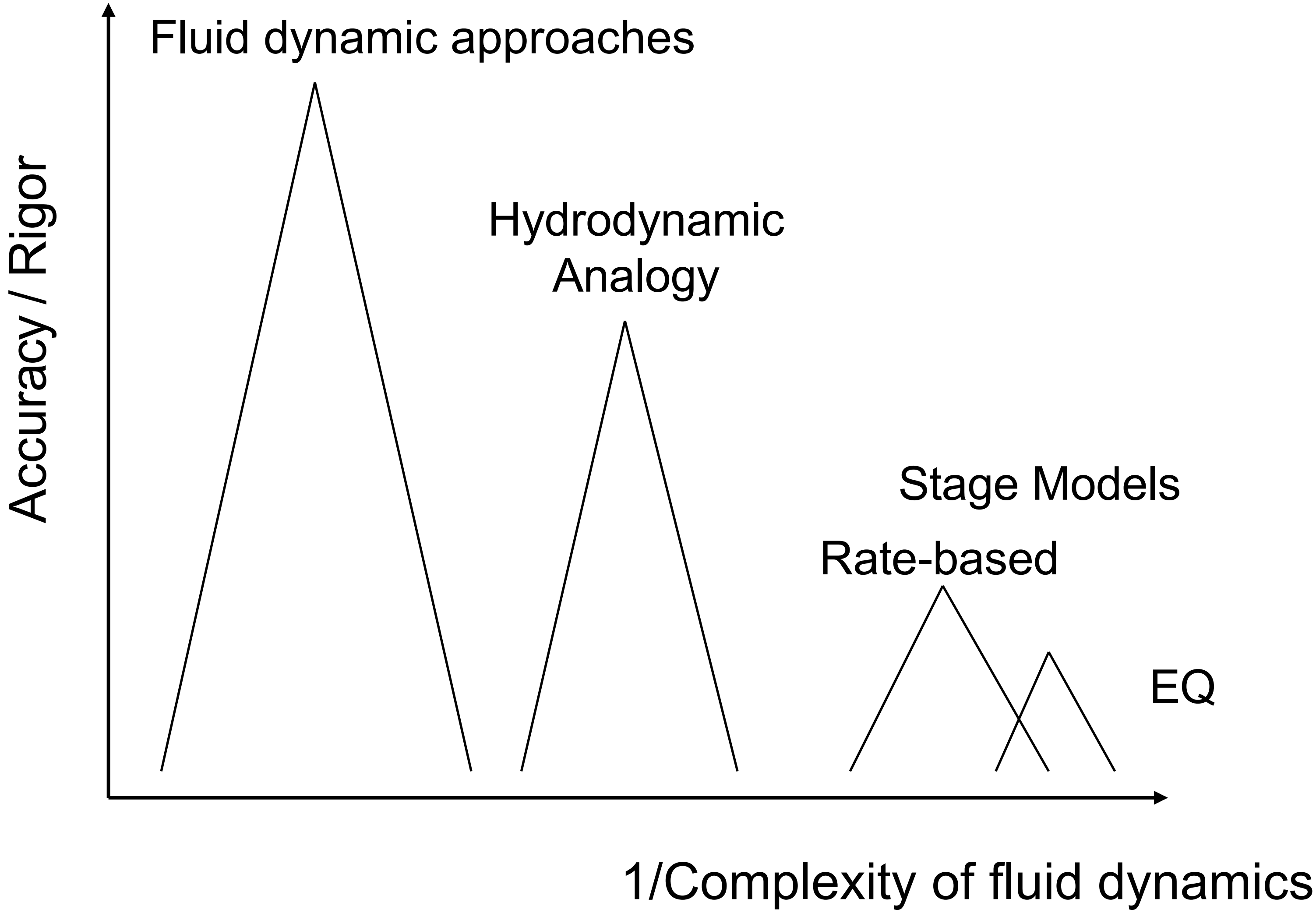
- **For each theoretical separation stage, the following variables are determined**
  - Temperature, pressure, vapor and liquid flow rates, concentration of the components in vapor and liquid

→ **Highly non-linear equation systems**

→ **Solution using appropriate mathematical methods**

- **Example 1: Wang-Henke method**
  - Solution of the material balance first, followed by the solution of the energy balance
  - Using substitution methods
- **Example 2: Naphtali-Sandholm method**
  - Simulatneous solution of the MESH equations
  - Using the introduction of a variable vector and a function vector

Classification of the methodological complexity according to Kenig (I)



Classification of the methodological complexity according to Kenig (II)

- **Stage models:**
  - Description of fluid dynamics through assumptions and simplifications
  - Equilibrium Stage Model: Lumped Parameters for HTU and NTU
  - Rate-Based: Describes mass transfer using the 2-film Model
- **Hydrodynamic Analogy:** Simplification of complex flow patterns into geometrically simple flows
- **Fluid Dynamic Approaches (CFD):**
  - Description of transport phenomena via partial differential equations (DGL)
  - Supplemented by initial and boundary conditions
  - Result: Local velocity, temperature and concentration fields
  - **But** requires the phase interface to be known at every point in time
- **Other models, e.g. cell models are also available**