[>>COnCEPT] Computer Optimization in Chemical Engineering Processes and Technologies

INTRODUCTION TO CHEMICAL PROCESS SIMULATORS

DWSIM Chemical Process Simulator

CAChemE

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October 2016

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Monday, October 3rd 2016

- Introduction to Sequential – Modular Steady State Process Simulators
- Get used to working with DWSIM and COCO

Monday, October 10th 2016

- Simulation of Chemical Reactors

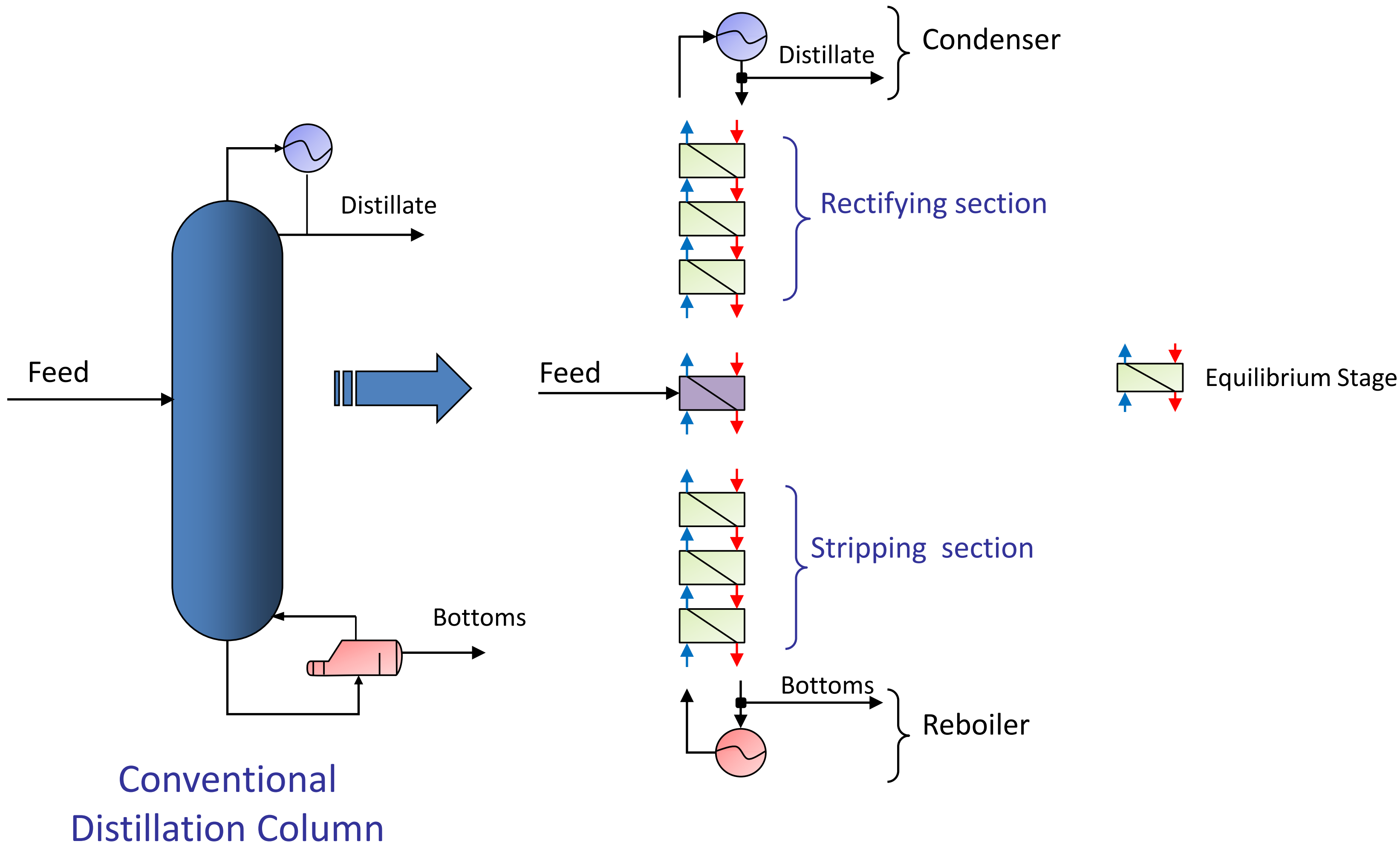
Monday, October 17th 2016

- Simulation of Distillation Columns

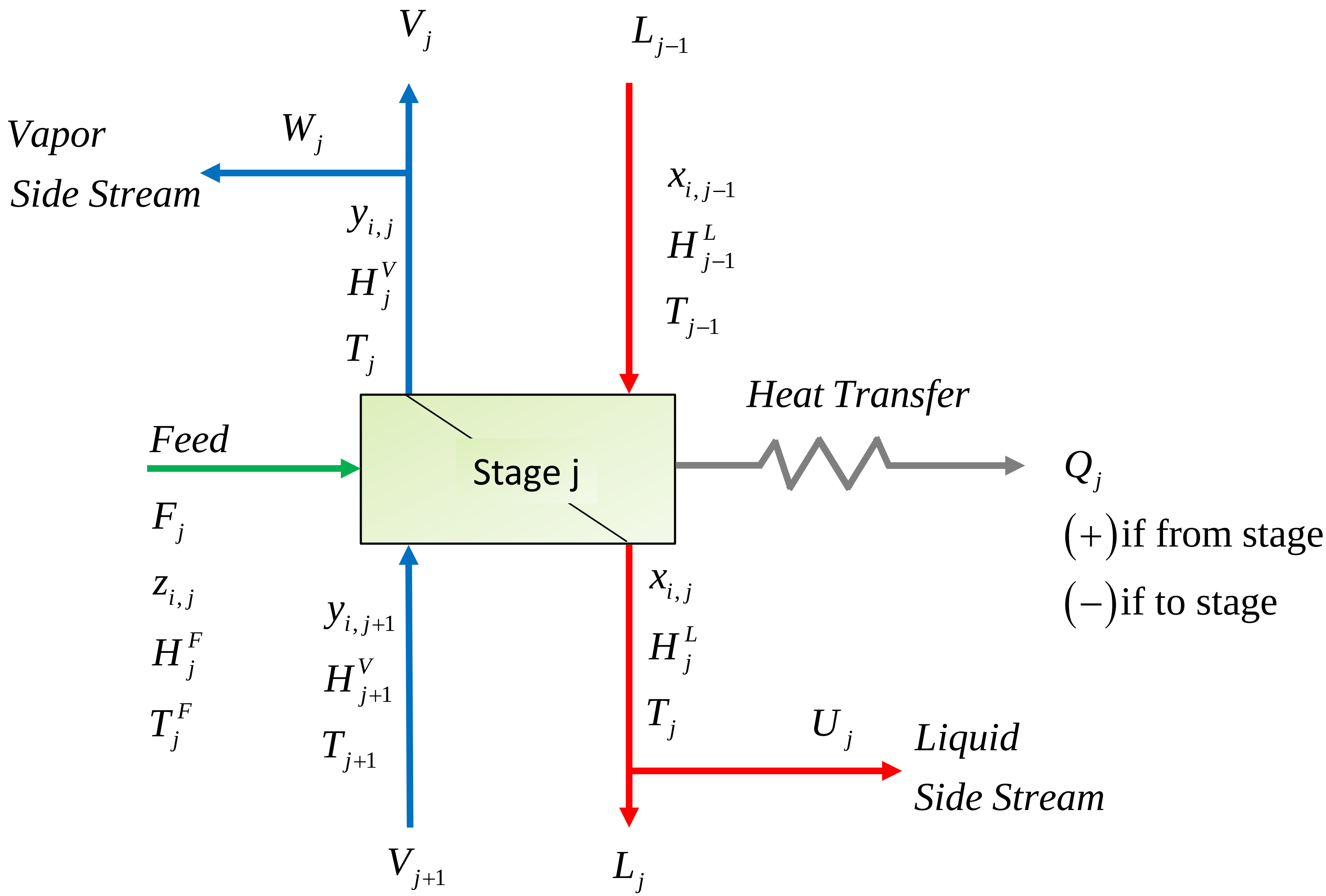
Monday, October 24th 2016

- Case studies

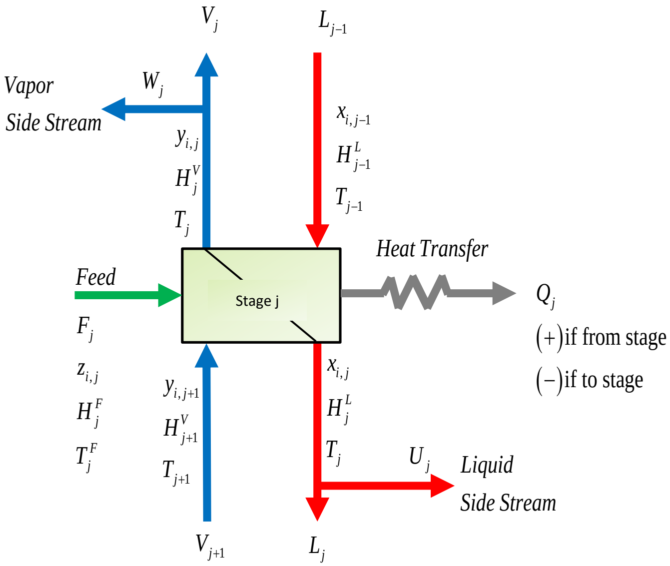
