

ChE 344
Winter 2011
Final Exam + Solution

Monday, April 25, 2011

Open Book, Notes, and Web

Name_____

Honor Code (Please sign in the space provided below)

"I have neither given nor received unauthorized aid on this examination, nor have I concealed any violations of the Honor Code."

(Signature)

The Basics

1) ____/ 5 pts

2) ____/ 5 pts

3) ____/ 5 pts

4) ____/ 5 pts

5) ____/ 5 pts

6) ____/ 5 pts

7) ____/ 5 pts

Applications

8) ____/ 5 pts

9) ____/ 10 pts

10) ____/ 10 pts

11) ____/ 10 pts

Professional

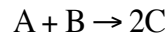
12) ____/ 10 pts

13) ____/ 20 pts

Total ____/ 100 pts

(5 pts) 1) Mole Balances, Chapter 1

The reaction



takes place in an unsteady CSTR. The feed is only A and B in equimolar proportions. Which of the following set of equations gives the correct mole balances on A, B and C. Species A and B are disappearing and Species C is being formed.

Circle the correct answer where all the mole balances are correct

(a)

$$F_{B0} - F_A - \int^V r_A dV = \frac{dN_A}{dt}$$

$$F_{B0} - F_B - \int^V r_A dV = \frac{dN_B}{dt}$$

$$-F_C + 2 \int^V r_A dV = \frac{dN_C}{dt}$$

Wrong sign for r_A , should be $+\int^V r_A dV$

(b)

$$F_{A0} - F_A + \int^V r_A dV = \frac{dN_A}{dt}$$

$$F_{A0} - F_B + \int^V r_A dV = \frac{dN_B}{dt}$$

$$-F_C - 2 \int^V r_A dV = \frac{dN_C}{dt}$$

All are correct.

(c)

$$F_{A0} - F_A + \int_0^V r_A dV = \frac{dN_A}{dt}$$

$$F_{A0} - F_B + \int^V r_A dV = \frac{dN_B}{dt}$$

$$F_C + \int^V r_C dV = \frac{dN_C}{dt}$$

Wrong sign for F_C , should be $-F_C$

(d)

$$F_{B0} - F_A - \int^V r_A dV = \frac{dN_A}{dt}$$

$$F_{B0} - F_B - \int^V r_A dV = \frac{dN_B}{dt}$$

$$-F_C + \int^V r_C dV = \frac{dN_C}{dt}$$

Wrong sign for $-r_A$, should be $+\int^V r_A dV$

Solution

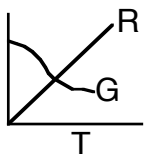
Answer is (b).

(5 pts) 2) Circle the correct answer, true (T), False (F) or (CT) Can't tell from the information given.

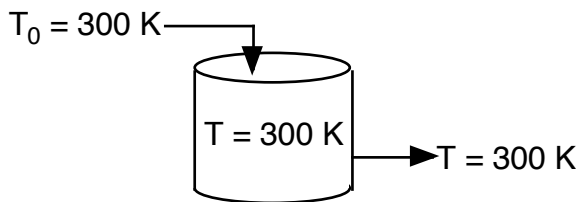
- T F CT (a) Multiple steady states can exist for an irreversible endothermic first order reactions.
- T F CT (b) A steady-state CSTR operates at 150°C. The reactor effluent is at the same temperature as the reactor contents. Is the reactor operating isothermally?
- T F CT (c) Multiple steady states can only exist for adiabatic reactions.
- T F CT (d) Reactor staging is only used for irreversible reactions.
- T F CT (e) The detrimental effect of pressure drop in gas phase reactions is more pronounced for adiabatic- exothermic reactions than for adiabatic endothermic reactions.

Solution

(a) False.



(b) Insufficient information to answer definitively. Need to know the feed temperature.



