1.Simulation for flash distillation

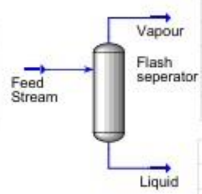
Feed Stream:

- ✓ Temperature: 115.6 ºC
- ✓ Pressure: 1896 kPa
- ✓ Molar Flow: 1748 kgmol/h
- ✓ Component Mole Fractions:
    - o Hydrogen: 0.004700
    - o Methane: 0.017600
    - o Ethane: 0.005400
    - o Benzene: 0.32900
    - o Toluene: 0.380900
    - o m-Xylene: 0.26200
- ✓ Vessel Pressure: 896.3 kPa

Question: Define suitable fluid package? Find out the vapor and liquid parameters.

Answer: Pheng-Robinson fluid package because of its characteristics. The parameters are given below.

Feed Stream		
Temperature	115.6	C
Pressure	1896	kPa
Molar Flow	1748	kgmole/h



Vapour		
Temperature	115.6	C
Pressure	999.7	kPa
Molar Flow	20.95	kgmole/h
Master Comp Mole Frac (Hydrogen)	0.262177	
Master Comp Mole Frac (Methane)	0.511430	
Master Comp Mole Frac (Ethane)	0.061301	
Master Comp Mole Frac (Benzene)	0.096851	
Master Comp Mole Frac (Toluene)	0.051708	
Master Comp Mole Frac (m-Xylene)	0.016532	

Liquid		
Temperature	115.6	C
Pressure	999.7	kPa
Molar Flow	1727	kgmole/h
Master Comp Mole Frac (Hydrogen)	0.001579	
Master Comp Mole Frac (Methane)	0.011617	
Master Comp Mole Frac (Ethane)	0.004724	
Master Comp Mole Frac (Benzene)	0.331949	
Master Comp Mole Frac (Toluene)	0.385047	
Master Comp Mole Frac (m-Xylene)	0.265084	

Is it possible for the sum of the mole fraction of methane and ethane in L. to be lower than 0.0005 and for the temperature of V to be 37.8 degree Celsius.?

Answer: No.

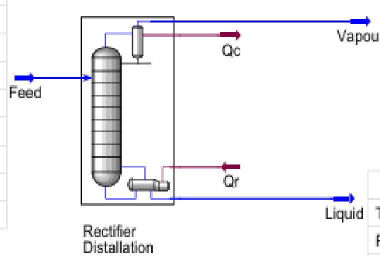
2. **Simulation for rectifier or multistage distillation**

Feed Stream:

- ✓ Temperature: 115.6 ºC
- ✓ Pressure: 1896 kPa
- ✓ Molar Flow: 1748 kgmol/h
- ✓ Component Mole Fractions:
  - o Hydrogen: 0.004700
  - o Methane: 0.017600
  - o Ethane: 0.005400
  - o Benzene: 0.32900
  - o Toluene: 0.380900
  - o m-Xylene: 0.26200
- ✓ Vessel Pressure: 896.3 kPa
- ✓ Extra Data:
  - o Real stages: (70% efficiency): 9 + partial reboiler+ full reflux condenser
  - o Feed stage: 2 (counting the condenser as 0), column pressure: 896.3 kPa
  - o Approximation: Distillate rate (D) = 49.4 kgmol/h; Reflux ratio (LD/D) = 2

Make it the sum of the mole fraction of methane and ethane in L. to be lower than 0.0005 and for the temperature of V to be 37.8 degree Celsius.?

Feed		
Temperature	115.6	C
Pressure	1896	kPa
Molar Flow	1748	kgmole/h
Master Comp Mole Frac (Hydrogen)	0.004702	
Master Comp Mole Frac (Methane)	0.017607	
Master Comp Mole Frac (Ethane)	0.005402	
Master Comp Mole Frac (Benzene)	0.329132	
Master Comp Mole Frac (Toluene)	0.381052	
Master Comp Mole Frac (m-Xylene)	0.262105	



Vapour		
Temperature	37.80	C
Pressure	896.3	kPa
Molar Flow	47.59	kgmole/h
Master Comp Mole Frac (Methane)	0.646377	
Master Comp Mole Frac (Ethane)	0.156125	

Liquid		
Temperature	200.2	C
Pressure	896.3	kPa
Molar Flow	1700	kgmole/h
Master Comp Mass Frac (Methane)	0.000002	
Master Comp Mass Frac (Ethane)	0.000391	

Rectifier Distallation	
Convergence	Converged
Number of Trays in Main Tray Section	9.000
Reflux Ratio	0.1955

