Process Simulation using DWSIM
A Free and Open Source Chemical Process Simulator

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Outline

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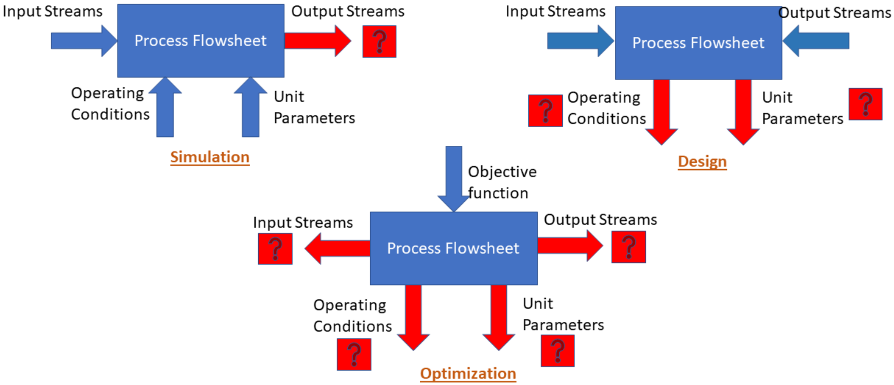
Design, Simulation & Optimization



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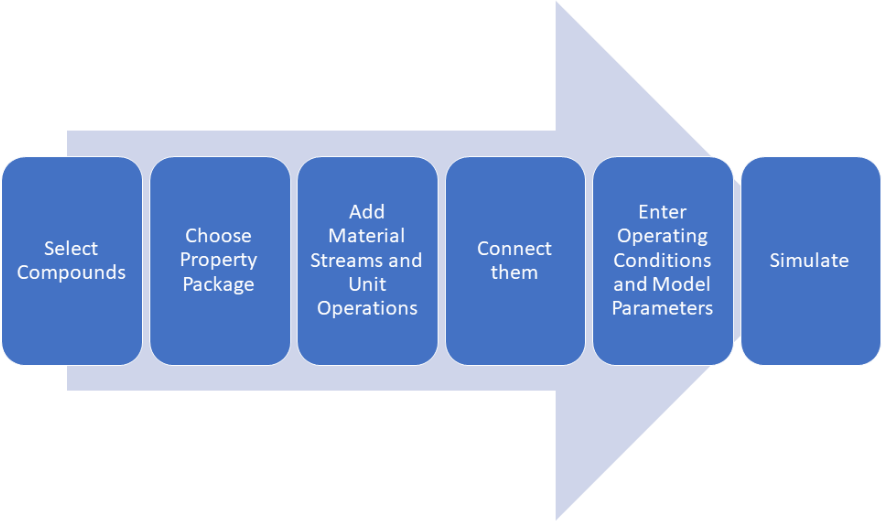
Simulating a Process Flowsheet



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Simulating a Material Stream

Important Properties to be specified in a Material Stream

- Flash Specification
- Flowrate
- Composition

Flash Specification

Flash Properties - Pressure, Temperature, Enthalpy, Entropy, Vapor Fraction

- Pressure and Temperature (TP)
- Pressure and Enthalpy (PH)
- Pressure and Entropy (PS)
- Pressure and Vapor Fraction (PVF)
- Temperature and Vapor Fraction (TVF)

Flow Rate

- Mass Flow Rate
- Molar Flow Rate
- Volumetric Flow Rate

Composition

- Mass Fraction
- Mole Fraction
- Mass Flows of Components
- Mole Flows of Components
- Molarities
- Molalities

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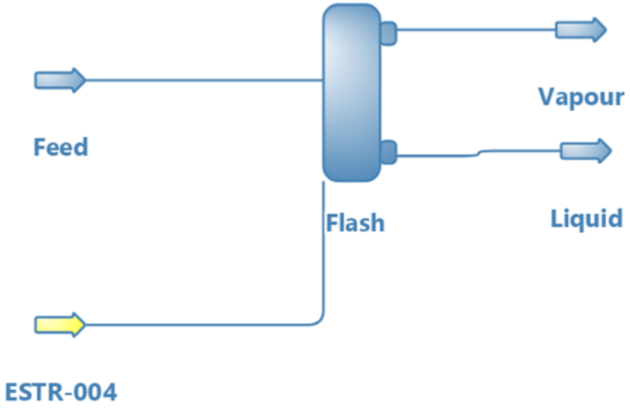
Problem 1: Simulation of a Flash Drum or Gas Liquid Separator

A 100 kmol/hr feed consisting of 10, 20, 30, and 40 mole% of propane, n-butane, n-pentane, and n-hexane, respectively, enters a flash chamber at 15 psia and 50°F. The flash drum is operated at 100 psia and 200° F. Applying the Raoult's law property package, compute the composition of the exit streams.

