CHEM-E7100, Engineering Thermodynamics, Separation Processes, part 2

Theory part

1.

How would you optimise the parameters of the activity coefficient model? The model alternatives are Wilson, NRTL and UNIQUAC. The system is the methyl isobutyl ketone and water that is a heterogenous minimum temperature boiling azeotrope with LLE split. This is not a calculation task.

2.

Explain the operation principle of counter-current multistage (for example 3 stage evaporator) evaporation of black liquor. The heat comes from the primary steam. What kind of thermophysical properties are needed?

CHEM-E7110, Engineering Thermodynamics, Separation Processes, part 2

Calculation Exam with Aspen and Excel, 15th December 2021

Name: _____ Student ID _____

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Answer the both questions, 6 points per each question, 12 points in total. Make a document (with screen captures) summarizing the way you solved the task into Word or Excel. Upload also the simulation files.

Duration: 4 hours, upload the files to MyCourses

Allowed material during the last 4 hours: The course material in MyCourses, books in paper or in electronic format for example in Knovel, any material found in web.

This exam is the personal exam, do it alone. As in the conventional exams regarding plagiarism, the same rules are valid in online exams
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Question 1

Upload files as "ETSPp2_exam15Dec2021_Task1_Familyname_Givenname.*" where * is the file type.

There is a review paper by Bejarano et al (2016) where one of the aqueous ternary systems is carbon dioxide + n-butanol + water. Luckily, there are some phase equilibrium data available for this system.

The data is already available in the Aspen-file "ETSPp2_exam_15Dec2021_CO2_nBuOH_W_template.apwz"

Select the components and then PC-SAFT model. In Components/Specifications/Enterprise Database move the "APV110 PC-SAFT" into the Selected databanks (already done, but check)

a) Data is CNVLE061 and CNVLE062. Optimize binary interaction parameter PCSKIJ of PC-SAFT for the system CO_2 + n-Butanol, plot the relevant phase equilibrium diagrams.

b) Data is CWVLE109 and CWVLE110. Optimize binary interaction parameter PCSKIJ of PC-SAFT for the system CO_2 + water, plot the relevant phase equilibrium diagrams.

c) Data is WNLLE045 and WNVLE069. Evaluate the system n-Butanol + water with the PCSKIJ = 0, plot the relevant phase equilibrium diagrams.

d) Calculate the LLE diagram of ternary system at 298 K and 9 MPa in Properties/Analysis. How many binary LLE systems there are?

There is an idea to remove n-Butanol from water rich phase using high pressure liquid CO_2 extraction process.

e) Please, simulate a counter-current multistage liquid-liquid extraction at 298 K and 9 MPa. The binary feed is 1 mol/s where mole fraction of n-Butanol is 0.02 and the rest is water. The pure CO_2 as a solvent is 1.5 mol/s. How many ideal stages are needed to get >95% of feed butanol into the extract.

f) Flash the extract from the high pressure extraction column to atmospheric pressure in two stage flash so that you get a gaseous CO_2 and a liquid mixture of n-Butanol and water. What is the mole fraction of the atmospheric flashed liquid extract compared to the feed of extraction column?

REF. Arturo Bejarano, Pedro C. Simões, José M. del Valle; Review: Fractionation technologies for liquid mixtures using dense carbon dioxide; *J. of Supercritical Fluids* 107 (2016) 321–348

Question 2

Upload files as "ETSPp2_ exam15Dec2021_Task2_Familyname_Givenname.*" where * is the file type

The components of the system are: methane, ethane, propane, n-butane, n-pentane and n-decane. The phase equilibrium model is PENG-ROB of Aspen with its default binary interaction parameters.

a) Why cubic equation of state is suitable model for this system?

There is an absorber to absorb butane and pentane of feed gas stream into high boiling lean oil. The purpose is to enrich methane, ethane and propane of the exit gas stream.

	lean oil	feed gas
flow/mol/s	20.79	100.8
T/K	305.4	313.7
p/MPa	2.76	2.76
mole fraction		
methane	0	0.2
ethane	0	0.4625
propane	0	0.3
n-butane	0.0003	0.031
n-pentane	0.005	0.006
n-decane	0.9947	0

b) How many ideal stages (equilibrium stages) you need to remove 93% of n-butane of feed gas? Absorber pressure is 2.76 MPa.

c) Give comments of the ratio of flows (L/G), temperature, mole fractions of liquid and gas phase and K-values (y_i/x_i) as a function of stage of column

See the details of the Sulzer packing on the next page.

d) Run the rate-based calculation of the absorption column and design the diameter of the column for 80% ± 5% of flooding. Assume that you have Sulzer Mellapak 250 Y as a structured packing. Aspen has its default parameters included.

