

Advanced Chemical Reaction Engineering

2004 PhD Qualification

(closed book)

1. A homogeneous gas-phase decomposition reaction  $4A \rightarrow R + 6S$  is proceeding in a plug flow reactor at  $1200^\circ\text{F}$  with first-order rate  $-r_A = kC_A$ , where  $k = 10/\text{hr}$ . What size of plug flow reactor operating at  $1200^\circ\text{F}$  and 4.6 atm can produce 80% conversion of a feed consisting of 4 lbmoles of pure A per hour. (10%)  
(Note: Gas constant  $R = 0.729 \text{ (ft}^3\text{)(atm)/(lbmole)(}^\circ\text{R)}$ )
2. A homogeneous liquid-phase reaction  $A \rightarrow R$   $-r_A = kC_A^2$  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  $A \rightarrow B$  for a feed of pure A at a rate of  $5 \text{ ft}^3/\text{h}$ . At the chosen operating T, the first-order rate constant  $k = 5.0/\text{h}$ . 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  $1000 \text{ ft}^3$  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 ( $n\text{-C}_5\text{H}_{12}$ ) is carried out catalytically at  $200^\circ\text{C}$ . The physical properties of the catalyst pellets are as follows: surface area =  $230\text{ m}^2/\text{g}$ , pore volume =  $0.35\text{ cm}^3/\text{g}$ , pellet density =  $1.2\text{ g/cm}^3$ , tortuosity = 2.

(a) Estimate the average pore diameter of the catalyst. (8%)

(b) Estimate the effective diffusivity (7%)

Additional information: To estimate Knudsen diffusivity  $D_{KA}$  ( $\text{cm}^2/\text{s}$ ):

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

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 ( $\text{C}_8\text{H}_{18}$ ) at  $450^\circ\text{C}$  give an apparent first-order irreversible rate constant,  $k_a$ , of  $0.25\text{ cm}^3/\text{s g-cat}$ . The data were obtained at 1 atm pressure with a spherical catalyst of 0.3 cm diameter. The density of the catalyst is  $1.2\text{ g/cm}^3$ . The effective diffusivity of the gas in the catalyst is  $5 \times 10^{-4}\text{ cm}^2/\text{s}$ . If the external diffusion resistance is negligible, estimate the intrinsic rate constant,  $k$ , in  $\text{cm}^3/\text{s g-cat}$ .

Additional information :

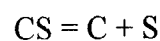
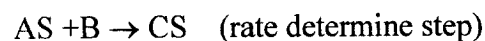
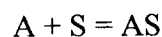
Effectiveness factor,  $\eta = \frac{3}{\phi^2} (\phi \coth \phi - 1)$ ; Thiele modulus,  $\phi = R \sqrt{\frac{k \rho_c}{D_e}}$

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

7. A catalytic reaction  $A + B \longrightarrow C$  was carried out at  $200^\circ\text{C}$  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  $100\text{ ml/min}$  at  $25^\circ\text{C}$  and 1 atm. The conversions of varied feed compositions are as follows:

run	Feed composition		Conversion $X_A$
	A (mol %)	B(mol%)	
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:



(20%)