Lecture # 14.1 CHE331A

Multiple Reactions Occur in the Chemical Industry

Categorization of Multiple Reactions

Parallel, Series, Complex and Independent Reactions

Definitions of instantaneous and overall Selectivity and Yields

Operating conditions and Reactor schemes for Multiple Reactions

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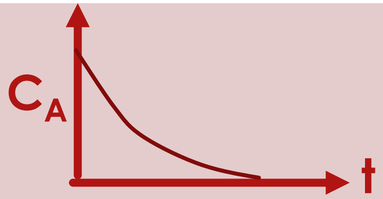
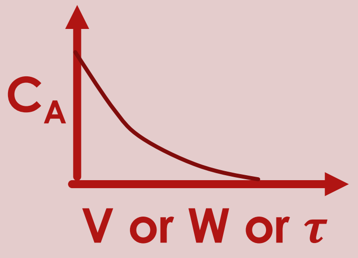
Basic design equations for ideal reactors revisited

Reactor	Design Eq^n	C_A vs. t or V or W
BR	$\frac{dN_A}{dt} = r_A . V$	
CSTR	$V = \frac{F_{A0} - F_A}{-r_A}$	Conc. is at the minimum
PFR	$\frac{dF_A}{dV} = r_A$	
PBR	$\frac{dF_A}{dW} = r'_A$	

Selection of Reactor type and conditions for Parallel reactions $A \xrightarrow{k_D} D$ and $A \xrightarrow{k_U} U$

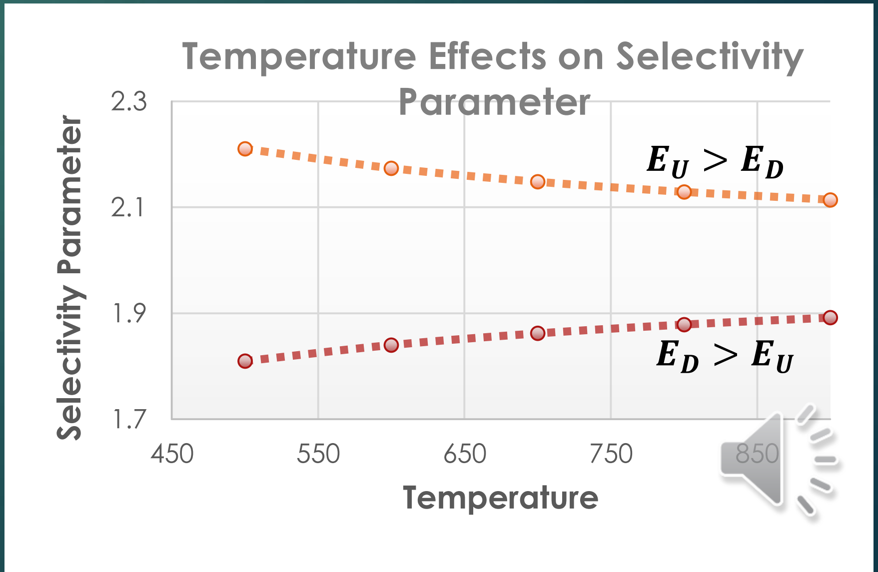
- Rate laws: $r_D = k_D C_A^{\alpha 1}$ and $r_U = k_U C_A^{\alpha 2}$
- Rate of disappearance of A: $-r_A = k_D C_A^{\alpha 1} + k_U C_A^{\alpha 2}$
- $S_{D/U} = \frac{r_D}{r_U} = \frac{k_D}{k_U} C_A^{\alpha 1 - \alpha 2}$ Methods to increase $S_{D/U}$ depends $\alpha 1 - \alpha 2$
- **Case I:** $\alpha 1 > \alpha 2$ and $\alpha 1 - \alpha 2 = a$ then $S_{D/U} = \frac{k_D}{k_U} C_A^a$
- To increase $S_{D/U}$, we need to keep C_A^a as high as possible
  - No inerts and operate at high pressures if gas phase reaction
  - Batch or PFR/PBR, instead of a CSTR, since conc is higher

Selection of Reactor type and conditions for Parallel reactions $A \xrightarrow{k_D} D$ and $A \xrightarrow{k_U} U$ continued