Simulation of Distillation Columns



Simulation of Distillation Columns



Simulation of Distillation Columns



MESH Equations

Material Balance

$$L_{j-1}x_{i,j-1} + V_{j+1}y_{i,j+1} + F_j z_{i,j} - \left(L_j + U_j\right)x_{i,j}$$
$$-\left(V_j + W_j\right)y_{i,j} = 0 \quad \forall i \in C,\ j \in NS$$

Vapor-Liquid Equilibrium Relation

$$f_{i,j}^{L} = f_{i,j}^{V}$$
$$f_{i,j}^{L} = f\left(T_j, P_j, x_{i,j}\right) \quad \forall i \in C,\ j \in NS$$
$$f_{i,j}^{V} = f\left(T_j, P_j, y_{i,j}\right)$$

Summation Equations

$$\sum_{i=1}^{C} y_{i,j} = 1, \quad \sum_{i=1}^{C} x_{i,j} = 0 \quad \forall j \in NS$$

Energy Balance

$$L_{j-1}H_{j-1}^{L} + V_{j+1}H_{j+1}^{V} + F_j H_j^{F} - \left(L_j + U_j\right)H_j^{L}$$
$$-\left(V_j + W_j\right)H_j^{V} - Q_j = 0 \quad \forall\ j \in NS$$
$$H_j^{L} = f\left(T_j, P_j, x_{i,j}\right)$$
$$H_j^{V} = f\left(T_j, P_j, y_{i,j}\right)$$

Simulation of Distillation Columns

MESH Equations fully describe the behavior of a distillation column.

- External to de column: these equations define the overall column total material balances, energy balances and product composition
- Internal to de column: they describe equilibrium conditions, internal component, total material and energy balances in each tray.

Nonlinear and Nonconvex algebraic system of equations

Rigorous Computational Methods

- Bubble-point methods (BP)
- Sum-rate methods (SR)
- 2N Newton methods
- Simultaneous correction methods (SC)
- Inside-out methods (IO)