3. **Distillation of a Multi-Component Hydrocarbon Feed**

Feed Stream:

Temperature: 98.2 ºC

Pressure: 1500 kPa

Molar Flow: 2100 kmol/h

Component Mole Fractions:

- Hydrogen: 0.0020
- Methane: 0.0150
- Ethane: 0.0090
- n-Butane: 0.0500
- Benzene: 0.4200
- Toluene: 0.3200
- Ethylbenzene: 0.1840

Column Information:

Real stages (75% efficiency): 10 + partial reboiler + full reflux condenser

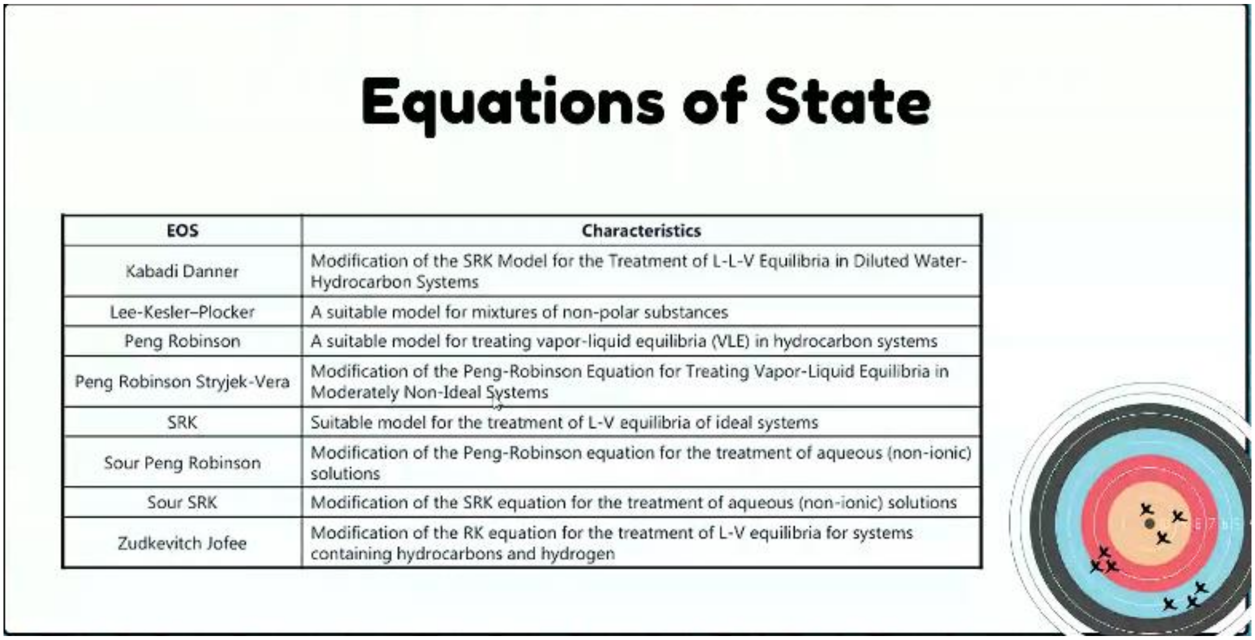
Feed stage: 2 (condenser counted as stage 0)

Column pressure: 1013 kPa

Approximation: D = 58.2 kmol/h; L/D = 2.5

Question:

Define suitable fluid package? Is it feasible for the sum of the mole fractions of hydrogen, methane, and ethane in the bottom product (L) to be lower than 0.001 and for the condenser vapor temperature (V) to be around 45.0 ºC? Justify your reasoning based on component volatilities and typical distillation behavior.

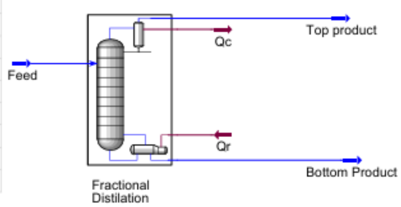


Equations of State

EOS	Characteristics
Kabadi Danner	Modification of the SRK Model for the Treatment of L-L-V Equilibria in Diluted Water-Hydrocarbon Systems
Lee-Kesler–Plocker	A suitable model for mixtures of non-polar substances
Peng Robinson	A suitable model for treating vapor-liquid equilibria (VLE) in hydrocarbon systems
Peng Robinson Stryjek-Vera	Modification of the Peng-Robinson Equation for Treating Vapor-Liquid Equilibria in Moderately Non-Ideal Systems
SRK	Suitable model for the treatment of L-V equilibria of ideal systems
Sour Peng Robinson	Modification of the Peng-Robinson equation for the treatment of aqueous (non-ionic) solutions
Sour SRK	Modification of the SRK equation for the treatment of aqueous (non-ionic) solutions
Zudkevitch Jofee	Modification of the RK equation for the treatment of L-V equilibria for systems containing hydrocarbons and hydrogen

Peng Robinson fluid package because of the all-feed input is mixed vapor- liquid hydrocarbon. Zudkevitch Jofee may also use for this case.

