Aspen Plus Assignment

Instructions

You need to complete the following tasks to meet part of the learning outcomes for course B49CG Process Design B.

Submission will take the form of uploading completed Aspen Plus simulation files and a single report, in word format, to the allocated submission folder on Canvas. The report should cover the questions asked in each task. Remember to format the simulation properly, using appropriate stream names.

Question 1 (15 marks)

A liquid feed of 150 mol/min at 405.3kPa and its bubble point is fed to a distillation tower to recover 90% of the n-pentane in the overhead and 90% of the n-hexane in the bottom. The composition of the liquid feed is given in table 1. The reboiler is operating at 405.3kPa and there is a pressure drop of 20kPa across the distillation column. Assume that the distillation column is operating at 1.14 times the minimum reflux ratio, R_{min} and the overhead product leaves the column as a liquid stream.

Table 1: Composition of liquid feed

Component in Liquid Feed	Mole Fraction
n-butane	0.40
n-pentane	0.25
n-hexane	0.20
n-heptane	0.15

You are required to model this distillation column using **short-cut distillation unit** in Aspen Plus and select Peng Robingson as the thermodynamic model. Note: Simulation file is required.

From the simulation result, determine:

1. The bubble point of liquid feed
2. The molar flow rate (in kmol/h) and molar composition of overhead and bottoms.
3. The minimum reflux ratio
4. The number of trays at 1.14 R_{min}

Question 2 (20 marks)

Ammonia, NH_3 can be synthesized by reacting nitrogen, N_2 with hydrogen, H_2 through the following reaction:

$$N_2(g) + 3H_2(g) \leftrightarrow 2NH_3(g)$$

A stream having a molar flow rate of 100 kmol/h, containing 25 mol% of N_2 and 75 mol% of H_2 at 300 K and 1 bar is fed to a reactor which operates at 300 K and 1 bar. Simulate the reaction process in an equilibrium reactor using Peng-Robinson property package. Hint: You can assume the temperature approach to equilibrium is 0 °C. Note: Simulation file is required.

From the simulation result, determine the following:

1. The equilibrium constant at 300K
2. The molar flow rate (kmol/h) and molar composition of each component in the reactor effluent stream
3. The fractional conversion of nitrogen at 300K

You are then tasked to investigate the effect of temperature from 280K to 500K on the equilibrium constant and the molar composition of NH_3 in reactor effluent. Based on your simulation model,

1. Comment on the effect of temperature on the molar composition of NH_3 in reactor effluent and equilibrium constant.
2. Generate a plot to show the effect of temperature ranging from 280K to 500K on the molar composition of NH_3 in the reactor effluent.
3. Tabulate a table for equilibrium constant at temperature ranging from 280K to 500K with the interval of 10K. From the tabulated table, determine the equilibrium constant at 400K.

Question 3 (15 marks)

AspenPlus is known for simulating fine chemical systems including solids. For this simulation question, create a new Aspen Plus simulation using the "solids" template and add in components Air, Water and Titanium Dioxide. The Titanium Dioxide is an in-soluble solid powder with a d50 size of 40 micron and a standard deviation of 38.

Explore solids separators including:

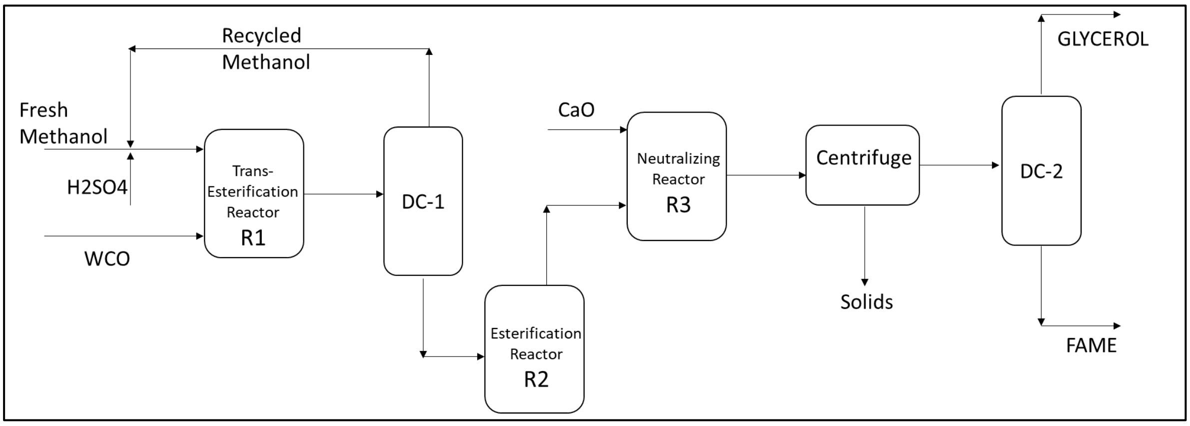
a. Cyclone for separating air/TiO2 mixtures. Choose sensible flowrates for each phase, but a suggestion is 1000 kg/hr TiO2, 20000 kg/hr of air, both at 5 deg C, 2 bar pressure. Start with a cyclone diameter of 2m, and see if you can detect a separation taking place as you would expect. Change the cyclone size to achieve a suitable differentiation in particle size from the two product streams.
b. Increase the moisture content of the feed stream to 10 wt% (wet basis) and repeat the cyclone separation. Identify where the water will go.
c. Install a dryer and see if you can bring the moisture content of the wet product from the cyclone down to 2 wt% (wet basis). Note you will have to select a "contact dryer", choose a sensible length and heat transfer properties.
d. Finally, recombine all streams together. Does the solids particle size distribution of the mixed product match with the feed stream?