- **Case 2:** $\alpha 2 > \alpha 1$ and $\alpha 2 - \alpha 1 = b$ then $S_{D/U} = \frac{k_D}{k_U}\frac{1}{C_A^b}$
- To increase $S_{D/U}$, we need to keep C_A^b as low as possible
  - Use inerts and operate at low pressures if gas phase reaction
  - Use a CSTR instead of Batch or PFR/PBR
  - Recycle reactor could also be used
- Temperature effects can be rationalized if the relative activation energies are known
  - Recommendations can be made for equal reaction orders

Temperature effects for Parallel reactions

- $r_D = k_D C_A^{\alpha 1}$ and $r_U = k_U C_A^{\alpha 1}$ $S_{D/U} = \frac{r_D}{r_U} = \frac{k_D}{k_U} = \frac{A_D}{A_U} exp\left[-\frac{(E_D - E_U)}{RT}\right]$
- Case 4’: $E_D > E_U$
  - k_D increases more rapidly with increase in temp compared to k_U
  - Reaction operated at the highest possible temp
- Case 5’: $E_U > E_D$
  - k_U increases more rapidly with increase in temp compared to k_D
  - Reaction should be operated at the lowest possible temp

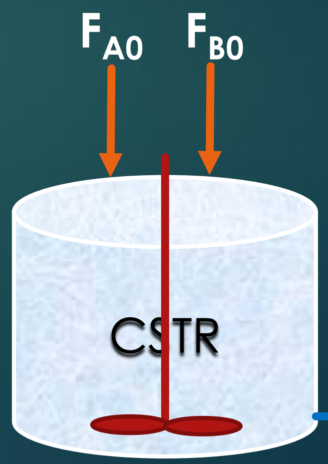


Parallel reactions for two reactants – Reactor selection

- $A + B \xrightarrow{k_D} D$ and $A + B \xrightarrow{k_U} U$ and $r_D = k_D C_A^{\alpha 1} C_B^{\beta 1}$ and $r_U = k_U C_A^{\alpha 2} C_B^{\beta 2}$
- $S_{D/U} = \frac{r_D}{r_U} = \frac{k_D}{k_U} C_A^{\alpha 1 - \alpha 2} C_B^{\beta 1 - \beta 2}$ is to be maximized $\rightarrow \alpha 1 - \alpha 2$ & $\beta 1 > \beta 2$
- Case I: $\alpha 1 > \alpha 2$ and $\beta 1 > \beta 2$
  - $\alpha 1 - \alpha 2 = a$ & $\beta 1 - \beta 2 = b \quad \rightarrow$
  - To maximize $S_{D/U} = \frac{k_D}{k_U} C_A^a C_B^b$ $\quad C_A$ *and* C_B should be high
  - Tubular reactor (PFR/PBR)
  - Batch reactor
  - High pressures and no inerts

Parallel reactions for two reactants – Reactor selection - Case II

- $S_{D/U} = \frac{r_D}{r_U} = \frac{k_D}{k_U} C_A^{\alpha1-\alpha2} C_B^{\beta1-\beta2}$ $\alpha1 - \alpha2$ and $\beta1 - \beta2$
- Case II: $\alpha2 > \alpha1$ and $\beta2 > \beta1$ $\rightarrow$ $\alpha2 - \alpha1 = a$ & $\beta2 - \beta1 = b$
  - To maximize $S_{D/U} = \frac{k_D}{k_U} \frac{1}{C_A^a C_B^b}$ C_A and C_B should be low
  - CSTR or a PFR/PBR with a large recycle
  - Low pressures (gas-phase) and use inerts



Parallel reactions for two reactants – Reactor selection - Case III/IV

- Case III: $\alpha 1 > \alpha 2$ and $\beta 2 > \beta 1 \quad \rightarrow \quad \alpha 1 - \alpha 2 = a \quad \& \quad \beta 2 - \beta 1 = b$
  - To maximize $S_{D/U} = \frac{k_D}{k_U}\frac{C_A^a}{C_B^b}$ $\quad C_A$ *should be high and* C_B *should be low*
  - Semi-Batch reactor with A initially present and B slowly fed
  - Tubular reactor (or membrane reactor) with side streams of B fed
  - Series of small CSTRs with A fed to the first reactor and B fed to each
- Case IV: is similar

$\alpha 2 > \alpha 1$ and

$\beta 1 > \beta 2$