Feed		
Temperature	98.20	C
Pressure	1500	kPa
Molar Flow	2100	kgmole/h
Master Comp Mole Frac (Hydrogen)	0.002000	
Master Comp Mole Frac (Methane)	0.015000	
Master Comp Mole Frac (Ethane)	0.009000	
Master Comp Mole Frac (n-Butane)	0.050000	
Master Comp Mole Frac (Benzene)	0.420000	
Master Comp Mole Frac (Toluene)	0.320000	
Master Comp Mole Frac (E-Benzene)	0.184000	



Fractional Distilation	
Number of Trays in Main Tray Section	10.00
Reflux Ratio	0.1432

Top product		
Temperature	45.00	C
Pressure	1013	kPa
Molar Flow	59.88	kgmole/h
Master Comp Mole Frac (Hydrogen)	0.070146	
Master Comp Mole Frac (Methane)	0.526087	
Master Comp Mole Frac (Ethane)	0.281532	

Bottom Product		
Temperature	186.8	C
Pressure	1013	kPa
Molar Flow	2040	kgmole/h
Master Comp Mole Frac (Hydrogen)	0.000000	
Master Comp Mole Frac (Methane)	0.000000	
Master Comp Mole Frac (Ethane)	0.001002	

It is feasible for the sum of the mole fractions of hydrogen, methane, and ethane in the bottom product (L) to be lower than 0.001 and for the condenser vapor temperature (V) to be around 45.0 ºC. If the reflux ratio, top product molar flow, and bottom product molar flow are 0.1432, 59.88 kgmol/h, and 2040 kgmol/h, respectively.

4. Separation of Light Hydrocarbons (C1–C4)

Feed Stream:

Temperature: 35.0 ºC

Pressure: 3000 kPa

Molar Flow Rate: 1000 kmol/h

Component Mole Fractions:

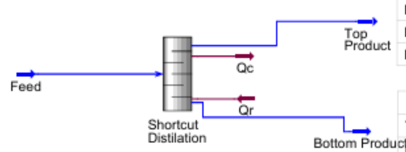
- Methane: 0.250
- Ethane: 0.400
- Propane: 0.250
- n-Butane: 0.100

Query:

Define suitable fluid package? If Propane Mole Fraction in distillate stream is 0.0120 (3000 kPa), Ethane Mole Fraction in bottom is 0.0250 (3000 kPa), and actual reflux ratio is 1.5 times higher to minimum reflux ratio, then is it feasible for the propane mole fraction in the distillate to be as low as 0.0120, and the ethane mole fraction in the bottoms to be as low as 0.0250, under the specified reflux ratio? Justify based on component volatility and shortcut distillation theory.

Answer: Peng-Robinson fluid package because of the all-feed input is mixed vapor- liquid hydrocarbon. The actual reflux ratio is 1.332. It is feasible for the propane mole fraction in the distillate to be as low as 0.0120, and the ethane mole fraction in the bottoms to be as low as 0.0250, under the specified reflux ratio.

Feed		
Temperature	35.00	C
Pressure	3000	kPa
Molar Flow	1000	kgmole/h
Master Comp Mole Frac (Methane)	0.250000	
Master Comp Mole Frac (Ethane)	0.400000	
Master Comp Mole Frac (Propane)	0.250000	
Master Comp Mole Frac (n-Butane)	0.100000	



Top Product		
Temperature	-56.12	C
Pressure	3000	kPa
Molar Flow	649.0	kgmole/h
Master Comp Mole Frac (Ethane)	0.602798	
Master Comp Mole Frac (Propane)	0.012000	

Bottom Product		
Temperature	89.77	C
Pressure	3000	kPa
Molar Flow	351.0	kgmole/h
Master Comp Mole Frac (Ethane)	0.024999	
Master Comp Mole Frac (Propane)	0.690094	