(c) False. See Equation 12-8

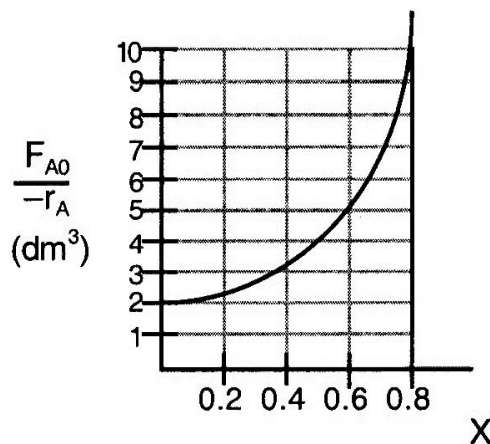
(d) False. See Figure 11-4

(e) True. $\frac{dy}{dW} = \frac{\alpha}{-2y} (1 + \epsilon X) \frac{T}{T_0}$

Exothermic $T \uparrow$ $y \downarrow$

Endothermic $T \downarrow$ $y \uparrow$

- (5 pts) 3) Circle the correct answer.
Consider the following Levenspiel plot



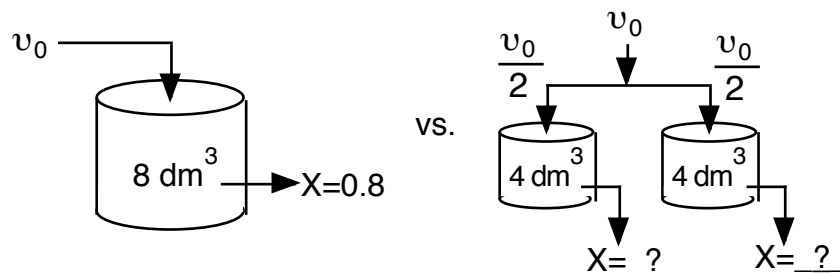
(1 pt) (a) The equilibrium conversion is

- (1) $X_e < 0.6$ (2) $X_e = 0.8$ (3) $X_e > 0.8$ (4) Can't tell from the information given

(1 pt) (b) The flow rate to an 8 dm³ CSTR corresponding to Figure E4-1 where 80% conversion is achieved is

- (1) $F_{A0} = 0.8$ mol/s (2) $F_{A0} = 10$ mol/s
(3) $F_{A0} = 1$ mol/s (4) Can't tell from the information given

(1 pt) (c) If the conversion achieved in a single 8 dm³ CSTR is 80%, what would the conversion be if the flow is equally divided into two CSTRs in parallel with first reactor having a volume of 4 dm³ each (same total volume).

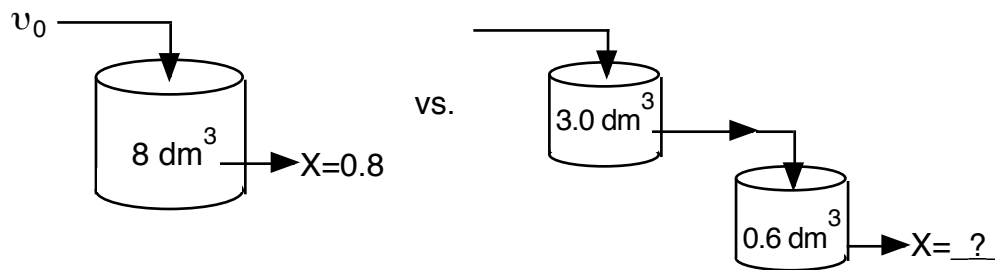


The total reactor volume is constant at 8 dm³.

The conversion for the two reactors in parallel is

- (1) $X > 0.8$ (2) $X < 0.8$ (3) $X = 0.8$ (4) Can't tell from the information given

(2 pts) (d) If the conversion achieved in a single 8 dm³ CSTR is 80%, what would the conversion be if two CSTRs are connected in series with first reactor having a volume of approximately 3.0 dm³ and the second reactor having a volume of 0.6 dm³.



