CHEM-E7100, Engineering Thermodynamics, Separation Processes, part 1

Extra Aspen Exam, Calculation part, 9th Dec 2019

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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) into a Word-file summarizing the way you solved the task. Upload Excel and Aspen files as supplementary files.

<u>Duration</u>: 3 hours, upload the files to MyCourses

<u>Allowed material during the last 3 hours</u>: The course material found in MyCourses including Lecture notes (book style text in 6 chapters), lecture slides (PowerPoint style), exercises, steam tables as a paper print (for example Keskinen, K. I., Kemian laitetekniikan…., or similar book), books in chemical engineering as a paper print or in Knovel, mathematical tables. You can use Internet and Aspen tutorials. The computer you have to use is the computer administered by the university in the computer class.

<u>NOT allowed material</u>: Discussing, e-mailing or use of social media applications in internet to communicate with other peoples are not allowed. Phone, tablet or own personal computer are not allowed and must be closed.

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Task 1

Upload files as “ETSPp1_exam9Dec2019_Task1_Familyname_Givenname.*” where * is the file type.

A long time ago (Pavasovic V, (1978), *Eur. Fed. Chem. Eng.*, Recomm. Syst. Liq. Extr. Stud., editor: T. Misek) there was an international project on liquid-liquid extraction. One of the test mixtures was separation of acetone (2-propanone) from water using toluene as a solvent. Liquid-liquid equilibrium is given in Table 1.

Table 1. LLE of ternary toluene + acetone + water, in mole fraction, data also as an xlsx-file in MC

Temperature 20 °C, atmospheric pressure					
x' (toluene)	x' (2-propanone)	x' (water)	x'' (toluene)	x'' (2-propanone)	x'' (water)
0.0001	0.01441	0.98549	0.95146	0.04353	0.00501
0.00021	0.0305	0.96929	0.88953	0.10314	0.00733
0.00021	0.03768	0.96211	0.85578	0.13458	0.00964
0.00034	0.06915	0.93051	0.71711	0.26473	0.01816
0.00048	0.09708	0.90244	0.60444	0.36546	0.0301
0.00101	0.1279	0.87109	0.48057	0.46721	0.05222
0.00171	0.1535	0.84479	0.39265	0.52777	0.07958
0.00388	0.20499	0.79113	0.26649	0.59343	0.14008
0.00673	0.24107	0.7522	0.20982	0.60701	0.18317
0.00817	0.25763	0.7342	0.18713	0.60153	0.21134

a) Verify the UNIFAC-Dortmund model against the given ternary data. Plot both measured and modelled acetone in extract as a function of acetone in raffinate. Give comments on the accuracy of UNIF-DMD.

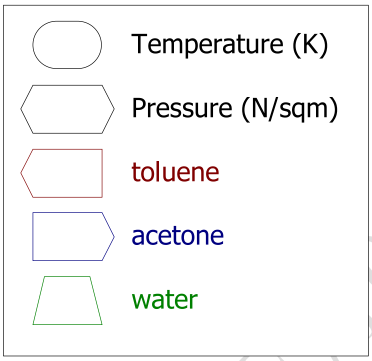
b) Assume, feed stream F contains toluene 0 mol/h, acetone 516.5 mol/h and water 3885.65 mol/h. Temperature of extraction is 20 °C and pressure is atmospheric. Solvent is pure toluene. Maximum mole fraction of acetone in raffinate is 0.025. What is the minimum solvent flow in mol/h based on the experimental data of Table 1.

Advise: (Because mole fraction of toluene in raffinate is very close to zero, graphically vertical axis and raffinate are almost overlapping)

c) Identical to b) but what is the minimum solvent flow in mol/h based on the UNIF-DMD data from Aspen.

d) Compare the consequence of minimum solvent rate to the design of extraction system if it is based on experimental or modelled LLE.

Use the following stream labels (composition in mole fraction) to help checking of answers



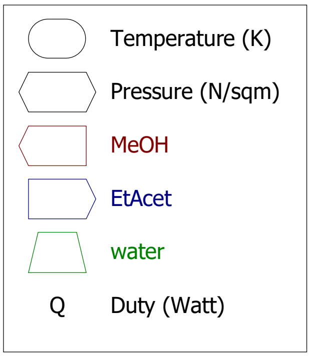
e) In practice it is better to have even smaller mole fraction in raffinate than the design specification in b). Make a graph of acetone mole fraction in raffinate as a function of ideal stages assuming the solvent flow of pure toluene is 1800 mol/h. Give comments on the composition profile, such as when increasing the number of stages gives only marginal effect of composition.

f) In the real process the solvent is recycled. What is the reason that prevents the acetone mole fraction in raffinate to be so low than in e)? Give comments on the density difference of the phases in this system.

Task 2

Upload files as “ETSPp1_exam9Dec2019_Task2_Familyname_Givenname.*” where * is the file type.

The ternary mixture of methanol + ethyl acetate + water is distilled at atmospheric pressure. Use the following stream labels (composition in mole fraction) to help checking of answers.



a) The feed into the distillation column is a mixture given in mole fraction methanol (z=0.15) + ethyl acetate (z=0.03) + water (z = 0.82) and at its boiling point. Assume the flow 0.001 kmol/s. Try to get one pure component (> 0.97 in mole fraction) out of the distillation column. Explain with the aid of distillation curve map (Distillation Synthesis is Aspen) what the bottom stream and the distillate streams can be and when the system is VLE or VLLE system.

b) Design and simulate the distillation column. Report the operating specifications, number of ideal stages, feed location, key component for the second liquid phase. Also plot the profiles, at least temperature, composition and flowrate.

c) Similar to a) but mixture is in mole fraction methanol (z=0.15) + ethyl acetate (z=0.67) + water (z = 0.18)

d) Similar to b)