Shortcut Distilation		
Minimum Reflux	0.8884	
Minimum Trays	7.377	
Actual Trays	14.77	
Optimal Feed	7.678	
Condenser Duty	1.575e+007	kJ/h
Reboiler Duty	8.047e+006	kJ/h
External Reflux	1.332	

5. Distillation of a Multi-Component Hydrocarbon Feed

Feed Stream:

Temperature: 132.5 ºC

Pressure: 2100 kPa

Molar Flow: 1600 kmol/h

Component Mole Fractions:

- Methane: 0.0120
- Ethane: 0.0180
- Propylene: 0.0450
- Benzene: 0.2800
- Toluene: 0.3300
- m-Xylene: 0.3150

Column Information:

Real stages (65% efficiency): 8 + partial reboiler + total reflux condenser

Feed stage: 3 (condenser counted as stage 0)

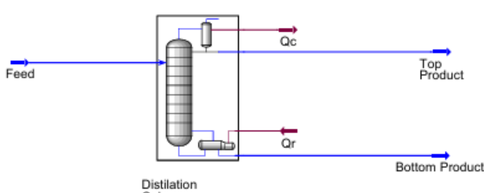
Column pressure: 1200 kPa

Approximation: D = 42 kmol/h; L/D = 1.8

Query:

Define suitable fluid package? Can the mole fraction of propylene in the bottom stream (L) be less than 0.003, and can the vapor temperature at the top of the column be about 55.0 ºC? Provide justification considering separation principles and boiling point trends.

Feed		
Temperature	132.5	C
Pressure	2100	kPa
Molar Flow	1600	kgmole/h
Master Comp Mole Frac (Methane)	0.012000	
Master Comp Mole Frac (Ethane)	0.018000	
Master Comp Mole Frac (Propene)	0.045000	
Master Comp Mole Frac (Benzene)	0.280000	
Master Comp Mole Frac (Toluene)	0.330000	
Master Comp Mole Frac (m-Xylene)	0.315000	



Top Product		
Temperature	-102.7	C
Pressure	1200	kPa
Molar Flow	42.01	kgmole/h

Bottom Product		
Temperature	185.0	C
Pressure	1200	kPa
Molar Flow	1558	kgmole/h
Master Comp Mole Frac (Propene)	0.040343	

Distilation Column	
Convergence	Converged
Number of Trays in Main Tray Section	8.000
Reflux Ratio	1.800

Fluid package: Pheng Robinson for hydrocarbon feed.

It is not possible to get the mole fraction of propylene in the bottom stream (L) be less than 0.003, and can the vapor temperature at the top of the column be about 55.0 ºC.

6. De-ethanizer Design in Ethylene Plant

Feed Stream:

Temperature: 45.2 ºC

Pressure: 2800 kPa

Molar Flow Rate: 850 kmol/h

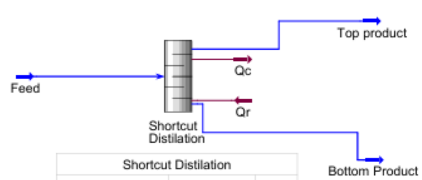
Component Mole Fractions:

- Methane: 0.180
- Ethylene: 0.420
- Ethane: 0.250
- Propane: 0.150

Query:

Define suitable fluid package? If Ethane Mole Fraction in distillate stream is 0.0070, Ethylene Mole Fraction in bottom is 0.0200, and actual reflux ratio is 1.8 times higher to minimum reflux ratio, then calculate the actual reflux ratio, and actual and minimum stages of column.

Feed		
Temperature	45.20	C
Pressure	2800	kPa
Molar Flow	850.0	kgmole/h
Master Comp Mole Frac (Ethane)	0.250000	
Master Comp Mole Frac (Propane)	0.150000	
Master Comp Mole Frac (Ethylene)	0.420000	
Master Comp Mole Frac (Methane)	0.180000	



Shortcut Distillation		
Minimum Reflux	3.316	
Minimum Trays	23.68	
Actual Trays	35.52	
Optimal Feed	19.93	
Condenser Duty	3.124e+007	kJ/h
Reboiler Duty	2.093e+007	kJ/h
External Reflux	5.969	

Top product		
Temperature	-57.08	C
Pressure	2800	kPa
Molar Flow	506.7	kgmole/h
Master Comp Mole Frac (Ethylene)	0.691034	

Bottom Product		
Temperature	25.49	C
Pressure	2800	kPa
Molar Flow	343.3	kgmole/h
Master Comp Mole Frac (Ethane)	0.608626	

Answer: Actual reflux ration: 5.969, actual stages of column; 35.52, and minimum stages of column: 23.68.

