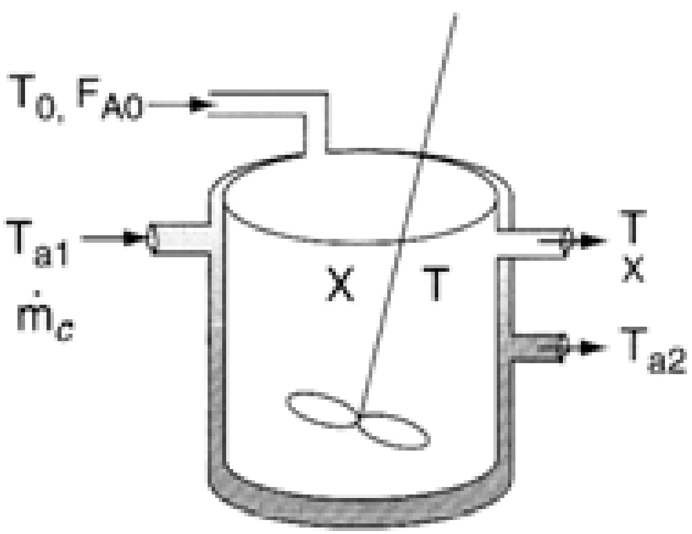
# 8. Steady-State Nonisothermal Reactor Design

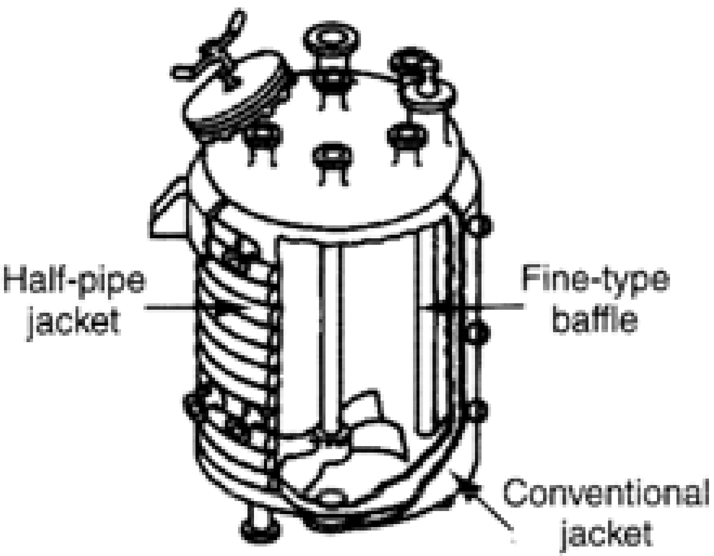
- Energy Balance
  - Overview of User Friendly Energy Balance Equations
  - Manipulating the Energy Balance, $\Delta H_{\mathrm{Rx}}$
- Reversible Reactions
- Adiabatic Reactions
- Applications of the PFR/PBR User Friendly Energy Balance Equations
- Interstage Cooling/Heating
- **Evaluating the Heat Exchanger Term**
- **Multiple Steady States**
- **Multiple Reactions with Heat Effects**

# 6. CSTR with Heat Effect I

- **Apply general energy balance to the CSTR at st st**

$$\dot{Q} - \dot{W}_s - F_{A0}\sum_{i=1}^{n}\Theta_i C_{Pi}\left[T - T_{i0}\right] - \Delta H_{Rx}(T) F_{A0} X = 0$$



# 6. CSTR with Heat Effect II

- **Algorithm for CSTR design 1**

Example: Elementary irreversible liquid-phase reaction

$$A \longrightarrow B$$

Given $F_{A0}$, $C_{A0}$, $k_0$, $E$, $C_{P_A}$, $\Delta H^\circ_{Rx}$, $\Delta C_P=0$, $\Theta_i=0$

CSTR

↓

Design equation $\quad V = \dfrac{F_{A0}X}{-r_A}$

Rate law $\quad -r_A = kC_A$

$$k = Ae^{-E/RT} = k_1 \exp\left[\frac{E}{R}\left(\frac{1}{T_1} - \frac{1}{T}\right)\right]$$

