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

Course Exam 26.10.2021

Theory Part:

1. Significance of supersaturation in industrial crystallization.

2. Explain the operation principle of pressure swing distillation with the aid of schematic process flow diagram and the vapor-liquid-equilibrium diagrams.

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Calculation Exam, 26th October 2021

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Answer in the 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 production processes of iso-propanol (2-propanol, CAS 67-63-0) involves typically the separation of iso-propanol from water (CAS 7732-18-5). Unfortunately, there is an azeotrope of iso-propanol and water. Select UNIQUAC of Aspen with the default parameters as you model and use NIST/TDE.

a) What is the azeotropic mole fraction of iso-propanol and azeotropic temperature at atmospheric pressure? How much azeotropic mole fraction changes as pressure changes? Is pressure swing distillation possible? What would you comment on the liquid-liquid-equilibrium?

One alternative as an entrainer is diisopropyl ether (CAS 108-20-3). You are asked to study the phase equilibrium of binary and ternary systems

b) What information can be found for the phase equilibrium iso-propanol and diisopropyl ether? Prepare some graphs/diagrams comparing data and model and explain.

c) What information can be found for the phase equilibrium water and diisopropyl ether? Prepare some graphs/diagrams comparing data and model and explain.

d) There is a supplementary file "*ETSPp1_Exam_26Oct2021_Q1.xlsx*" containing phase equilibrium and density of ternary system. It makes your work easier, no need to upload the original publication of Acre (2000) et al. Compare UNIQUAC to this data and explain your findings.

REF: Alberto Arce, Alberto Arce, José Martínez-Ageitos, Eva Rodil, Oscar Rodríguez, Ana Soto, Physical and equilibrium properties of diisopropyl ether+isopropyl alcohol+water system, *Fluid Phase Equilibria*, Volume 170, Issue 1, 2000, Pages 113-126, ISSN 0378-3812, https://doi.org/10.1016/S0378-3812(00)00328-9.

e) Calculate the distillation synthesis of Aspen at atmospheric pressure. Is the distillation curve map qualitatively correct? What are the distillation regions and is there any ternary azeotrope? Which one is the dense phase and which one the less dense phase?

Question 2

Upload files as "ETSPp1_exam26Oct2021_Q2_Familyname_Givenname.*" where * is the file type.

Dilute acetic acid (CAS 64-19-7) in water (CAS 7732-18-5) is a typical case in the liquid-liquid-extraction. There have been many studies of solvent selection along the past decades. One solvent is toluene (CAS 108-88-3), a common industrial solvent, that was studied in 1979 by Salem.

REF: Salem A.B., *J. Chem. Eng. Japan*, (1979), vol. 12 p. 236.

The LLE data at 30 °C is given in "*ETSPp1_Exam_26Oct2021_Q2.xlsx*". Feed mole fraction of acetic acid is x(acetic acid) = 0.1 and the rest is water. The solvent is assumed as pure toluene. The maximum mole fraction of acetic acid in raffinate $x(\text{acetic acid})_{RN} = 0.02$. Because of the very low solubility toluene in water the raffinate in equilibrium is given to you. It is x(toluene) = 0.000211; x(acetic acid) = 0.02 and the rest is water.

a) What is the minimum solvent to feed ratio, S_{min} / F. Note! Don't waste your time in modifying the Excel template and hunting the last digits of decimals. Graphical schematic drawing is enough to generate the S_{min}/F for the simulation.

b) If you use solvent to feed ration that is 1.2 times the minimum in a) and there are 10 ideal stages, can you meet the raffinate specification? You can assume feed 1 mol/s. What is the raffinate mole fraction of all three components?

c) What is the density difference of liquid phases at the extraction column top and column bottom?

d) How much you need to increase the solvent to reach $x(\text{acetic acid})_{RN} = 0.004$? What is the weakness of toluene as a solvent?