

Uva Wellassa University, Sri Lanka
Faculty of Science and Technology
Science and Technology Degree Programme
1st Semester Examination – March/April 2013



SCT 331-3 Materials Chemistry I

Instructions to candidates

Total number of questions = Four (04)

Answer all questions

Time allocation: Three (03) hours

Total marks allocated: 400

1.

- a. State the van der Waals equation of state for a real gas. Identify all terms therein. (20 marks)
- b. Plot the P-V isotherms of carbon dioxide at different temperatures. Your answer should show the variation of isotherms (i) Above the critical temperature, (ii) At the critical temperature, and (iii) Below the critical temperature of CO₂. (20 marks)
- c. Plot the same family of P-V curves of CO₂ accordance to van der Waals equation. Identify the van der Waals loop and show a method of correcting this effect (no mathematical derivations are required). (20 marks)
- d. The critical constants of CO₂ is given as $P_c = 73.843$ bar, $V_c = 0.094$ (L.mol⁻¹), and $T_c = 304.14$ K. Calculate the compressibility factor and the van der Waals parameters of CO₂. Briefly explain the answer you obtained for compressibility factor. (20 marks)
- e. State the law of corresponding state of gases. (20 marks)

2.

- a. Maxwell Boltzmann distribution of speeds of gas molecules is given by the following equation:

$$F(u)du = \left(\frac{m}{2\pi k_b T} \right)^{3/2} u^2 e^{-mu^2 / 2k_b T} du$$

Identify all terms therein. Plot the distribution of the velocity of a given gas according the Maxwell Boltzmann distribution.

(20 marks)



b. State the physical meaning of following expressions:

i. $\int_{v_1}^{v_2} uF(u).du$

ii. $\int_0^\infty F(u).du$

iii. $\int_0^\infty uF(u).du$

iv. $\int_0^\infty u^2F(u).du$

Write simplified expressions of the integrals (ii), (iii) and (iv) (no mathematical derivations are needed).
(20 marks)

c. Define following terms: (i). collision cross section, (ii). reactive collision cross section. Write mathematical expressions for each of these parameters.

(10 marks)

d. State two assumptions made in the formulation of transition state theory. Consider following reaction in gas phase:

Prove that $k = k_b/h K^\ddagger$ where k is the rate constant of $A + B = C + D$ where all symbols carry standard meanings.

(40 marks)

e. The E_a and pre-exponential factor for a reaction $A_2 + B_2 = 2AB$ are 15.5 kJ.mol^{-1} and $10.9 \times 10^{10} \text{ dm}^3\text{mol}^{-1}\text{sec}^{-1}$ respectively. Calculate $\Delta H^\ddagger$ and $\Delta S^\ddagger$ at 1000 K .

(10 marks)

3.

a. Define following terms:

i. Steady state diffusion

ii. Transient state of diffusion

(10 marks)

b. State Fick's 2nd law of diffusion. Define all terms.

(10 marks)

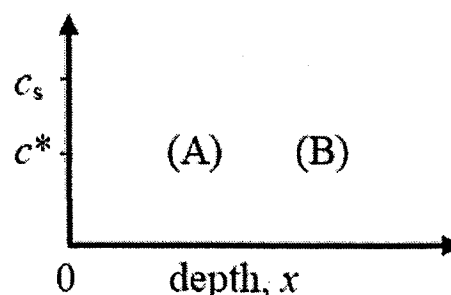
c. Fick's 2nd law has following solution

$$\frac{c_2 - c}{c_2 - c_2'} = \text{erf} \left(\frac{x}{2\sqrt{Dt}} \right)$$

State the initial and boundary conditions imposed to attain this solution. Simplify your answer when $\text{erf}(z) \sim z$.

(20 marks)

d. Specimens of steel are being surface hardened by the introduction of carbon. The concentration of carbon at the free surface of the steel is kept constant at c_s . Chemical analysis of a number of specimens indicates that after time, t , the carbon concentration has a value of c^* at a depth from the surface, x , shown below at (A), and that after time



$t_2 = 2t_1$, the carbon concentration has a value of c^* at a depth $x_2 = 2x_1$, shown below at (B).

Under these conditions, would you describe the rate of carburization as: *steady state diffusion*; *transient state diffusion*; or *not governed by diffusion*. i.e., rate limited by some other process.

Justify your choice. (Hint: plot concentration profiles at given times. Use the simplified derivation shown in section c)

(60 marks)

4.

- a. State the flux of current density, heat and mass transport according to Fick's 1st law.
(20 marks)
- b. Explain the process of self diffusion. How is this process experimentally measured?
(20 marks)
- c. Aluminum is to be diffused into a silicon single crystal. At what temperature will the diffusion constant (D) be $5 \times 10^{-11} \text{ cm}^2/\text{s}$? (Given: $E_A = 315 \text{ kJ/mole}$ and $D_0 = 1.70 \text{ cm}^2/\text{s}$).
(30 marks)
- d. Explain the role of catalytic convertor used in automobiles for pollution control.
(30 marks)