Results: Simulation of a Flash Drum or Gas Liquid Separator



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Problem 2: Computation of Bubble Point Temperature

Compute the bubble point temperature at 18 bar of the following hydrocarbon mixture using the Soave-Redlich-Kwong property package. Assume the mixture inlet temperature of 250°C, pressure of 5 bar and flow rate of 120 kmol/hr.

Component	Mole Fraction
C_1	0.05
C_2	0.1
C_3	0.15
i-C_4	0.1
n-C_4	0.2
i-C_5	0.25
n-C_5	0.15

Problem 3: Computation of Dew Point Temperature

Compute the dew point temperature at 1.5 bar of the following hydrocarbon mixture using the Soave-Redlich-Kwong property package. Assume the mixture inlet temperature of 250°C, pressure of 5 bar and flow rate of 120 kmol/hr.

Component	Mole Fraction
C_1	0.05
C_2	0.1
C_3	0.15
i-C_4	0.1
n-C_4	0.2
i-C_5	0.25
n-C_5	0.15

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Problem 4: T-xy and P-xy diagrams of a Binary Mixture

A binary mixture, consisting of 50 mole% ethanol and 50 mole% 1-propanol, is fed to a flash drum with a flow rate of 120 kmol/hr at 3.5 bar and 30^0C.

1. Produce T-xy plot at a constant pressure (1.013 bar)
2. Produce P-xy plot at a constant temperature (75^0C)
3. Produce xy plot based on the data obtained in Part (2)

Consider the Soave-Redlich-Kwong as a base property method.

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Problem Statement

100 kg/h of ethyl benzene at 260 $^\circ$C and 1.5 bar is decomposed to form styrene and hydrogen. Products are at 250 $^\circ$C and 1.2 bar. Assume the reaction to be vapour phase and 80% conversion of ethyl benzene takes place. Using Peng-Robinson model of thermodynamics, simulate the conversion reactor.

Repeat the above problem with conversion as function of temperature (where T is in K) provided as

$$f(T) = 0.0425(T + 248)$$

Input Data

- Components: Ethylbenzene-Styrene-Hydrogen
- Thermodynamic Property Package: Peng-Robinson
- Feed Mass Flow Rate: 100 kg/hr
- Feed Pressure: 1.52 bar
- Feed Temperature: 260°C
- Mole Fraction of Ethylbenzene: 1
- Mole Fraction of Styrene: 0
- Mole Fraction of Hydrogen: 0

Reaction and Reactor Input

- Reaction: Ethylbenzene $\rightarrow$Styrene $+$ Hydrogen
- $X_{ethylbenzene}$: 80
- Reactor Outlet Temperature: 250°C
- Reactor Pressure Drop: 0.3 bar

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Problem Statement

2000 kg/h of feed consisting of pure acetone at 100 °C and 2 bar enters a plug flow reactor (volume of 200 m^3 and 10 m length) to decompose into ketene and methane. The reaction rate is

$$-r_A = kP_{acetone} \frac{kmol}{m^3.hr}$$

where $P_{acetone}$ is the partial pressure of the Acetone in Pa. The reaction is assumed to follow arrhenius rate law where the pre-exponential factor is equal to 0.916 hr^{-1} and the activation energy is equal to 45000 $\frac{kJ}{kmol}$. The reactor is operated at 150 °C. Assuming the reaction to be in vapor phase and following Peng-Robinson property package, simulate a PFR.

Input Data

- Components: Acetone-Ketene-Methane
- Thermodynamic Property Package: Peng-Robinson
- Feed Mass Flow Rate: 2000 kg/hr
- Feed Pressure: 2 bar
- Feed Temperature: 100°C
- Mole Fraction of Acetone: 1
- Mole Fraction of Ketene: 0
- Mole Fraction of Methane: 0

Reaction and Reactor Input

- Reaction: Acetone $\rightarrow$Ketene + Methane
- Pre-exponential factor: 0.916 hr^{-1}
- Activation Energy: 45000 $\frac{kJ}{kmol}$
- Reactor Volume: 200 m^3
- Reactor Length: 10 m
- Reactor Outlet Temperature: 150°C

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Problem Statement

A 10000 kg/hr feed consisting 40% (by mole) Benzene and 60% Toluene enters a distillation column at 1.01325 bar and 80°C. The feed is to be separated such that composition of light key in bottoms is 1% (by mole) and composition of heavy key is 1% (by mole) in distillate. The column is operated at 1.4 times the minimum reflux ratio. The toal condenser pressure is 1.01325 bar and reboiler pressure is 1.01325 bar. Using Peng-Robinson property package, simulate the distillation column.

