

UNIVERSITY COLLEGE LONDON

University of London

EXAMINATION FOR INTERNAL STUDENTS

For The Following Qualifications:–

Coll Dip M.Eng.

Chemical Eng E875: Advanced Material Processes and Product Engineering

COURSE CODE : **CENGE875**

UNIT VALUE : **0.50**

DATE : **11-MAY-04**

TIME : **10.00**

TIME ALLOWED : **3 Hours**

Answer question 1 (PART A), one question from Part B and two questions from Part C; in total four questions.

*The maximum mark of question 1 (PART A) is 30 marks, distributed as indicated [].
The maximum mark of each question of Part B is 20 marks, distributed as indicated [].
The maximum mark of each question in Part C is 15 marks, distributed as shown [].
The total maximum mark is 80.*

PART A

1.

Derive the following equation for the solubility, expressed as mole-fraction, of a solid compound (2) in a supercritical fluid (1):

$$y_2 = \frac{P_2^{sat}}{P} \frac{\varphi_2^{sat} \exp\left\{ \int_{P_2^{sat}}^P \frac{v_2^s}{RT} dP \right\}}{\varphi_2}$$

where P_2^{sat} is the sublimation pressure of 2 at the temperature T , P is the total pressure, φ_2^{sat} is the fugacity coefficient of 2 as saturated vapour at temperature T , φ_2 is the fugacity coefficient of 2 in the supercritical phase at temperature T , v_2^s is the molar volume of component 2 as a solid and R is the universal gas constant ($R = 8.314 \text{ J mol}^{-1} \text{ K}^{-1} = 83.14 \text{ bar cm}^3 \text{ mol}^{-1} \text{ K}^{-1}$). [7]

The fugacity coefficient φ_2 is given by the following formula using the Peng - Robinson Equation of State:

$$\ln \varphi_2 = \frac{b_2}{b_{mix}} \left(\frac{pV_m}{RT} - 1 \right) - \ln \left(\frac{p(V_m - b_{mix})}{RT} \right) - \frac{a_{mix}}{2\sqrt{2}b_{mix}RT} \left(\frac{2 \sum_i y_i a_{i2}}{a_{mix}} - \frac{b_2}{b_{mix}} \right) \times \ln \left(\frac{V_m + (1 + \sqrt{2})b_{mix}}{V_m + (1 - \sqrt{2})b_{mix}} \right)$$

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1. continued

Making reasonable assumptions simplify this formula to the following one:

$$\ln \phi_2 = \ln \left(\frac{RT}{(V_m - b_1)P} \right) + \frac{b_2}{b_1} \left(\frac{PV_m}{RT} - 1 \right) - \frac{a_1}{2\sqrt{2}RTb_1} \left(\frac{2a_{12}}{a_1} - \frac{b_2}{b_1} \right) \times \ln \left(\frac{V_m + (1 + \sqrt{2})b_1}{V_m(1 - \sqrt{2})b_1} \right) \quad [4]$$

Use the equation for the solubility and the above simplified formula for ϕ_2 , in order to calculate the solubility of a component (2) with the following properties in supercritical CO₂ (1), at two temperature levels, 305 K and 315 K, and two pressures, 65 bar and 80 bar, each time (four sets of conditions):

$$P_2^{sat} \text{ at } 305 \text{ K: } 6.5 \times 10^{-6} \text{ bar, } P_2^{sat} \text{ at } 315 \text{ K: } 12.9 \times 10^{-6} \text{ bar,}$$

$$v_2^s = 138.2 \text{ cm}^3 \text{ mol}^{-1}$$

Critical Pressure and Temperature of component 2: 30 bar and 826 K

Accentric factor of component 2: $\omega_2 = 0.406$.

Additional Data: Critical Pressure and Temperature of CO₂: 73.8 bar and 304.1 K

Accentric factor of CO₂: $\omega_1 = 0.225$

Interaction coefficient between CO₂ and 2: $k_{12} = 0.09$

In order to calculate ϕ_2 you may use the PV plot for CO₂ on the following page.

[15]

Calculate the ratios of the solubility at 80 bar over this at 65 bar for both temperatures. Compare the ratios and comment on your results.

