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

Calculation Exam with Aspen and Excel, 9th December 2020

Name: _____ Student ID _____

****

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

<u>Duration</u>: 4 hours, upload the files to MyCourses

<u>Allowed material during the last 4 hours</u>: 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
****

Question 1

Upload files as "ETSPp2_exam9Dec2020_Task1_Familyname_Givenname.*" where
* is the file type.

There is a small laboratory process reported by Sako et al (1995) applying
compressed carbon dioxide to produce furfural from sugars at high pressure. The
components are carbon dioxide (1), furfural(2) and water(3). Sugars are out of scope
this time.

The data is already available in the file
"CO2_furf_water_HP_exam_9Dec_2020_template.apwz"

Select PC-SAFT model. Input manually the pure component parameters of furfural,
PCSFTM = 3.48414, PCSFTU = 297.025, PCSFTV = 3.20809

a) Optimize the system CO_2 + furfural, plot the relevant phase equilibrium diagrams.

b) Optimize the system CO_2 + water, plot the relevant phase equilibrium diagrams.

c) Optimize the system furfural + water, plot the relevant phase equilibrium diagrams.

d) There are three measurements on ternary VLLE at high pressure 5 MPa by Sako et al (1995)

Table 1. *VLLE at high pressure 5 MPa*

Pressure is 5 Mpa and composition in mole fraction								
	water-rich phase			furfural-rich phase			vapor phase		
T/K	CO2	furf	water	CO2	furf	water	CO2	furf	water
303	0.0187	0.008	0.9733	0.3716	0.4906	0.1378	0.9983	0.0005	0.0012
323	0.0351	0.0119	0.953	0.2521	0.5448	0.2031	0.997	0.001	0.002
343	0.0432	0.0159	0.9409	0.192	0.551	0.257	0.9911	0.0016	0.0073

Verify your model against this data. What is the average absolute percent deviation in mole fractions or plot modelled mole fraction vs. experimental mole fraction.

e) Try to simulate a single stage liquid liquid decanter process where the feed is 10 mol-% furfural and 90 mol-% water. The solvent is pure carbon dioxide and the molar ratio of feed to solvent is 1:1. The pressure range is 7 MPa $\pm$ 1 MPa and temperature range 298 K $\pm$ 5 K so that you have LLE system. What is the K-value of furfural? In the other words, is CO_2 extracting furfural well? How many percent of moles of furfural you get from feed to extract?

f) Try to simulate a counter-current multistage liquid-liquid extraction, where the feed, solvent, temperature and pressure are similar than in d). Discuss the number of ideal stages and calculate the moles of furfural in extract and in raffinate as a function of number of ideal stages at a couple of examples. How many percent of moles of furfural you get from feed to extract?

REF. Sako, T., Sugeta, T., Nakazawa, N., Otake, K., Sato, M., Ishihara, K., Kato, M., (1995), High pressure vapor-liquid and vapor-liquid-liquid equilibria for systems containing supercritical carbon dioxide, water and furfural, Fluid Phase Equilibria, **108**, 293-303,

Question 2

There is a gas stream 72.5 mol-% hydrogen, 25 mol-% methane and 2.5 mol-% ethane at the rate 16.84 kmol/s at 298 K and 2.76 MPa.

You are studying if **absorption** with pure liquid n-octane as an absorbent at the rate 13.31 kmol/s and at 298 K and 2.76 MPa can be used. In the other words, can you increase the mole fraction of hydrogen of the gas stream by removing the light hydrocarbons with absorption oil.

The absorption column is assumed to operate at the 2.76 MPa.

See the literature references on the second page

It's important to test the phase equilibrium model, in this case PSRK, for a couple of binary systems.

a) Test the binary system hydrogen + n-octane with the default parameters in the evaluation mode, dataset BVLE020, plot the relevant phase diagrams.

b) Test the binary system methane + n-octane with the default parameters in the evaluation mode, dataset BVLE011, BVLE012, BVLE013, plot the relevant phase diagrams.

c) Test the binary system ethane + n-octane with the default parameters in the evaluation mode, dataset BVLE004, plot the relevant phase diagrams.

