

Process Simulation using DWSIM

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CL308 - Course on Wheels
DWSIM Simulation
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Outline

- 1 Binary Column Distillation
- 2 Multicomponent Distillation
- 3 Conversion/Yield Reactor
- 4 Kinetic Reactor

Table of Contents

- 1 Binary Column Distillation
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Problem Statement

A binary mixture containing 40 mol% methanol and 60 mol% isopropanol is to be distilled. The mixture consists of equimolar amounts of vapor and liquid at a pressure of 1.01325 bar and a flowrate of 100 kmol/h. The desired purities are 99% methanol and 99% isopropanol. The column is operated at 1.4 times the minimum reflux ratio. The total condenser pressure is 1.01325 bar and reboiler pressure is 1.01325 bar.

Input Data

- Components: Methanol-Isopropanol
- Thermodynamic Property Package: NRTL
- Feed Molar Flow Rate: 100 kmol/hr
- Feed Pressure: 1.01325 bar
- Feed Vapor Phase Mol Fraction: 0.5
- Mole Fraction of Methanol: 0.4
- Mole Fraction of Isopropanol: 0.6

Column Input

- Mole Fraction of LK(Methanol) in Bottoms: 0.01
- Mole Fraction of HK(Isopropanol) 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: 3.84262
- Minimum Reflux Ratio: 2.74473
- Actual Number of Stages: 22
- Feed Stage Location: 10

Distillation Column Input

- Actual Number of Stages: 22
- Feed Stage Location: 10
- Reflux Ratio: 3.84262
- Bottoms Flow Rate: 60.204 kmol/h

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Problem Statement

A ternary mixture containing 30 mol% methanol, 30 mol% isopropanol and 40 mol% n-propanol is to be distilled. The mixture consists of equimolar amounts of vapor and liquid at a pressure of 1.01325 bar and a flowrate of 100 kmol/h. 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 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 column is operated at 1.4 times the minimum reflux ratio. The total condenser pressure is 1.01325 bar and reboiler pressure is 1.01325 bar.

Input Data

- Components: Methanol-Isopropanol-n-Propanol
- Thermodynamic Property Package: NRTL
- Feed Mass Flow Rate: 100 kmol/hr
- Feed Pressure: 1.01325 bar
- Feed Vapor Phase Mol Fraction: 0.5
- Mole Fraction of Methanol: 0.3
- Mole Fraction of Isopropanol: 0.3
- Mole Fraction of n-Propanol: 0.4

Column Input

- Mole Fraction of LK(Methanol) in Bottoms: 0.01
- Mole Fraction of HK(Isopropanol) 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-I Results

- Reflux Ratio: 4.36978
- Minimum Reflux Ratio: 3.12127
- Actual Number of Stages: 21
- Feed Stage Location: 10

Distillation Column-I Input

- Actual Number of Stages: 21
- Feed Stage Location: 10
- Reflux Ratio: 4.36978
- Bottoms Flow Rate: 70.4077 kmol/h

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Problem Statement

100 kg/h of ethyl benzene at 260 °C and 1.5 bar is decomposed to form styrene and hydrogen. Products are at 250 °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: $45000 \frac{\text{kJ}}{\text{kmol}}$
- Reactor Volume: 200 m^3
- Reactor Length: 10 m
- Reactor Outlet Temperature: 150°C

Thank you!