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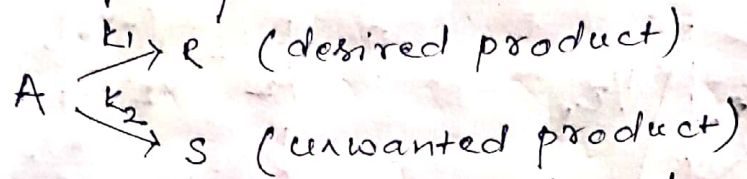
Unit: III

Topic: Parallel Reactions

# LECTURE: PARALLEL REACTIONS.

⇒ Qualitative analysis :-

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



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)

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

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  $\gg$  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.

$\Rightarrow$  PRODUCT DISTRIBUTION BY VARYING  $k_1/k_2$

$\rightarrow$  Product distribution can be controlled by varying  $k_1/k_2$  by

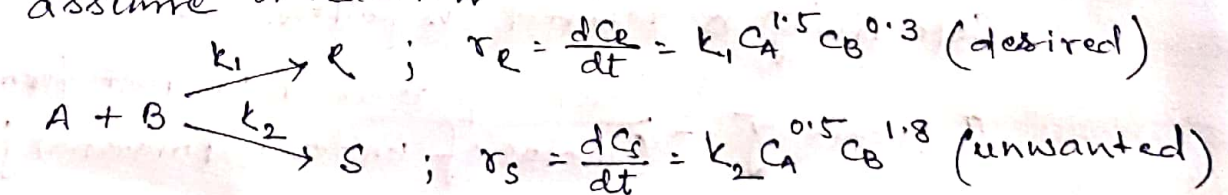
① By changing temperature [Activation energy varies]

② By using catalyst [Preferential catalysis/selectivity]

$\Rightarrow$  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.

$\Rightarrow$  CONTACTING PATTERNS FOR REACTIONS IN PARALLEL

Let us assume a reaction



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

Hence following pattern is required.

- |   |                    |                        |                                      |
|---|--------------------|------------------------|--------------------------------------|
| ① | Most desirable :-  | MFR used $\rightarrow$ | $C_A$ high ; $C_B$ low               |
| ② |                    | $\rightarrow$ Batch    | $\rightarrow$ $C_A$ low, $C_B$ low   |
| ③ |                    | $\rightarrow$ PFR      | $\rightarrow$ $C_A$ high, $C_B$ high |
| ④ | Least desirable :- | MFR                    | $\rightarrow$ $C_A$ low, $C_B$ high  |

## ⇒ QUANTITATIVE ANALYSIS :-

Let us introduce two terms  $\phi$  and  $\Phi$  where

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

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

$$\begin{aligned} \text{Hence for PFR: } \Phi_P &= \frac{-1}{C_{A0} - C_{Af}} \int_{C_{A0}}^{C_{Af}} \phi dC_A \\ &= \frac{1}{\Delta C_A} \int_{C_{A0}}^{C_{Af}} \phi dC_A \quad \text{--- (2)} \end{aligned}$$

$$\text{for MFR: } \Phi_M = \phi \text{ evaluated at } C_{Af} = \left( \frac{d\Phi_P}{dC_A} \right)_{\text{at } C_{Af}}$$

∴ 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 :-

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