Ph.D. Qualify Exam for Advanced Chemicai Reaction Engineering

(Department of Chemical Engineering, National Taiwan U of Science and Technology)

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Part I

1. (15%)

For a very rapid reaction taking place on a catalyst particle surface, (a) calculate the minimum mass flux of reactant A to a single catalyst pellet 1 cm in diameter suspended in a large body of liquid and (b) calculate the rate of reaction per unit surface area of catalyst. The reactant in the bulk fluid is 1 mol dm^{-3}, the diffusivity of A is 10^{-10} m^2 s^{-1}, and the kinematic viscosity of the continuous liquid phase is 0.5 cS.

2. (20%)

Propose and verify a gas-solid catalytic reaction mechanism that is consistent with the following experimentally observed reaction rate law for the reaction A + B ———> C.

$$-r_A' = k(P_A P_B - P_C/K)/(1 + K_A P_A + K_C P_C)$$

where $-r_A'$ is the rate of consumption of A per unit mass of catalyst, P_A, P_B and P_C are the partial pressures of A, B and C, respectively, k is an apparent reaction rate constant and K, K_A and K_C are equilibrium constants.

3. (15%)

(a) What is the physical meaning of the Thiele modulus? (b) What is the definition and physical meaning of internal effectiveness factor? (c) Comment on the values of the internal effectiveness factor when the Thiele modulus is greater than 30. Which step is the rate-limiting step in this gas-solid catalytic reaction system?

Part II.

4. (20%)

The elementary irreversible organic liquid-phase reaction

$$A + B \rightarrow C$$

is carried out adiabatically in a flow reactor. An equal molar feed in A and B enters at 27°C, and the volumetric flow rate is 2 dm^3/s.

Calculate the PFR and CSTR volumes necessary to achieve 85% conversion.

Additional information:

$H_A^0(273) = -20$ kcal/mol

$H_B^0(273) = -15$ kcal/mol

$H_C^0(273) = -41$ kcal/mol

$C_{A0} = 0.1$ kmol/m^3

$C_{PA} = C_{PB} = 15$ cal/mol.K $\qquad C_{PC} = 30$ cal/mol.K

$k = 0.01$ dm^3/mol.s at 300K $\qquad E = 10{,}000$ cal/mol

Hint: For adiabatic operation of a CSTR or a PFR with negligible stirring work, the energy balance equation can be written as

$$-X[\Delta \hat{H}^0_{RX}(T_R) + \Delta \tilde{C}_p(T-T_R)] = \Sigma\, \theta_i C_{pi}(T-T_{i0})$$

Show All Your Work.

5. (15%)

Compound A undergoes a reversible isomerization reaction, A ⇔ B, over a supported metal catalyst. Under pertinent conditions, A and B are liquid, miscible, and of nearly identical density; the equilibrium constant for the reaction (in concentration units) is 5.8. In a *fixed-bed isothermal flow reactor* in which backmixing is negligible (i.e. plug flow), a feed of pure A undergoes a net conversion to B of 55%. The reaction is elementary. If a second, identical flow reactor at the same temperature is placed downstream from the first, what overall conversion of A would you expect if the reactors are directly connected in series.

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6. (15%)

The following liquid-phase reactions were carried out in a CSTR at 325K.

3A → B+C	$-r_{1A} = k_{1A} C_A$	$k_{1A} = 0.7$ min^{-1}
2C + A → 3D	$r_{2D} = k_{2D} C_C^2 C_A$	$k_{2D} = 0.3$ dm^6/(mol^2.min)
4D+3C → 3E	$r_{3E} = k_{3E} C_D C_C$	$k_{3E} = 0.2$ dm^3/(mol.min)

The concentrations measured *inside* the reactor were $C_A = 0.10$, $C_B = 0.93$, $C_C = 0.51$, and $C_D = 0.049$ all in mol/dm^3.

(a) What are the net rates of formation of A, B, C, D, and E?

(b) The entering volumetric flow rate is 100 dm^3/min and the entering concentration of A is 3 M. What is the CSTR reactor volume?

Show All Your Work.