REAKTOR ALIR TANGKI BERPENGADUK (RATB)

Pertemuan 7, 8, dan 9

Sifat-sifat mendasar pada RATB

1. Pola alir adalah bercampur sempurna (back mixed flow atau BMF)

2. Meskipun aliran melalui RATB adalah kontinyu, tapi kec volumetris aliran pada pemasukan dan pengeluaran dapat berbeda, disebabkan oleh terjadinya perubahan densiti

3. BMF meliputi pengadukan yang sempurna dalam volume reaktor, yg berimplikasi pada semua sifat-sifat sistem menjadi seragam diseluruh reaktor

4. Pengadukan yg sempurna juga mengakibatkan semua komponen dlm reaktor mempunyai kesempatan yg sama utk meninggalkan reaktor

Sifat-sifat mendasar pada RATB (Lanjut)

5. Sebagai akibat poin 4, terdapat distribusi kontinyu dari waktu tinggal

6. Sebagai akibat dari poin 4, aliran keluaran mempunyai sifat-sifat sama dengan fluida dalam reaktor

7. Sebagai akibat dari 6, terdapat satu langkah perubahan yg menjelaskan perubahan sifat-sifat dari input dan output

8. Meskipun terdapat perubahan distribusi waktu tinggal, pencampuran sempurna fluida pada tingkat mikroskopik dan makroskofik membimbing utk merata-rata sifat-sifat seluruh elemen fluida

Keuntungan dan Kerugian Menggunakan RATB

- **Keuntungan**
  - Relatif murah untuk dibangun
  - Mudah mengontrol pada tiap tingkat, karena tiap operasi pada keadaan tetap, permukaan perpindahan panas mudah diadakan
  - Secara umum mudah beradaptasi dg kontrol otomatis, memberikan respon cepat pada perubahan kondisi operasi (misal: kec umpan dan konsentrasi)
  - Perawatan dan pembersihan relatif mudah
  - Dengan pengadukan efisien dan viskositas tidak terlalu tinggi, dalam praktek kelakuan model dapat didekati lebih tepat untuk memprediksi unjuk kerja.
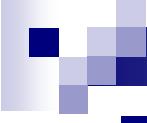
- **Kerugian**
  - Secara konsep dasar sangat merugikan dari kenyataan karena aliran keluar sama dengan isi vesel
  - Hal ini menyebabkan semua reaksi berlangsung pada konsentrasi yang lebih rendah (katakan reaktan A, C_A) antara keluar dan masuk
  - Secara kinetika normal r_A turun bila C_A berkurang, ini berarti diperlukan volume reaktor lebih besar untuk memperoleh konversi yg diinginkan
  - (Untuk kinetika tidak normal bisa terjadi kebalikannya, tapi ini tidak biasa, apakah contohnya dari satu situasi demikian?)
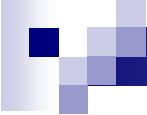
Persamaan perancangan untuk RATB

Pertimbangan secara umum:

- ☐ Neraca masa
- ☐ Neraca Energi

Perancangan proses RATB secara khas dibangun untuk menentukan volume vesel yang diperlukan guna mencapai kecepatan produksi yang diinginkan
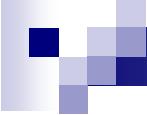
Parameter yang dicari meliputi:

- Jumlah stage yg digunakan untuk operasi optimal
- Fraksi konversi dan suhu dalam tiap stage
- Dimulai dengan mempertimbangkan neraca massa dan neraca energi untuk tiap stage

Neraca massa, volume reaktor, dan kecepatan produksi
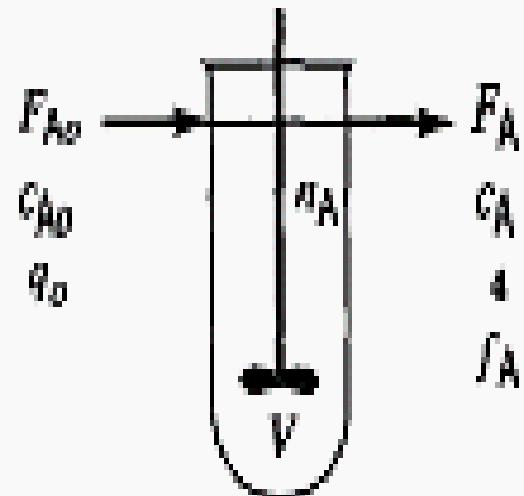
Untuk operasi kontinyu dari RATB vesel tertutup, tinjau reaksi:

$$A + \ldots \rightarrow \nu_C \, C + \ldots$$

dengan kontrol volume didefinisikan sebagai volume fluida dalam reaktor

$$\begin{pmatrix} \text{rate of} \\ \text{input of} \\ \text{A by flow} \end{pmatrix} - \begin{pmatrix} \text{rate of} \\ \text{output of} \\ \text{A by flow} \end{pmatrix} - \begin{pmatrix} \text{rate of} \\ \text{disappearance} \\ \text{of A by} \\ \text{reaction} \end{pmatrix} = \begin{pmatrix} \text{rate of} \\ \text{accumulation} \\ \text{of A within} \\ \text{the control} \\ \text{volume} \end{pmatrix} \qquad (1)$$

Secara operasional:

$$F_{A0} - F_A - (-r_A)V = dn_A/dt \qquad (2)$$

Dalam term kecepatan volumetrik:

$$c_{A0}q_0 - c_A q - (-r_A)V = dn_A/dt \qquad (3)$$

Dalam term konversi A, dengan hanya A yg tidak bereaksi dalam umpan ($f_{A0} = 0$):

$$F_{A0}f_A - (-r_A)V = dn_A/dt \qquad (4)$$

Untuk opersasi tunak (steady state) → $dn_A/dt = 0$

$$V = (c_{Ao}q_o - c_A q)/(-r_A)$$ (5)

$$= F_{Ao}f_A/(-r_A)$$ (6)

Residence time: $\quad\quad \bar{\tau} = V/q$ (7)

Space time: $\quad\quad\quad\quad\quad\quad\quad\quad$ (8)

$$\tau = V/q_o$$
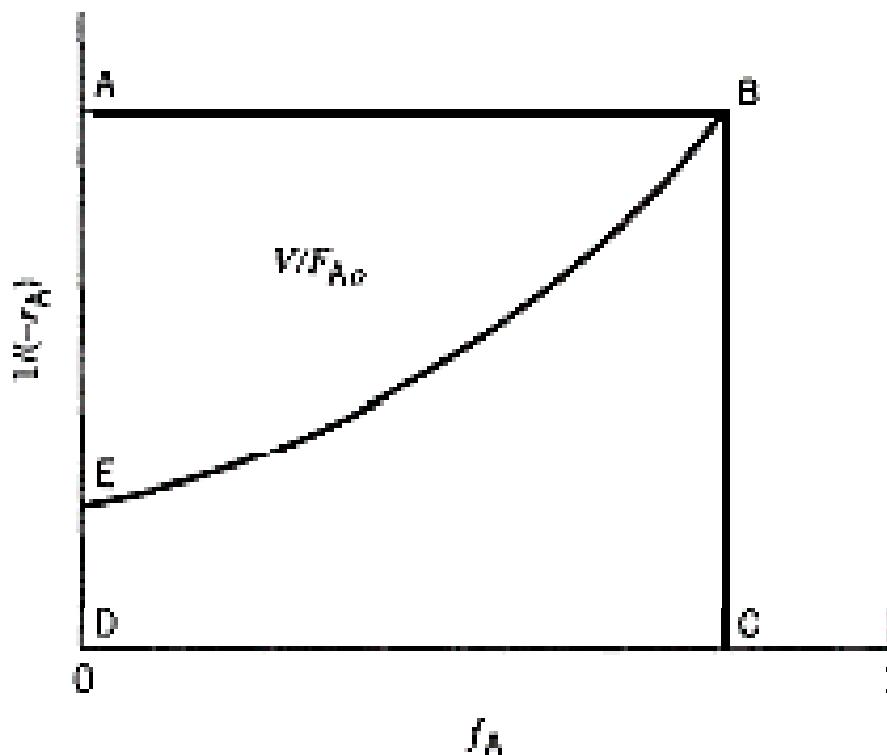
Kecepatan produksi:

$$Pr(C) = F_C = \nu_C F_{Ao} f_A = c_C q \quad\quad (9)$$

Neraca Energi

- Untuk reaktor alir kontinyu seperti RATB, neraca energi adalah neraca entalpi (H), bila kita mengabaikan perbedaan energi kinetik dan energi potensial dalam aliran, dan kerja shaft antara pemasukan dan pengeluaran

- Akan tetapi, dalam perbandingannya dengan BR, kesetimbangan harus meliputi entalpi masuk dan keluar oleh aliran

- Dalam hal berbagai transfer panas dari atau menuju kontrol volume, dan pembentukan atau pelepasan entalpi oleh reaksi dalam kontrol volume.

- Selanjutnya persamaan energi (entalpi) dinyatakan sbg:

$$\begin{pmatrix} \text{rate of} \\ \text{input of} \\ \text{enthalpy by} \\ \text{flow, heat} \\ \text{transfer or} \\ \text{reaction} \end{pmatrix} - \begin{pmatrix} \text{rate of} \\ \text{output} \\ \text{of enthalpy by} \\ \text{flow, heat} \\ \text{transfer or} \\ \text{reaction} \end{pmatrix} = \begin{pmatrix} \text{rate of} \\ \text{accumulation} \\ \text{of enthalpy} \\ \text{within control} \\ \text{volume} \end{pmatrix}$$

$$\left.\right|_{T_{ref}}^{T_o} \dot{m}_o c_{Po} dT - \left.\right|_{T_{ref}}^{T} \dot{m} c_p dT + UA_c(T_c - T), + (-\Delta H_{RA})(-r_A)V = dH/dt \qquad (10)$$

$$= d(m_t c_p T)/dt$$

Untuk operasi tunak $m = m_0$

$$\dot{m} c_p (T_o - T) + UA_c(T_c - T) + (-\Delta H_{RA})(-r_A)V = 0 \qquad (11)$$

Substitusi $F_{A0}\, f_A$ untuk (-r$_A$)V

$$\dot{m} c_p (T_o - T) + UA_c(T_c - T) + (-\Delta H_{RA})F_{Ao} f_A = 0 \qquad (12)$$

Hubungan f_A dengan suhu reaksi (T)

$$f_A = \frac{\dot{m}c_P T_o + UA_c T_c}{(-\Delta H_{RA})F_{Ao}} + \left[\frac{\dot{m}c_P + UA_c}{(-\Delta H_{RA})F_{Ao}} \right] T \qquad (13)$$
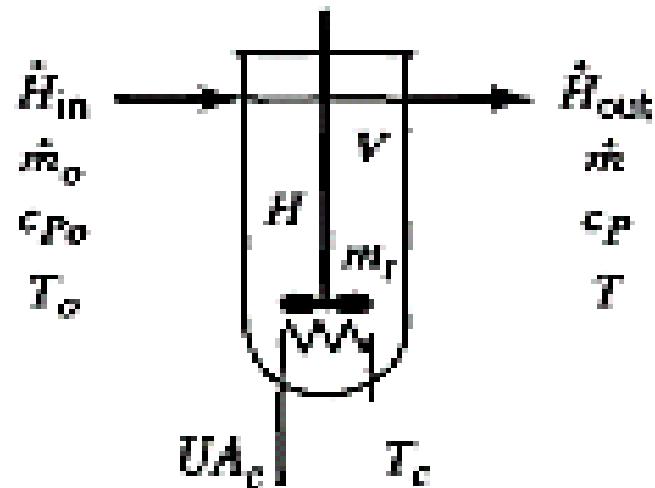
Sistem densiti konstan

Untuk sistem densiti konstan, beberapa hasil penyederhanaan antara lain:

Pertama, tanpa memperhatikan tipe reaktor, fraksi konversi limiting reactant, f_A, dapat dinyatakan dalam konsentrasi molar

$$f_A = (c_{Ao} - c_A)/c_{Ao} \quad \text{(constant density)} \tag{14}$$

Kedua, untuk aliran reaktor seperti RATB, *mean residence time* sama dengan *space time,* karena $q = q_0$

$$\bar{t} = \tau \quad \text{(constant density)} \tag{15}$$

Ketiga, untuk RATB, term akumulasi dalam persamaan neraca massa menjadi:

$$dn_A/dt = V\,dc_A/dt \qquad (\text{constant} \quad \text{density}) \qquad (16)$$

Terakhir, untuk RATB, persamaan neraca massa keadaan tunak dapat disederhanakan menjadi:

$$V = (c_{Ao} - c_A)q/(-r_A) \qquad (\text{constant} \quad \text{density}) \qquad (17)$$

Operasi keadaan tunak pada temperatur T

Untuk operasi keadaan tunak, term akumulasi dalam pers neraca massa dihilangkan

$$dn_A/dt = 0 \qquad (\text{steady-state})$$

Atau, untuk densiti konstan

$$dc_A/dt = 0 \qquad (\text{steady-state, constant density})$$

Bila T tertentu, V dapat dihitung dari pers neraca massa tanpa melibatkan neraca energi

Contoh 1.

For the liquid-phase reaction A + B → products at 20°C suppose 40% conversion of A is desired in steady-state operation. The reaction is pseudo-first-order with respect to A, with k_A = 0.0257 h^{-1} at 20°C. The total volumetric flow rate is 1.8 m^3 h^{-1}, and the inlet molar flow rates of A and B are F_{AO} and F_{BO} mol h^{-1}, respectively. Determine the vessel volume required, if, for safety, it can only be filled to 75% capacity.

Contoh 2.

A liquid-phase reaction A → B is to be conducted in a CSTR at steady-state at 163°C. The temperature of the feed is 20°C and 90% conversion of A is required. Determine the volume of a CSTR to produce 130 kg B h^{-1}, and calculate the heat load (Q) for the process. Does this represent addition or removal of heat from the system?

