

PHEN 612

SPRING 2008

WEEK 2

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Chapter 4*

Isothermal Reactor Design

We focus on the design of various types of reactors

Part I. Mole balances in terms of conversion

4.1 Design structure for isothermal reactors

How do we approach a problem?

1) Use the general mole balance equation:

$$\frac{d(N_A)}{dt} = F_{A0} - F_A + \int_V r_A dV$$

*Elements of Chemical Reaction Engineering – Fourth Edition
by H. Scott Fogler, Prentice Hall, 2006

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2) Derive designs equations for the specific reactor:

Batch:
$$N_{A0} \frac{dX}{dt} = -r_A V$$

CSTR:
$$V = F_{A0} (1/r_A) X$$

Plug flow:
$$\frac{F_{A0} dX}{dV} = -r_A$$

Packed bed:
$$\frac{F_{A0} dX}{dW} = -r_A'$$

3) We need $-r_A = f(X)$

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- 4) $f(X)$ is not known. We need to derive $-r_A = f(C_A, C_B, \dots)$
- 5) Concentration as a function of X

4.2 Scale-up of liquid-phase batch reactor data to the design of a CSTR

4.2.1 Batch operator: $V = V_0$ (ct volume)

$$\frac{1}{V} \frac{d(N_A)}{dt} = r_A$$

Or $\frac{d(C_A)}{dt} = r_A; \quad -\frac{d(C_A)}{dt} = -r_A$

We can use measured variables (i.e., C_A) to get r_A

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- Typical problem: estimate t necessary to achieve a conversion X : $A \rightarrow B$

1) Mole balance:
$$N_{A0} \frac{dX}{dt} = -r_A V$$

2) Rate law:
$$-r_A = kC_A^2$$

3) From stoichiometry:
$$C_A = C_{A0}(1-X)$$

4) The equations are combined to give:

$$t = \frac{1}{kC_{A0}} \left(\frac{X}{1-X} \right) \quad \text{Also called reaction time}$$

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- If we change the rate law to

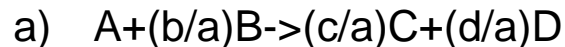
$$-r_A = kC_A$$

- The reaction time is: $t = \frac{1}{k} \ln\left(\frac{1}{1-X}\right)$

- In reality, the cycle time is the sum of the time to fill, the time to heat, the time to clean, and the reaction time.

- Example 4.1 shows how one can get the rate law from the data.

- Note on batch reactors



b) $N_A = N_{A0} - N_{A0}X = N_{A0}(1-X)$

c) Moles of B reacted = [(moles of B reacted)/(moles of A reacted)] * moles of A reacted = $(b/a) (N_{A0}X)$

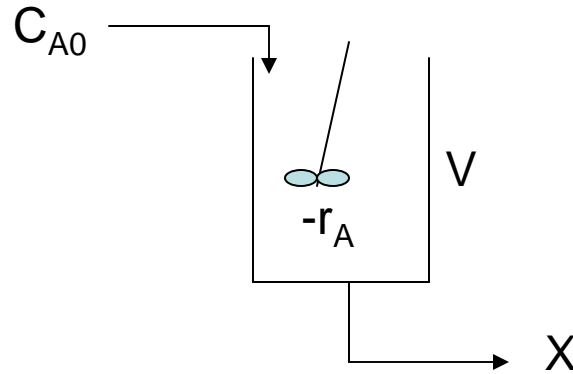
d) $C_A = (N_A/V) = N_{A0}(1-X)/V$; $C_B = (N_B/V) = [N_{B0} - (b/a) (N_{A0}X)]/V$;

$C_C = (N_C/V) = [N_{C0} + (c/a) (N_{A0}X)]/V$; $C_D = (N_D/V) = [N_{D0} + (d/a) (N_{A0}X)]/V$

$$\Theta_i = \frac{N_{i0}}{N_{A0}} = \frac{C_{i0}}{C_i} \quad \text{As a result: } C_B = \frac{N_{A0} \left(\Theta_B - \frac{b}{a} X \right)}{V} \quad \text{etc...}$$