The conversion for the two reactors in series is

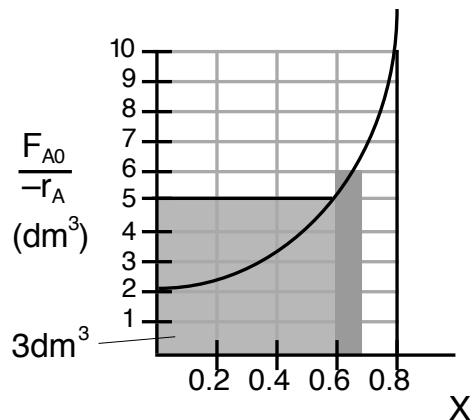
- (1) $X > 0.8$ (2) $X < 0.8$ (3) $X = 0.8$ (4) Can't tell from the information given

Solution

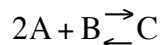
- (a) Ans. (3) $X_c > 0.8$
 (b) Ans. (d) Can't tell from information given
 (c) Ans. (3) $X = 0.8$. See p161.
 (d) Ans. (2) $X < 0.8$. Try $X = 0.6$

$$3 \text{ dm}^3 = 5 \text{ dm}^3 \times 0.6 = 3 \text{ dm}^3 \text{ checks}$$

$$\text{Try } \Delta V = 0.1 \text{ between } X = 0.6 \text{ and } 0.7 \quad V = 0.1 \times 6 \text{ dm}^3 = 0.6 \text{ dm}^3 \text{ checks}$$



(5 pts) 4) Consider the following reaction for parts (a), (b) and (c)



Write the rate law in terms of the specific reaction rate and species concentration when

(a) The reaction is irreversible and second order in A, and independent of the concentration of C, and overall first order.

$$-r_A = \underline{\hspace{2cm}}$$

(b) The reaction is elementary and reversible

$$-r_A = \underline{\hspace{2cm}}$$

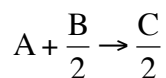
(c) Now consider the case when the reaction is first order in A and first order in B at high concentrations of A and B and is first order in A and second order in B at low concentrations of B. The rate law is

$$-r_A = \underline{\hspace{2cm}}$$

(d) What is the rate law for the reaction $\text{CH}_3\text{CHO} \rightarrow \text{CH}_4 + \text{CO}$?

$$-r_{\text{CH}_3\text{CHO}} = \underline{\hspace{2cm}}$$

Solution



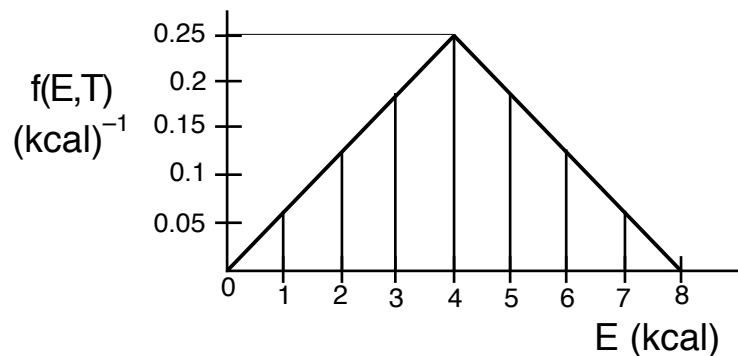
$$(a) \quad -r_A = k_A \frac{C_A^2}{C_B}$$

$$(b) \quad -r_A = k_A \left[C_A^2 C_B - \frac{C_C}{K_C} \right]$$

$$(c) \quad -r_A = \frac{k_1 C_A C_B^2}{1 + k_2 C_B}$$

$$(d) \quad -r_A = k C_A^{3/2} \text{ (see page 80)}$$

- (5 pts) 5) The following figure shows the energy distribution function at 300 K for the reaction $A + B \rightarrow C$



- (a) What fraction of the collisions have energies between 3 and 5 kcal?
 (b) What fraction of collisions have energies greater than 5 kcal?

