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Ex/MET/T/314/2017(S)

Bachelor of Metallurgical Engineering 3rd Year 1st Semester Examination, 2017
(Supplementary)

Chemical Kinetics and Mass Transfer

Time: Three Hours | Full Marks-100

Answer any Five questions.

1. i) The rate of a 2nd-order reaction is given as

$$r_A = 4\ C_A^2,\ \text{mol/liter.hr}$$ 5

What is the value and unit of the rate constant? If the rate is expressed in mol/cm^3.sec and concentration in mol/cm^3, how will the value and unit of the rate constant change?

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

$$2AB \xrightarrow{k} A_2B_2$$ 7

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

iii) After 8 minutes in a batch reactor, reactant (C_{A0} = 1 mol/liter) is 80% converted; after 18 minutes, conversion is 90%. Find a rate equation representing this reaction. (Note, A trial and error solution may be necessary.) 8

2. i) Consider a gas phase reaction 2A + B → A_2B which takes place according to the following 2-step mechanism:

i. $$A + B \underset{k_2}{\overset{k_1}{\rightleftarrows}} AB^*$$

ii. $$AB^* + A \xrightarrow{k_3} A_2B$$

If the initial concentrations are C_{A0} = 10 mol/m^3 and C_{B0} = 5 mol/m^3, find the value of C_{A2B} at t = 30 sec, when the reaction is carried out in a constant-volume batch reactor at temperature T. Given, k_1 = 0.02 m^3/mol.sec, k_2 = 3 sec^{-1} and k_3 = 6 m^3/mol.sec. 15

ii) Establish the following design equations for a steady-state mixed flow reactor:

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \frac{X_A}{-r_A}.$$ 5

3. i) Consider the following 2nd-order homogeneous reaction:

$$A + B \xrightarrow{k} AB$$ 5

Using the following data, determine the activation energy (E) of the reaction.

T, K	C_A, mol/lit	C_B, mol/lit	$-dC_A/dt$, mol/lit.min
1000	5	3	0.3
1500	5	2	1.0

ii) Consider the evaporation of liquid Zn taken in a rectangular tube into the stagnant film of argon formed by pure argon flowing over the tube at 764 ^{0}C and 1 atm. Given, the saturated vapor pressure of liquid Zn at 764 ^{0}C is 0.5 atm, $Z_2 - Z_1 = 0.02$ m, and $D_{Zn\text{-}Ar}$ (at 764 ^{0}C) = 1.43×10^{-4} m^2/s. Find

a) $J^*_{Ar(-Z),Z1}$
b) $V_{Zn,Z,Z1}$ 15

4. Consider the reduction of a dense cylindrical FeO sample ($L>>r$)) with a flowing mixture of CO-CO_2 mixture, which is controlled by 1-dimensional pore diffusion in the r-direction though the product (Fe) layer. The reduction reaction is

$$FeO\ (s) + CO\ (g) = Fe(s) + CO_2\ (g).$$

i) Show that the molar rate of reduction of FeO, $-dn_{FeO}/dt$, can be expressed as follows:

$$-dn_{FeO}/dt = \frac{2\pi L(C_{CO,b} - C_{CO,e})D_{pore}}{\ln(r^0_{FeO}/r_{FeO})},$$

where r^0_{FeO} is the initial radius of the cylinder having the length L. 10

ii) Show that the progress of the reduction can be expressed as

$$X_{FeO} + (1 - X_{FeO})\ln(1 - X_{FeO}) = \frac{4D_{pore}(C_{CO,b} - C_{CO,e})t}{\rho_{m,FeO}.(r^0_{FeO})^2}.$$ 10

5\. i) The following table shows the data for the half-life period ($t_{1/2}$) versus the initial concentration of reactant A (C_{A0}) for the reaction, A → Products.

$\log C_{A0}$	10	20	30
$\log t_{1/2}$	30	35	40

Find the order of the reaction. 5

ii) Refer to the problem of dissolution of a flat plate (A) in a flowing fluid (B). If the local Sherwood Number at x = 0.5 m is 1000 and D_{AB} = 1.2 × 10^{-8} m^2/s, determine the steady rate of dissolution W_{A_P} (mole/time) of the plate. Given,

L = 1 m W (width of the plate) = 0.3 m
C_{As} = 40mol/m^3 $C_{A\infty}$ = 0. 7

iii) Considering the following 1st-order reversible reaction

$$A \underset{k_b}{\overset{k_f}{\rightleftarrows}} B, \quad M = C_{B0} / C_{A0},$$

derive the rate equation 8

$$-\ln \left(\frac{C_A - C_{Ae}}{C_{A0} - C_{Ae}} \right) = At, \text{ where } A = f(k_f, C_{A0}, M, C_{Ae}).$$

6\. i) Give the two basic postulates, one thermodynamic and the other kinetic, of the activated complex theory. 3

ii) Give one metallurgical example for
   (a) series reactions
   (b) parallel reactions 3

iii) Give an example in which the term "order" does not apply in the rate equation of the reaction. 3

iv) Superimpose the ln k vs $1/T$ plots for the two reactions, P → Q and M → N, for each of the following two cases:

(a) $A_{P \to Q} = A_{M \to N}$, $E_{P \to Q} < E_{M \to N}$

(b) $E_{P \to Q} = E_{M \to N}$, $A_{P \to Q} < A_{M \to N}$. 5

v) Consider the half-order nonelementary homogeneous reaction

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

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. 6