Note: Simulation file is required.

The video in the URL will help you set up the solid and particle size distribution "https://www.youtube.com/watch?v=aLBE3JFsJwM"

Question 4 (50 marks)

Figure below shows a biodiesel production scheme via an acid-catalyzed process using waste cooking oil (WCO) which has a feed flow of 920 kg/h to produce biodiesel (FAME) with glycerol ($C_3H_8O_3$) as a by-product. Triglyceride with triolein 90 wt% ($C_{57}H_{104}O_6$) and free fatty acid by oleic acid ($C_{18}H_{34}O_2$) 10 wt% are used to represent the composition in the WCO. Methyl oleate or oleic acid methyl ester ($C_{19}H_{36}O_2$) are chosen for the biodiesel (FAME). Fresh methanol, WCO and H_2SO_4, CaO feeds are at 25°C and 1 bar. In transesterification reactor R1, the feed molar ratio of oil: methanol: H_2SO_4 are 1:50:1.35. WCO is pumped to 4 bar and heated to 60 °C before entering the reactor. The recycled methanol stream combines with fresh methanol and H_2SO_4 acid, pumped to 4 bar prior feeding into the reactor R1.



Transesterification take place in R1 assuming that 97% of the triglyceride is converted into FAME (the main product) and glycerol. The liquid product of the reactor consists of glycerol, methyl oleate and unreacted methanol, acid, and oil, which enter the distillation tower (DC-1). DC-1 recovers the excess liquid methanol (99.9wt%) in the distillate, cooled down to 30 °C before recycled to R1. The bottom product stream from DC-1 is cooled to 70 °C and transferred into the esterification reactor, R2. All oleic acid is converted into methyl oleate in R2 as shown in reaction eq(1):

Methanol + Oleic Acid → Methyl Oleate + Water *Eq(1)*

It is aimed to remove all the acid catalyst in the neutralizing reactor R3. Sulfuric acid is completely removed by neutralizing and adding CaO(s) by forming $CaSO_4$ precipitate and water as shown in reaction eq(2).

$H2SO_4$ (aq) + CaO(s) → $CaSO_4$ (s)+ Water (aq) *Eq(2)*

The output stream of R3 is sent to a centrifuge to separate all the solids from the liquid stream. The liquid stream is further sent to the second distillation column DC-2 operating at vacuum condition. In DC-2, the target is to separate the lighter compounds water, glycerol from the FAME (main product) and obtain biodiesel purity of at least 95 wt%.

Further information of the operating conditions of reactors and distillation columns are provided below:

Transesterification reactor R1	Esterification reactor R2	Neutralizing reactor R3**
Temperature: 80 °C Pressure: 4 bar	Temperature: 70 °C Pressure: 2 bar	Temperature: 40 °C Pressure: 2 bar

**If there are missing parameters of $CaSO_4$, add the free energy of formation (DHFORM and DHAQFM) = -338.7 kcal/mol under Parameters-Pure components- New- Scalar.

DC-1 Configuration	DC-2 Configuration	Centrifuge
Reflux ratio: 2 Condenser Pressure: 190 kPa Reboiler Pressure: 200 kPa	No of stages: 6 (estimate) Condenser Pressure: 20 kPa Reboiler Pressure: 30 kPa	Pressure: 1 bar Temperature change: 0 ^{o}C

You are required to simulate the above process in Aspen Plus using the NRTL model. From your simulation, determine the following:

a) The molar flow and composition of recycled methanol stream
b) The amount of CaO(s) required
c) The reboiler and condenser duty (in kW) of DC-2
d) The FAME product stream mass flow and compositions

Note: Simulation file is required.

Full marks will be awarded with use of Aspen Plus advanced features, example RadFrac distillation column than a DSTWU column or splitter. *Hint: Do the recycle stream at the end.*