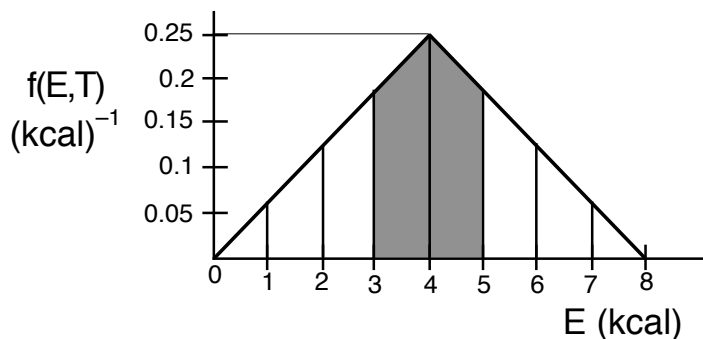
Solution

- (a) Between 0 and 4 kcal

$$f(E,T) = \left(\frac{0.25}{4}\right)E$$

- Between 4 and 8 kcal

$$f(E,T) = \frac{0.5 - 0.25}{4}E$$

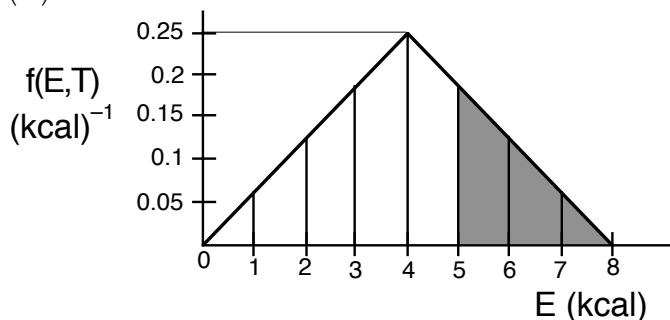


$$\text{at } E = 3 \quad f(E,T) = \frac{3}{4} \cdot 0.25 = 0.188$$

$$\text{at } E = 5 \quad f(E,T) = \frac{3}{4} \cdot 0.25 = 0.188$$

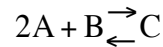
$$\begin{aligned} \text{Area} &= 1 \times (0.25) + (1) \frac{3}{4} \cdot 0.25 \\ &= 0.44 = 44\% \end{aligned}$$

- (b) $\left(\frac{3}{4}\right)(.25)$



$$\begin{aligned} \text{Area} &= \left(\frac{3}{4}\right)(.25) \times 3 \times \frac{1}{2} = \\ &= 0.28 = 28\% \end{aligned}$$

(5 pts) 6) Consider the following elementary gas phase reaction



Write $-r_A$ solely as a function of conversion (i.e., evaluating all symbols) when the reaction is an elementary, reversible, gas phase, isothermal reaction with no pressure drop with an equal molar feed with $C_{A0} = 2.0$, $k_A = 2$ and $K_C = 0.5$ all in proper units.

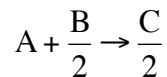
$$-r_A = \underline{\hspace{2cm}}$$

Solution

Elementary

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

A is the limiting reactant



$$y_{A0} = \frac{1}{2} \text{ (Equimolar)}$$

$$\varepsilon = y_{A0} \delta = \frac{1}{2} \left(\frac{1}{2} - \frac{1}{2} - 1 \right) = -\frac{1}{2}$$

$$C_A = \frac{C_{A0}(1-X)}{(1+\varepsilon X)}, \quad C_B = \frac{C_{A0} \left(\Theta_B - \frac{X}{2} \right)}{(1+\varepsilon X)}, \quad C_C = \frac{C_{A0} \frac{X}{2}}{(1+\varepsilon X)}$$

$$-r_A = k \left[\frac{C_{A0}^3 (1-X)^2 \left(\Theta_B - \frac{X}{2} \right)}{(1+\varepsilon X)^3} - \frac{C_{A0} X}{2K_C (1+\varepsilon X)} \right]$$