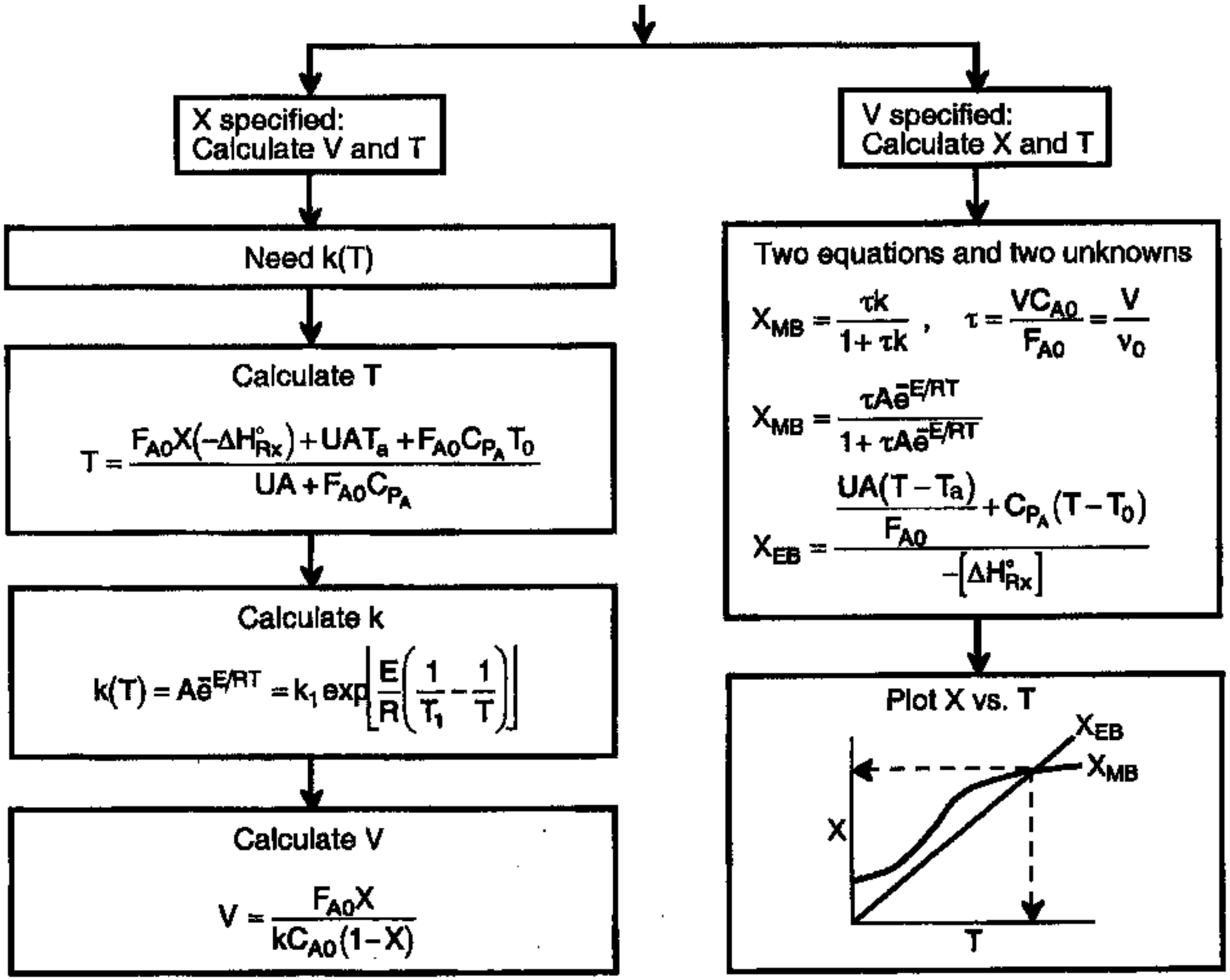
Stoichiometry $\quad C_A = C_{A0}(1-X)$

Combining $\quad V = \dfrac{F_{A0}X}{kC_{A0}(1-X)}$

↓

# 6. CSTR with Heat Effect III

- **Algorithm for CSTR design 2**



# 6. CSTR with Heat Effect IV

## ○ Algorithm for CSTR design 3

**A**

Specify $X$

Find $V$ and $T$

↓

Calculate $T$ From Eqn. (8-56)

↓

Calculate $k$

$k = Ae^{-E/RT}$

(e.g., $-r_A = kC_{A0}(1 - X)$)

↓

Calculate $-r_A(X,T)$

↓

Calculate $V$

$$V = \frac{F_{A0}X}{-r_A}$$

**B**

Specify $T$

Find $X$ and $V$

↓

Calculate $X$ From Eqn. (8-55)

↓

Calculate $k$

$k = Ae^{-E/RT}$

(e.g., $-r_A = kC_{A0}(1 - X)$)

↓

Calculate $-r_A(X,T)$

↓

Calculate $V$

$$V = \frac{F_{A0}X}{-r_A}$$

**C**

Specify $V$

Find $X$ and $T$

↓

Use Eqn. (8-55) to plot $X_{EB}$ vs. $T$

↓

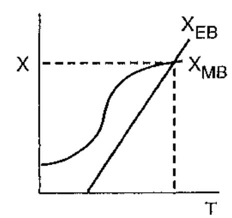
Solve Eqn. (8-53) for $X_{MB} = f(T)$ to find $X_{MB}$ vs. $T$

(e.g., $X_{MB} = \dfrac{\tau A \exp[-E/(RT)]}{1 + \tau A \exp[-E/(RT)]}$ )

↓

Plot $X_{EB}$ and $X_{MB}$ as a function of $T$

↓

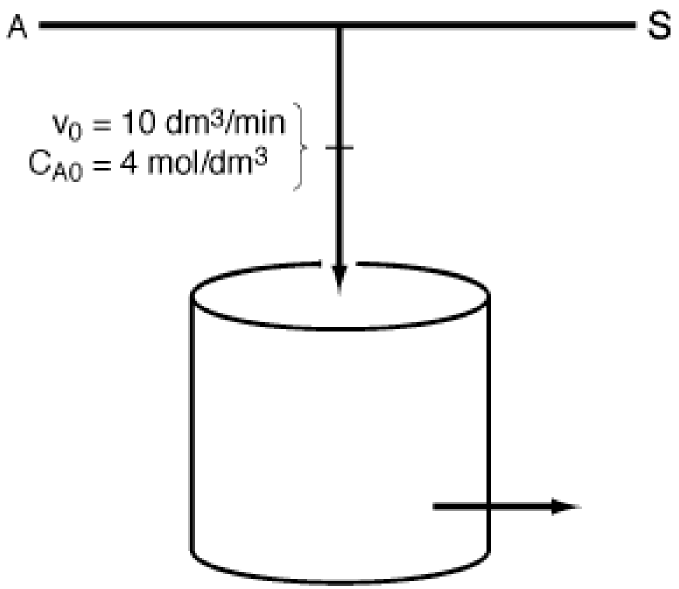



$X_{MB}$ = conversion calculated from the mole balance

$X_{EB}$ = conversion calculated from the energy balance

# 6. CSTR with Heat Effect V

- **Given X ☞ Find T and V**
  - ☜ **Linear progression of calc T ⇒ calc k ⇒ calc $K_C$ ⇒ calc $-r_A$ ⇒ calc V**
  - **- Second order reaction in CSTR, adiabatically, acid-catalyzed irreversible liquid-phase reaction at 300 K**




