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Reactor design

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Example & Problem

PFR & MFR

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- 5.2. In an isothermal batch reactor 70% of a liquid reactant is converted in 13 min. What space-time and space-velocity are needed to effect this conversion in a plug flow reactor and in a mixed flow reactor?

Prob 2

for batch $t = 13$ min and $x_A = 70\%$

for rate $\epsilon_A = 0$ and $\Sigma_A = 0$ and first order reaction \Rightarrow $\ln(1-x_A) = -kt$

$$\therefore -r_A = k C_A \Rightarrow \ln(1-x_A) = -kt$$

$$-\ln(1-0.7) = k(13) \Rightarrow k = 0.0926 \text{ min}^{-1}$$

for PFR & MFR $\tau = t$

for PFR

$$k\tau = -(1-\Sigma_A) \ln(1-x_A) - \Sigma_A x_A \quad \text{at any } \Sigma_A$$

when $\Sigma_A = 0$

$$k\tau = -\ln(1-x_A) \Rightarrow 0.0926 \times \tau = -\ln(1-0.7)$$

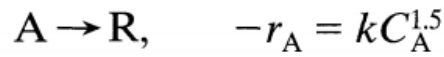
$\therefore \tau = 13$ min the same time for batch

for CSTR

$$\tau = \frac{C_{A0} x_A}{-r_A} = \frac{C_{A0} x_A}{k C_A} = \frac{C_{A0} x_A}{k C_{A0} (1-x_A)}$$

$$= \frac{0.7}{0.0926 (1-0.7)} = 25.19 \text{ min}$$

5.4. We plan to replace our present mixed flow reactor with one having double the volume. For the same aqueous feed (10 mol A/liter) and the same feed rate find the new conversion. The reaction kinetics are represented by



and present conversion is 70%.

Prob 4

$$C_{A0} = 10 \text{ mol/lit } \quad \xi_A = 0$$

$$-r_A = k C_A^{1.5}$$

$$\text{at } V_1 \Rightarrow \chi_{A1} = 0.7$$

$$\text{at } V_2 \Rightarrow \chi_{A2} = ?$$

$$V_2 = 2V_1 \quad \left. \vphantom{V_2 = 2V_1} \right\} \text{ at MFR}$$

$$\tau = \frac{V_1}{\nu} = \frac{C_{A0} \chi_{A1}}{-r_A} \quad \text{for Case 1}$$

$$\frac{V_1}{\nu} = \frac{10 \times 0.7}{k C_{A0}^{1.5} (1 - \chi_{A1})^{1.5}} \Rightarrow \frac{V_1}{\nu} = \frac{10 \times 0.7}{k \times 5.196}$$

$$\frac{V_1}{\nu} = \frac{1347}{k} \quad \Rightarrow \quad k = \frac{1347}{\frac{V_1}{\nu}}$$

for Case 2

$$\tau = \frac{V_2}{\nu} = \frac{C_{A0} \chi_{A2}}{k C_{A0}^{1.5} (1 - \chi_{A2})^{1.5}} = \frac{0.316 \chi_{A2}}{k (1 - \chi_{A2})^{1.5}}$$

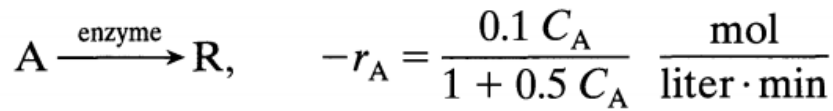
sub k and ν

$$\frac{2V_1}{\nu} = \frac{0.316 \chi_{A2}}{(1 - \chi_{A2})^{1.5}} \times \frac{V_1}{\nu \times 1347}$$

canceling $\frac{V_1}{\nu}$ and χ_{A2} and rearranging

$$\therefore \chi_{A2} \approx 0.8 \quad \Rightarrow \quad \text{conversion when } V_2 = 2V_1 \Rightarrow 80\%$$

5.9. A specific enzyme acts as catalyst in the fermentation of reactant A. At a given enzyme concentration in the aqueous feed stream (25 liter/min) find the volume of plug flow reactor needed for 95% conversion of reactant A ($C_{A0} = 2$ mol/liter). The kinetics of the fermentation at this enzyme concentration is given by



Prob. 9

$$V = 25 \text{ liter/min} \quad \xi_A = 0 \quad C_{A0} = 2 \text{ mol/lit}$$

$$-r_A = \frac{0.1 C_A}{1 + 0.5 C_A} \quad \text{when } X_A = 95\% \quad V = ? \quad \text{PFR}$$

$$\frac{V}{V_0} = C_{A0} \int_0^{X_A} \frac{dX_A}{-r_A} = - \int_{C_{A0}}^{C_A} \frac{dC_A}{-r_A}$$

$$C_A = C_{A0}(1 - X_A) = 2(1 - 0.95) = 0.1$$

$$\frac{V}{V_0} = - \int_2^{0.1} \frac{1 + 0.5 C_A}{0.1 C_A} dC_A = - \left[\frac{10}{C_A} dC_A + 5 dC_A \right]$$

$$= - \left[10 \ln C_A \Big|_2^{0.1} + 5 C_A \Big|_2^{0.1} \right]$$

$$\frac{V}{25} = - \left[10 \ln \frac{0.1}{2} + 5(0.1 - 2) \right]$$

$$\therefore V = 25 \times 39.45 = 986.25 \text{ lit}$$

كذلك يمكن حل السؤال
بواسطة طريقة Simpson's
rule

5.10. A gaseous feed of pure A (2 mol/liter, 100 mol/min) decomposes to give a variety of products in a plug flow reactor. The kinetics of the conversion is represented by



Find the expected conversion in a 22-liter reactor.

