Ex/MET/T/314/2019

Bachelor of Metallurgical Engineering 3rd Year 1st Semester Examination, 2019

Chemical Kinetics and Mass Transfer

Time: Three Hours Full Marks-100

Answer question no. 1 and any four from the rest

1. a) Considering the following reaction to be an elementary one,

$$AlCl_3\,(g) + H_2\,(g) \underset{k_b}{\overset{k_f}{\rightleftarrows}} 2HCl\,(g) + AlCl\,(g)$$

(both k_f and k_b refer to $AlCl_3$)

Find the expression for r_{HCl}. 2

b) The total pressure in a closed reactor in which pure AB fed at 1 atm undergoes the 2nd-order irreversible reaction

$$2AB \xrightarrow{k} A_2B_2$$

decreases to 0.8 atm in 5 mintes at 500 K. Determine k. 4

c) According to the activated complex theory for the gas-phase reaction

$$A\,(g) + B\,(g) \xrightarrow{k} AB\,(g) \qquad (1),$$

the two-step reaction mechanism is

i) $A\,(g) + B\,(g) \overset{eqbm}{\leftrightarrow} AB^*\,(g)$

ii) $AB^*\,(g) \xrightarrow{k'} AB\,(g)$

If the thermodynamic equilibrium constants, K_e, for step i) are 10^{-10} and 10^{-8} at 1000 K and 1200 K, respectively, find the (approximate) value of the activation energy of Reaction (1). 4

d) Distinguish between

i) integral and differential methods of batch reactor data analysis
ii) plug flow reactor and mixed flow reactor 4

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e) Consider the following nonelementary homogeneous reaction with order n = 1/3:

$$A \xrightarrow{k} B.$$

Find its integrated form of rate equation (X_A vs t). Explain with the help of a suitable plot how you will find out the rate constant k. 4

f) Consider the following 2-step series reaction taking place in gas phase:

i) $2A \overset{eqbm}{\leftrightarrow} R + S \qquad K_c = 4$

ii) $R + S \rightarrow 2T$

Consider that the reaction starts with $C_{A0} = 10$ mol/m^3, $C_{R0} = C_{S0} = 2$ mol/m^3, and $C_{T0} = 0$. Plot C_A, C_R, C_S and C_T each vs t in four separate figures. Range the concentration scale (y-axis) from 0 to 20 mol/m^3 and time scale (x-axis) from zero to (tending to) infinity. 6

g) Under what physico-chemical conditions of the system does a steady state diffusion occur? Why do we consider a semi-infinite sample for an unsteady state diffusion? How will you contrast a steady state, pseudo steady state, and unsteady state diffusion? 5

h) How many minimum data points are required to ascertain a rate controlling mechanism of a gas-solid reaction with the help of i) a conventional linearity plot and ii) reduced time plot? Give the most distinct advantage of each plot over the other. 4

i) Write the equation of continuity in 3-dimensionsal mass transfer in the rectangular co-ordinate system (x, y, z). Give the physical significance of the equation. 3

j) Consider the unidirectional carburization of iron at 1000 ^{0}C in which the surface of the initially pure iron is brought in contact with a carburizing gas at time t = 0,which instantaneously raises the concentration of carbon in the iron at the surface to C_{is}. The value of C_i / C_{is} is found to be 0.28 at x=5 mm after 1 hr of carburization. Find C_i / C_{is} at x=9 mm after 2 hr of carburization.
Given, erfc (0.761) = 0.28 4

2. Refer to the problem of diffusion-controlled evaporation of liquid A (say, Zn) into a stagnant inert gas B (say, Ar). See Figure 1. If the tube is not replenished for the liquid

lost through evaporation, the liquid level will continuously go down. Show that the time required for the whole liquid to evaporate is given by

$$t_{z1=0} = \frac{\rho_{m,A}\left[z_2 z_{1(0)} - \frac{z_{1(0)}^{\;2}}{2}\right]}{cD_{AB} \ln \frac{x_{B2}}{x_{B1}}},$$

where $z_{1(0)}$ is the z_1 at t = 0 and $\rho_{m,A}$ is the molar density of liquid A. The system is under constant temperature and pressure. 15