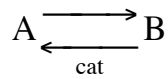
$$-r_A = k \left[\frac{C_{A0}^2 (1-X)^2}{\left(1 - \frac{1}{2} X \right)^2} \cdot \frac{C_{A0} \left(1 - \frac{1}{2} X \right)}{\left(1 - \frac{1}{2} X \right)} - \frac{C_{A0} X}{2K_C \left(1 - \frac{1}{2} X \right)} \right]$$

$$-r_A = 2 \left[\frac{C_{A0}^3 (1-X)^2}{\left(1 - \frac{1}{2} X \right)^2} - \frac{C_{A0} X}{2K_C \left(1 - \frac{1}{2} X \right)} \right]$$

$$k = 2 \left(\frac{\text{dm}^3}{\text{mol} \cdot \text{s}} \right)^2, \quad C_{A0} = 2 \frac{\text{mol}}{\text{dm}^3}, \quad \Theta_B = 1, \quad K_C = 0.5 \left(\frac{\text{dm}^3}{\text{mol}} \right)^2$$

$$-r_A = 2 \left[\frac{8(1-X)^2}{\left(1 - \frac{1}{2}X\right)^2} - \frac{2X}{\left(1 - \frac{1}{2}X\right)} \right]$$

(5 pts) 7) The elementary gas phase isomerization exothermic reaction



is carried out isothermally at 400K in a PBR where the pressure drop occurs with $\alpha = 0.001 \text{ kg}^{-1}$. The flow is laminar. Currently 50% conversion is achieved. The equilibrium constant at this temperature is 3.0.

(a) For a fixed mass flow rate $\dot{m}$, if the reactor diameter is increased by a factor of 4, the conversion X is

- (1) $X > 0.5$ (2) $X < 0.5$ (3) $X = 0.5$ (4) insufficient information to tell.

(b) For a fixed mass flow rate $\dot{m}$, the equilibrium conversion X_e is

- (1) $X_e = 0.5$ (2) $X_e = 0.667$ (3) $X_e = 0.75$ (4) insufficient information to tell.

(c) For a fixed mass flow rate $\dot{m}$, if the reactor diameter is increased by a factor of 2, the equilibrium conversion X_e will

- (1) increase (2) decrease (3) remain the same (4) insufficient information to tell

(d) For a fixed mass flow rate $\dot{m}$, if the particle size is increased the equilibrium conversion X_e will

- (1) increase (2) decrease (3) remain the same (4) insufficient information to tell

(e) Consider the case where an adiabatic endothermic reaction becomes “frozen” in a PFR [cf. p.541]. The actual conversion, X , can be greater than the equilibrium conversion, X_e , near the point where the reaction becomes frozen.

- (1) True (2) False (3) Depends on feed condition

Solution

(a) Ans. (1) $X > 0.5$

$$\alpha \sim \frac{1}{D^2}$$

Increase D , decrease α , increase X .

(b) Ans. (3) $X_e = 0.75$

$$X_e = \frac{K_C}{1 + K_C} = \frac{3}{1 + 3} = 0.75$$

(c) Ans. (3) remain the same

$$K_C = \frac{C_A}{C_{Ae}} = \frac{C_{A0}(1 - X_e)y}{C_{A0}X_e y} = \frac{1 - X_e}{X_e}$$

X_e is not a function of pressure drop parameter α .

(d) Ans. (3) or (4)

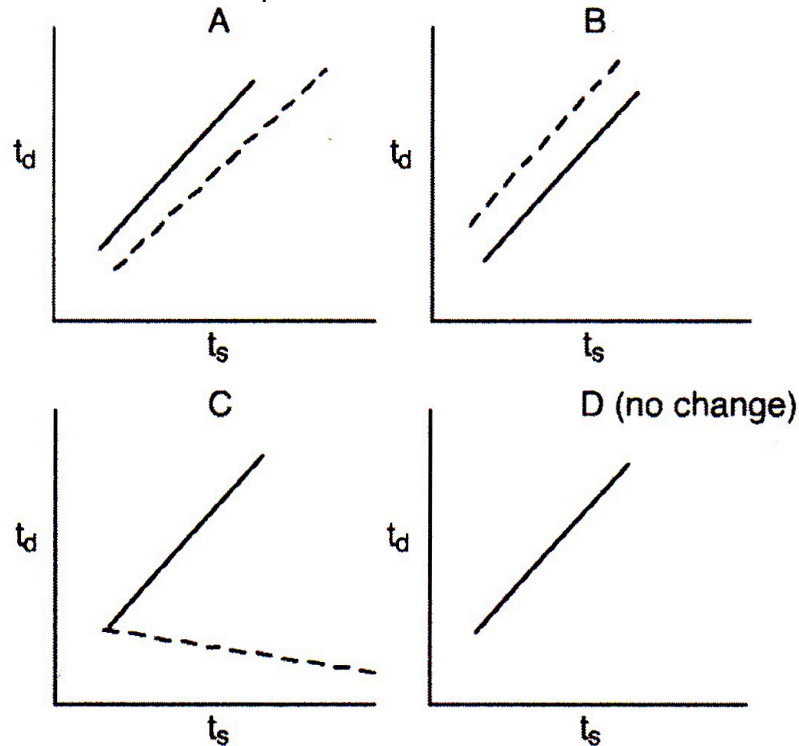
Exothermic $D_p \uparrow$ then $K \downarrow$ then $X_e \downarrow$

