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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 $X_A = 70\%$

في هذا السؤال يجب ان نجد order التفاعل لايجاد معادلة rate
لذلك يجب ان يحددوا المادة المتفاعلة
(*) سوف نفرض ان التفاعل first order and $\varepsilon_A = 0$

$\therefore -r_A = K C_A^1 \Rightarrow -\ln(1 - X_A) = Kt$

$-\ln(1 - 0.7) = K(13) \Rightarrow K = 0.0926 \ \frac{1}{min}$

الان نجد τ لـ PFR & MFR

for PFR

$K\tau = -(1 - \varepsilon_A)\ln(1 - X_A) - \varepsilon_A X_A$ at any ε_A

when $\varepsilon_A = 0$

$K\tau = -\ln(1 - X_A) \Rightarrow 0.0926 * \tau = -\ln(1 - 0.7)$

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

for CSTR

$$\tau = \frac{C_{A0} X_A}{-r_A} = \frac{C_{A0} X_A}{K C_A^1} = \frac{C_{A0} X_A}{K C_{A0}(1 - X_A)}$$

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

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

$$A \rightarrow R, \qquad -r_A = kC_A^{1.5}$$

and present conversion is 70%.

Prob 4

$C_{A0} = 10$ mol/lit $\varepsilon_A = 0$ $-r_A = K C_A^{1.5}$

at $V_1 \Rightarrow X_{A_1} = 0.7$

at $V_2 \Rightarrow X_{A_2} = ?$ $V_2 = 2V_1$ } at MFR

$\tau = \frac{V_1}{v} = \frac{C_{A0} X_{A_1}}{-r_A}$ for Case 1

$\frac{V_1}{v} = \frac{10 * 0.7}{K C_{A0}^{1.5} (1-X_A)^{1.5}} \Rightarrow \frac{V_1}{v} = \frac{10 * 0.7}{K * 5.196}$

$\frac{V_1}{v} = \frac{1.3447}{K}$ --- ① $\Rightarrow K = \frac{1.3447 \, v}{V_1}$

for Case 2

$\tau = \frac{V_2}{v} = \frac{C_{A0} X_{A2}}{K C_{A0}^{1.5} (1-X_{A2})^{1.5}} = \frac{0.316 \, X_{A2}}{K (1-X_{A2})^{1.5}}$

sub K and V_2

$\frac{2V_1}{v} = \frac{0.316 \, X_{A2}}{(1-X_{A2})^{1.5}} * \frac{V_1}{v * 1.347}$

هذا معادله بدلاله متغير واحد X_{A2} فقط نجد قيمته

$\therefore X_{A2} \cong 0.8 \Rightarrow$ 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

$$A \xrightarrow{\text{enzyme}} R, \qquad -r_A = \frac{0.1\, C_A}{1 + 0.5\, C_A} \quad \frac{\text{mol}}{\text{liter} \cdot \text{min}}$$

Prob. 9

$v = 25$ liter/min $\quad \varepsilon_A = 0 \quad C_{A0} = 2$ mol/lit

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

$$\frac{V}{v_0} = C_{A0} \int_0^{X_A} \frac{dX_A}{-r_A} = -\int_{C_{A0}}^{C_{Af}} \frac{dC_A}{-r_A}$$

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

$$\frac{V}{v_0} = -\int_2^{0.1} \frac{1 + 0.5\, C_A}{0.1\, C_A}\, dC_A = -\left[\int \frac{10}{C_A}\, dC_A + \int 5\, dC_A\right]$$

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

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

$\therefore V = 25 \times 39.45 = 986.25$ lit

كذلك يمكن حل السؤال

بطريقة 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

$$A \rightarrow 2.5\text{ (products)}, \qquad -r_A = (10\ \text{min}^{-1})C_A$$

Find the expected conversion in a 22-liter reactor.

Prob 10

gaseous $\varepsilon_A \neq 0$ $\quad C_{A0} = 2$ mol/lit $\quad F_{A0} = 100$ mol/min

$V = 22$ lit $\quad X_A = ?$ $\quad A \rightarrow 2.5\,P$ $\quad$ PFR

$\varepsilon_A = \frac{2.5-1}{1} = 1.5$ $\qquad -r_A = 10\,C_A = 10\,C_{A0}\left(\frac{1-X_A}{1+\varepsilon_A X_A}\right)$

$\tau = \frac{V}{v_0} = \frac{V C_{A0}}{F_{A0}} = C_{A0}\int_0^{X_{Af}} \frac{dX_A}{-r_A}$

$$\frac{V}{F_{A0}} = \frac{1}{10\,C_{A0}}\int_0^{X_{Af}} \frac{1+\varepsilon_A X_A}{1-X_A}\,dX_A$$

$$\frac{22 \times 10 \times 2}{100} = \int \frac{1}{1-X_A}\,dX_A + 1.5\int \frac{X_A}{1-X_A}\,dX_A$$

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

$$4.4 = -2.5\ln(1-X_A) - 1.5X$$

$\Rightarrow X_A \simeq 0.9$

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

$$2A \rightarrow R, \qquad -r_A = 0.05\, C_A^2 \ \frac{\text{mol}}{\text{liter} \cdot \text{sec}}$$

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

Prob 15

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

$2A \rightarrow R$ $-r_A = 0.05\, C_A^2 \ \frac{\text{mol}}{\text{lit/sec}}$

$C_{Af} = 0.5$ $v_0 = ?$

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

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

$$X_A = \frac{C_{A0} - C_A}{C_{A0} + \varepsilon_A C_A} = 0.666$$

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

$$v_0 = \frac{V * -r_A}{C_{A0}\, X_A}$$

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

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

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:

$$A \xrightarrow{+A} R \xrightarrow{+A} S \xrightarrow{+A} T \ldots$$

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

$$A \xrightarrow{\text{enzyme}} R, \qquad -r_A = \frac{0.1\, C_A}{1 + 0.5\, C_A} \; \frac{\text{mol}}{\text{liter} \cdot \text{min}}$$

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

$$4PH_3 \rightarrow P_4(g) + 6H_2, \qquad -r_{\text{phos}} = (10\ \text{hr}^{-1})C_{\text{phos}}$$

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:

$$A \rightarrow 3R, \qquad -r_A = (0.6\ \text{min}^{-1})C_A$$

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
C_A, mmol/liter	30	60	80	105

$A \rightarrow 3R$