

Lecture # 10.1 CHE331A

- Basics of reactions and ideal reactors
- Design/Analysis of CSTRs, PFRs, PBRs, Batch and Semi-batch in terms of conversions and molar flow rates or concentrations
- Collection and Analysis of Rate Data

Batch Reactor

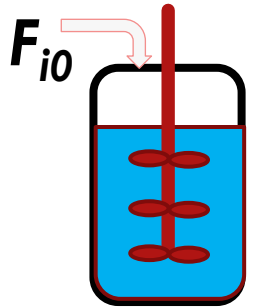
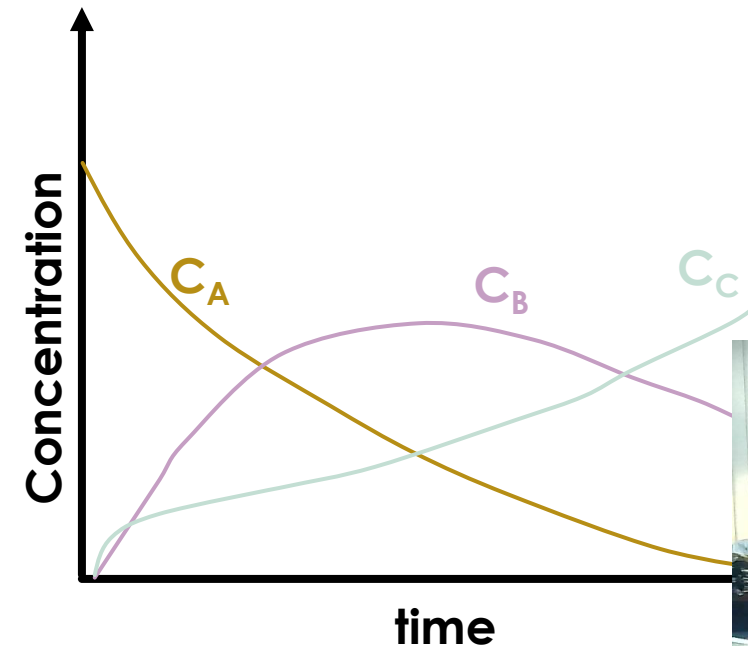
$$-r_A = k \cdot C_A^2$$

$$t_R = \frac{1}{k \cdot C_{A0}} \frac{(1 + \varepsilon)X}{(1 - X)} - \varepsilon \ln \frac{1}{1 - X}$$

$$t_T = t_R + t_C + t_F + t_E$$

Semi-Batch Reactor

$$\frac{dC_A}{dt} = r_A - \frac{C_A \cdot \dot{v}_0}{V(t)}; \quad \frac{dC_B}{dt} = r_B + \frac{(C_{B0}^{in} - C_B) \dot{v}_0}{V(t)}; \quad \frac{dC_C}{dt} = r_C - \frac{C_C \dot{v}_0}{V(t)}$$



There are a number of ways we analyze Rate data

► Purpose is to:

- Determine rates of different species → rate of disappearance, formation
- Develop rate laws → dependency on concentration/pressure of the different species
- Determine values of rate constant and (apparent) activation energy

► Methods used for analysis:

- Differential method
- Integral method
- Methods of half-life
- Least-square method



Data analysis procedure to determine rate data usually depends on the type of reaction

- ▶ Homogeneous reactions:
 - Often obtained using a batch reactor
 - Obtain concentration versus time data
- ▶ Heterogeneous (gas-solid) reactions:
 - Often obtained using a PBR operating in the differential mode
 - Obtain rate versus partial pressure data
- ▶ Assume a rate law, then apply mole balance equation
- ▶ Determine parameters associated with the rate law



Batch Reactor data analysis can be done in three ways

- ▶ Differential method, integral method or nonlinear regression
- ▶ For irreversible reactions it is possible to determine the reaction order and specific rate constants
 - Single reactant dependent, e.g., $-r_A = k \cdot C_A^\alpha$
 - Multiple concentration dependent (method of excess), $-r_A = k \cdot C_A^\alpha C_B^\beta$

Excess B so that $C_B \sim \text{constant}$: $-r_A = k' \cdot C_A^\alpha$, $k' = k \cdot C_B^\beta \approx k \cdot C_{B0}^\beta$

Similarly take excess A so that $-r_A = k \cdot C_A^\alpha C_B^\beta = k'' \cdot C_B^\beta$, $k'' \approx k \cdot C_{A0}^\alpha$



Differential method of analysis involves differentiating concentration versus time data

► Mole balance for a batch reactor: $r_A = \frac{dC_A}{dt}$

► Rate law: $-r_A = k \cdot C_A^\alpha \Rightarrow -\frac{dC_A}{dt} = k \cdot C_A^\alpha$

► Thus,

$$\ln \left(-\frac{dC_A}{dt} \right) = \ln k + \alpha \cdot \ln C_A$$

► Plotting $\ln \left(-\frac{dC_A}{dt} \right)$ versus $\ln C_A \rightarrow \text{slope} = \alpha$

► k obtained from specific values of $-\frac{dC_A}{dt}$ and C_A

► Thus, from the C_A versus t data we need to determine $\frac{dC_A}{dt}$



The differential of concentration versus time can be obtained in a number of ways

► Methods to determine $\frac{dC_A}{dt}$ are:

- Graphical differentiation
- Numerical differentiation
- Differentiation of a polynomial fit

► Graphical method:

- Disparities in data can be seen and remedial actions can be taken
- Involves plotting of $-\frac{\Delta C_A}{\Delta t}$ versus t
- Equal-area differentiation to obtain $\frac{dC_A}{dt}$

time (min)	C(EG)	$\Delta(t)$	$\Delta(C)$	$\Delta C/\Delta t$	$D(CEG)/dt$
0	0				0.315
		0.5	0.145	0.29	
0.5	0.145				0.265
		0.5	0.125	0.25	
1	0.270				0.225
		0.5	0.106	0.212	
1.5	0.376				0.200