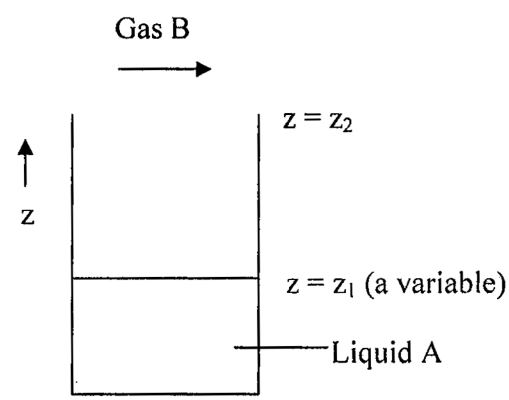

Fig. 1

3. Consider the following homogeneous, elementary reactions taking place in series. The reactions are carried out in a constant-volume batch reactor, at temperature T, in which A is initially charged with the concentration C_{A0}.

$$A \xrightarrow{k_1} R \xrightarrow{k_2} S$$

Derive an expression for each of i) C_S, ii) dC_S/dt, and iii) d^2C_S/dt^2 in terms of k_1, k_2, C_{A0}, and t. Also, plot each of the above three vs t. 15

4. A dense, spherical FeO pellet with 0.02 m initial diameter is reduced by a stream of 80% CO-20% CO_2 mixture at 940 K and 1 atm total pressure. Consider that the reduction is rate controlled by pore diffusion. The C_{CO} vs 1/r plot, in the range $1/r^0_{FeO}$ to $1/r_{FeO}$, yields a slope of -0.1 mol/m^2 at time $t = t_1$. Find, at $t = t_1$,

i) fractional reduction of FeO
ii) the mass of the reduced pellet
iii) the individual mass of Fe and FeO each in the reduced pellet.

Data: i. $FeO(s) + CO(g) = Fe(s) + CO_2(g)$, $\Delta G^0 = -22800 + 24.26\,T$ J
ii. Mass density of FeO = 5.7 gm/cc. 15

5. a) Consider the 2-dimensional mass transfer problem of the dissolution of a flat plate (A) in a flowing liquid (B), with limited solubility of A in B. Derive an expression for the local mass transfer coefficient ($h_{m,x}$) in terms of the diffusivity (D_{AB}), Schmidt No. (Sc), average velocity of the mixture (v_x^*), kinematic viscosity (ν), and location (x). 9

b) Derive the following 3-dimensional equation of diffusion with convection for A in binary mixture A-B in terms of cylindrical co-ordinates (r, θ, z):

$$\frac{\partial C_A}{\partial t} = -\left[\frac{1}{r}\frac{\partial}{\partial r}(rN_{Ar}) + \frac{1}{r}\frac{\partial N_{A\theta}}{\partial \theta} + \frac{\partial N_{Az}}{\partial z}\right]$$ 6

6. i) Show that the molar flux of a species in a mass transfer system can be expressed as the product of concentration and velocity of the species. 3

ii) Consider the steady state evaporation of liquid A taken in a rectangular tube into the stagnant film of B formed by pure B flowing over the tube. The concentration profiles (C_i vs z) of A and B are found to be nonlinear. Explain under what condition the profiles can be approximately linear. Find the relation between N_{Az} and J^*_{Az} under this condition. 4

iii) At 773 K, a diffusion experiment indicates that 3 out of 10^{10} atoms have enough activation energy to jump out of the lattice site into an interstitial position. At 873 K, 4 out of 10^8 acquire the same. What is the activation energy for this jump? 3

iv) In the following 1st-order irreversible series reaction

$$A \rightarrow R \rightarrow S,$$

the input concentration C_{A0} in a constant-volume reactor can be written in terms of the instantaneous concentrations as

$$C_{A0} = C_A + C_R + C_S.$$

How will you express the C_{A0} if the reaction stoichiometry changes to

$$A \rightarrow \alpha R \rightarrow \beta S\ ?$$ 3

v) Find the unit of the rate constant of a half-order homogeneous reaction. 2