X_e is not a function of particle size or any other geometry. But will a change in pressure drop affect the achievable conversion, and therefore temperature? X_e is a function of temperature. So probably accept unchanged OR Can't tell

(e) Ans. (2)

X_e can never be less than X , (i.e., X can never be greater than X_e).

- (5 pts) 8) Suppose inerts are added to the system in Example 13-2. The dashed line represents the relationship after the inerts were added. Which figure represents how the relationship between the line the reactor failed after start up, t_r , and the down time, t_d , would change? The solid line represents the case without inerts?



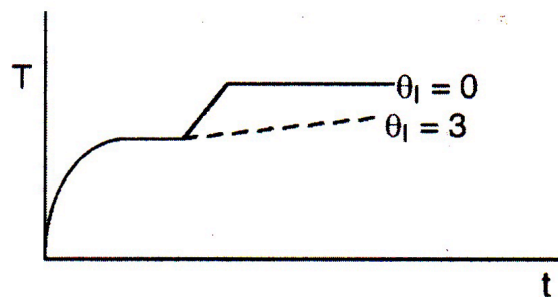
Solution

Answer: B

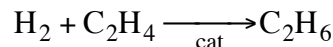
Explanation:

$$\frac{dT}{dt} = \frac{Qg - Qr}{\sum N_i C_{P_i}} = \frac{Qg - Qr}{N_A C_{P_A} + N_B C_{P_B} + N_C C_{P_C} + N_I C_{P_I}}$$

We see the rate of temperature increase, $\frac{dT}{dt}$, decreases as the amount of inert, N_I , increases. Therefore, the temperature will not rise as rapidly during the adiabatic period (down time, t_d) and we can have longer down times without having an explosion.



(10 pts) 9) **P10-5. Study Problem.** The rate law for the hydrogenation (H) of ethylene (E) to form ethane (A)



over a cobalt-molybdenum catalyst [*Collection Czech. Chem. Commun.*, 51, 2760 (1988)] is

$$-r'_E = \frac{kP_E P_H}{1 + K_E P_E}$$

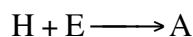
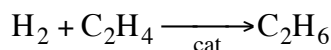
Suggest a mechanism and rate-limiting step consistent with the rate law and then derive the rate law.

Solution

H = H₂

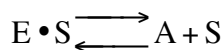
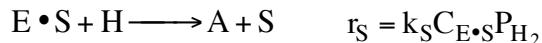
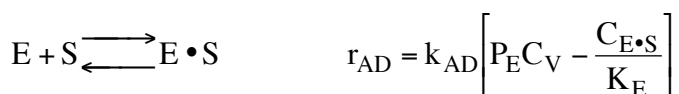
E = Ethylene

A = Ethane



Because neither H₂ or C₂H₆ are not in the denominator of the rate law they are either not adsorbed or weakly adsorbed. Assume H₂ in the gas phase reacts with C₂H₄ adsorbed on the surface and ethane goes directly into the gas phase. Then check to see if this mechanism agrees with the rate law