Data: $M_A = M_B = 200$ g mol^{-1}; cp = 2.0 J g^{-1}K^{-1}; $\rho = 0.95$ g cm^{-3}; $\Delta H_{RA} = -87$ kJ mol^{-1}; $k_A = 0.80$ h^{-1} at 163°C

Contoh 3

Consider the startup of a CSTR for the liquid-phase reaction A → products. The reactor is initially filled with feed when steady flow of feed (q) is begun. Determine the time (t) required to achieve 99% of the steady-state value of f_A.
Data: V = 8000 L; q = 2 L s^{-1}; C_{Ao} = 1.5 mol L^{-1}; k_A = 1.5 x l0^{-4} s^{-1}.
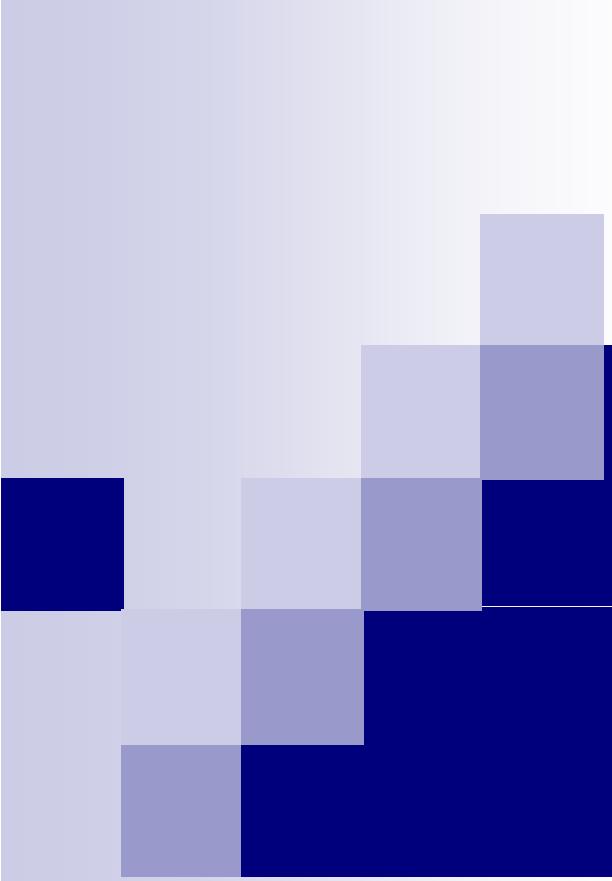
REAKTOR ALIR TANGKI BERPENGADUK (RATB)

Pertemuan 8

TINJAU ULANG NERACA ENERGI SISTEM ALIR

$$Q$$

$F_i|_{in}$
$H_i|_{in}$
$E_i|_{in}$

system

W_s

$F_i|_{out}$
$H_i|_{out}$
$E_i|_{out}$
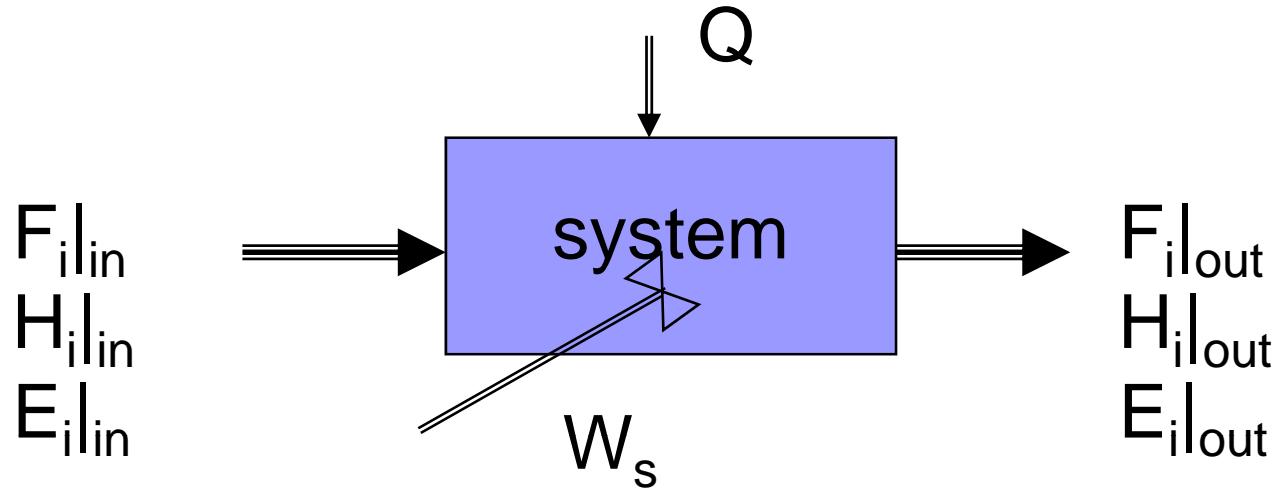
Neraca Energi

$$R_{in} - R_{out} + R_{gen} = R_{acc}$$

$$\dot{Q} - \dot{W} + \sum_{i=1}^{n} F_i E_i \bigg|_{in} - \sum_{i=1}^{n} F_i E_i \bigg|_{out} = \left(\frac{dE}{dt} \right)_{System} \qquad (8\text{-}1)$$

E_i = Energy of component i

$$\dot{W} = \dot{W}_s - \underbrace{\sum_{i=1}^{n} F_i PV_i \bigg|_{in} + \sum_{i=1}^{n} F_i PV_i \bigg|_{out}}_{} \qquad \text{(8-2)}$$

Work do to flow velocity

For chemical reactor K$_i$, P$_i$, and "other" energy are neglected so that:

$$E_i = U_i \qquad \text{(8-3)}$$

and

$$H_i = U_i + PV_i \qquad \text{(8-4)}$$

Combined the eq. 8-4, 8-3, 8-2, and 8-1 be result,

$$\dot{Q} - \dot{W}_s + \sum_{i=1}^{n} F_i H_i \bigg|_{in} - \sum_{i=1}^{n} F_i H_i \bigg|_{out} = \left(\frac{dE}{dt}\right)_{System} \qquad \text{(8-5)}$$

General Energy Balance:

$$\dot{Q} - \dot{W}_s + \sum F_{io} H_{io} - \sum F_i H_i = \frac{dE_{system}}{dt}$$

For steady state operation:

$$\dot{Q} - \dot{W}_s + \sum F_{io} H_{io} - \sum F_i H_i = 0$$

We need to put the above equation into a form that we can easily use to relate X and T in order to size reactors. To achieve this goal, we write the molar flow rates in terms of conversion and the enthalpies as a function of temperature. We now will "dissect" both Fi and Hi.

Flow Rates, Fi

For the generalized reaction:

$$A + \frac{b}{a}B \rightarrow \frac{c}{a}C + \frac{d}{a}D$$
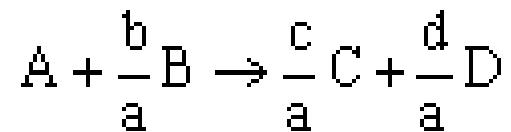
$$F_A = F_{A0}(1-X), \quad F_B = F_{A0}\left(\Theta_B - \frac{b}{a}X\right)$$

In general,

$$F_i = F_{A0}\left(\Theta_i + \upsilon_i X\right)$$

$$\upsilon_A = -1, \quad \upsilon_B = -\frac{b}{a}, \quad \upsilon_C = \frac{c}{a}, \quad \upsilon_D = \frac{d}{a}$$

Enthalpies, Hi
Assuming no phase change:

$$H_i = H_i^\circ(T_R) + \int_{T_R}^{T} C_{Pi}\, dT \qquad\qquad \sum \upsilon_i H_i = \Delta H_R(T) = \Delta H_R^\circ(T_R) + \int_{T_R}^{T} \Delta C_P\, dT$$

$$\boxed{\Delta H_{RX} = \frac{d}{a} H_D + \frac{c}{a} H_C - \frac{b}{a} H_B - H_A}$$

$$C_{Pi} = \alpha_i + \beta_i T + \chi_i T^2 \qquad\qquad \Delta C_P = \frac{d}{a} C_{PD} + \frac{c}{a} C_{PC} - \frac{b}{a} C_{PB} - C_{PA}$$

Mean heat capacities:

$$\tilde{C}_{Pi} = \frac{\int_{T_R}^{T} C_{Pi}\, dT}{(T - T_R)} \qquad\qquad \tilde{C}_{Pi} = \frac{\int_{T_{io}}^{T} C_{Pi}\, dT}{(T - T_{io})}$$

$$H_i = H_i^\circ(T_R) + \hat{C}_{Pi}(T - T_R)$$

$$\Delta H_R(T) = \Delta H_R^\circ(T_R) + \Delta \hat{C}_P(T - T_R)$$

$$\sum \upsilon_i \hat{C}_{Pi} = \Delta \hat{C}_P = \frac{d}{a}\hat{C}_{PD} + \frac{c}{a}\hat{C}_{PC} - \frac{b}{a}\hat{C}_{PB} - \hat{C}_{PA}$$

Self Test

Calculate ΔH_{Rx}°, ΔC_p, and $\Delta H_{Rx}(400)$

for the reaction, $A \rightarrow 2B + C$

There are inerts **I** present in the system.

Additional Information:

$$H_A^0(298) = -100 \ \text{kcal/mol} \quad A \qquad \tilde{C}_{P_A} = 80 \ \text{cal/mol} \ {}^\circ C$$

$$H_B^0(298) = -40 \ \text{kcal/mol} \quad B \qquad \tilde{C}_{P_B} = 20 \ \text{cal/mol} / {}^\circ C$$

$$H_C^0(298) = -30 \ \text{kcal/mol} \quad C \qquad \tilde{C}_{P_C} = 30 \ \text{cal/mol} \ {}^\circ C$$

$$H_I^0(298) = -100 \ \text{kcal/mol} \quad I \qquad \tilde{C}_{P_I} = 190 \ \text{cal/mol} \ {}^\circ C$$

Solution

$$\Delta H_{Rx}^0(298) = H_C^0 + 2H_B^0 - H_A^0 = (-30) + 2(-40) - (-100) = -10 \frac{\text{kcal}}{\text{mole} \ A}$$

$$\Delta \hat{C}_P = \tilde{C}_{P_C} + 2\tilde{C}_{P_B} - \tilde{C}_{P_A} = 30 + 2(20) - 80 = -10 \frac{\text{cal}}{\text{mol} \ {}^\circ C}$$

$$\Delta H_{Rx}(T) = \Delta H_{Rx}^{\odot}(298) + \Delta C_P(T - T_R)$$

$$= -10\,\frac{\text{kcal}}{\text{mole}\ \ A} + (-10)(T - 298)$$

$$\Delta H_R(400) = -10\,\frac{\text{kcal}}{\text{mole}\ \ A} - 10(400 - 298) = -10,000 - (10)(102)$$

$$= -11,200\,\frac{\text{cal}}{\text{mole}\ \ A}$$

Note: The inerts do not come into these claculations of $\Delta H_{Rx}^{\odot}$ or $\Delta \hat{C}_P$.

Energy Balance with "dissected" enthalpies:

$$\dot{Q} - \dot{W}_s - F_{A0} \int_{T_R}^{T} \sum \Theta_i C_{Pi} \, dT - F_{A0} X \left[\Delta H_R^{\circ}(T_R) + \int_{T_R}^{T} \Delta C_P \, dT \right] = 0$$

For constant or mean heat capacities:

$$\dot{Q} - \dot{W}_s - F_{A0} X \left[\Delta H_R^{\circ}(T_R) + \Delta \hat{C}_P (T - T_R) \right] = F_{A0} \sum \Theta_i \tilde{C}_{Pi} (T - T_{i0})$$

Adiabatic Energy Balance:

$$T = T_0 - \frac{X \left[\Delta H_R^{\circ}(T_R) + \Delta \hat{C}_P (T_0 - T_R) \right]}{\sum \Theta_i \tilde{C}_{Pi} + X \Delta \hat{C}_P} = T_0 - \frac{X \left[\Delta H_R(T_0) \right]}{\sum \Theta_i \tilde{C}_{Pi} + X \Delta \hat{C}_P}$$

Adiabatic Energy Balance for variable heat capacities:

$$X = \frac{\sum \Theta_i \alpha_i (T_0 - T) + \frac{1}{2}\sum \Theta_i \beta_i (T_0^2 - T^2) + \frac{1}{3}\sum \Theta_i \chi_i (T_0^3 - T^3)}{\Delta H_R(T_R) + \Delta\alpha(T - T_R) + \frac{1}{2}\Delta\beta(T^2 - T_R^2) + \frac{1}{3}\Delta\chi(T^3 - T_R^3)}$$

CSTR Algorithm (Section 8.3 Fogler)

1.) Given X

Find T and V

Solution: linear progression of calc $T \rightarrow$ cal $k \rightarrow$ calc $K_C \rightarrow$ calc $-r_A \rightarrow$ calc V

2.) Given T

Find X and V

Solution: linear progression: calc $k \rightarrow$ cal $K_C \rightarrow$ calc $X \rightarrow$ calc $-r_A \rightarrow$ calc V

3.) Given V

Find X

Solution: plot X_{EB} vs. T and X_{MB} vs. T on the same graph:
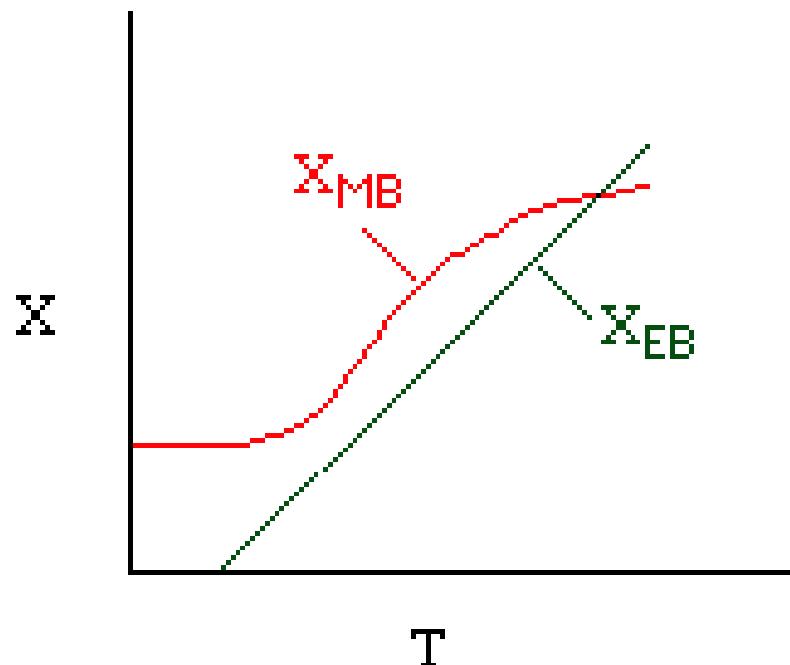
Self Test

For and adiabatic reaction with $\dot{W}_s$ and $\Delta C_P = 0$, sketch conversion as a function of temperature.