$$\Delta H_{Rx}(300\,K) = -3300\ cal/mol \cdot {}^{\circ}C$$

$$C_{P_A} = 15\ cal/mol \cdot {}^{\circ}C$$

$$C_{P_B} = 15\ cal/mol \cdot {}^{\circ}C$$

$$C_{P_S} = 18\ cal/mol \cdot {}^{\circ}C$$

$$k(300\,K) = 0.0005\ dm^3/mol \cdot min$$

$$E = 15{,}000\ cal/mol$$

# 6. CSTR with Heat Effect VI

- **Given X ☞ Find T and V 2**

**(a) What CSTR reactor volume is necessary to achieve 80% conversion?**

**1. CSTR Design Equation:**

$$V = \frac{F_{A0}X}{-r_A}$$

**2. Rate Law:**

$$-r_A = kC_A^2$$

**3. Stoichiometry:**

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

**4. Combine:**

$$V = \frac{\upsilon_0 X}{kC_{A0}(1-X)^2}$$

$$V = \frac{F_{A0}X}{kC_A^2} = \frac{C_{A0}\upsilon_0 X}{k[C_{A0}(1-X)]^2}$$

# 6. CSTR with Heat Effect VII

- **Given X ☞ Find T and V 3**

**5. Determine T: adiabatic energy balance**

$$T = \frac{X\left[-\Delta H_{Rx}(T_R)\right] + \sum \Theta_i \tilde{C}_{P_i} T_0 + X\Delta\hat{C}_P T_R}{\sum \Theta_i \tilde{C}_{P_i} + X\Delta\hat{C}_P}$$

$$\Delta\hat{C}_P = C_{P_B} - C_{P_A} = (15 - 15)\text{cal/mol}\cdot{}^{\circ}\text{C} = 0$$

$$T = \frac{X\left[-\Delta H_{Rx}(T_R)\right] + \sum \Theta_i \tilde{C}_{P_i} T_0}{\sum \Theta_i \tilde{C}_{P_i}}$$

$$T = T_0 + \frac{X\left[-\Delta H_{Rx}(T_R)\right]}{\sum \Theta_i \tilde{C}_{P_i}}$$

# 6. CSTR with Heat Effect VII

○ **Given X ☞ Find T and V 3**

**5. Determine T: adiabatic energy balance**

**- Substituting for known values and solving for T**

$$T = 300\ \text{K} + \frac{(0.8)[-(-3300\ \text{cal/mol})]}{[(15+18)(\text{cal/mol}\cdot{}^{\circ}\text{C})]} \qquad T = 380\ \text{K}$$

**6. Solve for the Rate Constant (k) at T = 380 K:**

$$k(T) = k(T_1)\exp\left[\frac{E}{R}\left(\frac{1}{T_1} - \frac{1}{T}\right)\right]$$

$$k(380\ \text{K}) = \left(0.0005\,\frac{\text{dm}^3}{\text{mol}\cdot\text{min}}\right)\exp\left[\frac{\left(15{,}000\,\frac{\text{cal}}{\text{mol}}\right)}{\left(1.987\,\frac{\text{cal}}{\text{mol}\cdot\text{K}}\right)}\left(\frac{1}{300\text{K}} - \frac{1}{380\text{K}}\right)\right]$$

$$k = 0.1\ \text{dm}^3/\text{mol}\cdot\text{min}$$

# 6. CSTR with Heat Effect VIII

- **Given X ☞ Find T and V 4**

**7. Calculate the CSTR Reactor Volume (V):**

$$V = \frac{\upsilon_0 X}{kC_{A0}(1-X)^2}$$

$$V = \frac{\left(10\frac{dm^3}{min}\right)(0.8)}{\left(0.1\frac{dm^3}{mol \cdot min}\right)\left(4\frac{mol}{dm^3}\right)(1-0.8)^2}$$

$$\boxed{V = 500\ dm^3}$$

# 6. CSTR with Heat Effect IX

- **Given V ☞ Find X and T**

**(b) What conversion can be achieved in a 1000 dm $^3$ CSTR? What is the new exit temperature?**

**1. CSTR Design Equation:**

$$V = \frac{F_{A0}X}{-r_A}$$

**2. Rate Law:**

$$-r_A = kC_A^2$$

**3. Stoichiometry:**

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

**4. Combine:**

$$V = \frac{\upsilon_0 X}{kC_{A0}(1-X)^2}$$

$$V = \frac{F_{A0}X}{kC_A^2} = \frac{C_{A0}\upsilon_0 X}{k[C_{A0}(1-X)]^2}$$

# 6. CSTR with Heat Effect X

- Given V ☞ Find X and T 2

  More convenient to work with this equation in terms of space time, rather than volume

$$\tau = \frac{1}{kC_{A0}}\frac{X}{(1-X)^2}$$

**5. Solve the Energy Balance for $X_{EB}$ as a function of T:**

$$X_{EB} = \frac{\sum \Theta_i \tilde{C}_{P_i}(T - T_0)}{-\Delta H_{Rx}(T_R)}$$

$$X_{EB} = \frac{(C_{P_A} + C_{P_S})(T - T_0)}{-\Delta H_{Rx}(T_R)}$$

# 6. CSTR with Heat Effect XI

- **Given V ☞ Find X and T 3**

**6. Solve the Mole Balance for $X_{MB}$ as a function of T:**

$$\tau k C_{A0} = \frac{X}{(1-X)^2}$$

$$X_{MB} = \frac{(2\tau k C_{A0}+1) - \sqrt{4\tau k C_{A0}+1}}{2(\tau k C_{A0})}$$