Advise: Number of stages (mathematical) of rate base is three times the ideal stages in b)

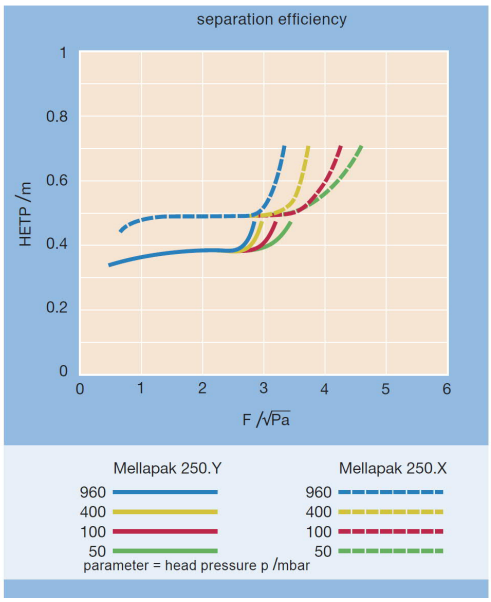
Advise: It is easier to start in the rating-mode to get it converging. You can manually update the diameter and section packing height. Or you can switch from the rating-mode to the design-mode to find out the diameter but the section packing height you need to update manually.

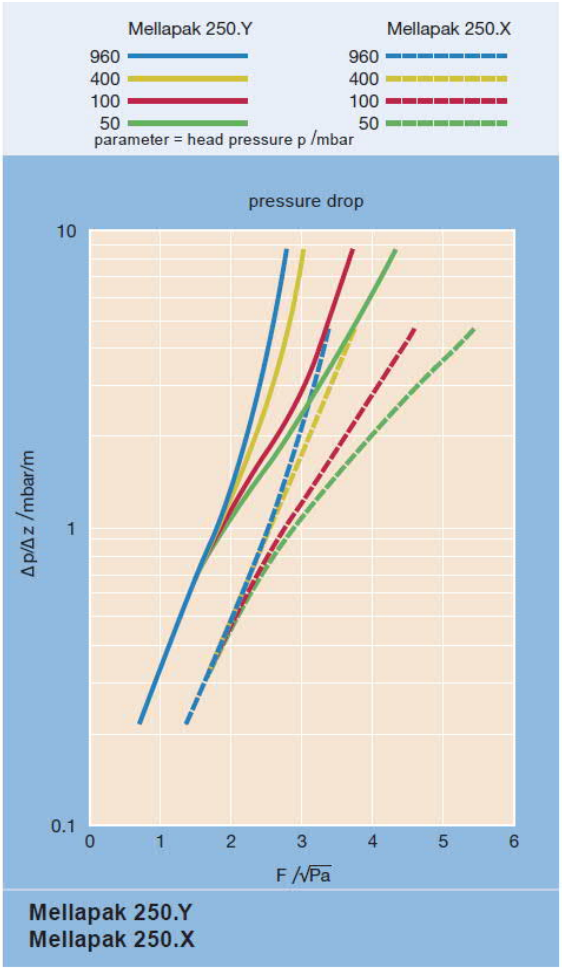
e) Design the packing height of the column so that you get close to the specification of b)

Mellapak 250.Y/X
A highly versatile packing type

0602 2510

Mellapak is the most widely used structured packing worldwide. It has proven excellent performance in columns with diameters up to 15 m. It is supplied in sheet metal thicknesses from 0.1 mm up.





where the term F is

F	F factor = $w_G \cdot \sqrt{\rho_G}$	m/s $\sqrt{kg/m^3}$ = $\sqrt{Pa}$	0.8197	ft/s $\sqrt{lbm/ft^3}$
w_G	Superficial gas velocity (related to empty column)	m/s	3.281	ft/s
ρ_G	Gas density	kg/m^3	0.06243	lb/ft^3