Prob 10

gaseous $\Sigma_A \neq 0$ $C_{A0} = 2 \text{ mol/liter}$ $F_{A0} = 100 \frac{\text{mol}}{\text{min}}$

$V = 22 \text{ liter}$ $x_A = ?$ $A \rightarrow 2.5 P$ PFR

$$\Sigma_A = \frac{2.5 - 1}{1} = 1.5 \quad -r_A = 10 C_A = 10 C_{A0} \left(\frac{1 - x_A}{1 + \Sigma_A x_A} \right)$$

$$\frac{V}{F_{A0}} = \tau = \frac{V C_{A0}}{F_{A0}} = C_{A0} \int_0^{x_A} \frac{dx_A}{-r_A}$$

$$\frac{V}{F_{A0}} = \frac{1}{10 C_{A0}} \int_0^{x_A} \frac{1 + \Sigma_A x_A}{1 - x_A} dx_A$$

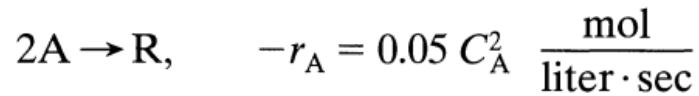
$$\frac{22 \times 10 \times 2}{100} = \int \frac{1}{1 - x_A} dx_A + 1.5 \int \frac{x_A}{1 - x_A} dx_A$$

$$4.4 = -\ln(1 - x_A) + 1.5 \left[-x_A - \ln(1 - x_A) \right]$$

$$4.4 = -2.5 \ln(1 - x_A) - 1.5 x_A$$

$$\Rightarrow x_A \approx 0.9$$

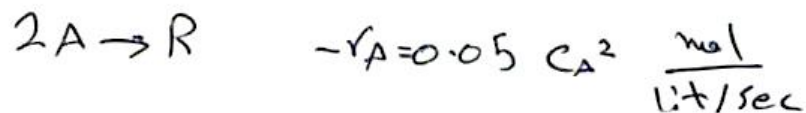
5.15. A gaseous feed of pure A (1 mol/liter) enters a mixed flow reactor (2 liters) and reacts as follows:



Find what feed rate (liter/min) will give an outlet concentration $C_A = 0.5$ mol/liter.

Prob 15

gaseous $C_{A0} = 1 \text{ mol/lit}$ $V = 2 \text{ lit}$



$$C_{AF} = 0.5 \quad v_0 = ?$$

$$\Sigma_A = \frac{1-2}{2} = -0.5$$

$$\frac{V}{v_0} = \frac{C_{A0} \chi_A}{-r_A}$$

$$v_0 = \frac{V \cdot -r_A}{C_{A0} \chi_A}$$

$$= \frac{2 \text{ lit} \cdot 0.0125 \text{ mol/lit} \cdot \text{sec}}{1 \text{ mol/lit} \cdot 0.666} = 0.037 \text{ lit/sec}$$

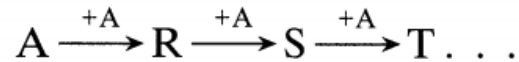
$$\chi_A = \frac{C_{A0} - C_A}{C_{A0} + \Sigma_A C_A} = 0.666$$

$$\begin{aligned} -r_A &= 0.05 (0.5)^2 \\ &= 0.0125 \frac{\text{mol}}{\text{lit} \cdot \text{sec}} \end{aligned}$$

$$v_0 = 0.0375 \frac{\text{lit}}{\text{sec}} \cdot \frac{60 \text{ sec}}{1 \text{ min}} = 2.25 \text{ lit/min}$$

H.W. Problem

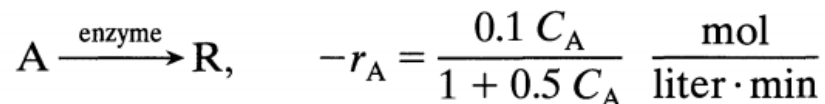
5.3. A stream of aqueous monomer A (1 mol/liter, 4 liter/min) enters a 2-liter mixed flow reactor, is radiated therein, and polymerizes as follows:



In the exit stream $C_A = 0.01$ mol/liter, and for a particular reaction product W, $C_W = 0.0002$ mol/liter. Find the rate of reaction of A and the rate of formation of W.

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5.11. Enzyme E catalyses the fermentation of substrate A (the reactant) to product R. Find the size of mixed flow reactor needed for 95% conversion of reactant in a feed stream (25 liter/min) of reactant (2 mol/liter) and enzyme. The kinetics of the fermentation at this enzyme concentration are given by



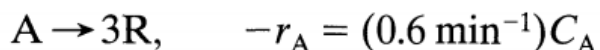
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5.13. At 650°C phosphine vapor decomposes as follows:



What size of plug flow reactor operating at 649°C and 11.4 atm is needed for 75% conversion of 10 mol/hr of phosphine in a 2/3 phosphine–1/3 inert feed?

5.16. Gaseous reactant A decomposes as follows:



Find the conversion of A in a 50% A–50% inert feed ($v_0 = 180$ liter/min, $C_{A0} = 300$ mmol/liter) to a 1 m^3 mixed flow reactor.

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5.19. Pure gaseous A at about 3 atm and 30°C (120 mmol/liter) is fed into a 1-liter mixed flow reactor at various flow rates. There it decomposes, and the exit concentration of A is measured for each flow rate. From the following data find a rate equation to represent the kinetics of the decomposition of A. Assume that reactant A alone affects the rate.

v_0 , liter/min	0.06	0.48	1.5	8.1	A \rightarrow 3R
C_A , mmol/liter	30	60	80	105	