Solution

$$\dot{Q} - \dot{W}_s - F_{A0}X\left[\Delta H^{\circ}_{Rx}(T_R) + \Delta \hat{C}_P(T - T_R)\right] = F_{A0}\sum \theta_i C_{P_i}(T - T_0)$$

$$\dot{Q} = 0, \dot{W}_s = 0, \Delta \hat{C}_P = 0 \quad \therefore \Delta H_{Rx} = \Delta H^{\circ}_{Rx}$$

$$X\left[-\Delta H_{Rx}(T_R)\right] = \left(\sum \theta_i C_{P_i}\right)(T - T_0)$$

$$X_{EB} = \frac{\left[\sum \theta_i C_{P_i}\right]}{\left[-\Delta H_{Rx}\right]}\left[T - T_0\right]$$

A. <u>For an exothermic reaction,</u> ΔH_{RX} is negative (-), X_{EB} increases with increasing T.

[e.g., $\Delta H_{RX}= -100$ kJ/mole A]

$$X_{EB} = \frac{\left(\sum \theta_i C_{P_i}\right)\left(T - T_0\right)}{+\left[a\;positive\;number\quad\right]}$$
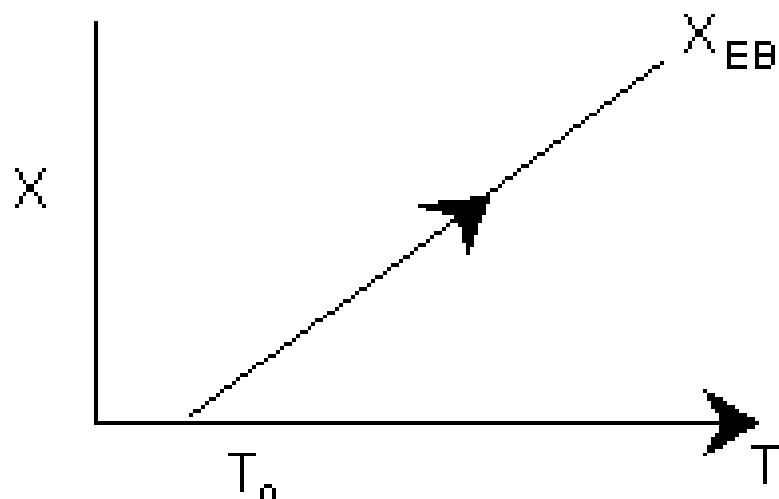
B. <u>For an endothermic reaction,</u> ΔH_{RX} is positive (+), X_{EB} increases with decreasing T. [e.g., ΔH_{RX}= +100 kJ/mole A]

$$X = \frac{\left[\sum \theta_i C_{P_i}\right]\left[T - T_0\right]}{-\left[\Delta H_{Rx}\right]} = \frac{\left[\sum \theta_i C_{P_i}\right]\left[T - T_0\right]}{\left[a \; negative \; number\right]}$$
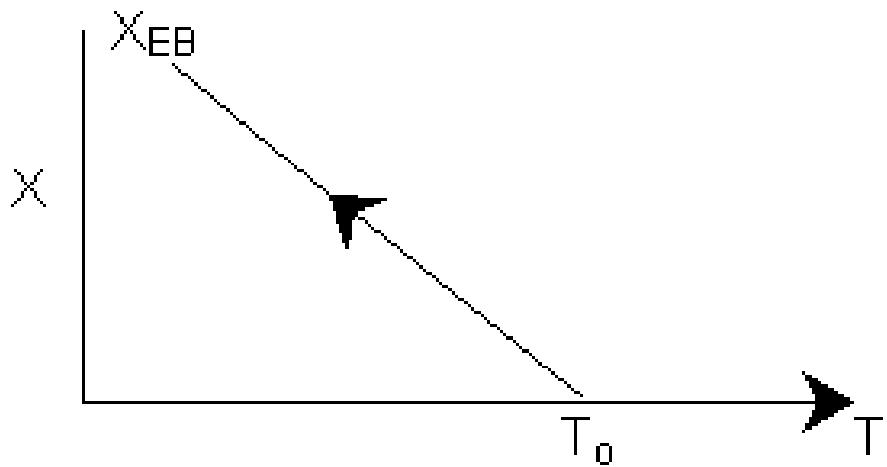
For a first order reaction, $\quad X_{MB} = \dfrac{\tau k}{1 + \tau k} = \dfrac{\tau A e^{-E/RT}}{1 + \tau A e^{-E/RT}}$
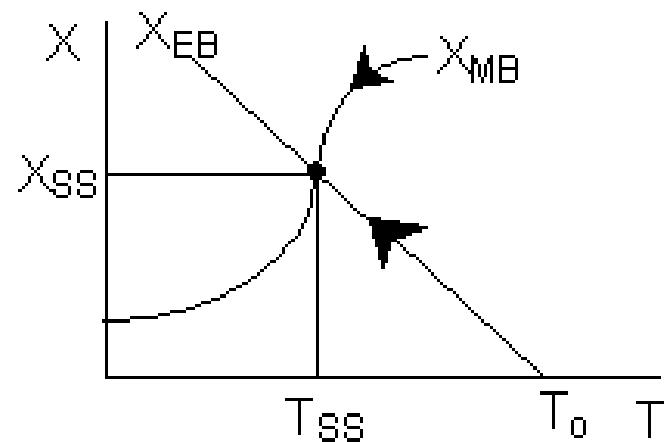
Both the mole and energy balances are satisfied when $X_{MB} = X_{EB}$. The steady state temperature and conversion are T_{SS} and X_{SS}, respectively, for an entering temperature T_O.

Evaluating the Heat Exchange Term, Q
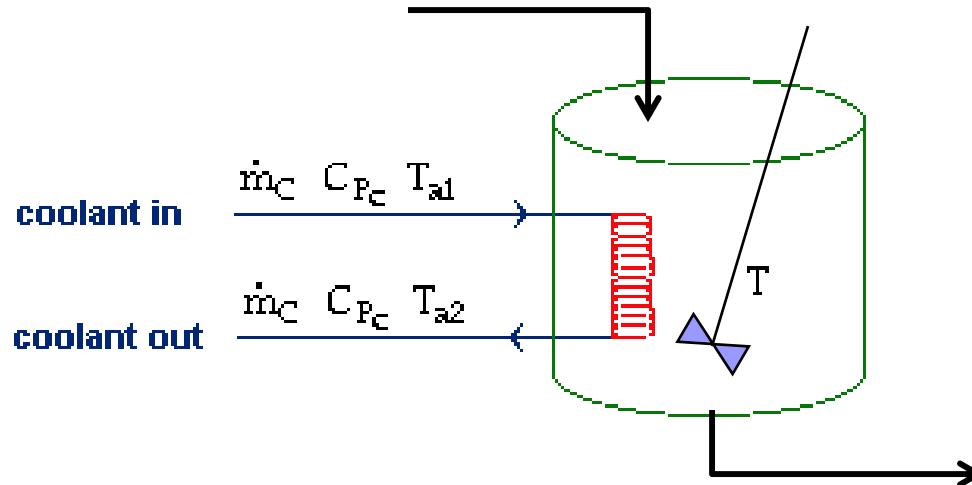
Energy transferred between the reactor and the coolant:

$$\dot{Q} = \dot{m}_C C_{Pc} \left(T_{a1} - T_{a2} \right)$$

Assuming the temperature inside the CSTR, T, is spatially uniform:

Manipulating the Energy Exchange Term

Combining: $\dot{Q} = \dot{m}_C C_{Pc}(T_{a1} - T_{a2}) = UA \dfrac{(T_{a1} - T_{a2})}{\ln\left(\dfrac{T_{a1} - T}{T_{a2} - T}\right)}$

$$\ln\left(\frac{T_{a1} - T}{T_{a2} - T}\right) = \frac{UA}{\dot{m}C_{Pc}} \frac{(T_{a1} - T_{a2})}{(T_{a1} - T_{a2})} = \frac{UA}{\dot{m}C_{Pc}}$$

$$\left(\frac{T_{a1} - T}{T_{a2} - T}\right) = \exp\left(\frac{UA}{\dot{m}C_{Pc}}\right)$$

$$(T_{a1} - T)\exp\left(-\frac{UA}{\dot{m}C_{Pc}}\right) = (T_{a2} - T)$$

$$T_{a2} = T + (T_{a1} - T)\exp\left(-\frac{UA}{\dot{m}C_{Pc}}\right)$$

$$\dot{Q} = \dot{m}_C C_{Pc}(T_{a1} - T_{a2}) = \dot{m}_C C_{Pc}\left[T_{a1} - T - (T_{a1} - T)\exp\left(-\frac{UA}{\dot{m}C_{Pc}}\right)\right]$$

$$\dot{Q} = \dot{m}_C C_{Pc} \left[(T_{a1} - T) - (T_{a1} - T)\exp\left(-\frac{UA}{\dot{m}C_{Pc}} \right) \right]$$

$$\dot{Q} = \dot{m}_C C_{Pc} (T_{a1} - T) \left[1 - \exp\left(-\frac{UA}{\dot{m}C_{Pc}} \right) \right]$$

At high coolant flowrates the exponential term will be small, so we can expand the exponential term as a Taylor Series, where the terms of second order or greater are neglected, then:

$$\dot{Q} = \dot{m}_C C_{Pc} (T_{a1} - T) \left[1 - \exp\left(-\frac{UA}{\dot{m}C_{Pc}} \right) \right]$$

$$\dot{Q} = \dot{m}_C C_{Pc} \left(T_{a1} - T \right) \left[1 - \left(1 - \frac{UA}{\dot{m}C_{Pc}} \right) \right] = \dot{m}_C C_{Pc} \left(T_{a1} - T \right) \left(\frac{UA}{\dot{m}C_{Pc}} \right)$$

$$\dot{Q} = UA \left(T_{a1} - T \right)$$

Since the coolant flowrate is high, $T_{a1} \cong T_{a2} \cong T_a$:

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

Reversible Reactions (Chp8 Fogler, Appendix C)

For Ideal gases, K_C and K_P are related by

$$K_P = K_C(RT)^\delta$$

$$\delta = \Sigma \, \nu_i$$

$$K_C = \frac{K_P}{(RT)^\delta}$$

$$\frac{d\ln K_P}{dT} = \frac{\Delta H_R(T)}{RT^2} = \frac{\Delta H_R^0(T_R) + \Delta \hat{C}_P(T - T_R)}{RT^2}$$

endothermic reaction

exothermic reaction
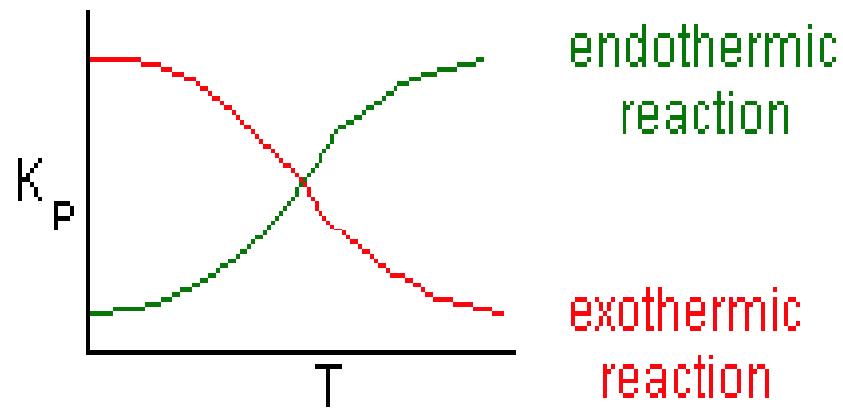
For the special case of $\Delta \hat{C}_P = 0$:

$$K_P(T_2) = K_P(T_1)\exp\left[\frac{\Delta H_R^0(T_R)}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)\right]$$

Algorithm for Adiabatic Reactions:

1. Choose X → calc T → calc k → (if gas, calc To/T) → calc K_C → calc $-r_A$

2. Increment X and then repeat calculations.

3. When finished, plot $\dfrac{F_{A0}}{-r_A}$ vs. X or use some numerical technique to find V.
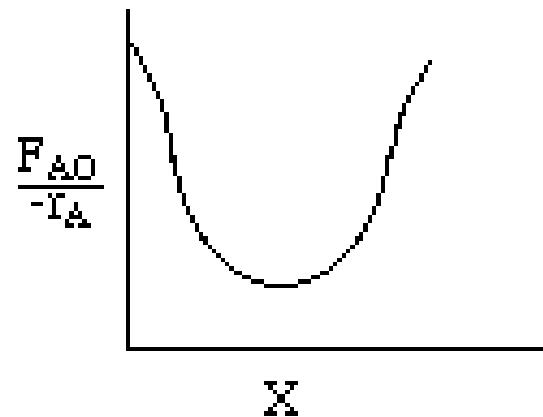
Levenspiel Plot for an
exothermal, adiabatic reaction.

PFR ──▷〔▭〕──▶ (The shaded area in the plot is the volume.)

For an exit conversion of 40%

For an exit conersion of 70%

$$\frac{F_{A0}}{-r_A}$$

0.4

$$\frac{F_{A0}}{-r_A}$$

0.7
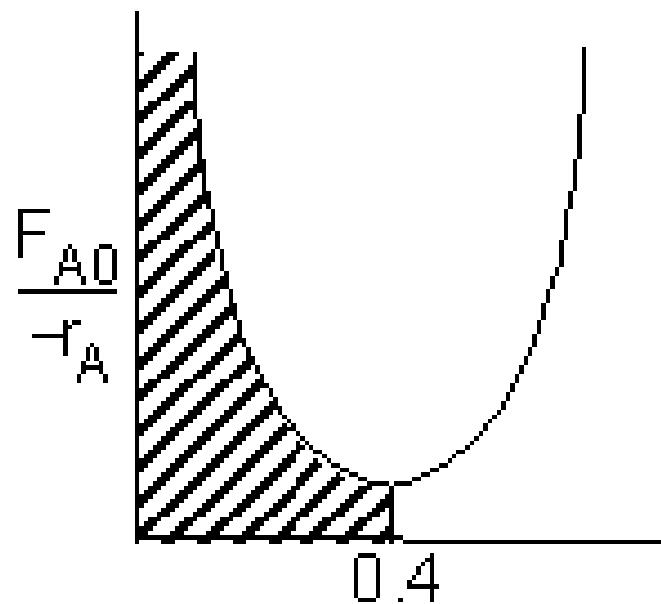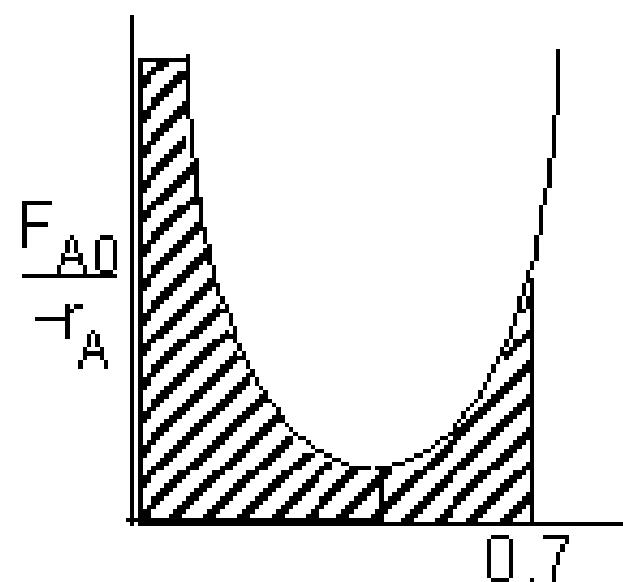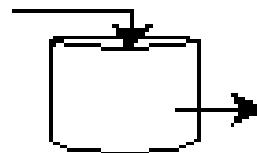
CSTR Shaded area is the reactor volume.

