

UNIVERSITY COLLEGE LONDON

University of London

EXAMINATION FOR INTERNAL STUDENTS

For The Following Qualification:–

M.Eng.

Chemical Eng E875: Advanced Material Processes and Product Engineering

COURSE CODE : CENGE875

UNIT VALUE : 0.50

DATE : 19–MAY–06

TIME : 10.00

TIME ALLOWED : 3 Hours

Please answer **Question 1 (Part A)**, **one question from Part B** and **two questions from Part C**; in total four questions. Only the first 4 questions answered will be marked.

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 indicated.
The total maximum mark is 80.
 Graph Paper Provided

PART A

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

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

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]

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

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

CONTINUED

Making reasonable assumptions simplify this formula to the following one:

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

- iii) 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 (four sets of conditions):

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

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

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

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

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

Acentric 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 in the following page. [15]

- iv) 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:

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

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

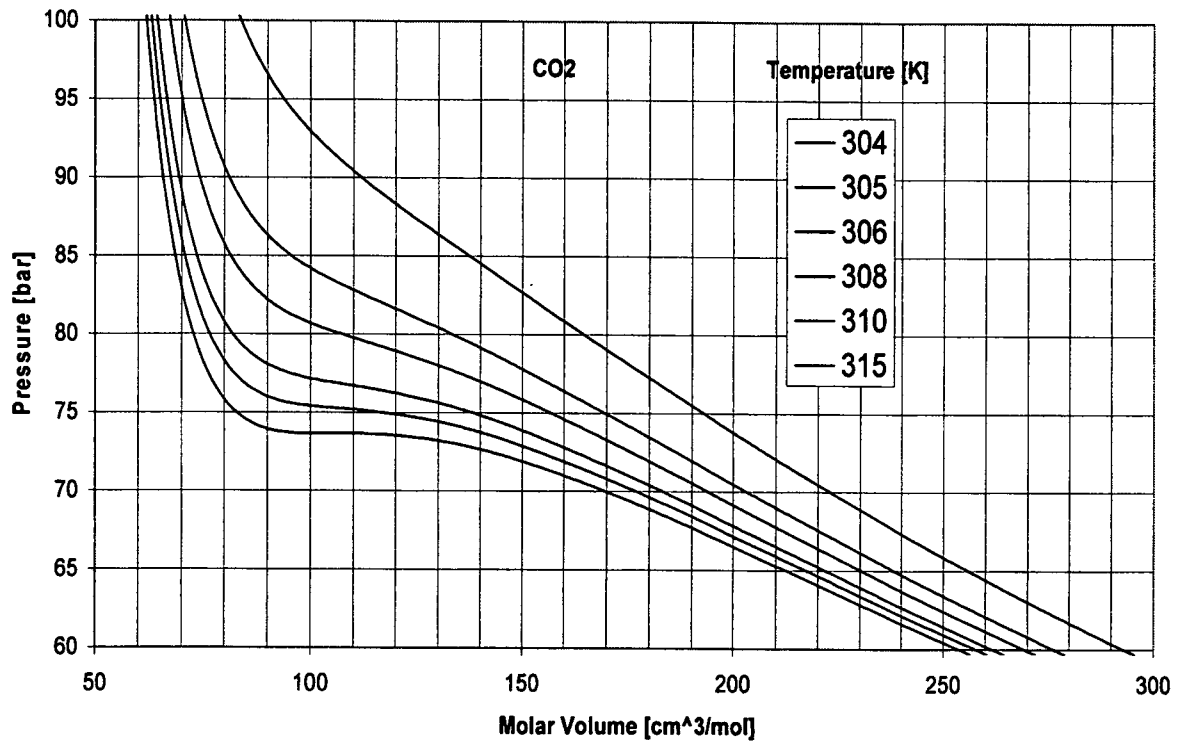
$$f\omega = 0.37464 + 1.54226\omega - 0.26992\omega^2$$

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

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

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

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



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PART B

2.

- i) What is the kinetic effect of pressure on chemical reactions? Explain its origin and name the characteristic quantity that determines the kinetic effect. [5]
- ii) Explain the solvent effect of pressure on chemical reactions and its origin. Based on that, explain the dramatic effect of pressure on chemical reactions in near critical and supercritical media. [5]
- iii) Describe the mechanism of intumescence in flame retardant coatings. [10]

3.

- i) Explain the principle of lithography, as well as the terms positive and negative resist. [5]
- ii) Draw a typical sensitivity curve and define the term contrast for both resist types. [5]
- iii) Present a schematic model of polymer dissolution and formulate the differential equations describing the process. [10]

PART C

4.

- i) Name and briefly describe the steps of concept generation. [10]
- ii) Expand further on concept classification tree and concept combination table. [5]

5.

- i) Name and briefly describe the steps of concept screening and concept scoring. Explain the differences between the corresponding steps. [10]
- ii) Give a schematic overview of the Design for Manufacturing (DFM) methodology. [5]

6.

- i) Name and briefly explain the ways of prototypes classification. [4]
- ii) Name and briefly discuss the five principles of prototyping. [7]
- iii) Name and briefly discuss the steps in planning for prototypes. [4]

END OF PAPER