Eley Rideal



Assume surface reaction

$$C_{\text{E} \cdot \text{S}} = K_E P_E C_V$$

$$r_S = k_S [C_{\text{E} \cdot \text{S}} P_H]$$

$$C_T = C_V + C_{\text{E} \cdot \text{S}}$$

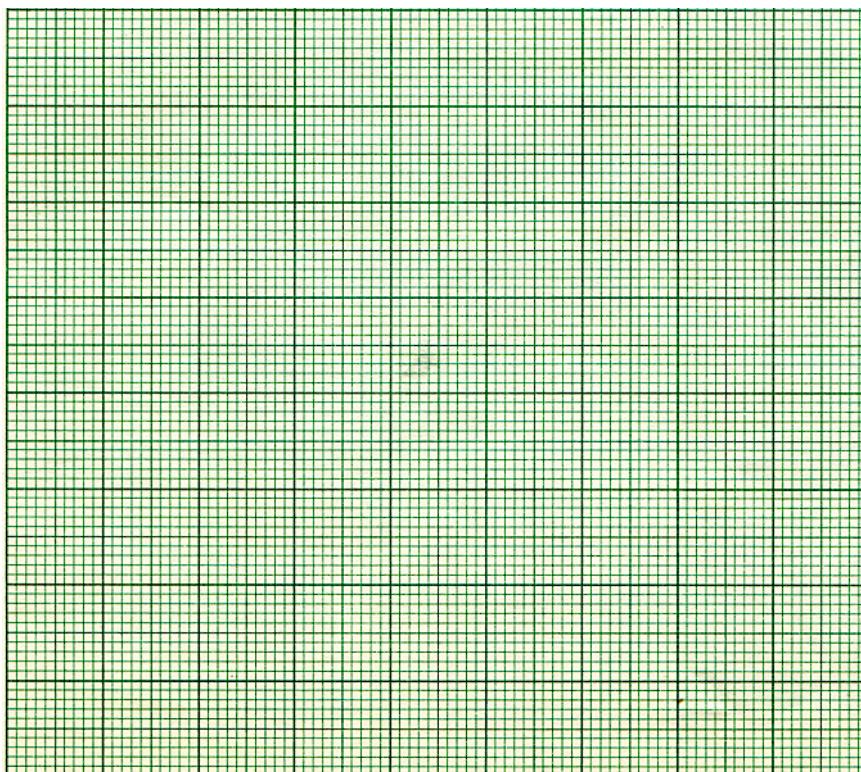
$$-r'_A = k_S K_E C_T \left[\frac{P_E P_H}{1 + K_E P_E} \right]$$

(10 pts) 10) P7-10. **Study Problem.** In order to study the photochemical decay of aqueous bromine in bright sunlight, a small quantity of liquid bromine was dissolved in water contained in a glass battery jar and placed in direct sunlight. The following data were obtained at 25°C:

Time (min)	0	10	20	30	40	50	60
Ppm Br ₂ , C _A	3.45	2.45	1.74	1.23	0.88	0.62	0.44

- Determine whether the reaction rate is zero, first, or second order in bromine, and calculate the reaction rate constant in units of your choice. (Hint: Preliminary calculations suggest the reaction may be first order.)
- Assuming identical exposure conditions, calculate the required hourly rate of injection of bromine (grams per hour) into a very large sunlit body of water, 25,000 gal (94,600 dm³) in volume, in order to maintain a sterilizing level of bromine of 1.0 ppm.

Note: ppm = parts of bromine per million parts of brominated water by weight. In dilute aqueous solutions, 1 ppm = 1 milligram per liter.)
(From California Professional Engineers' Exam.)



Solution

P7-10 (a)

Photochemical decay of bromine in bright sunlight:

