Advanced Chemical Reaction Engineering

2004 PhD Qualification

(closed book)

1. A homogeneous gas-phase decomposition reaction 4A --->R + 6S is proceeding in a plug flow reactor at 1200°F with first-order rate $-r_A = kC_A$, where k = 10/hr. What size of plug flow reactor operating at 1200°F and 4.6 atm can produce 80% conversion of a feed consisting of 4 lbmoles of pure A per hour. (10%)
(Note: Gas constant R = 0.729 (ft^3)(atm)/(lbmole)(°R))

2. A homogeneous liquid-phase reaction A ---> R $-r_A = kC_A^2$ takes place with 50% conversion in a mixed reactor. What will be the conversion if the original reactor is replaced by a plug flow reactor of equal size --- all else remaining unchanged? (10%)

3. An isothermal, constant-pressure PFR is design to give a conversion of 63.2% of A to B for the first-order gas-phase decomposition A ----> B for a feed of pure A at a rate of 5 ft^3/h. At the chosen operating T, the first-order rate constant k = 5.0/h. However, after the reactor is installed and in operation, it is found that conversion is only 92.7% of the desired conversion. This discrepancy is thought to be due to a flow disturbance in the reactor that gives rise to a zone of intense backmixing. Assuming that this zone behaves like a CSTR in series and in between two PFRs, what fraction of the total reactor volume is occupied by this zone? (15%)

4. A total of 2500 gal/h of metaxylene is being isomerized to a mixture of orthoxylene, metaxylene, and paraxylene in a reactor containing 1000 ft^3 of catalyst. The reaction is being carried out at 750 F and 300 psig. Under these conditions, 37% of the metaxylene fed to the reactor is isomerized. At a flow rate of 1667 gal/h, 50% of the metaxylene is isomerized at the same T and P. It is now proposed that a second plant be built to process 5500 gal/h of metaxylene at the same T and P. What size of reactor is required if conversion in the new plant is to be 46% instead of 37%? (15%)

5. The isomerization of n-pentane (n-C_5H_{12}) is carried out catalytically at 200℃. The physical properties of the catalyst pellets are as follows: surface area = 230 m^2/g, pore volume = 0.35 cm^3/g, pellet density = 1.2 g/cm^3, tortuosity = 2.
   (a) Estimate the average pore diameter of the catalyst. (8%)
   (b) Estimate the effective diffusivity (7%)
   Additional information: To estimate Knudsen diffusivity D_{KA} (cm^2/s) :

$$D_{KA} = 9.70 \times 10^{-3} \bar{r} \sqrt{\frac{T}{M_A}}$$

where $\bar{r}$ = the ave. pore radius, cm; T = temperature, K;
M_A = molecular weight, g/g-mol

6. Rate data for the pyrolysis of normal octane (C_8H_{18}) at 450℃ give an apparent first-order irreversible rate constant, k_a, of 0.25 cm^3/s g-cat. The data were obtained at 1 atm pressure with a spherical catalyst of 0.3 cm diameter. The density of the catalyst is 1.2 g/cm^3. The effective diffusivity of the gas in the catalyst is 5x10^{-4} cm^2/s. If the external diffusion resistance is negligible, estimate the intrinsic rate constant, k, in cm^3/s g-cat.
   Additional information：

   Effectiveness factor, $\eta = \frac{3}{\phi^2}(\phi \coth \phi - 1)$; Thiele modulus, $\phi = R\sqrt{\frac{k\rho_c}{D_e}}$

   [hint: you may need to use trial-and-error for solution] (15%)

7. A catalytic reaction A + B $\longrightarrow$ C was carried out at 200℃ and 1 atm in a packed bed reactor. The reactor was loaded with 10 g of catalyst. The total volumetric rate to the reactor was 100 ml/min at 25℃ and 1 atm. The conversions of varied feed compositions are as follows:

run	Feed composition		Conversion
	A (mol %)	B(mol%)	X_A
1	23.6	76.4	0.096
2	47.3	52.7	0.046
3	77.9	22.1	0.014

   Show that the following mechanism can well describe the experimental results:

   A + S = AS

   AS +B $\rightarrow$ CS (rate determine step)

   CS = C + S

   (20%)