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4.3 Design of CSTRs



From Chapter 2:

$$V = F_{A0} (1/-r_A)_{\text{exit}} X$$

$$F_{A0} = v_0 C_{A0} \quad V = v_0 C_{A0} X / (-r_A)$$

$$\text{Space time: } \tau = \frac{V}{v_0} = \frac{C_{A0} X}{-r_A}$$

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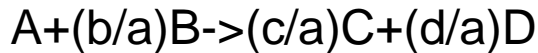
4.3.1 A single CSTR

$$-r_A = kC_A$$

$$C_A = C_{A0}(1-X) \quad \tau = \frac{C_{A0}X}{-r_A}; \quad \tau = \frac{C_{A0}X}{kC_A} = \frac{C_{A0}X}{kC_{A0}(1-X)} = \frac{X}{k(1-X)}$$

$$X = \frac{\tau k}{1 + \tau k}$$

- Note on CSTRs



$$C_A = (F_A/v) = F_{A0}(1-X)/v; \quad C_B = (F_B/v) = [F_{B0} - (b/a)(F_{A0}X)]/v;$$

$$C_C = (F_C/v) = [F_{C0} + (c/a)(F_{A0}X)]/v; \quad C_D = (F_D/v) = [F_{D0} + (d/a)(F_{A0}X)]/v$$

$$v = v_0$$

$$C_A = C_{A0}(1-X); \quad C_B = C_{A0}(\Theta_B - (b/a)X); \quad \text{etc...}$$

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As a result:

$$C_A = C_{A0} (1 - X) = C_{A0} \left(1 - \frac{\tau k}{1 + \tau k} \right) = \frac{C_{A0}}{1 + \tau k}$$

For first-order reactions, τk is the reaction Damkohler number: Da

In general $Da = \frac{-r_{A0}V}{F_{A0}}$ = (Rate of reaction at entrance)/(entering flow rate of A)

- For a first-order system, we have $Da = \frac{kC_{A0}V}{v_0C_{A0}} = \tau k$
- For a second-order system, we have $Da = \frac{kC_{A0}^2V}{v_0C_{A0}} = \tau kC_{A0}$

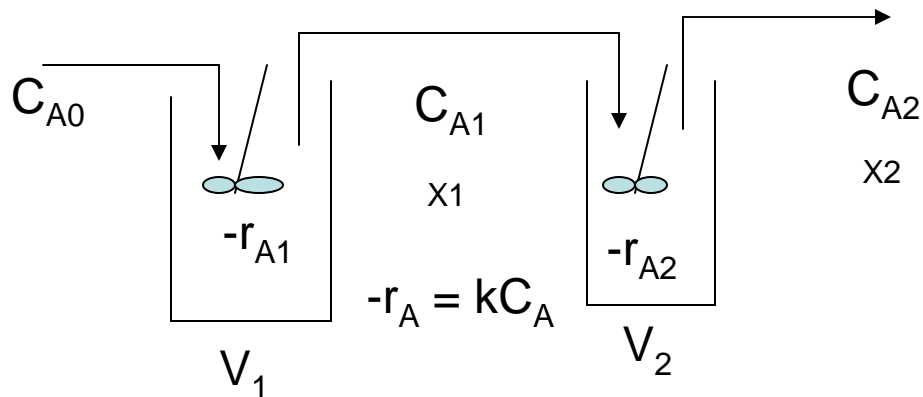
Rule of thumb: $Da < 0.1 \rightarrow X < 0.1$

$Da > 10 \rightarrow X > 0.9$

- For first-order systems: $X = \frac{Da}{1 + Da}$

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4.3.2 CSTRs in series



$$V_2 = (F_{A1} - F_{A2}) / (-r_{A2}) = v_0 (C_{A1} - C_{A2}) / (k_2 C_{A2})$$

We can solve for C_{A2} :
$$C_{A2} = \frac{C_{A1}}{1 + \tau_2 k_2} = \frac{C_{A0}}{(1 + \tau_1 k_1)(1 + \tau_2 k_2)}$$

If $\tau_1 = \tau_2 = \tau$ and $k_1 = k_2 = k$:
$$C_{A2} = \frac{C_{A0}}{(1 + \tau k)^2}$$

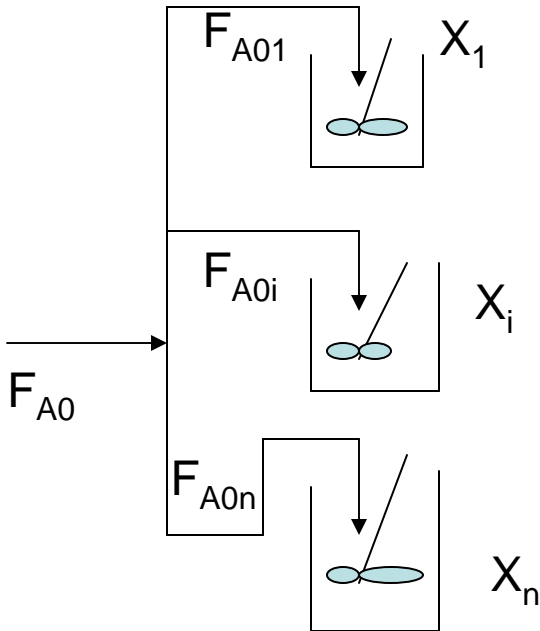
In general:
$$C_{An} = \frac{C_{A0}}{(1 + \tau k)^n} = \frac{C_{A0}}{(1 + Da)^n}$$

