Ph.D. Qualifying Examination

Advanced Chemical Reaction Engineering (Part I)

1. Derive a reactor design equation for the continuous stirred tank reactor (CSTR) and plug flow reactor (PFR), respectively, based on the general mole balance equation $F_{j0} - F_j + \int r_j \, dV = dN_j/dt$. Indicate all the assumptions used in the derivation. (10%)

2. The elementary reaction $A_{(l)} + B_{(l)} \xrightarrow{k} C_{(l)} + D_{(l)}$ is carried out in a reaction system comprising a CSTR (1) and a PFR (2) in series. Size this system provided that $C_{A0} = 0.01$ mol/L, $C_{B0} = 1$ mol/L, $v_0 = 1$ L/s, $F_{A1} = 0.005$ mol/s, $X_2 = 0.8$ and $k = 0.01$ L/mol-s. (15%)

3. Derive a reaction rate law for the formation of HBr ($H_2 + Br_2 \longrightarrow 2HBr$) based on the following mechanism:

   Initiation: $Br_2 \xrightarrow{k1} 2\,Br^*$

   $Br^* + H_2 \xrightarrow{k2} HBr + H^*$

   Propagation: $H^* + Br_2 \xrightarrow{k3} HBr + Br^*$

   $H^* + HBr \xrightarrow{k4} H_2 + Br^*$

   Termination: $2\,Br^* \xrightarrow{k5} Br_2$

   where Br* and H* are free radicals. (20%)

4. For batch, semibatch and CSTR systems, list their average residence time in decreasing order. (5%)

5. A slug of dye is placed in the feed stream to a stirred reaction vessel operating at steady state. The dye concentration in the effluent stream was monitored as a function of time to generate the data in the table below. Time is measured relative to that at which the dye was injected. Determine the average residence time of the fluid for this system. (16%)

Time, t (s)	Tracer concentration (g/m^3)
0	0.0
120	6.5
240	12.5
360	12.5
480	10.0
600	5.0
720	2.5
840	1.0
960	0.0
1080	0.0

6. The first order reaction A$\longrightarrow$B was carried out over two different-sized pellets. The pellets were contained in a spinning basket reactor that was operated at sufficiently high rotation speeds that external mass transfer resistance was negligible. The results of two experimental runs made under identical conditions are as given in the following table. Estimate the Thiele modulus for each pellets.(18%)

	Measured rate (obs) (mol/g cat·s) x 10^{5}	Pellet radius (m)
Run 1	3.0	0.01
Run 2	15.0	0.001

$$\frac{-r'_{A(obs)} R^2 \rho_c}{D_e C_{As}} = \eta \phi_1^2$$

$$\eta \phi_1^2 = 3(\phi_1 \coth \phi_1 -$$

$$\phi_1 \equiv R\sqrt{\frac{-r'_{As}\rho_c}{D_e C_{As}}}$$

7. The elementary irreversible gas-phase catalytic reaction

$$A \xrightarrow{k_1} B$$

$$-\frac{dX_A}{dt} = \frac{-r'_A W}{C_{A0} V_0}$$

is carried out isothermally in a batch reactor. The catalyst deactivation follows a first-order decay law and is independent of the concentration of both A and B

. Derive an expression for conversion as a function of time, the reactor parameters and the catalyst parameters. (16%)