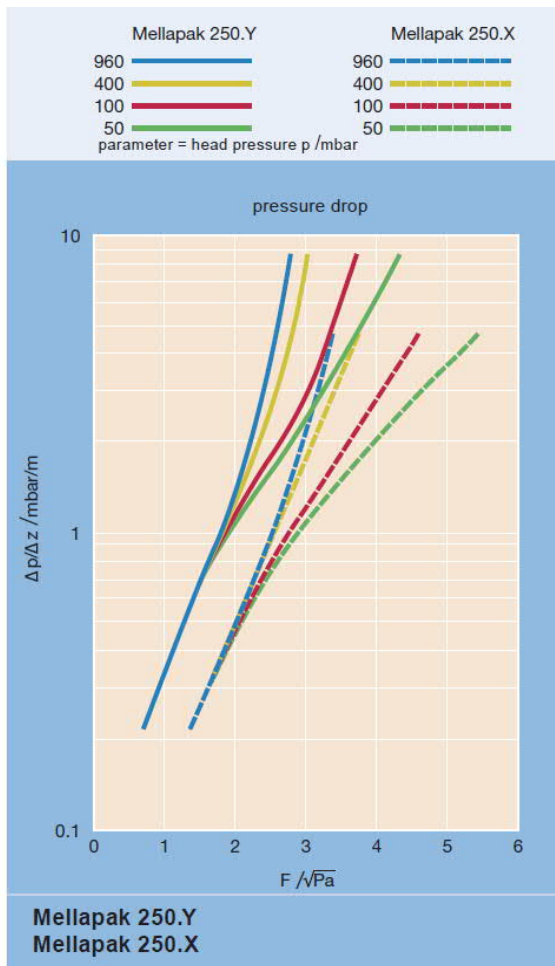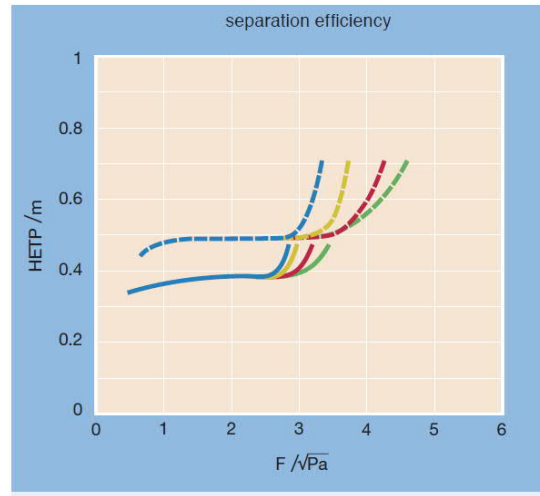Give your comments of the accuracy of the PSRK based on a) – c)

d) Run the simulation where there are 10 and 20 ideal stages. Does it have any effect on the mole fraction of exit gas. Your comments, is this simulation efficient in enriching hydrogen?

e) Run the rate based simulation to find out the diameter of the column. Sulzer Mellapak 250 Y is the structured packing, use the default parameters of the packing. What is the pressure drop across the packing?

See the details of packing on the next page.

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

0602 2510

separation efficiency

Mellapak 250.Y   Mellapak 250.X
960 ————   960 ————
400 ————   400 ————
100 ————   100 ————
50 ————   50 ————
parameter = head pressure p /mbar

pressure drop

Mellapak 250.Y
Mellapak 250.X

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/m³	0.06243	lb/ft³

BVLE020 =
Kim, K. J.; Way, T. R.; Feldman Jr., K. T.; Razani, A. J. Chem. Eng. Data, 1997, 42, 214-215 Solubility of Hydrogen in Octane, 1-Octanol, and Squalane

BVLE011, BVLE012, BVLE013 =
Velikovskii, A. S.; Stepanova, G. S.; Vybornova, Ya. I. Gaz. Prom., 1964, 9, 1-6 Phase equilibria of binary mixtures of methane with hydrocarbons of the normal paraffin series

BVLE004 =
Rodriguez, A. B. J.; Mccaffrey, D. S.; Kohn, J. P. J. Chem. Eng. Data, 1968, 13, 164-168 Heterogeneous Phase and Volumetric Equil. in the Ethane-n-Octane System system