Using conversion X , we have:

$$X = 1 - \frac{1}{(1 + Da)^n} = 1 - \frac{1}{(1 + \tau k)^n}$$

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4.3.3 CSTRs in parallel



$$V_i = F_{A0i} [X_i / (-r_{Ai})]$$

If $V_1 = V_i = V_n$, same T , and identical feed rate

We have: $X_1 = X_2 = X_n = X$;

$$-r_{A1} = -r_{A2} = -r_{An} = -r_A;$$

$$V_i = V/n; F_{A0i} = F_{A0}/n$$

$$V = F_{A0} X_i / (-r_{Ai}) = F_{A0} X / (-r_A)$$

The conversion in any of the reactors is identical to what we would achieve if the reactant were fed in one stream to a large reactor of volume V .

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4.3.4 A second-order reaction in CSTR

- We start with the rate law and design equation:

$$V = F_{A0} X_i / (-r_{Ai}) = F_{A0} X / (kC_A^2)$$

- Using stoichiometry and $v = v_0$, we have

$$C_A = C_{A0} (1 - X)$$

- Also: $F_{A0} X = v_0 C_{A0} X$

- As a result
$$V = \frac{v_0 C_{A0} X}{kC_{A0}^2 (1 - X)^2}$$

- Since $\tau = \frac{V}{v_0}$ we have $\tau = X / [kC_{A0} (1 - X)^2]$

$$X = [(1 + 2 Da) - (1 + 4 Da)^{1/2}] / (2 Da) \quad \text{with } Da = \tau k C_{A0}$$

Example 4.2 on page 163 illustrates these concepts

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4.6 Synthesizing the design of a chemical plant

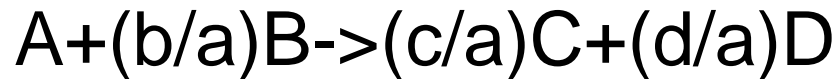
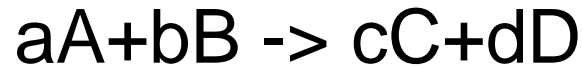
The design of a chemical plant requires knowledge of several process units, in addition to the reactor. It is also critical to address profit from the chemical plant.

4.7 Mole balances on CSTRs, PFRs, PBR, and batch reactors

4.7.1 Liquid phase

We need to monitor the concentration of species.

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$$\text{Batch: } dC_A/dt = r_A; \quad dC_B/dt = (b/a) r_A$$

$$\text{CSTR: } V = v_0(C_{A0} - C_A)/-r_A; \quad V = v_0(C_{B0} - C_B)/(-(b/a)r_A)$$

$$\text{PFR: } v_0 dC_A/dV = r_A; \quad v_0 dC_B/dV = (b/a) r_A$$

$$\text{PBR: } v_0 dC_A/dW = r'_A; \quad v_0 dC_B/dW = (b/a) r'_A$$

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4.7.2 Gas phase

We need to use the number of moles.

Batch: $dN_A/dt = r_A V$; $dN_B/dt = r_B V$; $dN_C/dt = r_C V$; $dN_D/dt = r_D V$

CSTR: $V = (F_{A0} - F_A)/-r_A$; $V = (F_{B0} - F_B)/-r_B$;
 $V = (F_{C0} - F_C)/-r_C$; $V = (F_{D0} - F_D)/-r_D$

PFR: $dF_A/dV = r_A$; $dF_B/dV = r_B$; $dF_C/dV = r_C$;
 $dF_D/dV = r_D$

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- **Notes on gas phase (variable v)**

$$C_T = F_T/v = P/(ZRT); F_T = C_T v$$

Z: compressibility factor

$$C_{T0} = F_{T0}/v_0 = P_0/(Z_0RT_0);$$

With $z = z_0$, $v = v_0(F_T/F_{T0})(P_0/P)(T/T_0)$

As a result: $C_j = F_j/v = C_{T0}(F_j/F_T)(P/P_0)(T_0/T)$