

Lecture # 14.2 CHE331A

Multiple Reactions
Occur in the
Chemical Industry

Categorization as
Parallel, Series,
Complex and
Independent
Reactions

Definitions of
instantaneous and
overall Selectivity
and Yields

Choice of Reactors
and Reactor
Schemes for Parallel
Reactions

**Operating
conditions for Series
Reactions**

GOUTAM DEO

CHEMICAL ENGINEERING DEPARTMENT

IIT KANPUR



For series reactions it is important to choose space-time or real-time

- ▶ In parallel reactions the undesired product was minimized by choosing a proper reactor and adjusting reaction conditions (e.g., conc.)
- ▶ For series reactions the space-time (for a flow reactor) or real-time (for a batch reactor) is important
- ▶ For series reaction: $A \xrightarrow{k_1} D \xrightarrow{k_2} U$ to maximize D we need 1st reaction to be favored and 2nd reaction not to be favored
 - Can be achieved in a flow reactor and batch reactor
 - For batch reactor a short reaction time will favor formation of D
 - For PFR/PBR a short length of reactor will favor formation of D



Quantitative analysis provides more definite answers

- ▶ Reaction: $A \xrightarrow{k_1} D \xrightarrow{k_2} U$
- ▶ Reactor: PFR with $C_A = C_{A0}$ at $V = 0$
- ▶ Mole balance on A: $\frac{dF_A}{dV} = r_A$
- ▶ Rate law: $-r_A = k_1 C_A$ Assume: $F_A = C_A \dot{V}_0$ and $F_D = C_D \dot{V}_0$
- ▶ Thus, $\dot{V}_0 \frac{dC_A}{dV} = -k_1 C_A$ and with $\tau = \frac{V}{\dot{V}_0}$
$$C_A = C_{A0} \exp(-k \cdot \tau)$$



Mole balance can also be done on species D

► Mole balance on D: $\frac{dF_D}{dV} = r_D$

► Rate law: $r_D = r_{D1} + r_{D2} = k_1 C_A - k_2 C_D$

► $\dot{v}_0 \frac{dC_D}{dV} = k_1 C_A - k_2 C_D$ and with $C_A = C_{A0} \exp(-k_1 \tau)$

$$\frac{dC_D}{d\tau} + k_2 C_D = k_1 C_{A0} \exp(-k_1 \tau)$$

► Using the integrating factor $\frac{d(C_D e^{k_2 \tau})}{d\tau} = k_1 C_{A0} \exp[(k_2 - k_1)\tau]$

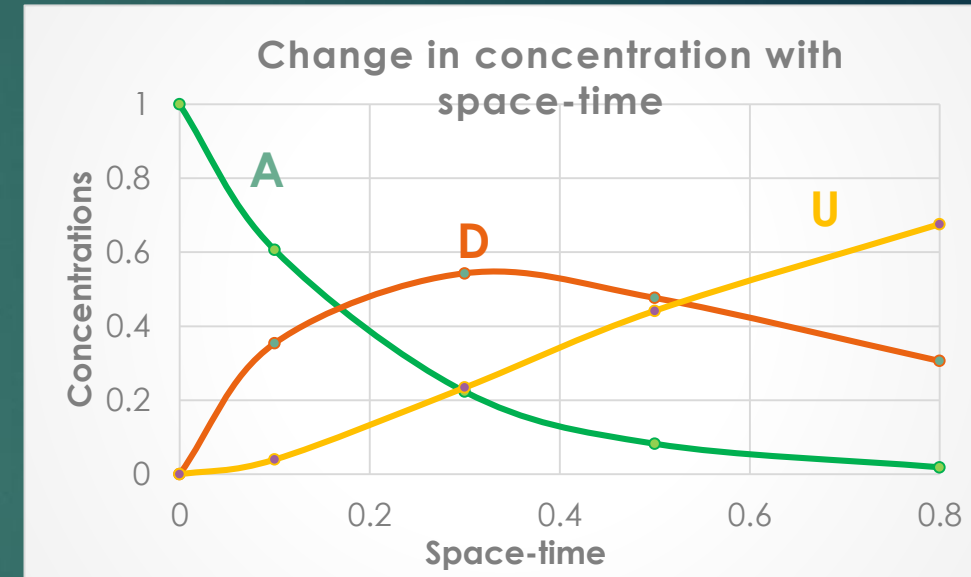
$$C_D = k_1 C_{A0} \left[\frac{e^{-k_1 \tau} - e^{-k_2 \tau}}{k_2 - k_1} \right]$$



The concentration of the (intermediate) desired product depends on the space-time

- ▶ $C_D = k_1 C_{A0} \left[\frac{e^{-k_1 \tau} - e^{-k_2 \tau}}{k_2 - k_1} \right]$
- ▶ C_D reaches a maximum $\rightarrow \frac{dC_D}{d\tau} = 0$
- ▶ Thus, $\tau_{opt} = \frac{1}{k_1 - k_2} \ln \left(\frac{k_1}{k_2} \right) \rightarrow V_{opt} \text{ (or } W_{opt})$
- ▶ $X_{opt} = 1 - \exp(-k_1 \tau_{opt})$
- ▶ $X_{opt} = 1 - \exp \left[-\ln \left(\frac{k_1}{k_2} \right)^{k_1 / (k_2 - k_1)} \right]$

$$X_{opt} = 1 - \left(\frac{k_1}{k_2} \right)^{k_1 / (k_2 - k_1)}$$



Summary

- ▶ Multiple Reactions: classified into four basic reactions
 - Parallel, Series, Complex and Independent
- ▶ Define selectivity and yield
- ▶ Parallel reactions:
 - Choice of reactors/reactor scheme and operating conditions
- ▶ Series reactions:
 - Choice of optimum space-time or reaction-time

