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

Calculation Exam with Aspen and Excel, 24th February 2021

Name: ___________________________________ Student ID _________________

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

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

<u>Allowed material during the last 4 hours</u>: This is the open book exam. You can for example use the course material in MyCourses, books in paper or in electronic format for example in Knovel, any material found in the www.

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

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One technique to produce acetone is hydration of propylene to 2-propanol and then dehydrogenation of 2-propanol to acetone. (Ullmann's encyclopedia) In this case we study the binary system of isopropanol (2-propanol) and acetone (2-propanone).

Imagine that you are at the R&D department to screen the simulation techniques and got the following tasks. The purpose is to validate the phase equilibrium model and transport property correlations.

a) Check the UNIQUAC binary interaction parameters based on the VLE datasets VLE011, VLE018 and excess enthalpy HX003. [there is an error message in Aspen because DCPLS is outside its limits. You can fix it by setting the DCPLS = 101821 J/kmol-K in the pure component parameters REVIEW-matrix]. Draw the relevant graphs.

b) Optimize the better parameters based on VLE and excess enthalpy. What are the parameter values and their standard deviation? Draw the relevant graphs.

c) Calculate the excess molar volume for the dataset DEN004

d) Optimize the binary interaction parameter of Grunberg-Nissan model based on dataset VIS001. What is the average absolute deviation? Draw the relevant graphs.

e) Test the Li's thermal conductivity model based on the dataset TCR001. What is the average absolute deviation? Draw the relevant graphs.

Question 2

Upload files as "ETSPp2_exam24Feb2021_Task2_Familyname_Givenname.*" where * is the file type

Sulfur dioxide (SO_2) as an impurity in air (air is the mixture of nitrogen N_2 and oxygen O_2, mole ratio 79/21) is absorbed into pure water. The mole fraction of SO_2 is 0.016 and the rest of the gas stream is air.

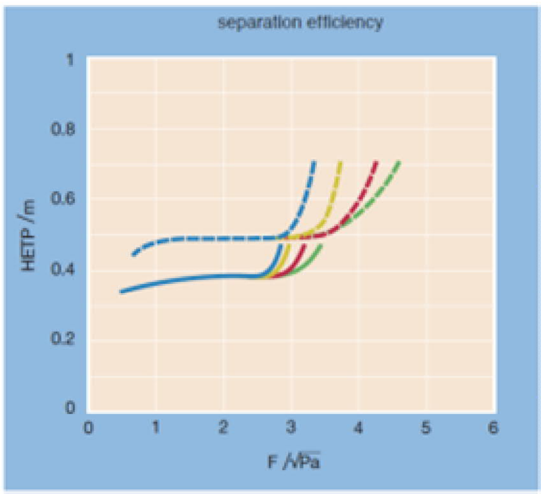
The temperature of liquid water and the temperature of gas feed is 30 °C, the both are at atmospheric pressure. The absorption column operates at the atmospheric pressure. The liquid water flow is 2.2 kmol/s and SO_2 flow is 0.062 kmol/s.

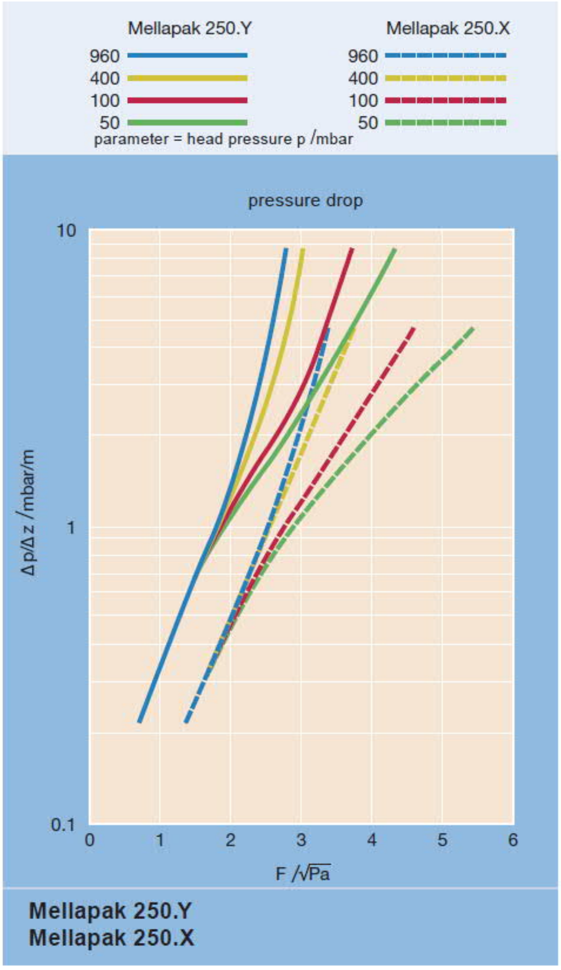
a) Find SO_2 + water binary VLE data from Aspen's NIST database. Evaluate the PSRK equation of state against the NIST data. Plot the relevant VLE graphs.

b) Build a simulation model for absorption assuming the ideal stage model. Test step by step to find how many ideal stages are needed to get the SO_2 mole fraction in the exit gas stream to 0.004. Make a table of the tests and plot the exit gas mole fraction of SO_2 as a function of ideal stages.

c) Build a simulation model for absorption assuming the rate based model. It is known that the packed height is 3.5 m. Size the diameter that the column runs at 85 % of the flooding limit. The structured packing is Sulzer's Mellapak 250 Y.

d) Find the pressure drop across the packing. How much the mole fractions of the exit flows deviate from the ideal stages assumption? Discuss the temperature profile inside the absorber. Comment the density of the liquid phase based on the PSRK model.





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