Simulation of Distillation Columns

Main Steps for the Simulation of a Conventional Distillation Column

1. Component Selection

2. Fluid package Selection

3. Flash Algorithm Selection

4. Add *Distillation Column* Object

5. Set Column Properties
- Condenser & Reboiler Pressure
- Condenser type
- Condenser & Reboiler Specifications

6. Set Number of Stages

7. Set Column Pressure Profile

8. Edit Column Connections

9. Solving Method Selection

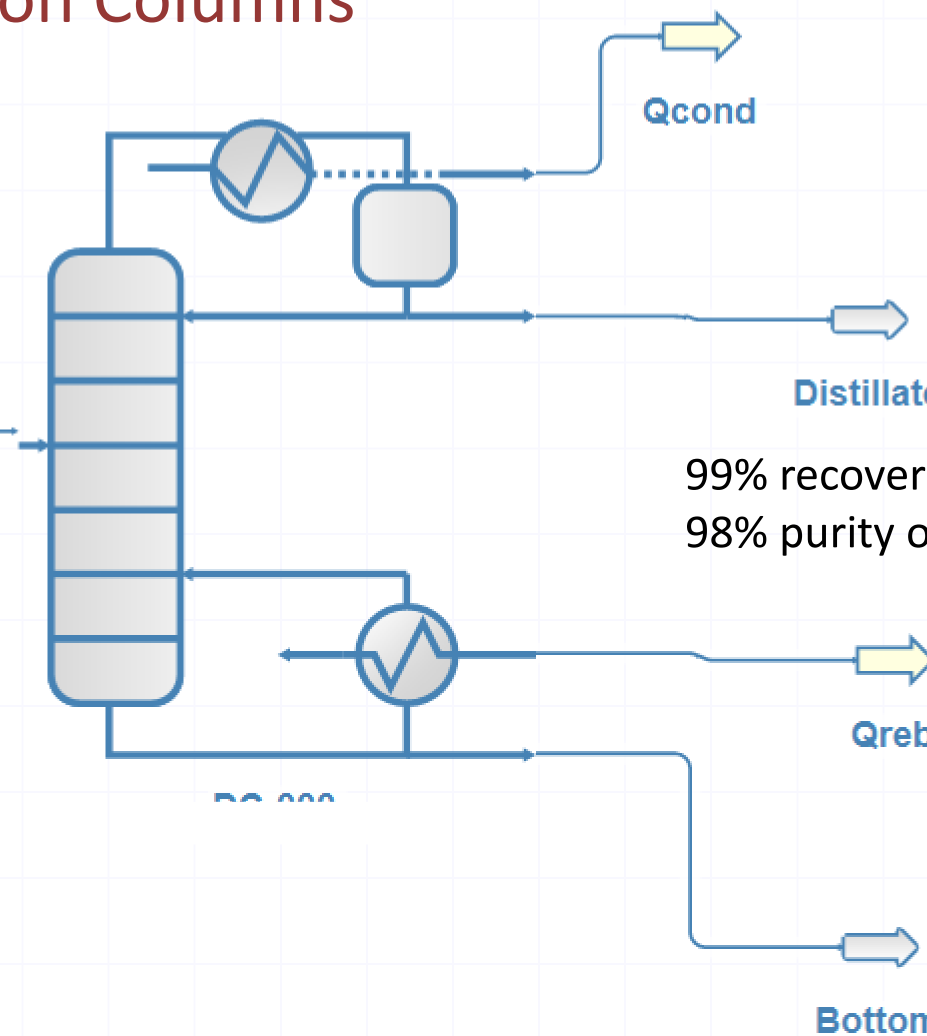
10. Run Model

Simulation of Distillation Columns

Example

Feed

Molar Flow 200 kmol/h
Pressure 1.1 bar
Vapor fraction 0



99% recovery of Bz
98% purity of Bz

Molar Composition

x_{Bz} = 0.35
x_{T} = 0.29
$x_{M\text{-}xy}$ = 0.12
$x_{O\text{-}xy}$ = 0.12
$x_{P\text{-}xy}$ = 0.12

Column Diameter Estimation

[R. Smith. Chemical Process Design and Integration]
[H. Kister. Distillation Design]

$$F_{LV} = \frac{L}{V}\sqrt{\frac{\rho_V}{\rho_L}\frac{M_L}{M_V}}$$

- F_{LV} ➔ Liquid-Vapor flow parameter
- L, V ➔ Liquid/Vapor molar flowrate [kmol s^{-1}]
- M_L,M_V ➔ Liquid/Vapor molar mass [kg $kmol^{-1}$]
- ρ_L, ρ_V ➔ Liquid/Vapor density [kg m^{-3}]

$$K_T = \left(\frac{\sigma}{20}\right)^{0.2} \exp\left[-2.979 - 0.717\ln F_{LV} - 0.0865\left(\ln F_{LV}\right)^2 + 0.997\ln H_T - 0.07973\ln F_{LV}\ln H_T + 0.256\left(\ln H_T\right)^2\right]$$

- KT ➔ Parameter for terminal velocity [m s^{-1}]
- σ ➔ Surface tension [dyne cm^{-1}]
- HT ➔ Tray spacing [m] (0,25 – 0,6 m)

$$v_T = f_F\, K_T\sqrt{\frac{\rho_L - \rho_V}{\rho_V}}$$

$$D_{column} = \sqrt{\frac{4 M_V V}{f_A\, \pi\, \rho_V\, f_S\, v_T}}$$

- v_T ➔ Vapor flooding velocity [m s^{-1}]
- f_F ➔ Foaming factor

  Low/ Moderate foaming ~ [0,9 - 0,85]

- f_A ➔ Net area factor (~0,9)
- f_S ➔ Flooding velocity safety factor (~0,8)