Lecture # 13 CHE331A

Introduction and Design equations for Ideal reactors

(BR, CSTR, PFR, PBR)

Basic Concepts in Chemical kinetics (types of reactions, rate and equilibrium constants)

Isothermal Reactor Design (CSTR, PFR, PBR), Constant volume and Variable volume, EG production

Collection and Analysis of Data (Differential, Integral, Non-linear regression, Differential reactor)

Design of Multiple Reactions in Isothermal Reactors

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Often Multiple reactions occur in Reactors in the Chemical Industry

- Some reactions are desirable and others undesirable
- There is a need to minimize undesirable reactions to enhance the profitability of a process
- Reactions can be classified into four basic reactions
  - Parallel
  - Series
  - Complex
  - Independent

Parallel and Series Reactions differ in the way the reactants are consumed

- In parallel reactions the reactant is consumed in different reaction pathways

$$A \xrightarrow{k_1} D \text{ (desired)}, \qquad A \xrightarrow{k_2} U \text{ (undesired)}$$

$$C_2H_4 + O_2 \xrightarrow{k_1} C_2H_4O \text{ (desired)}, \qquad C_2H_4 + O_2 \xrightarrow{k_2} CO_2 + H_2O \text{ (undesired)}$$

- In series reactions an intermediate desirable product is formed, which reacts to form another product

$$A \xrightarrow{k_1} D \text{ (desired)} \xrightarrow{k_2} U \text{ (undesired)}$$

$$C_2H_4O + NH_3 \rightarrow HOCH_2CH_2NH_2 \xrightarrow{+EO} (HOCH_2CH_2)_2NH_2 \text{ (desired)} \xrightarrow{+EO} (HOCH_2CH_2)_3NH_2 \text{ (undesired)}$$

Independent reactions involve different reactants reacting at the same time

- Reactants nor products react with each other

(i) $A \rightarrow B + C$ (ii) $D \rightarrow E + F$

- Example,

Cracking of crude oil to form petrol

$$C_{15}H_{32} \rightarrow C_{12}C_{26} + C_3H_6$$

$$C_8H_{18} \rightarrow C_6C_{14} + C_2H_4$$

Complex reactions involve the combination of series, parallel and independent reactions

$$\boldsymbol{A} + B \rightarrow \boldsymbol{C} + D \qquad \boldsymbol{A} + \boldsymbol{C} \rightarrow E$$

- Combination of series and parallel reactions is seen in the formation of butadiene from ethanol

$$C_2H_5OH \rightarrow C_2H_4 + H_2O$$

$$C_2H_5OH \rightarrow CH_3CHO + H_2$$

$$C_2H_4 + CH_3CHO \rightarrow C_4H_6 + H_2O$$

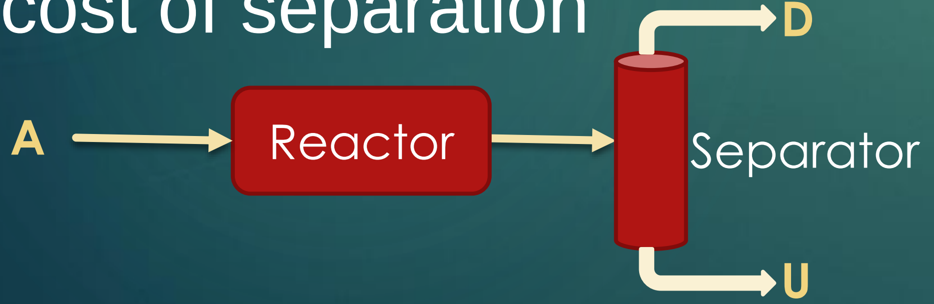
Desired and Undesired Reactions and decisions to make