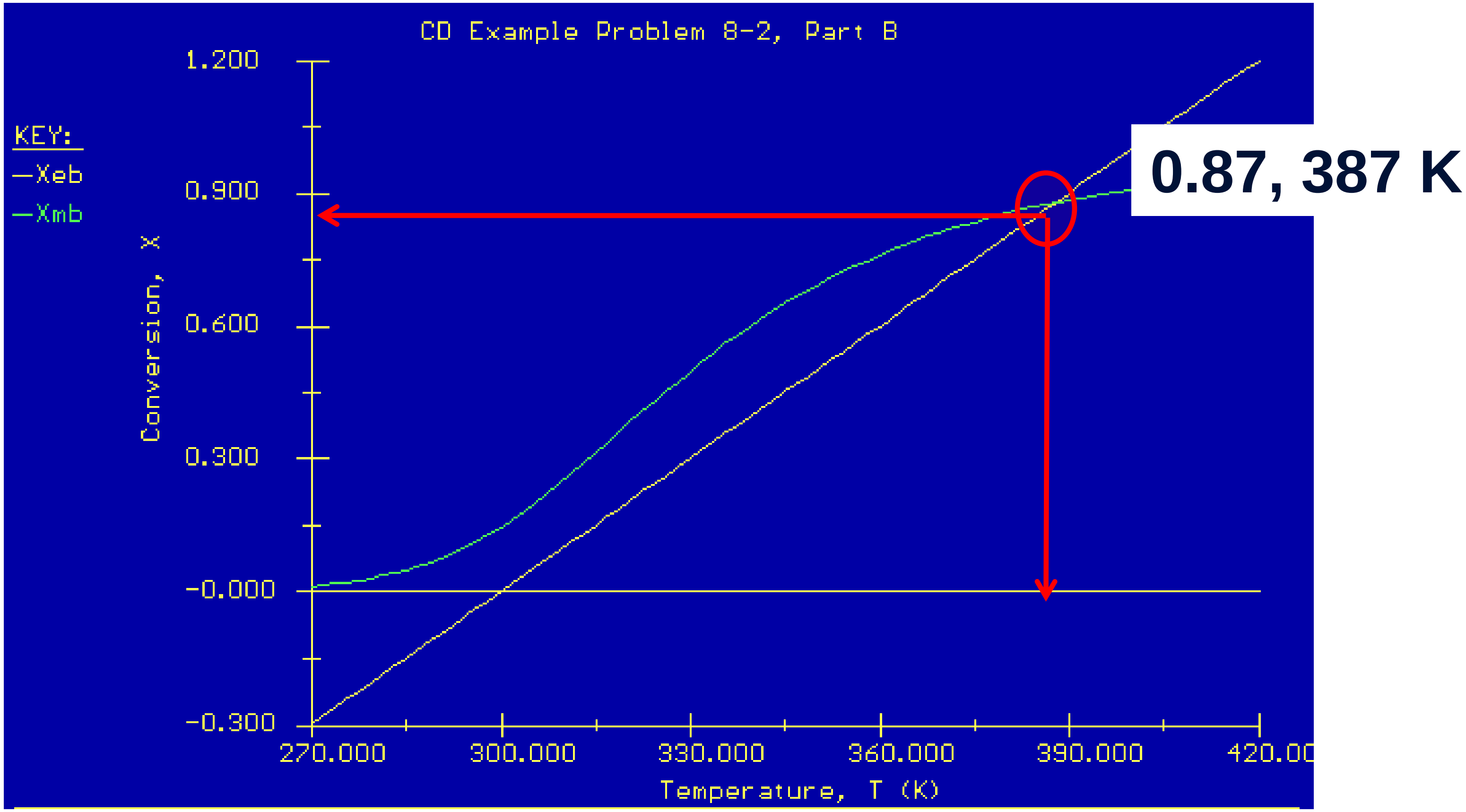
$$Da = \tau k C_{A0}$$

$$X_{MB} = \frac{(2Da+1) - \sqrt{4Da+1}}{2(Da)}$$

# 6. CSTR with Heat Effect XII

○ **Given V ☞ Find X and T 4**

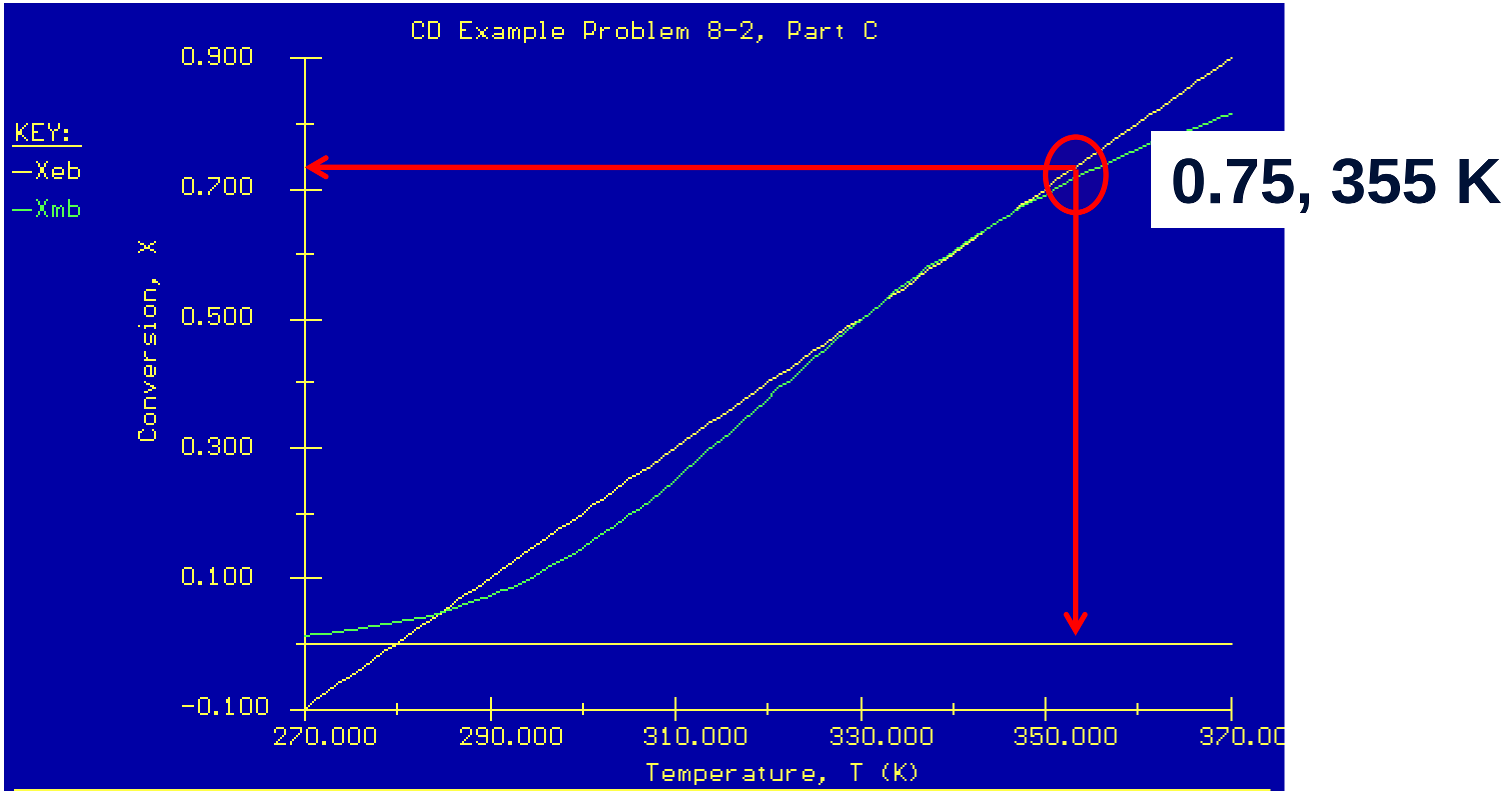
**7. Plot $X_{EB}$ and $X_{MB}$ :**



# 6. CSTR with Heat Effect XIII

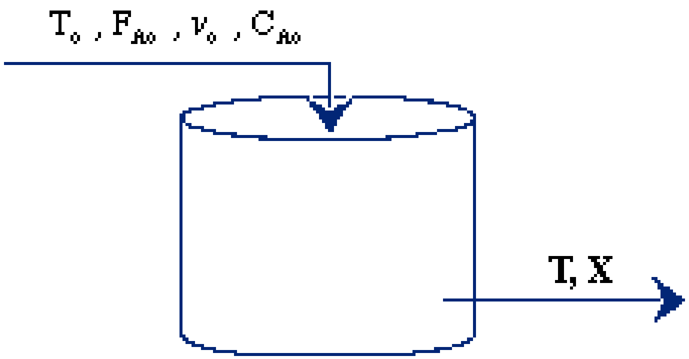
- **Given V ☞ Find X and T 5**

**(c) How would your answers to part (b) change, if the entering temperature of the feed were 280 K?**



# 6. CSTR with Heat Effect XIV

- **Given T ☞ Find X and V**
  - ☜ **Linear progression of calc k ⇒ calc $K_C$ ⇒ calc X ⇒ calc $-r_A$ ⇒ calc V**
  - **- First order reaction in CSTR, adiabatically, acid-catalyzed irreversible liquid-phase reaction**
  - **- Also given $k$, $E$, $C_{PA}=C_{PB}$, $\Delta H_{Rx}$ , $C_{Ao}$, and $v_o$**



# 6. CSTR with Heat Effect XV

- **Given T ☞ Find X and V 2**

$$\text{Mole Balance :}\quad V = \frac{F_{Ao}X}{-r_A}$$

$$\text{Rate Law :}\quad -r_A = kC_A$$

$$k = Ae^{-E/RT}$$

