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Subject: Chemical Reaction Engineering

Unit: III

Topic: Parallel Reactions

LECTURE: PARALLEL REACTIONS.

⇒ Qualitative analysis :—

→ Let a reactant A decompose into 2 products by either one of 2 paths.

$$A \xrightarrow{k_1} R \text{ (desired product)}$$
$$A \xrightarrow{k_2} S \text{ (unwanted product)}$$

Let corresponding rate equations be

$$r_R = \frac{dC_R}{dt} = k_1 C_A^{a_1} \; ; \; r_S = \frac{dC_S}{dt} = k_2 C_A^{a_2}$$

∴ Relative rate of formation :—

$$\frac{r_R}{r_S} = \frac{dC_R}{dC_S} = \frac{k_1}{k_2} C_A^{a_1 - a_2} \quad \text{— (1)}$$

⇒ The ratio should be large

⇒ In the equation, C_A can be controlled only.

⇒ C_A is kept low by :

1. using MFR
2. maintaining high conversions
3. increasing inerts in feed
4. decreasing pressure in gas-phase systems.

⇒ C_A is kept high by :—

1. using batch reactor or PFR
2. low conversions
3. remove inerts
4. increasing pressure

⇒ Consider equation (1)

(1) if $a_1 > a_2$ (desired reaction order > unwanted reaction)

$$\therefore \frac{r_R}{r_S} = K' C_A^{a_1} \qquad [K' = k_1/k_2]$$

for $\frac{r_R}{r_S}$ to be large ; C_A should be large.

Hence for $a_1 > a_2$; a batch reactor or PFR should be used.

Also minimum reactor size is needed.

② if $a_2 > a_1$ [unwanted >> desired]

$$\frac{r_R}{r_S} = K' C_A^{-a_2} = \frac{K'}{C_A^{a_2}} \quad [K' = k_1/k_2]$$

for $\frac{r_R}{r_S}$ to be large ; C_A should be low

Hence large volume MFR is needed.

③ if $a_1 = a_2$

$$\frac{r_R}{r_S} = K' \cdot C_A^0 = K' = k_1/k_2 = \text{constant}$$

unaffected by type of reactor used.

⇒ PRODUCT DISTRIBUTION BY VARYING k_1/k_2

→ Product distribution can be controlled by varying k_1/k_2 by

① By changing temperature [Activation energy varies]

② By using catalyst [Preferential catalysis / selectivity]

⇒ SUMMARY :- In parallel reactions, concentration level of reactants is key to control product distribution. High concentration favors high order reaction and vice-versa. However concentration level has no effect on equal order reactions.

⇒ CONTACTING PATTERNS FOR REACTIONS IN PARALLEL

Let us assume a reaction

$$A + B \xrightarrow{k_1} R \; ; \quad r_R = \frac{dC_R}{dt} = k_1 C_A^{1.5} C_B^{0.3} \text{ (desired)}$$

$$A + B \xrightarrow{k_2} S \; ; \quad r_S = \frac{dC_S}{dt} = k_2 C_A^{0.5} C_B^{1.8} \text{ (unwanted)}$$

$$\therefore \frac{r_R}{r_S} = \frac{k_1}{k_2} C_A \cdot C_B^{-1.5} \quad \text{[should be kept as large as possible]}$$

Hence following pattern is required

① Most desirable :- MFR used → C_A high ; C_B low

② ← Batch → C_A low, C_B low

③ ← PFR → C_A high, C_B high

④ Least desirable :- MFR → C_A low, C_B high

⇒ QUANTITATIVE ANALYSIS :-

Let us introduce two terms φ and Φ where

$$\varphi = \frac{(\text{moles R formed})}{(\text{moles A reacted})} = \frac{dC_R}{-dC_A} \quad \text{[instantaneous fractional yield]}$$

and

$$\Phi = \frac{(\text{all R formed})}{(\text{all A reacted})} = \frac{C_{Rf}}{C_{A0} - C_{Af}} = \frac{C_{Rf}}{(-\Delta C_A)} \quad \text{[overall fractional yield]}$$

Hence for PFR:

$$\Phi_P = \frac{-1}{C_{A0} - C_{Af}} \int_{C_{A0}}^{C_{Af}} \varphi \, dC_A$$

$$= \frac{1}{\Delta C_A} \int_{C_{A0}}^{C_{Af}} \varphi \, dC_A \quad \text{--- (2)}$$

for MFR:

$$\Phi_m = \varphi_{\text{evaluated at } C_{Af}} = \left(\frac{d\Phi_P}{dC_A}\right)_{\text{at } C_{Af}}$$

∴ We have 2 equations :-

$$\Phi_M = \left(\frac{d\Phi_P}{dC_A}\right)_{C_{Af}}$$

$$\Phi_P = \frac{1}{\Delta C_A} \int_{C_{A0}}^{C_{Af}} \Phi_M \, dC_A$$

⇒ SELECTIVITY :-

Selectivity is defined as follows :-

$$\text{Selectivity} = \frac{(\text{moles of desired product formed})}{(\text{moles of undesired material formed})}$$