For an exit conversion of 40%

For an exit conersion of 70%

$$\frac{F_{A0}}{-r_A}$$

0.4

$$\frac{F_{A0}}{-r_A}$$
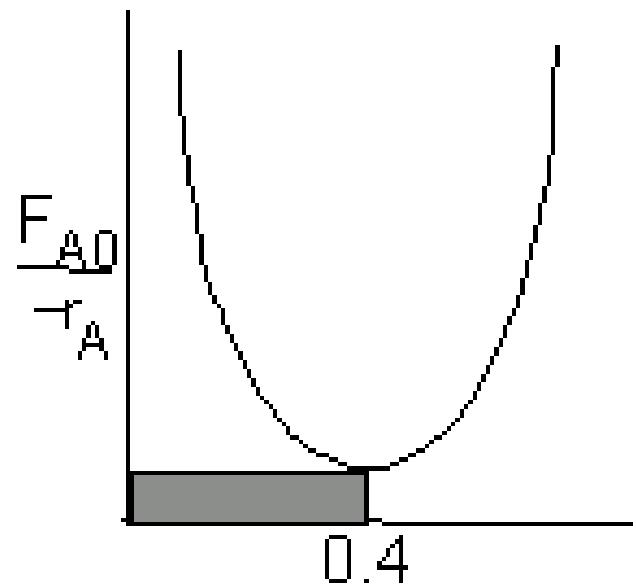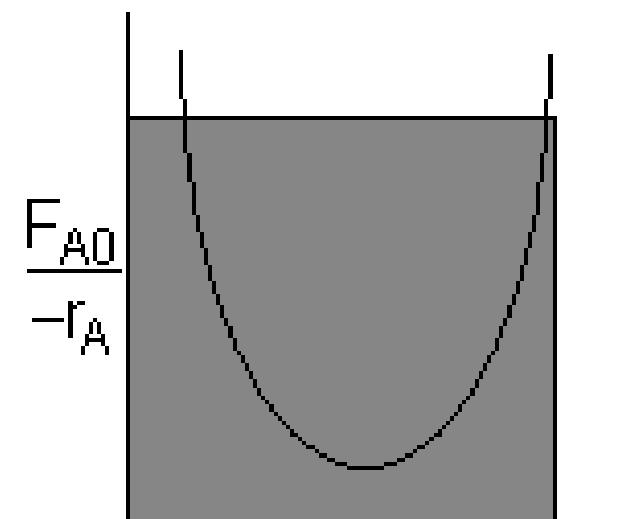
CSTR+PFR
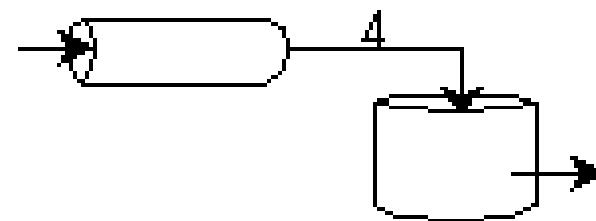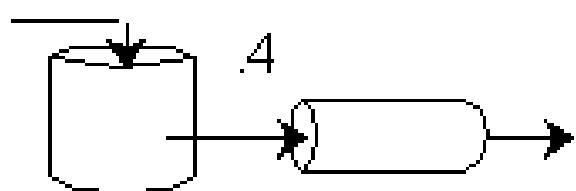
For an intermediate conversion of 40% and exit conversion of 70%
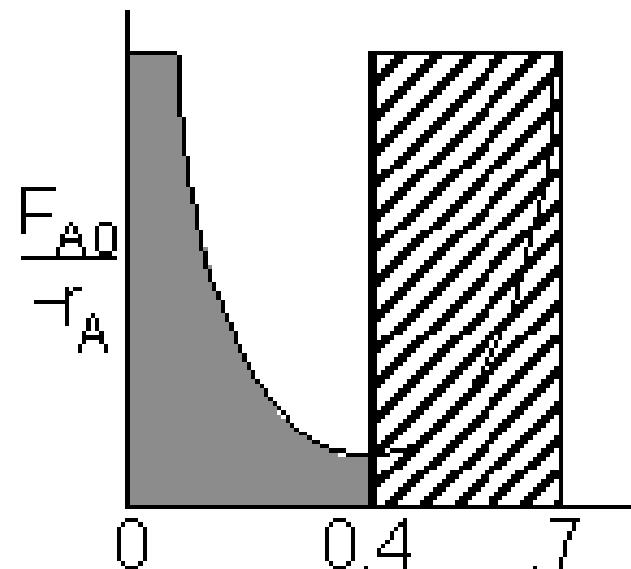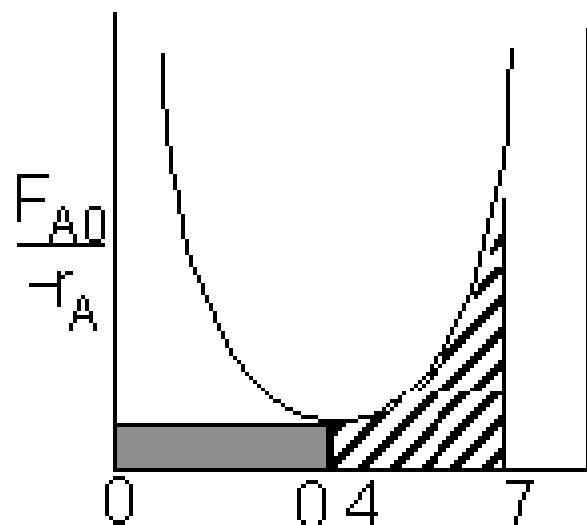
Example: Exothermic, Reversible Reaction

Why is there a maximum in the rate of reaction with respect to conversion (and hence, with respect to temperature and reactor volume) for an adiabatic reactor?

Rate Law:
$$-r_A' = k\left[C_A C_B - \frac{C_C^2}{K_C} \right]$$

$$-r_A' = \underbrace{\left[A\exp\left(-\frac{E}{RT}\right) \right]}_{A} \underbrace{\left[C_{A0}^2 \left((1-X)(2-X) - \frac{4X^2}{K_C} \right)\left(\frac{T_0}{T}y\right)^2 \right]}_{B}$$

$$T = T_0 - \frac{X\Delta H_{RX}}{\Sigma\Theta_i C_{Pi} + X\Delta C_p}$$
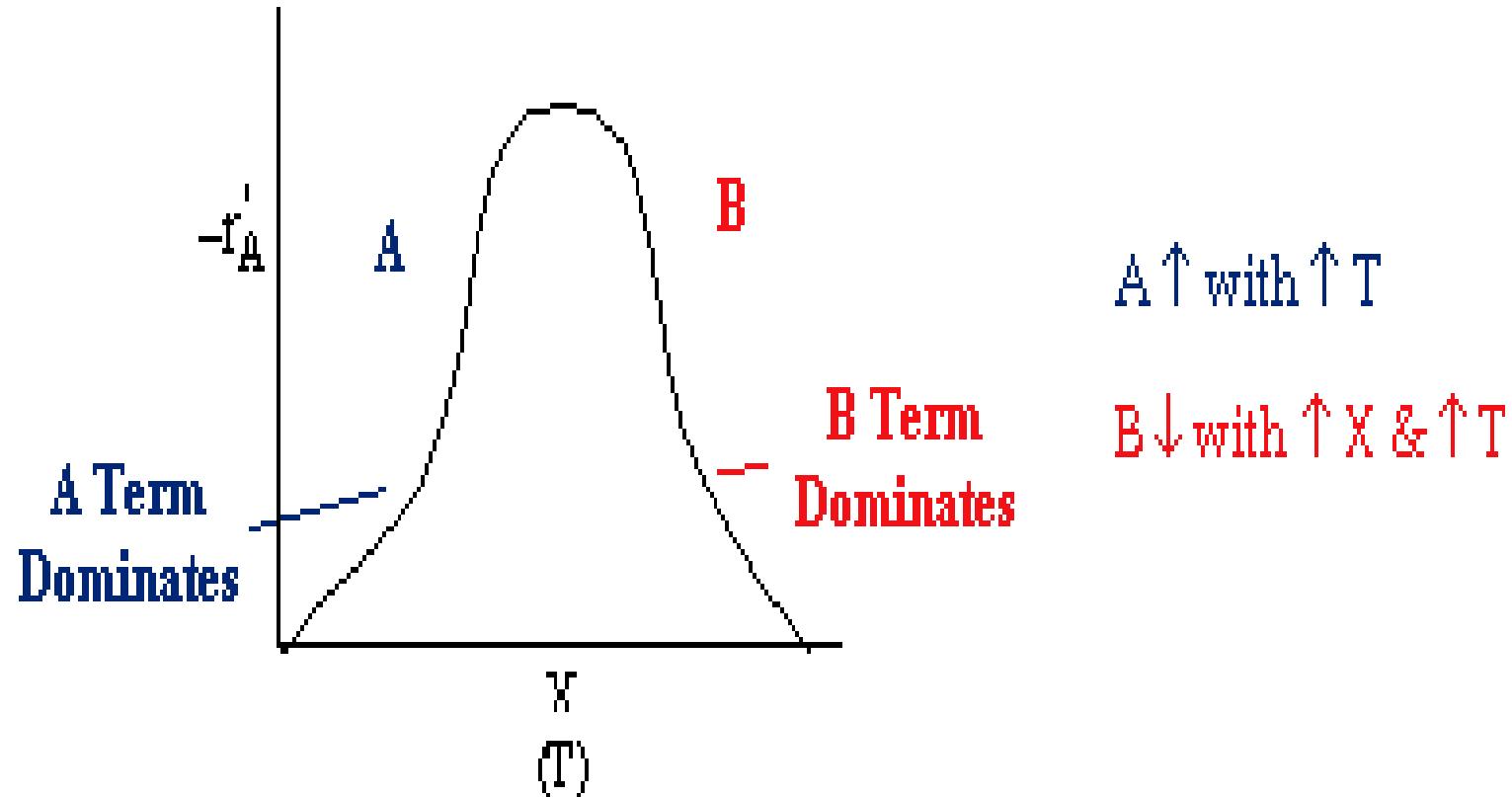
Reactor Inlet Temperature and Interstage Cooling

Optimum Inlet Temperature:

Fixed Volume Exothermic Reactor

$$A + B \Leftrightarrow 2C$$
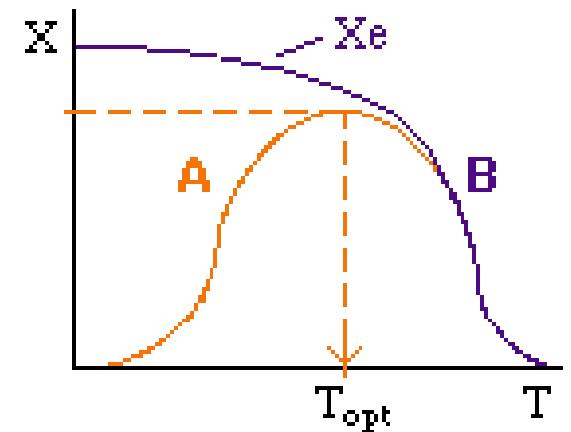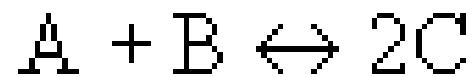
**Curve A:** Reaction rate slow, conversion dictated by rate of reaction and reactor volume. As temperature increases rate increases and therefore conversion increases.

Curve B: Reaction rate very rapid. Virtual equilibrium reached in reaction conversion dictated by equilibrium conversion.

Interstage Cooling:
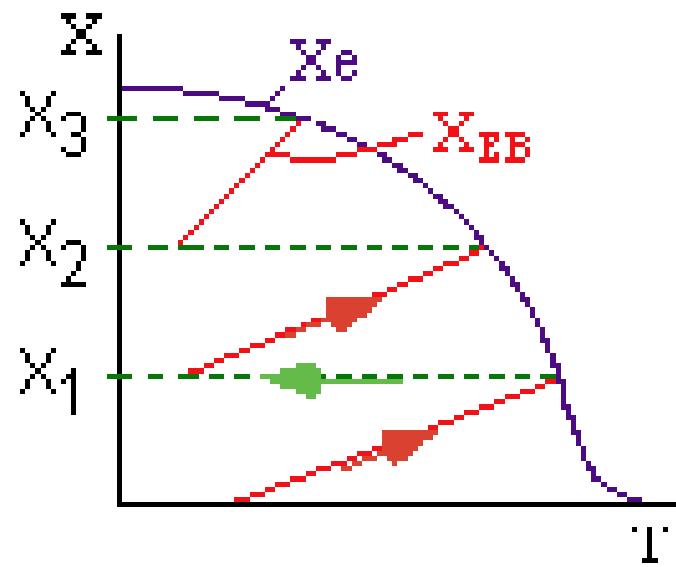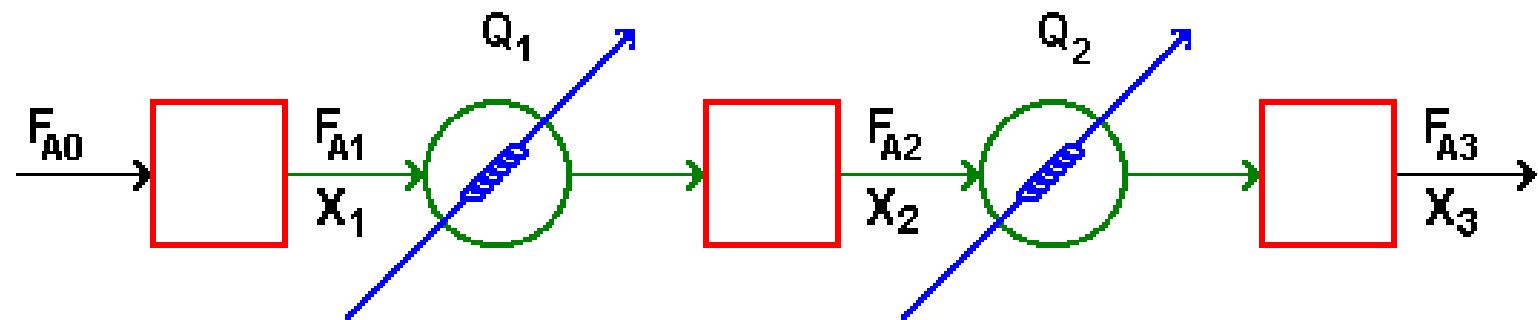
Self Test