[4]

For any part of question 1, you may use the following equations:

$$\ln \phi_2 = \int_0^P \left[\frac{v_2}{RT} - \frac{1}{P} \right] dP$$

Peng - Robinson Equation of State:

$$P = \frac{RT}{V_m - b} - \frac{a}{V_m^2 + 2bV_m - b^2}$$

$$\text{where } a = \frac{0.45724RT_c^2}{P_c} \left(1 + f\omega \left(1 - \sqrt{\frac{T}{T_c}} \right) \right)^2$$

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1. continued

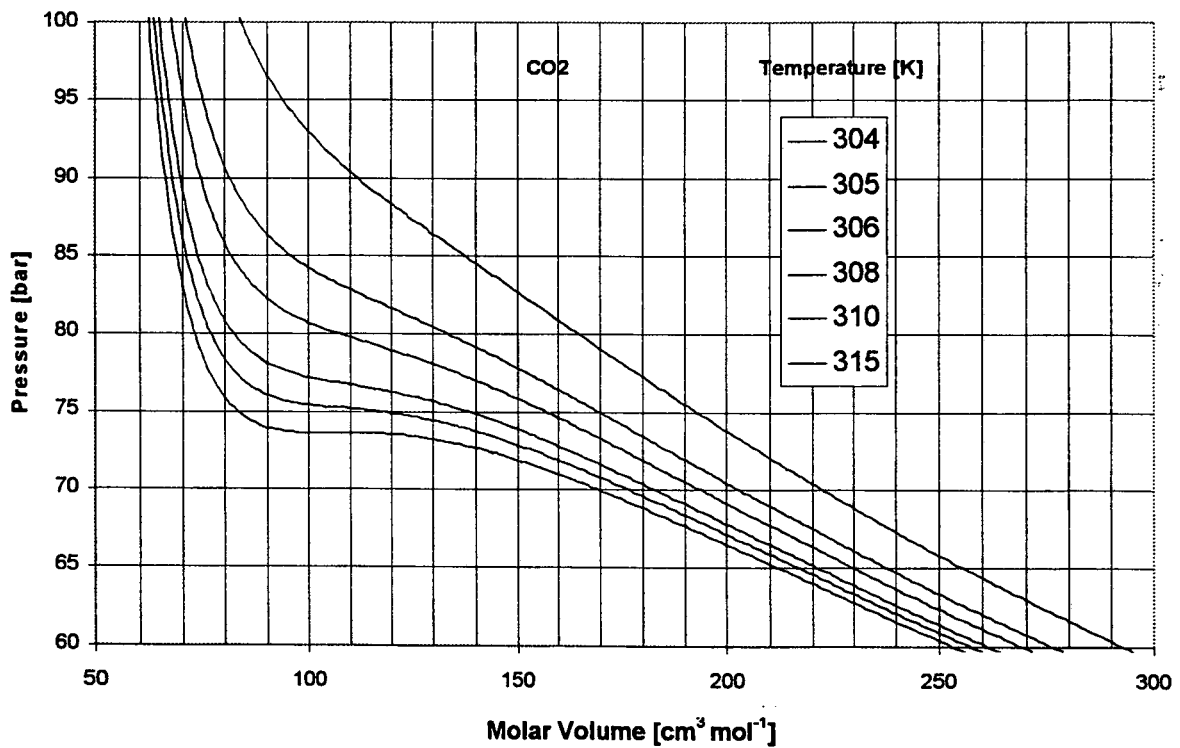
$$f\omega = 0.37464 + 1.54226\omega - 0.26992\omega^2$$

$$b = \frac{0.07780RT_c}{P_c}$$

$$b_{mix} = \sum_i y_i b_i$$

$$a_{mix} = \sum_i \sum_j y_i y_j a_{ij} (1 - k_{ij})$$

$$a_{ij} = (a_i a_j)^{1/2}$$



PLEASE TURN OVER

PART B

2.

How do red phosphorus and phosphorus compounds act as a flame retardant? [6]

Halogen-containing formulations are widely used as flame retardants. Explain their retardation mechanism and why attempts are being made to replace them. [6]

Describe the general mechanisms involved in polymer decomposition. [4]

What is meant by the following terms in relation to chain-scission mechanisms:

- i) Intramolecular H-Transfer
- ii) Intermolecular H-Transfer

Use reaction schemes in your answer. [4]

3.

Explain the principle of lithography, as well as the terms positive and negative resist. [6]

Draw a typical sensitivity curve and define the term contrast for both resist types. [4]

Derive an equation describing the dependence of the average molar mass of the resist upon the radiation dose in lithography. [7]

Define the characteristic quantity G and explain how it can be estimated. [3]

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PART C

- 4.
- a) What is a concept combination table? Explain how it works, its usefulness and useful guidelines. [5]
 - b) Name and briefly describe the steps of concept screening and concept scoring. Explain the differences between the corresponding steps. [10]
- 5.
- a) Name and briefly explain the ways of prototypes classification. [4]
 - b) Name and briefly discuss the five principles of prototyping. [7]
 - c) Name and briefly discuss the steps in planning for prototypes. [4]
- 6.
- a) Give a schematic overview of the Design for Manufacturing (DFM) methodology. [5]
 - b) In the framework of DFM, describe briefly the methodology for estimating manufacturing costs. Explain the terms of fixed costs and variable costs. What is the bill of materials? [10]

END OF PAPER