$$\text{Stoichiometry :}\quad C_A = C_{Ao}(1-X)$$

$$\text{Combine :}\quad V = \frac{C_{Ao}v_o X}{kC_{Ao}(1-X)} \Rightarrow \tau = \frac{1}{k}\frac{X}{(1-X)}$$

$$\text{Energy Balance :}\quad T = T_o - \frac{(-\Delta H_{rx})X}{C_{pA}}$$

# 6. CSTR with Heat Effect XVI

- **Given T ☞ Find X and V 3**

Given T

1) Calculate $X = \frac{C_{pA}(T-T_o)}{\Delta H_{rx}}$

2) Calculate $k = Ae^{-E/RT} = k_1(T_1)\exp\left[\frac{E}{R}\left(\frac{1}{T_1}-\frac{1}{T}\right)\right]$

3) Calculate $\tau = \frac{1}{k}\frac{X}{(1-X)}$

4) Calculate $V = v_o \tau$

# 7. Multiple Steady States (MSS)

○ **CSTR with Heat Effects**

$$\dot{Q} - \dot{W}_s - F_{A0}\sum_{i=1}^{n}\Theta_i C_{P_i}(T - T_{i0}) - [\Delta H^\circ_{Rx}(T_R) + \Delta C_P(T - T_R)]F_{A0}X = 0$$

**- For very large coolant rate, $T_a$ is constant**

$$\dot{Q} = UA(T_a - T)$$

**- $\Delta C_P = 0$**

$$\frac{UA}{F_{A0}}(T_a - T) - \Sigma\Theta_i C_p(T - T_0) - \Delta H^\circ_{Rx}X = 0$$

$$T = \frac{F_{A0}X(-\Delta H_{Rx}) + UA\ T_a + F_{A0}C_{P_A}T_0}{UA + F_{A0}C_{P_A}}$$