An inert **I** is injected at the points shown below:
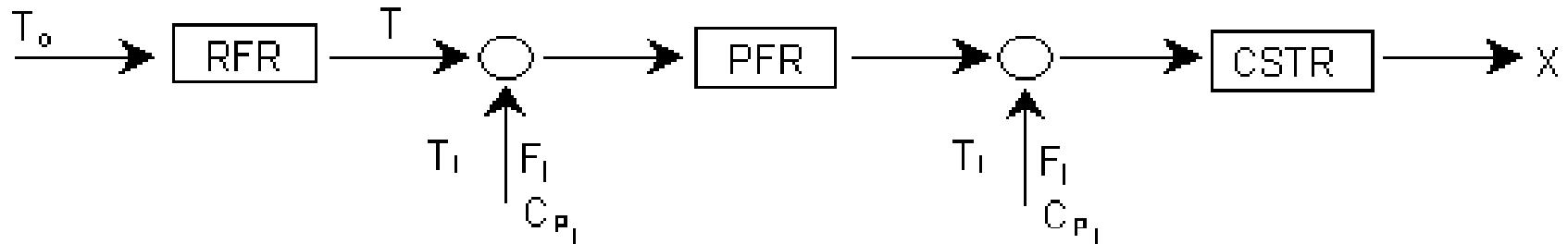
Sketch the conversion-temperature trajectory for an endothermic reaction.
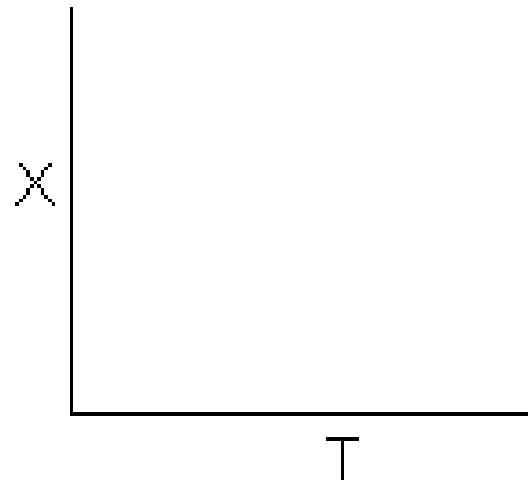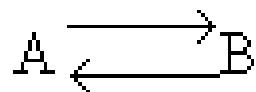
Solution

For an endothermic reaction, the equilibrium conversion increases with increasing T.

For $\dfrac{\Delta H^{\circ}_{Rx}}{R} = +10000 \ \mathrm{K}^{-1}$ and $K_{eq}=.1$ and T_2

$$K_{eq} = \exp\left[10000\left[\frac{1}{T_2} - \frac{1}{T}\right]\right]$$
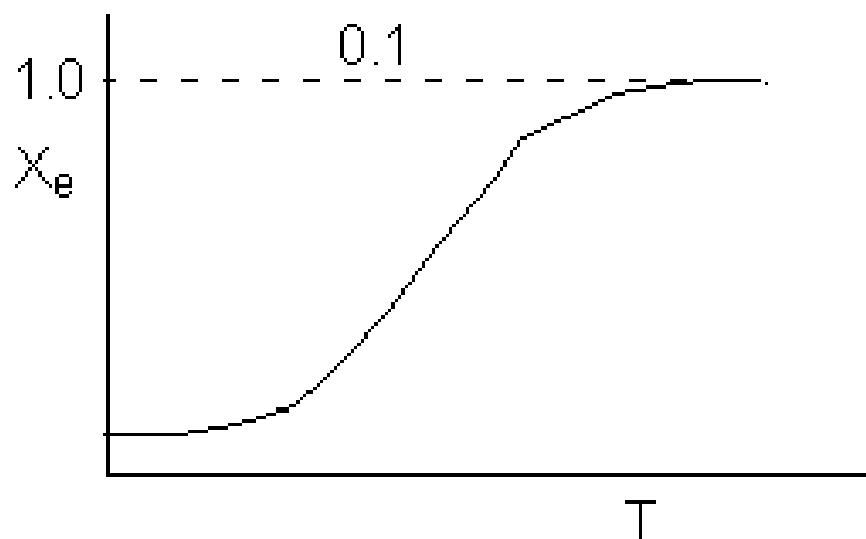
# From the energy balance we know the temperature decreases with increasing conversion.

$$T = T_0 - X\frac{\Delta H_{Rx}}{C_{P_A}}$$

$F_A = F_{A0}(1-X_1)$

$F_B = F_{A0}(X_1)$

F_I

$F_A = F_{A0}(1-X_1)$

$F_B = F_{A0}X_1$

F_I

$T_1 \quad T_2$

T_I
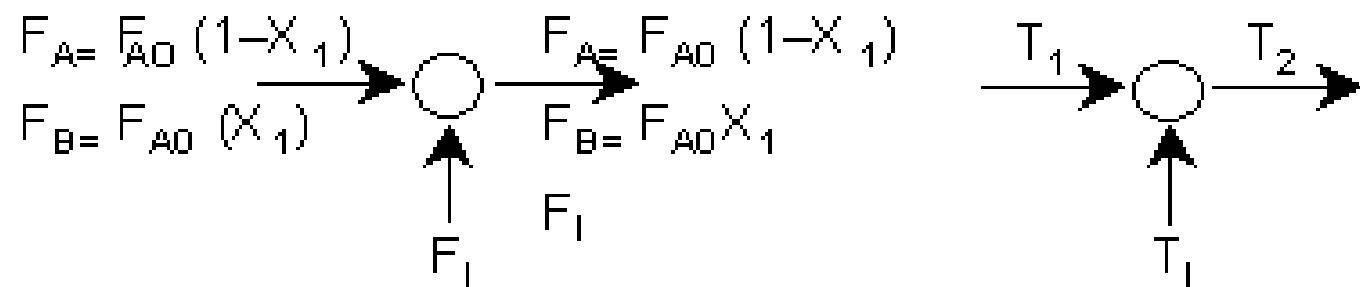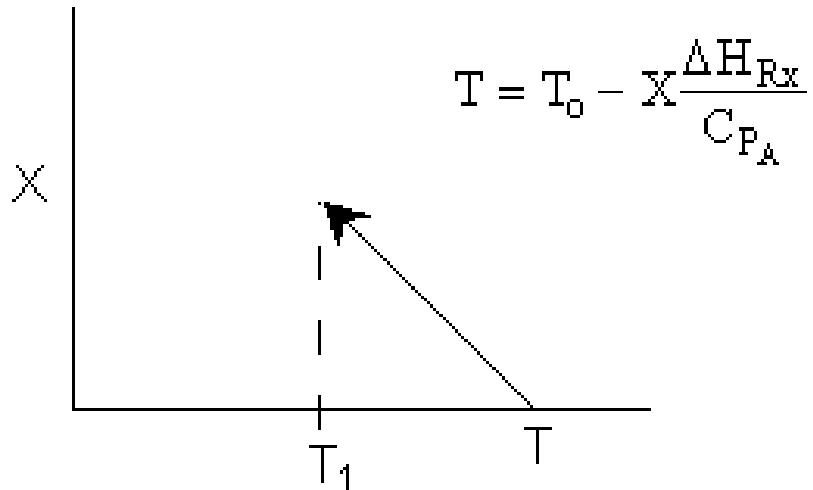
Energy Balance around junction:

$$F_A C_{P_A}(T_1 - T_R) + F_B C_{P_B}(T_1 - T_R) + F_I C_{P_I}(T_I - T_R)$$

$$= F_A C_{P_A}(T_2 - T_R) + F_B C_{P_B}(T_2 - T_R) + F_I C_{P_I}(T_2 - T_R)$$

Solving T2

$$T_2 = T_R + \frac{F_{A0} C_{P_A}(1 - X_1)(T_1 - T_R) + F_{A0} C_{P_B} X_1(T - T_R) + F_I C_{P_I}(T_I - T_R)}{F_{A0} C_P (1 - X_1) + F_{A0} C_{P_B} X_1 + F_I C_{P_I}}$$
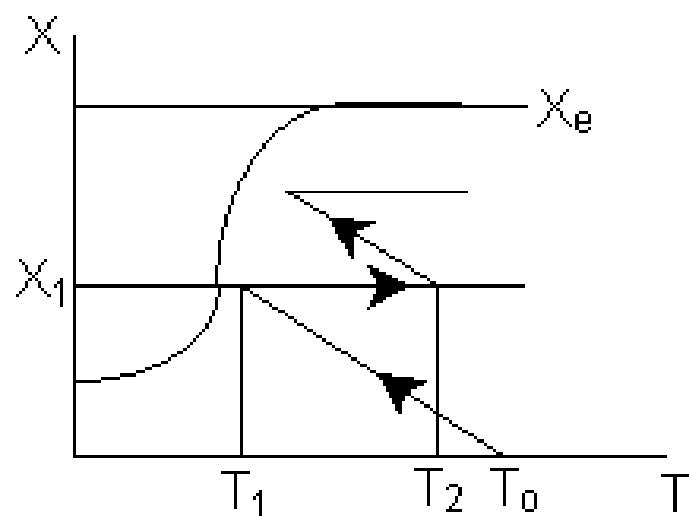
Example CD8-2
Second Order Reaction Carried Out Adiabatically in a CSTR

The acid-catalyzed irreversible liquid-phase reaction

$$A \longrightarrow B$$

is carried out adiabatically in a CSTR.

A ———————————————— S

$v_0 = 10$ dm³/min
$C_{A0} = 4$ mol/dm³
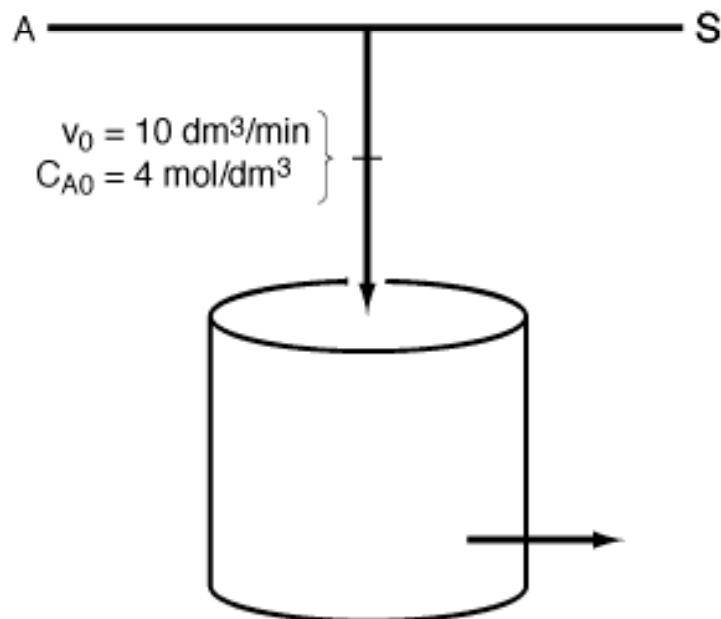
The reaction is second order in A. The feed, which is equimolar in a solvent (which contains the catalyst) and A, enters the reactor at a total volumetric flowrate of 10 dm^3/min with the concentration of A being 4M. The entering temperature is 300 K.

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

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

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

Additional Information:

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

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

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

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

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

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

Example CD8-2 Solution, Part A
Second Order Reaction Carried Out Adiabatically in a CSTR

(a) We will solve part (a) by using the nonisothermal reactor design algorithm discussed in Chapter 8.

1. CSTR Design Equation: $\quad V = \dfrac{F_{A0}X}{-r_A}$

2. Rate Law: $\quad -r_A = kC_A^2$

3. Stoichiometry: $\quad$ liquid, $\upsilon = \upsilon_0$

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

4. Combine:

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

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

Given conversion (X), you must first determine the reaction temperature (T), and then you can calculate the reactor volume (V).

5. Determine T:

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

For this problem:

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

which leaves us with:

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

After some rearranging we are left with:

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

Substituting for known values and solving for T:

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

$$T = 380\,K$$

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

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

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

$$k = 0.1 \, dm^3 / mol \cdot min$$

7. Calculate the CSTR Reactor Volume (V):

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

Substituting for known values and solving for V:

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

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

Example CD8-2 Solution, Part B
Second Order Reaction Carried Out Adiabatically
in a CSTR

(b) For part (b) we will again use the
nonisothermal reactor design algorithm
discussed in Chapter 8. The first four steps of
the algorithm we used in part (a) apply to our
solution to part (b). It is at step number 5,
where the algorithm changes.

NOTE: We will find it more convenient to work with
this equation in terms of space time, rather than
volume:

Space time is defined as: $\tau = \dfrac{V}{\upsilon_0}$

After some rearranging: $\dfrac{V}{\upsilon_0} = \dfrac{1}{kC_{A0}} \dfrac{X}{(1-X)^2}$

Substituting: $\tau = \dfrac{1}{kC_{A0}} \dfrac{X}{(1-X)^2}$

Given reactor volume (V), you must solve the energy balance and the mole balance simultaneously for conversion (X), since it is a function of temperature (T).

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

From the adiabatic energy balance (as applied to CSTRs):

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

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

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

We'll rearrange our combined equation from step 4 to give us:

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

Rearranging gives:

$$\tau k C_{A0} - 2\tau k C_{A0}X + \tau k C_{A0}X^2 = X$$

$$\tau k C_{A0} - (2\tau k C_{A0} + 1)X + \tau k C_{A0}X^2 = 0$$

Solving for X gives us:

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

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

After some final rearranging we get:

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

Let's simplify a little more, by introducing the Damköhler Number, Da:

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

We then have:

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

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

You want to plot XEB and XMB on the same graph (as functions of T) to see where they intersect. This will tell you where your steady-state point is. To accomplish this, we will use Polymath (but you could use a spreadsheet).