Input Data

- Components: Benzene-Toluene
- Thermodynamic Property Package: Peng-Robinson
- Feed Mass Flow Rate: 10000 kg/hr
- Feed Pressure: 1.01325 bar
- Feed Temperature: 80°C
- Mole Fraction of Benzene: 0.4
- Mole Fraction of Toluene: 0.6

Column Input

- Mole Fraction of LK(Benzene) in Bottoms: 0.01
- Mole Fraction of HK(Toluene) in Distillate: 0.01
- Condenser Type: Total
- Condenser Pressure: 1.01325 bar
- Reboiler Pressure: 1.01325 bar
- $\frac{R}{R_{min}} = 1.4$

Shortcut Column Results

- Reflux Ratio: 2.19366
- Minimum Reflux Ratio: 1.5669
- Actual Number of Stages: 19
- Feed Stage Location: 9

Distillation Column Input

- Actual Number of Stages: 19+1
- Feed Stage Location: 9
- Reflux Ratio: 2.19
- Bottoms Flow Rate: 69.5776 kmol/h

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Problem Statement

A 10000 kg/hr feed consisting 50% (by mole) Benzene, 30% Toluene and 20% p-Xylene enters a distillation column at 1.01325 bar and 80°C. The feed is to be separated through a sequence of columns such that in the first column, the composition of light key in bottoms is 0.1% (by mole) and composition of heavy key is 1% (by mole) in distillate. In the second column, the composition of light key in bottoms is 1% (by mole) and composition of heavy key is 1% (by mole) in distillate. The columns are operated at 1.3 times the minimum reflux ratio. For both the columns, the toal condenser pressure is 1.01325 bar and reboiler pressure is 1.01325 bar. Using Peng-Robinson property package, simulate the sequence of distillation column.

Input Data

- Components: Benzene-Toluene-p-Xylene
- Thermodynamic Property Package: Peng-Robinson
- Feed Mass Flow Rate: 10000 kg/hr
- Feed Pressure: 1.01325 bar
- Feed Temperature: 80°C
- Mole Fraction of Benzene: 0.5
- Mole Fraction of Toluene: 0.3
- Mole Fraction of P-xylene: 0.2

Column Input

- Mole Fraction of LK(Benzene) in Bottoms: 0.001
- Mole Fraction of HK(Toluene) in Distillate: 0.01
- Condenser Type: Total
- Condenser Pressure: 1.01325 bar
- Reboiler Pressure: 1.01325 bar
- $\frac{R}{R_{min}} = 1.3$

Shortcut Column-I Results

- Reflux Ratio: 1.31455
- Minimum Reflux Ratio: 1.01119
- Actual Number of Stages: 26
- Feed Stage Location: 16

Distillation Column-I Input

- Actual Number of Stages: 26+1
- Feed Stage Location: 16
- Reflux Ratio: 1.31455
- Bottoms Flow Rate: 56.3513 kmol/h

Shortcut Column-II Results

- Reflux Ratio: 1.86416
- Minimum Reflux Ratio: 1.43397
- Actual Number of Stages: 26
- Feed Stage Location: 14

Distillation Column-II Input

- Actual Number of Stages: 26+1
- Feed Stage Location: 14
- Reflux Ratio: 1.86
- Bottoms Flow Rate: 22.6424 kmol/h

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Problem 11: Simulation of Heat Exchanger

A heat exchanger is to be used to transfer heat to a toluene feed stream from a styrene product stream. The toluene enters the exchanger at a flow rate of 125000 lb/hr at 100^0F and 90 psia. The styrene enters at a flow rate of 150000 lb/hr at 300^0F and 50 psia. Overall heat transfer coefficient is 55 BTU/[ft^2 h R] and the area of the heat exchanger is 3000 ft^2. Calculate the fluid outlet temperatures, total heat exchanged, thermal efficiency and LMTD.

Important Links

FOSSEE DWSIM Webpage:
https://dwsim.fossee.in/

DWSIM Flowsheeting Project:
https://dwsim.fossee.in/flowsheeting-project

DWSIM Spoken Tutorials: https://spoken-tutorial.org/tutorial-search/?search_foss=DWSIM&search_language=English

DWSIM Developer's Webpage: http://dwsim.inforside.com.br/

References

- Fogler, H. Scott (2005), *Elements of Chemical Reaction Engineering*, 3rd ed., Prentice-Hall of India, New Delhi.
- Seider, W.D., J.D. Seider and D.R. Lewin (1998), *Process Design Principles: Synthesis, Analysis, and Evaluation*, 1st ed., John Wiley & Sons, New York.
- Jana, Amiya K. *Process Simulation and Control Using Aspen*, PHI Learning, 2014.

For any queries

contact-dwsim@fossee.in

Thanks

for your time and patience