# 7. Multiple Steady States II

- **CSTR with Heat Effects 2**

$$X = \frac{\frac{UA}{F_{A0}}(T - T_a) + \Sigma\Theta_i C_{p_i}(T - T_0)}{[-\Delta H^\circ_{Rx}(T_R)]}$$

**- In general**

$$[X(-\Delta H_{Rx})] - \left[\Sigma\Theta_i C_{P_i}(T - T_0) + \frac{UA}{F_{A0}}(T - T_A)\right] = 0$$

$$\begin{bmatrix}\text{Heat Generated}\\ G(T)\end{bmatrix} - \begin{bmatrix}\text{Heat Removed}\\ R(T)\end{bmatrix} = 0$$

$$C_{P_0} = \Sigma\Theta_i C_{P_i}$$

$$X(-\Delta H_{Rx}) = C_{P_0}\left[T - T_0 + \frac{UA}{F_{A0}C_{P_0}}(T - T_a)\right]$$

# 7. Multiple Steady States III

- **CSTR with Heat Effects 3**

$$\text{Let } \kappa = \frac{UA}{F_{A0}C_{P_0}}$$

$$X(-\Delta H_{Rx}) = C_{P_0}(T + \kappa T - T_0 - \kappa T_a)$$

$$= C_{P_0}(1+\kappa)\left(T - \frac{T_0 + \kappa T_a}{1+\kappa}\right)$$

$$= C_{P_0}(1+\kappa)(T - T_C)$$

$$T_C = \frac{T_0 + \kappa T_a}{1+\kappa}$$

$$\boxed{V = \frac{F_{A0}X}{-r_A(X,T)}}$$

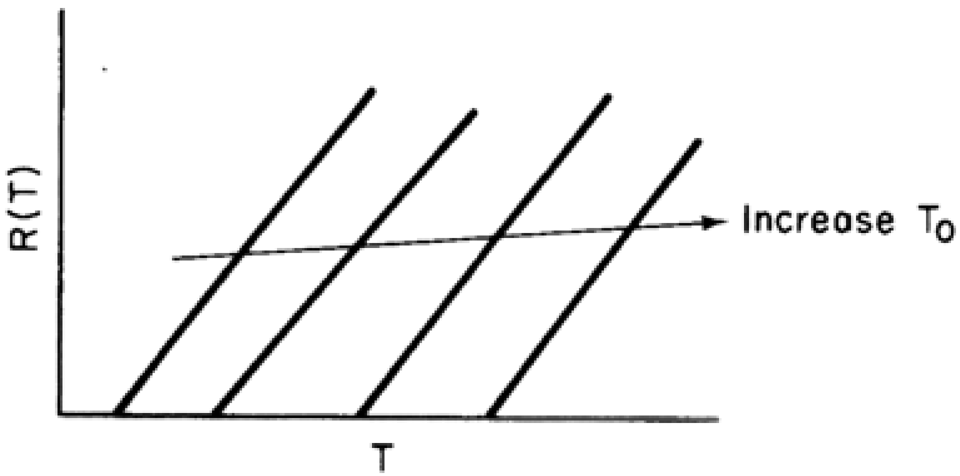