7. Debutanizer Column Design

Feed Stream:

Temperature: 52.5 ºC

Pressure: 2600 kPa

Molar Flow Rate: 900 kmol/h

Component Mole Fractions:

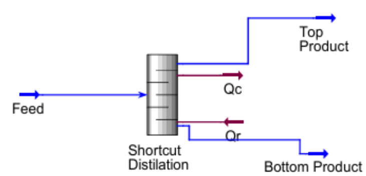
- Propane: 0.100
- n-Butane: 0.400
- i-Butane: 0.250
- n-Pentane: 0.180
- i-Pentane: 0.070

Query:

Define suitable fluid package? If n-Pentane Mole Fraction in distillate stream is 0.0100, i-Butane Mole Fraction in bottom is 0.0210, and actual reflux ratio is 2 times higher to minimum reflux ratio, then calculate the actual reflux ratio, actual and minimum stages of column, and give some observation on influencing parameters of short cut distillation column.

Answer: Peng-Robinson for organic compounds. Actual reflux ration: 3.820, actual stages of column; 20.94, and minimum stages of column: 14.06.

Feed		
Temperature	52.50	C
Pressure	2600	kPa
Molar Flow	900.0	kgmole/h
Master Comp Mole Frac (Propane)	0.100000	
Master Comp Mole Frac (n-Butane)	0.400000	
Master Comp Mole Frac (i-Butane)	0.250000	
Master Comp Mole Frac (n-Pentane)	0.180000	
Master Comp Mole Frac (i-Pentane)	0.070000	



Top Product		
Temperature	116.7	C
Pressure	2600	kPa
Molar Flow	686.7	kgmole/h

Bottom Product		
Temperature	172.8	C
Pressure	2600	kPa
Molar Flow	213.3	kgmole/h

Shortcut Distillation	
Minimum Reflux	1.910
Minimum Trays	14.06
Actual Trays	20.94
Optimal Feed	7.354
External Reflux	3.820

8. Distillation of a Multi-Component Hydrocarbon Feed

Feed Stream:

Temperature: 125 ºC

Pressure: 1800 kPa

Molar Flow: 2000 kmol/h

Component Mole Fractions:

- Methane: 0.0100
- Ethane: 0.0075
- Benzene: 0.3050
- Toluene: 0.2900
- m-Xylene: 0.2800
- o-Xylene: 0.1075

Column Information:

Real stages (72% efficiency): 12 + partial reboiler + total reflux condenser

Feed stage: 4 (condenser counted as stage 0)

Column pressure: 1000 kPa

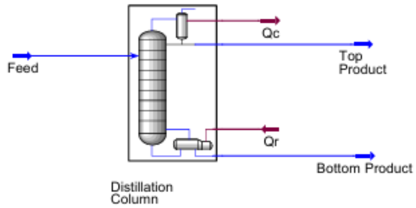
Approximation: D = 60 kmol/h; L/D = 3.0

Query:

Define suitable fluid package? Is it possible for the total mole fraction of ethane and methane in the distillate stream (V) to exceed 0.015, and for the condenser temperature to be around 41.5 ºC? Explain your answer based on the separation profile and volatility characteristics.

Answer: Peng-Robinson fluid package. It is not possible for the total mole fraction of ethane and methane in the distillate stream (V) to exceed 0.015, but it is possible for the condenser temperature to be around 41.5 ºC for changing molar flow rate.

Feed		
Temperature	125.0	C
Pressure	1800	kPa
Molar Flow	2000	kgmole/h
Master Comp Mole Frac (Methane)	0.010000	
Master Comp Mole Frac (Ethane)	0.007500	
Master Comp Mole Frac (Benzene)	0.305000	
Master Comp Mole Frac (Toluene)	0.290000	
Master Comp Mole Frac (m-Xylene)	0.280000	
Master Comp Mole Frac (o-Xylene)	0.107500	



Top Product		
Temperature	41.51	C
Pressure	1000	kPa
Molar Flow	911.1	kgmole/h

Bottom Product		
Temperature	238.6	C
Master Comp Mole Frac (Methane)	0.000000	
Master Comp Mole Frac (Ethane)	0.000000	

Distillation Column		
Number of Trays in Main Tray Section	12.00	
Reflux Ratio	3.000	
Molar Flow (Molar Flow_1)	2000	kgmole/h
Molar Flow (Molar Flow_2)	911.1	kgmole/h
Molar Flow (Molar Flow_3)	1089	kgmole/h