CD Example Problem 8-2, Part B

KEY:
— Xeb
— Xmb

Conversion, X

1.200

0.900

0.600

0.300

-0.000

-0.300

270.000   300.000   330.000   360.000   390.000   420.00

Temperature, T (K)

X = 0.87 and T = 387 K
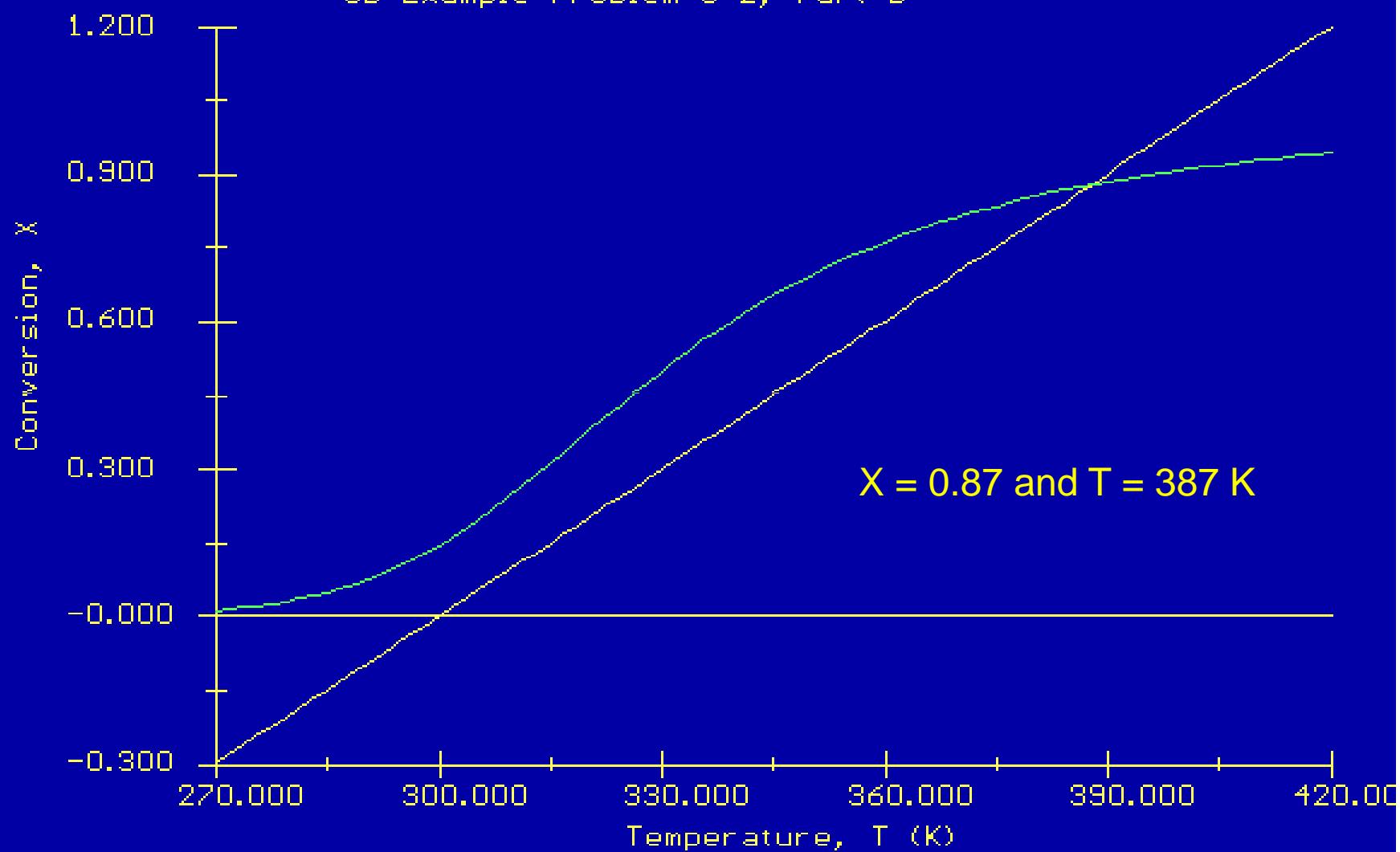
GRAPH OPTIONS

s.   Change X axis scale.   S.   Change Y axis scale.

l.   Add label to X axis.   L.   Add label to Y axis.   t. change graph title.

F3   to print the graph   F8 for display options.

Our corresponding Polymath program looks like this:

```
                 CD Example Problem 8-2, Part B
Equations                                              Initial values

d(T)/d(t)=2                                                270

k=0.0005*exp(15000/1.987*(1/300-1/T))

Cao=4

Cpa=15

Cps=18

DeltaH=-3300

To=300

V=1000

v=10

tau=V/v

Xeb=(Cpa+Cps)*(T-To)/(-DeltaH)

Da=tau*k*Cao

Xmb=(2*Da+1-(4*Da+1)^0.5)/(2*Da)

t_0 = 0,     t_f = 75
```

NOTE: Our use of d(T)/d(t)=2 in the above program is merely a way for us to generate a range of temperatures as we plot conversion as a function of temperature.

Example CD8-2 Solution, Part C
Second Order Reaction Carried Out Adiabatically in a CSTR

(c) For part (c) we will simply modify the Polymath program we used in part (b), setting our initial temperature to 280 K. All other equations remain unchanged.

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

We see that our conversion would be about 0.75, at a temperature of 355 K.

Multiple Steady States

Pertemuan ke 9

Multiple Steady States

$$\dot{Q} - \dot{W}_S - F_{A0} \sum \theta_i \breve{C}_{Pi}(T - T_0) + (r_A V)(\Delta H_R(T)) = 0$$

$$\dot{W}_S \cong 0$$

$$\overbrace{C_{P0}}$$
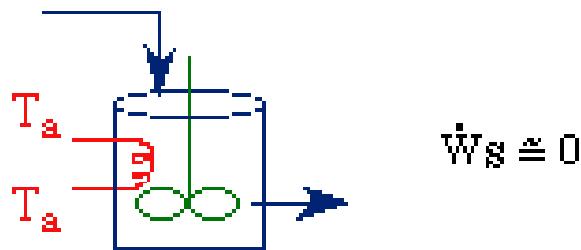
$$UA(T_A - T) - F_{A0} \sum \theta_i \hat{C}_{Pi}(T - T_0) + (r_A V)(\Delta H_R(T)) = 0$$

Factor $F_{A0}\, C_{P0}$ and then divide by F_{A0}

$$-C_{P0}\left[(T - T_0) + \frac{UA}{F_{A0}C_{P0}}(T - T_A)\right] + \left[\frac{(r_A V)(\Delta H_R)}{F_{A0}}\right] = 0$$

$$\kappa = \frac{UA}{F_{A0}C_{P0}}, \quad T_C = \frac{T_0 + \kappa T_A}{1 + \kappa}$$

$$\left[\frac{(r_A V)(\Delta H_R(T))}{F_{A0}}\right] - \left[C_{P0}(1+\kappa)(T-T_C)\right] = 0$$

For a CSTR: $F_{A0}X = -r_A V$

$$\left[X(-\Delta H_R(T))\right] - \left[C_{P0}(1+\kappa)(T-T_C)\right] = 0$$

$$G(T) - R(T) = 0$$

where

$$G(T) = \left(\frac{-r_A V}{F_{A0}}\right)(-\Delta H_R(T)) = X(-\Delta H_R(T))$$

$$R(T) = C_{P0}(1+\kappa)(T-T_C)$$
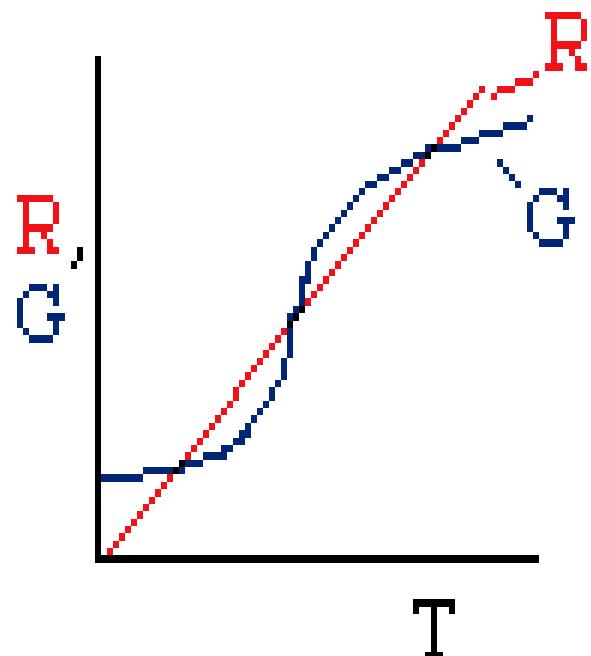
R > G: Temp. will decrease

R < G: Temp. will increase

Self Test

Can there be multiple steady states (MSS) for a irreversible first order endothermic reaction?

Solution

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

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

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

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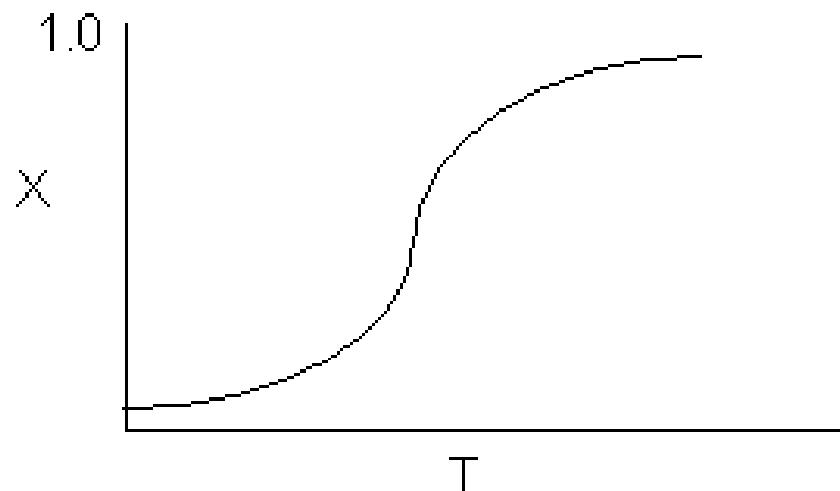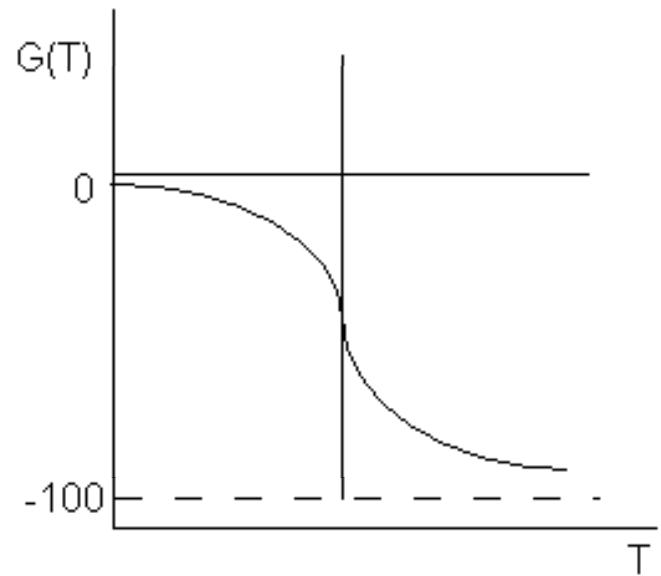
$$G = -\Delta H_{RX}$$

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

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

$$T_c = \frac{T_o + \kappa T_a}{1+\kappa}$$
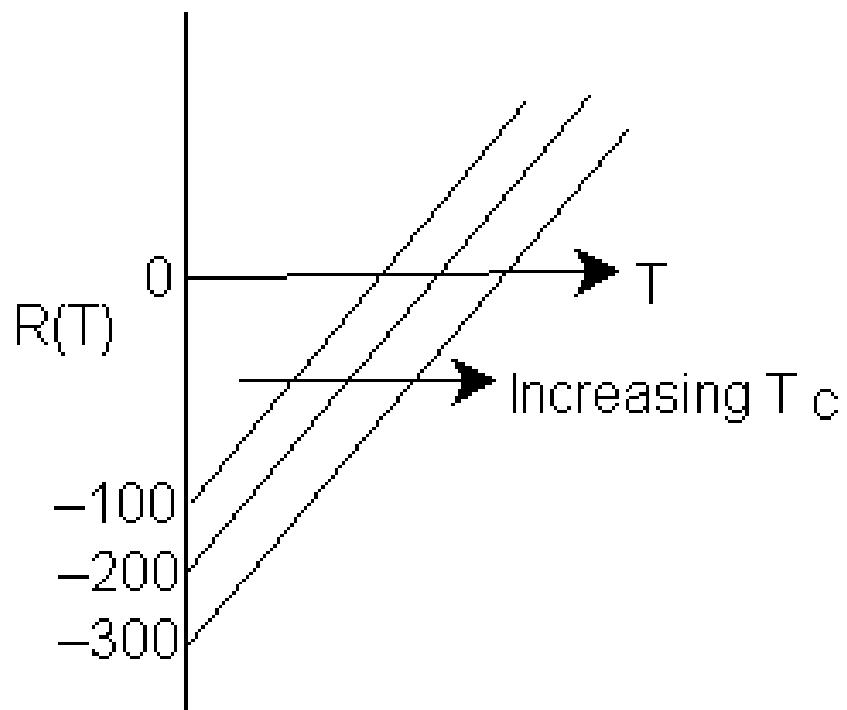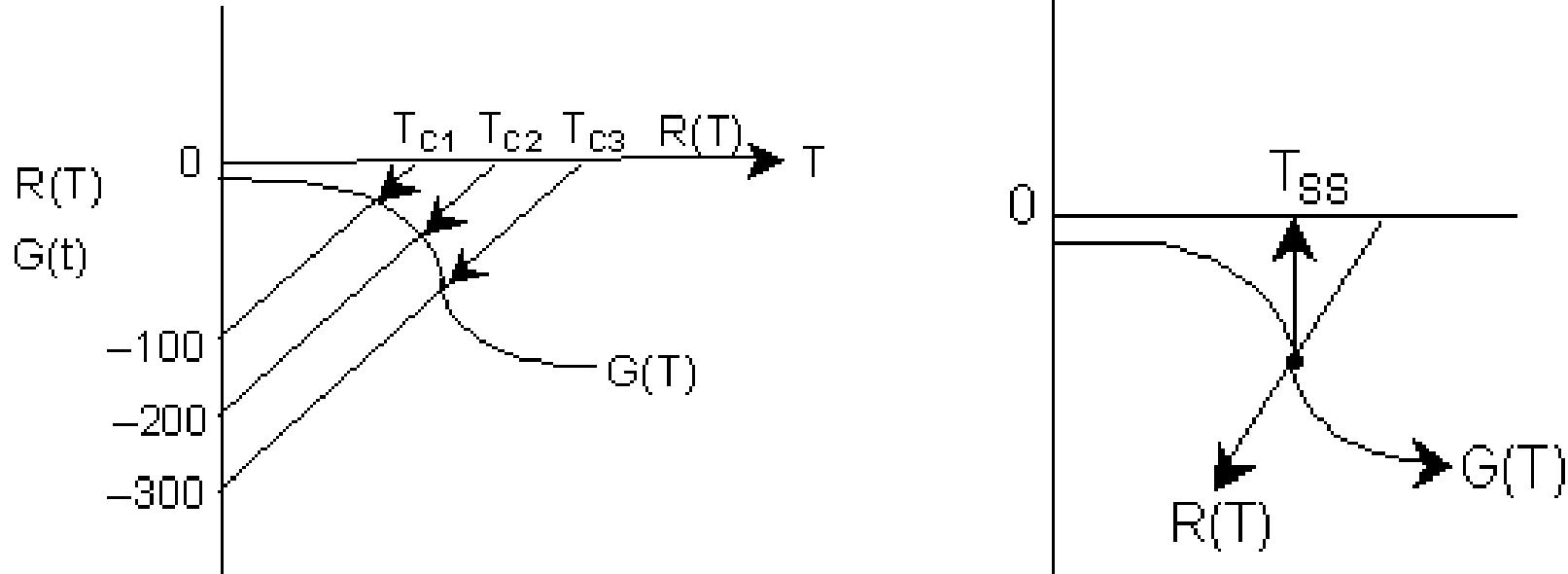
There are no multiple steady states for an endothermic, irreversible first order reactor. The steady state reactor temperature is T_S. Will a *reversible* endothermic first order reaction have M_{SS}?

