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

Calculation Exam, 17th October 2022

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Answer both of the questions, 6 points per each question, 12 points in total.

Duration: 3 hours

Allowed material during the last 3 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

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The topic of removal of dilute acetic acid (abbr. HAc) in water is studied for several decades. One of the studies proposes butyl acetate (abbr. BuAcet) as solvent and data is given in Table 1. The reference is İnce and Kõrbaşlar, Liquid-liquid equilibria of the water-acetic acid-butyl acetate system, *Brazilian Journal of Chemical Engineering*, Vol. 19, No. 02, pp. 243 - 254

Table 1. *One row is a tie-line, data given in mole fractions. (given in Excel in MyCourses also)*

x'(BuAcet)	x'(HAc)	x'(water)	x"(BuAcet)	x"(HAc)	x"(water)	T/K	p/kPa
0.0032	0.0332	0.9636	0.7712	0.0872	0.1416	298.15	101.325
0.0035	0.0640	0.9325	0.6250	0.1561	0.2189	298.15	101.325
0.0054	0.0922	0.9024	0.5269	0.2079	0.2652	298.15	101.325
0.0088	0.1227	0.8685	0.4114	0.2466	0.3420	298.15	101.325
0.0178	0.1626	0.8195	0.3106	0.2768	0.4126	298.15	101.325
0.0272	0.1914	0.7814	0.2159	0.2774	0.5068	298.15	101.325

The feed into the continuous multistage counter current liquid-liquid extraction column is given in mole fractions. The feed is a mixture of acetic acid and water where x(acetic acid) = 0.1 and x(water) = 0.9. Solvent is pure butyl acetate.

a) Draw the Kinney-diagram where solvent is the horizontal axis and acetic acid the vertical axis.

b) The column is isothermal at 25 °C. The target mole fraction of acetic acid in raffinate is maximum x(acetic acid,raff) = 0.01. What is the minimum solvent to feed ratio into the column?

c) Select the UNIQ-HOC phase equilibrium model and import the following parameters into your Aspen simulation, shown in Table 2. The system is simulated at 298.15 K and at atmospheric pressure.

Table 2. *UNIQUAC model binary interaction parameters (given in Excel in MyCourses also)*

comp i	comp j		T unit	Aij	Aji	Bij	Bji
N-BUT-01	ACETI-01		K	0	0	-536.897	228.7023
N-BUT-01	WATER		K	0.978554	-1.53917	-805.444	313.9847
ACETI-01	WATER		K	1.235868	-2.89057	-88.7288	283.4795

Compare UNIQ-HOC model to the given data using Aspen software and draw the Kinney-diagram. The McCabe diagram (acetic acid in raffinate in horizontal and acetic acid in extract in vertical axis) in Excel is easier to draw. Does the model give more or less ideal stages for a specified solvent to feed rate than the experimental data?

d) If the feed is 1.0 mol/s, solvent 0.3 mol/s and the same raffinate specification applies, can you reach the raffinate specification with less or equal than 5 ideal (≤ 5) stages?

e) If you have an existing extraction column having 5 ideal stages, what would be the solvent flow to reach raffinate specification. Please, make a table of your testing to reach the raffinate specification.

f) We had the raffinate specification in b) due to graphical reasons. If you could have a 10 ideal stage column and solvent 0.4 mol/s, what would be the raffinate mole fraction and how many percent of moles of input acetic acid you would get into the extract?

Question 2

Design a continuous vacuum evaporative crystallization process for sucrose. Use Excel in Task (i) and Aspen Plus in Task (ii).

A saturated sucrose solution with total mass flow rate of 100 kg/h at 40 °C is fed to a MSMPR crystallizer. Crystal shape is cubic. Crystallizer volume is 2.5 m³. Use 74 mbar (boiling point approximately 40 °C) as pressure and 10 kW as heat duty (latent heat of evaporation about 2256 kJ/kg water). Kinetic parameters are $K_b = 1.6 \cdot 10^{10}$, $i = 0.92$, and $j = 1$ in $B = K_b\, G^i\, M_T^j$.

      i)   Calculate the vapor flow rate and product rate.
      ii)   Calculate crystal growth rate and dominate crystal size.

Solubility of sucrose (Mullin's *Crystallization*).

T, °C	c*, g of sucrose /100 g water
0	179
10	190
20	204
30	219
40	238
60	287
80	362
100	487