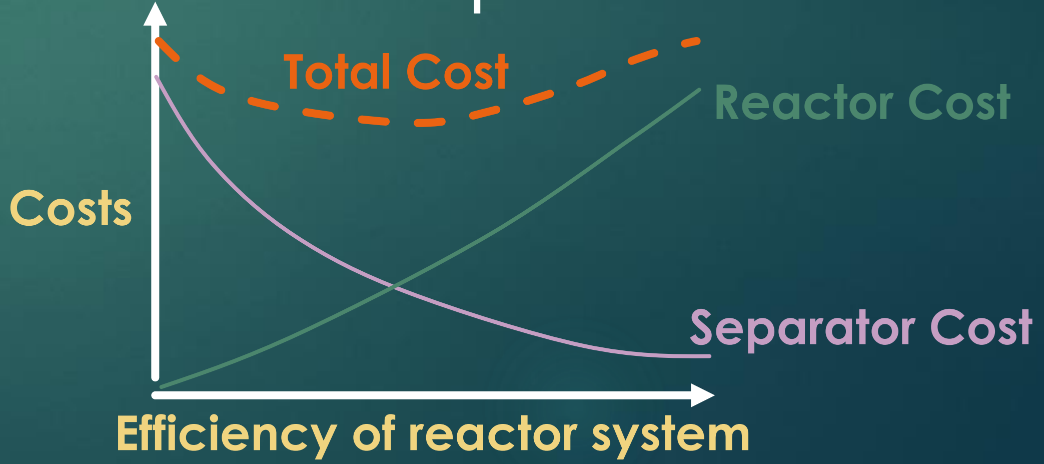
- Focus is to maximize the desired product formed and minimize the amount of undesired formed

Parallel reactions: $A \xrightarrow{k_D} D$ $A \xrightarrow{k_U} U$

Series reactions: $A \xrightarrow{k_D} D \xrightarrow{k_U} U$

Usually, the greater the amount of undesirable product more is the cost of separation





Selectivity and yield are useful parameters that are required to describe Multiple reactions

- Selectivity: Provides information about the formation of one product over another – two types of selectivity defined in literature
  - Instantaneous selectivity: $S_{D/U} = \frac{r_D}{r_U} = \frac{rate\ of\ formation\ of\ D}{rate\ of\ formation\ of\ U}$
  - Overall selectivity: $\bar{S}_{D/U} = \frac{F_D}{F_U} = \frac{exit\ molar\ flrow\ rate\ of\ D}{exit\ molar\ flow\ rate\ of\ U}$ (Flow reactor)

    (Batch reactor) $\bar{S}_{D/U} = \frac{N_D}{N_U} = \frac{Number\ of\ moles\ of\ D\ at\ the\ end\ of\ reation}{Number\ of\ moles\ of\ U\ at\ the\ end\ of\ reaction}$
- For CSTR: $A \xrightarrow{k_D} D$ and $A \xrightarrow{k_U} U \Rightarrow \bar{S}_{D/U} = \frac{F_D}{F_U} = \frac{r_D V}{r_U V} = \frac{r_D}{r_U} = S_{D/U}$
- Thus, for a CSTR: $\bar{S}_{D/U} = S_{D/U}$ (try this for a series reaction)

Similar to selectivity, the yield also has two definitions

- Instantaneous Yield, Y_D : $\quad Y_D = \frac{r_D}{-r_A} = \frac{rate\ of\ formation\ of\ D}{rate\ of\ disappearance\ of\ A}$
- Overall selectivity, $\bar{Y}_D$:
  - (Flow reactor) $\quad \bar{Y}_D = \frac{F_D}{F_{A0}-F_A} = \frac{exit\ molar\ flow\ rate\ of\ D}{moles\ of\ A\ converted}$
  - (Batch reactor) $\quad \bar{Y}_D = \frac{N_D}{N_{A0}-N_A} = \frac{Number\ of\ moles\ of\ D\ formed\ at\ the\ end\ of\ reation}{Number\ of\ moles\ of\ A\ consumed\ at\ the\ end\ of\ reaction}$

- Similar to selectivity, for a CSTR: $\quad Y_D = \bar{Y}_D$
- Overall selectivities and yields are important for determining profits, whereas rate-based parameters help in reactor selection and reactor scheme