Now we need to find X. We do this by combining the mole balance, rate law, Arrhenius Equation, and stoichiometry.

For the first-order, irreversible reaction A $\rightarrow$ B, we have:

$$X = \frac{\tau k}{1 + \tau k}$$ where $$\tau k = \left(\frac{V}{v_0}\right) A e^{-E/RT}$$

At steady state:

$$\underbrace{\frac{\tau k}{1 + \tau k}(-\Delta H_R)}_{G(T)} = \underbrace{C_{P0}(1 + \kappa)\ (T - T_C)}_{R(T)}$$
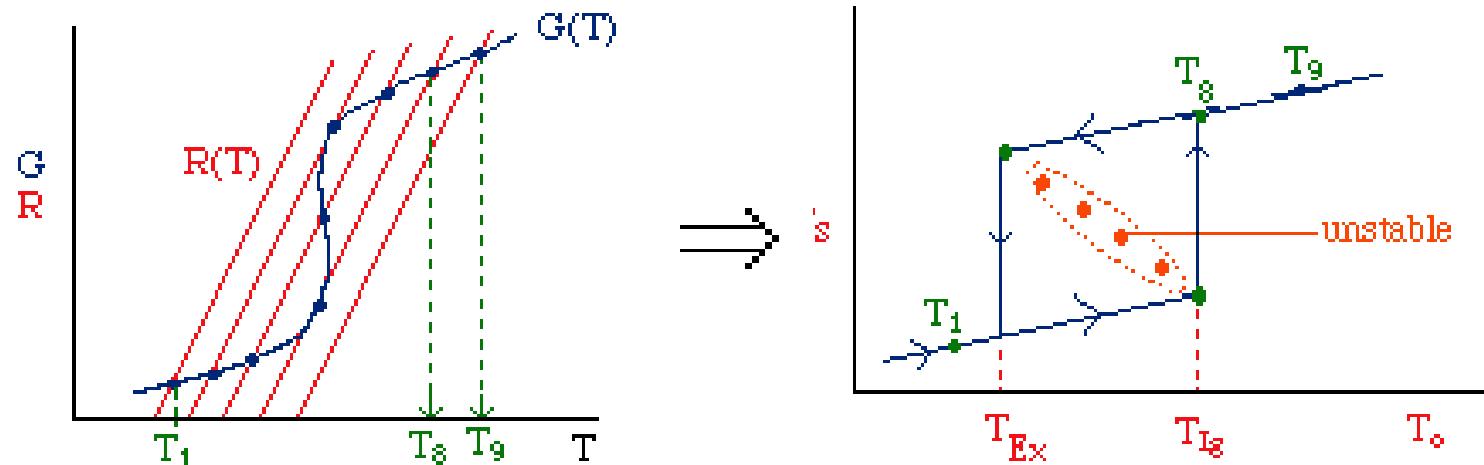
Unsteady State CSTR

Balance on a system volume that is well-mixed:

$$\dot{Q} - \dot{W}_S + \Sigma F_{io}H_{io} - \Sigma F_iH_i = \frac{dE_{sys}}{dt} = \frac{d\Sigma N_iE_i}{dt} = \frac{d\Sigma N_iH_i}{dt} = \Sigma H_i\frac{dN_i}{dt} + \Sigma N_i\frac{dH_i}{dt}$$

$$F_{io} - F_i + r_iV = \frac{dN_i}{dt} \qquad\qquad \frac{dH_i}{dt} = C_{P_i}\frac{dT}{dt}$$

$$\dot{Q} - \dot{W}_S + \Sigma F_{io}H_{io} - \Sigma F_iH_i = \Sigma H_i(F_{io} - F_i + r_iV) + \Sigma N_i C_{P_i}\frac{dT}{dt} = \Sigma H_i F_{io} - \Sigma H_iF_i + \Sigma r_iV H_i + \Sigma N_i C_{P_i}\frac{dT}{dt}$$

$$r_i = \upsilon_i(-r_A)$$

$$\dot{Q} - \dot{W}_S + \Sigma F_{io}(H_{io} - H_o) = -r_AV \Sigma \upsilon_iH_i + \Sigma N_i C_{P_i}\frac{dT}{dt}$$

$$\boxed{\dot{Q} - \dot{W}_S + (r_AV)|\Delta H_R(T)| = \Sigma F_{io}(H_i - H_{io}) + \Sigma N_i C_{P_i}\frac{dT}{dt}}$$

$$\boxed{\dot{Q} - W_S - F_{AO} \Sigma \theta_i \tilde{C}_{P_i}(T - T_o) + (r_A V)|\Delta H_R(T)| = \Sigma N_i C_{P_i}\frac{dT}{dt}}$$

RATB Bertingkat (Multistage)

- RATB bertingkat terdiri atas 2 atau lebih reaktor tangki berpengaduk yang disusun seri

- Keuntungan RATB bertingkat dua atau lebih, untuk mencapai hasil yg sama? ukuran/ volume reaktor lebih kecil dibandingkan RATB tunggal

- Kerugian utama RATB bertingkat beroperasi pada konsentrasi yang lebih rendah diantara pemasukan dan pengeluaran

- Untuk RATB tunggal, berarti bahwa beroperasi pada konsentrasi dalam sistem serendah mungkin, dan untuk kinetika normal, diperlukan volume reaktor semakin besar

- Bila 2 tangki (beroperasi pd T sama) disusun seri, yang kedua beroperasi pada konsentrasi sama spt tangki tunggal diatas, tapi yg pertama beroperasi pada konsentrasi lebih tinggi, jadi volume total kedua tangki lebih kecil daripada tangki tunggal

Rangkaian RATB bertingkat N
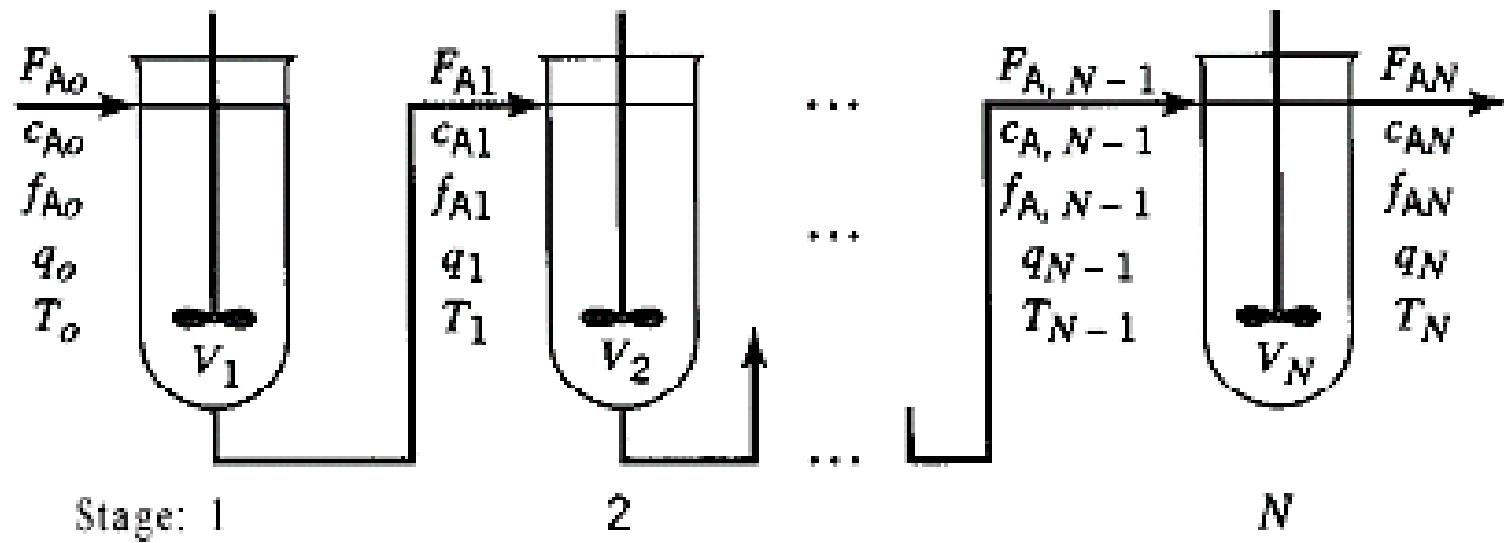
Pers neraca massa pada RATB ke i

$$V_i = F_{Ao}(f_{Ai} - f_{A,i-1})/(-r_A)_i \qquad (14.4\text{-}1)$$

Grafik ilustrasi operasi 3 RATB seri
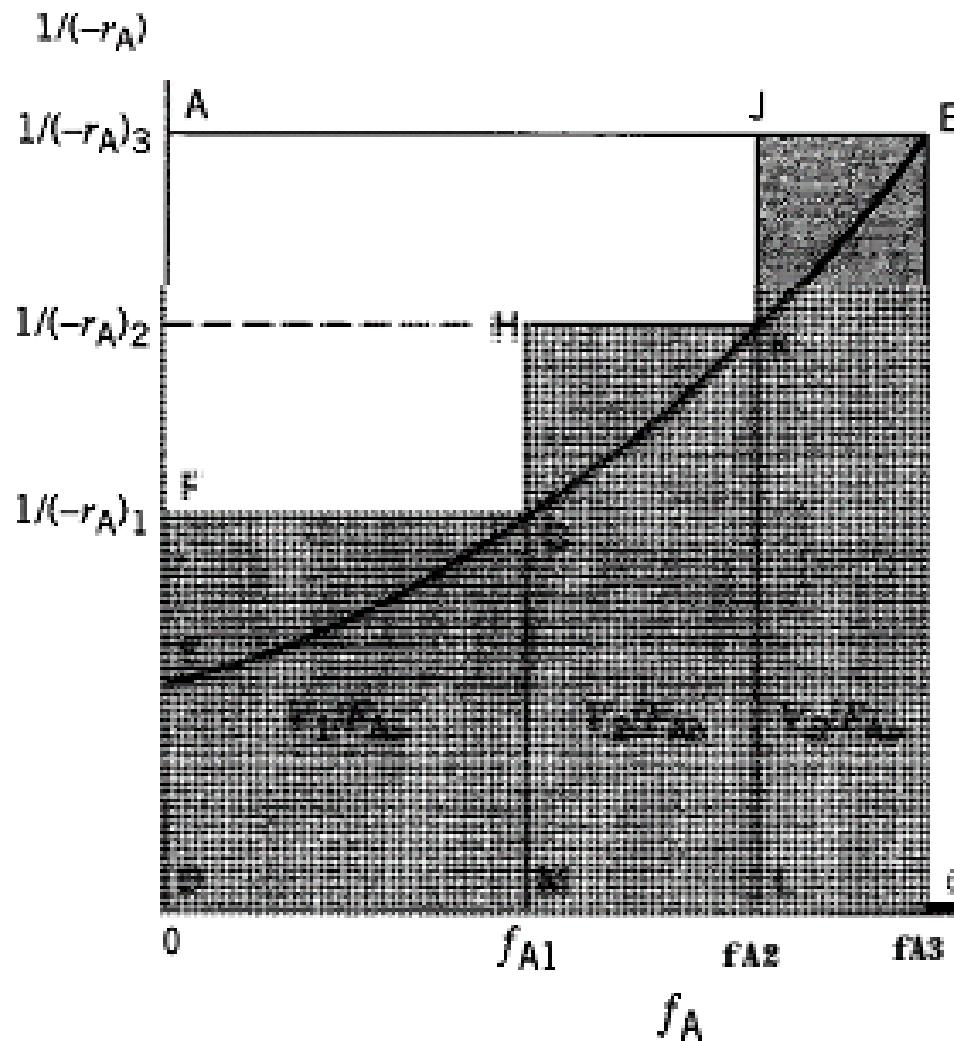
Penyelesaian pers 14.4-1 untuk mencari V (diberi f_A) atau mencari f_A (diberi V) dapat dilakukan secara grafik atau secara analitis. Cara grafik dapat digunakan untuk mencari f_A, atau bila bentuk analitis ($-r_A$) tidak diketahui