# 7. Multiple Steady States IV

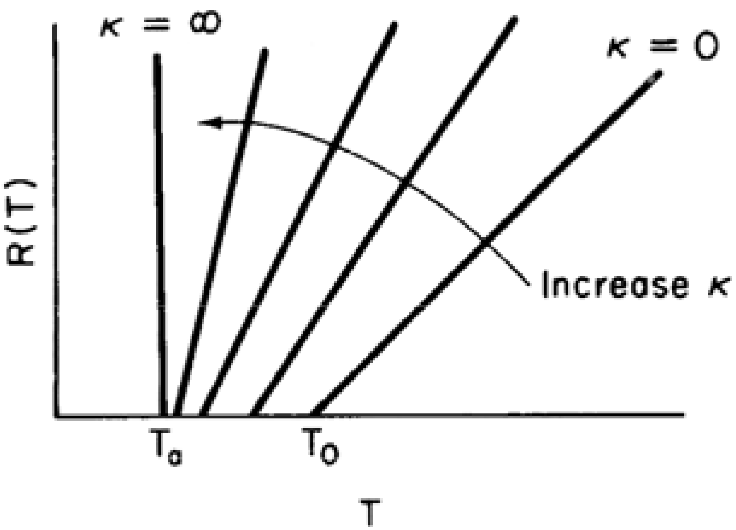
- **CSTR with Heat Effects 4**

$$-X\Delta H^\circ_{Rx} = C_{P_0}(1+\kappa)(T-T_c)$$

$$X = \frac{C_{P_0}(1+\kappa)(T-T_c)}{-\Delta H^\circ_{Rx}}$$

$$T = T_c + \frac{(-\Delta H^\circ_{Rx})(X)}{C_{P_0}(1+\kappa)}$$



# 7. Multiple Steady States V

- **Heat of generation**

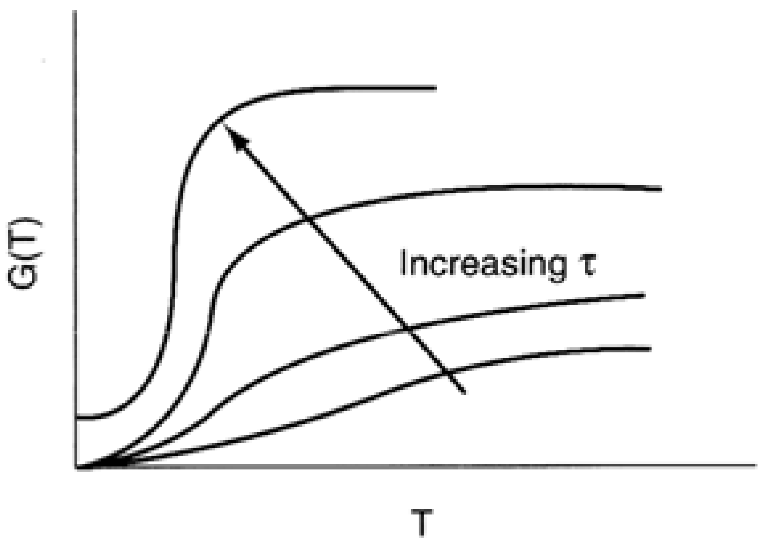
  **- First-order liquid-phase reaction**

$$V = \frac{F_{A0}X}{kC_{A0}(1-X)} = \frac{C_{A0}\upsilon_0 X}{kC_{A0}(1-X)}$$

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

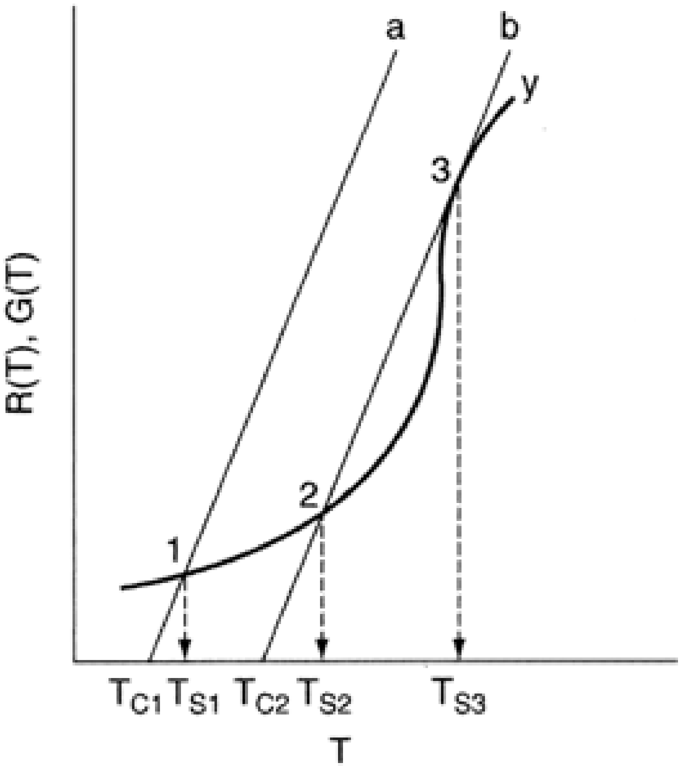
$$X = \frac{\tau k}{1+\tau k} = \frac{\tau A e^{-E/RT}}{1+Ae^{-E/RT}}$$

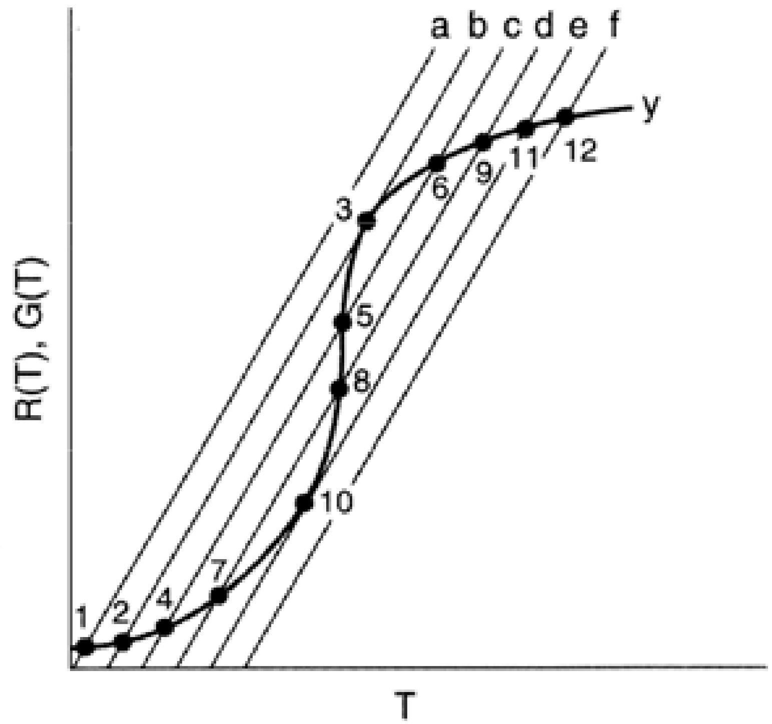
$$G(T) = X(-\Delta H_{Rx}) = \frac{\tau A e^{-E/RT}}{1+Ae^{-E/RT}}(-\Delta H_{Rx})$$



# 7. Multiple Steady States VI

- **Heat of generation**



# ※ Self Test

- **MSS for an Endothermic Reaction**
  - **Can there be multiple steady states (MSS) for a irreversible first order endothermic reaction?**

**Sol)**

$$G(T) = (X)(-\Delta H_{Rx})$$

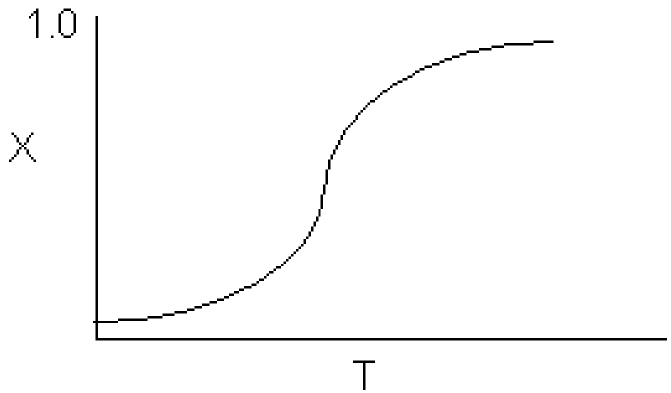
- **For an endothermic reaction $H_{RX}$ is positive, (e.g., $H_{RX}$ = +100 kJ/mole).**

$$G(T) = -100\ X$$

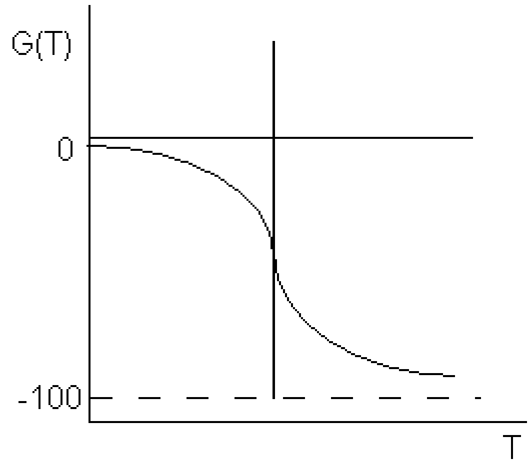
$$X = \frac{\tau k}{1+\tau k} = \frac{\tau A e^{-E/RT}}{1+\tau A e^{-E/RT}}$$

# ※ Self Test

## ○ MSS for an Endothermic Reaction 2

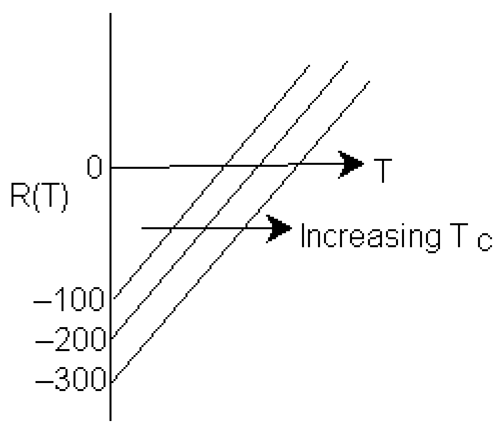


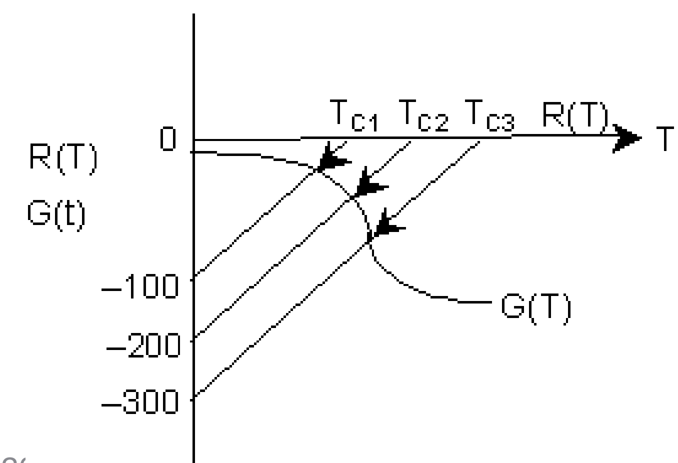

$$R(T) = C_{P_0}(1+K)(T - T_C)$$




$$G = -\Delta H_{RX} X$$

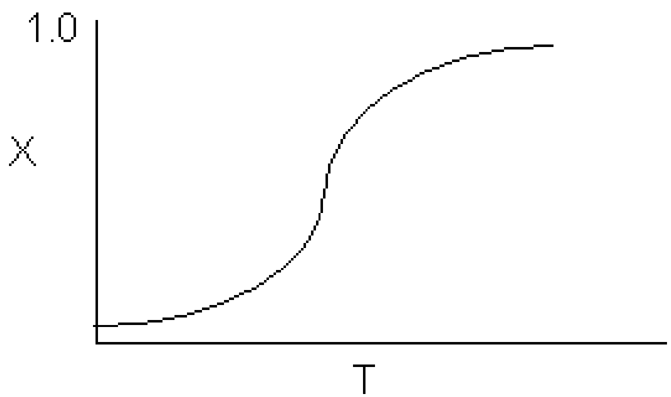
$$G = -100 \frac{\tau A e^{-E/RT}}{1 + \tau A e^{-E/RT}}$$

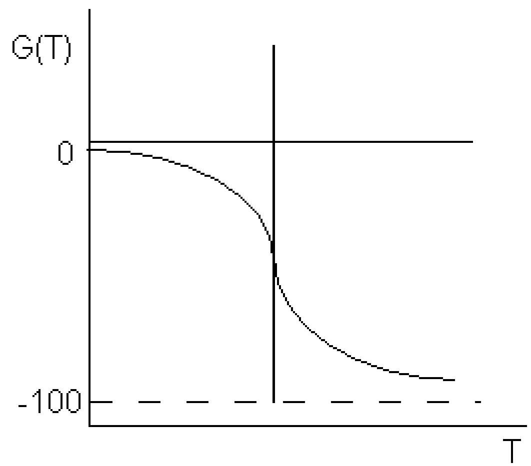


# ※ Self Test 2

- **MSS for an Endothermic Reaction 2**




$$G = -\Delta H_{RX} X$$

$$G = -100 \frac{\tau A e^{-E/RT}}{1 + \tau A e^{-E/RT}}$$

$$R(T) = C_{P_0}(1+K)(T - T_C)$$