Penyelesaian grafis untuk N = 2

Untuk stage 1:
$$(-r_A)_1 = (F_{Ao}/V_1)f_{A1}$$

Untuk stage 2:
$$(-r_A)_2 = (F_{Ao}/V_2)(f_{A2} - f_{A1})$$
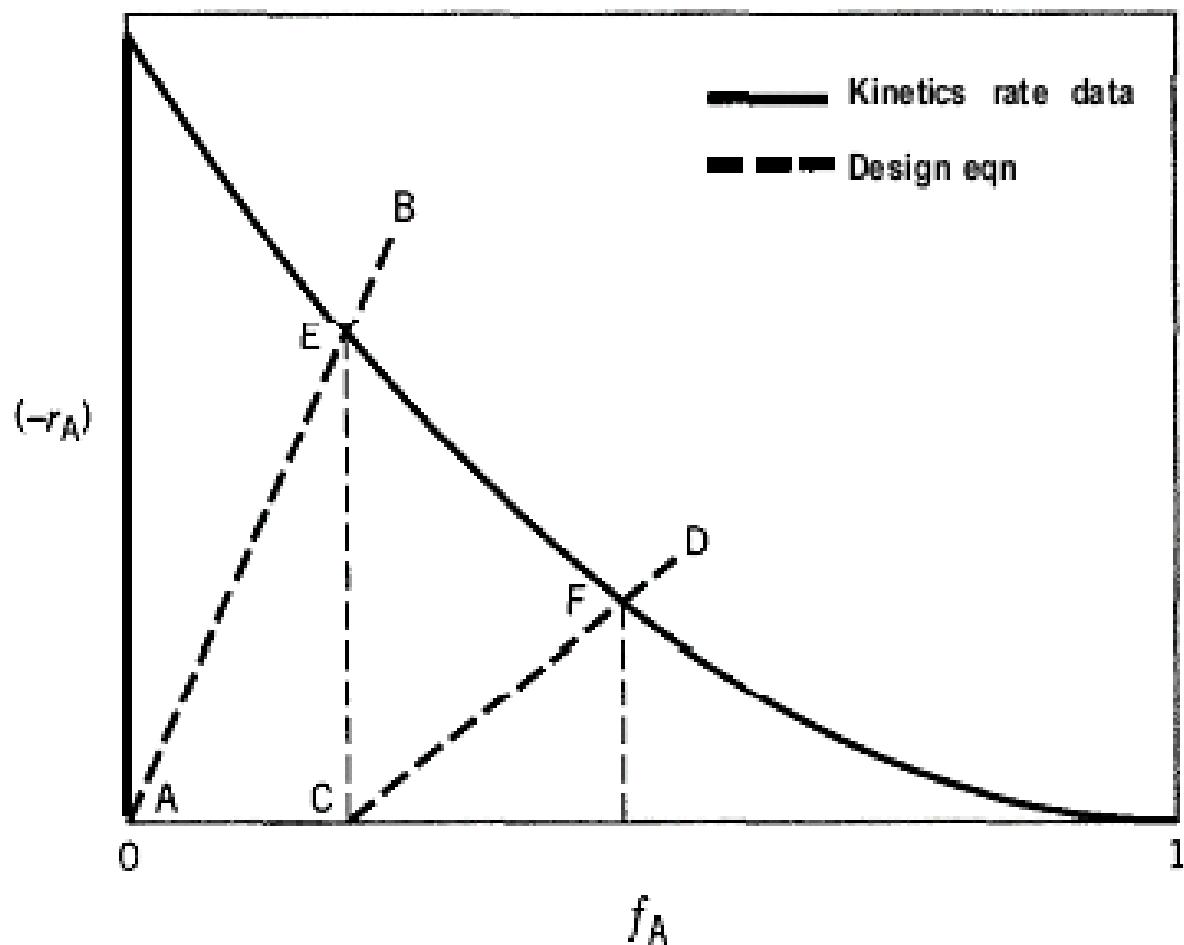
Figure 14.11 Basis for graphical solution for multistage CSTR (for A + ... → products)

Example 14-9

A three-stage CSTR is used for the reaction A $\rightarrow$ products. The reaction occurs in aqueous solution, and is second-order with respect to A, with k_A = 0.040 L mol^{-1} min^{-1}. The inlet concentration of A and the inlet volumetric flow rate are 1.5 mol L^{-1} and 2.5 L min^{-1}, respectively. Determine the fractional conversion (f_A) obtained at the outlet, if V_1 = 10 L, V_2 = 20 L, and V_3 = 50 L, (a) analytically, and (b) graphically.

Solusi

Untuk stage 1 dari persamaan kecepatan

$$(-r_A)_1 = k_A c_{A1}^2 = k_A c_{Ao}^2 (1 - f_{A1})^2$$

Karena densitas konstan

$$(-r_A)_1 = (F_{Ao}/V_1)(f_{A1} - 0)$$

Lakukan pengaturan sehingga diperoleh pers kwadrat

$$f_{A1}^2 - \left(\frac{F_{Ao}}{k_A c_{Ao}^2 V_1} + 2 \right) f_{A1} + 1 = 0$$

Atau dengan memasukkan bilangan numerik

$$f_{A1}^2 - 6.167 f_{A1} + 1 = 0$$

- Diperoleh $f_{A1} = 0.167$
- Similarly, for stages 2 and 3, we obtain $f_{A2} = 0.362$, and $f_{A3} = 0.577$, which is the outlet fractional conversion from the three-stage CSTR.

Penyelesaian cara grafis sbb
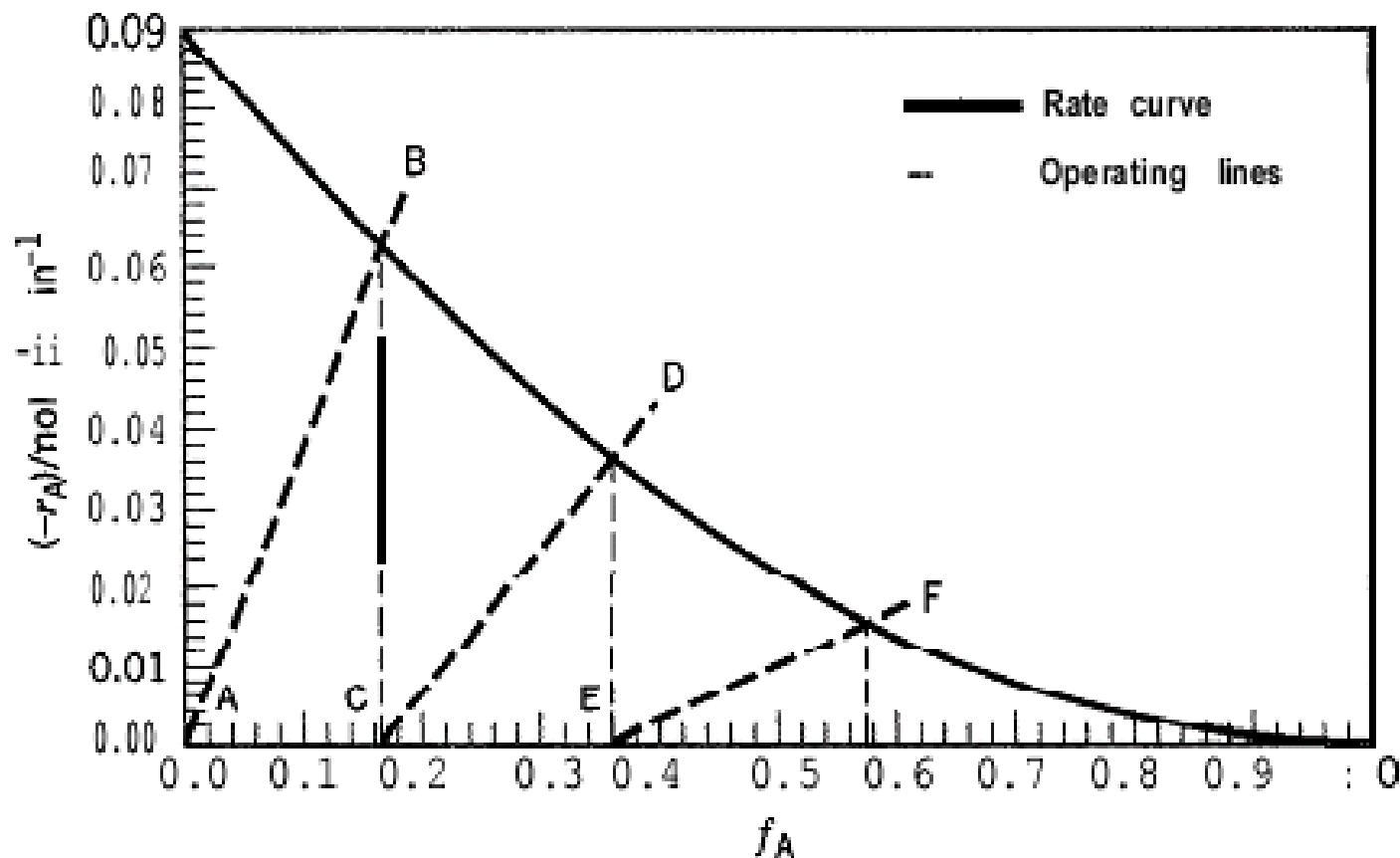
Figure. 14.12 Graphical solution of Example 14-9

(b) The graphical solution is shown in Figure 14.12. The curve for $(-r_A)$ from the rate law is first drawn. Then the operating line AB is constructed with slope $F_{A0}/V_1 = c_{A0}q_0/V_1 = 0.375$ mol $L^{-1}min^{-1}$ to intersect the rate curve at $f_{A1} = 0.167$; similarly, the lines CD and EF, with corresponding slopes 0.1875 and 0.075, respectively, are constructed to intersect 0.36 and $f_{A3} = 0.58$, respectively. These are the same the rate curve at the values $f_{A2} =$ values as obtained in part (a).

Optimal Operation

The following example illustrates a simple case of optimal operation of a multistage CSTR to minimize the total volume. We continue to assume a constant-density system with isothermal operation

Exp. 14-10

Consider the liquid-phase reaction A + . . . → products taking place in a two-stage CSTR. If the reaction is first-order, and both stages are at the same T, how are the sizes of the two stages related to minimize the total volume V for a given feed rate (F_{Ao}) and outlet conversion (f_{A2})?

Solusi

From the material balance, equation 14.4-1, the total volume is

$$V = V_1 + V_2 = F_{Ao}\left[\frac{f_{A1} - 0}{(-r_A)_1} + \frac{f_{A2} - f_{A1}}{(-r_A)_2}\right] \qquad \text{A}$$

From the rate law,

$$(-r_A)_1 = k_A c_{Ao}(1 \qquad f_{A1}) \qquad \text{B}$$
$$(-r_A)_2 = k_A c_{Ao}(1 - f_{A2}) \qquad \text{C}$$

Substituting (B) and (C) in (A), we obtain

$$V = \frac{F_{Ao}}{k_A c_{Ao}}\left(\frac{f_{A1}}{1 - f_{A1}} + \frac{f_{A2} - f_{A1}}{1 - f_{A2}}\right) \qquad \text{D}$$

$$\left(\frac{\partial V}{\partial f_{A1}}\right)_{f_{A2,T}} = 0 \qquad\qquad \text{E}$$

From (E) and (D), we obtain

$$\frac{\partial V}{\partial f_{A1}} = \frac{F_{Ao}}{k_A c_{Ao}} \left[\frac{1}{(1-f_{A1})^2} - \frac{1}{1-f_{A2}} \right] = 0$$

from which $\qquad f_{A2} = f_{A1}(2 - f_{A1})$

If we substitute this result into the material balance for stage 2 (contained in the last term in (D)), we have

$$V_2 = \frac{F_{Ao}}{k_A c_{Ao}}\left(\frac{f_{A2} - f_{A1}}{1 - f_{A2}}\right) = \frac{F_{Ao}}{k_A c_{Ao}}\left(\frac{f_{A1}}{1 - f_{A1}}\right) = V_1$$

- That is, for a first-order reaction, the two stages must be of equal size to minimize V.

- The proof can be extended to an N-stage CSTR. For other orders of reaction, this result is approximately correct. The conclusion is that tanks in series should all be the same size, which accords with ease of fabrication.

- Although, for other orders of reaction, equal-sized vessels do not correspond to the minimum volume, the difference in total volume is sufficiently small that there is usually no economic benefit to constructing different-sized vessels once fabrication costs are considered.

Example 11

A reactor system is to be designed for 85% conversion of A (fA) in a second-order liquid phase reaction, A → products; k_A = 0.075 L mol^{-1} min^{-1}, q_0 = 25 L min^{-1}, and C_{A0} = 0.040 mol L^{-1}. The design options are:

(a) two equal-sized stirred tanks in series;

(b) two stirred tanks in series to provide a minimum total volume.

The cost of a vessel is $290, but a 10% discount applies if both vessels are the same size and geometry. Which option leads to the lower capital cost?

Solusi

Case (a). From the material-balance equation 14.4-1 applied to each of the two vessels 1 and 2,

$$V_1 = F_{Ao}f_{A1}/k_A c_{A1}^2 = F_{Ao}f_{A1}/k_A c_{Ao}^2(1 - f_{A1})^2 \qquad \text{(A)}$$

$$V_2 = F_{Ao}(f_{A2} - f_{A1})/k_A c_{Ao}^2(1 - f_{A2})^2 \qquad \text{(B)}$$

Equating V_1 and V_2 from (A) and (B), and simplifying, we obtain

$$(f_{A2} - f_{A1})/(1 - f_{A2})^2 = f_{A1}/(1 - f_{A1})^2$$

This is a cubic equation for f_{A1} in terms of f_{A2}:

$$f_{A1}^3 - (2 + f_{A2})f_{A1}^2 + (2 + f_{A2}^2)f_{A1} - f_{A2} = 0$$

$$f_{A1}^3 - 2.85 f_{A1}^2 + 2.7225 f_{A1} - 0.85 = 0$$

❑This equation has one positive real root, f_{A1} =0.69, which can be obtained by trial.
❑This corresponds to $V_1 = V_2 = 5.95 \times 10^4$ L (from equation (A) or (B)) and a total capital cost of 0.9(290)(5.95 X 104)2/1000 = $31,000 (with the 10% discount taken into account)

Case (b). The total volume is obtained from equations (A) and (B):

$$V = V_1 + V_2 = \frac{F_{Ao} f_{A1}}{k_A c_{Ao}^2 (1 - f_{A1})^2} + \frac{F_{Ao} (f_{A2} - f_{A1})}{k_A c_{Ao}^2 (1 - f_{A2})^2}$$

For minimum V,

$$\left(\frac{\partial V}{\partial f_{A1}}\right)_{f_{A2}} = \frac{F_{Ao}}{k_A c_{Ao}^2}\left[\frac{1 + f_{A1}}{(1 - f_{A1})^3} - \frac{1}{(1 - f_{A2})^2}\right] = 0$$

This also results in a cubic equation for f_{A1}, which, with the value $f_{A2} = 0.85$ inserted, becomes

$$f_{A1}^3 - 3f_{A1}^2 + 3.0225\,f_{A1} - 0.9775 = 0$$

Solution by trial yields one positive real root: $f_{A1} = 0.665$. This leads to $V_1 = 4.95 \times 10^4$ L, $V_2 = 6.84 \times 10^4$ L, and a capital cost of \$34,200.

Conclusion:

The lower capital cost is obtained for case (a) (two equal-sized vessels), in spite of the fact that the total volume is slightly larger (11.9×10^4 L versus 11.8×10^4 L).