t (min)	0	10	20	30	40	50	60
C _A (ppm)	3.45	2.45	1.74	1.23	0.88	0.62	0.44

Mole balance: constant V

$$\frac{dC_A}{dt} = r_A = -kC_A^\alpha$$

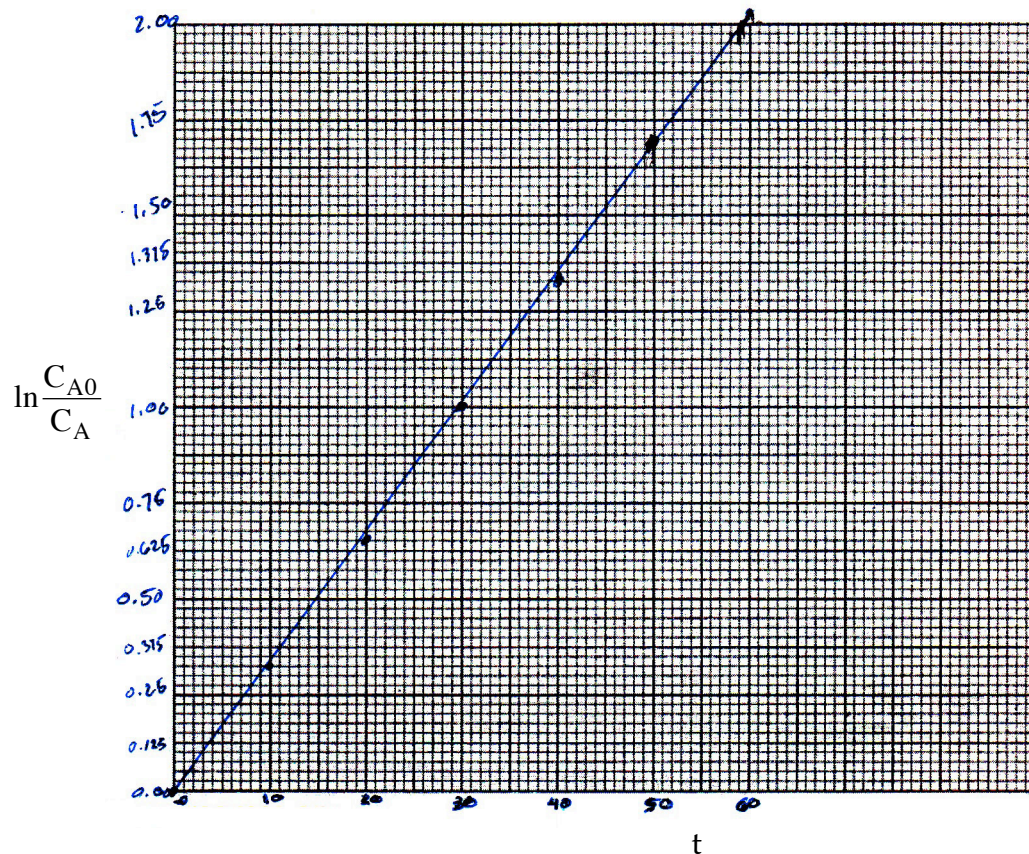
$$\alpha = 1, \text{ therefore } \frac{dC_A}{dt} = -kC_A$$

$$\frac{dC_A}{dt} = -kC_A, \ln \frac{C_{A0}}{C_A} = kt$$

After plotting and differentiating by equal area

Time (min)	0	10	20	30	40	50	60
Ppm Br ₂ , C _A	3.45	2.45	1.74	1.23	0.88	0.62	0.44
-dC _A /dt		0.082	0.061	0.042	0.030	0.0215	0.014
ln(-dC _A /dt)		-2.501	-2.797	-3.170	-3.507	-3.840	-4.269
ln C _A		0.896	0.554	0.207	-0.128	-0.478	-0.821
ln C _{A0} /C _A	0	0.34	0.68	1.03	1.34	1.72	2.05

First order



Slope of Plot of $\ln (C_{A0}/C_A)$ versus t

$$\text{Slope} = \frac{2.0}{58 \text{ min}}$$

$$k = 0.0345 \text{ min}^{-1}$$

P7-10 (b)

$$\frac{dN_A}{dt} = V r_A$$

$$\frac{dN_A}{dt} = F_{A0} - 0 + r_A V$$

$$\text{Steady state } \frac{dN_A}{dt} = 0$$

$$F_{A0} = -r_A V$$

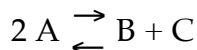
$$\text{at } C_A = 1 \text{ ppm}$$

$$r_A = -0.344 \frac{\text{ppm}}{\text{min}} = -0.344 \frac{\text{mg}}{\text{l min}}$$

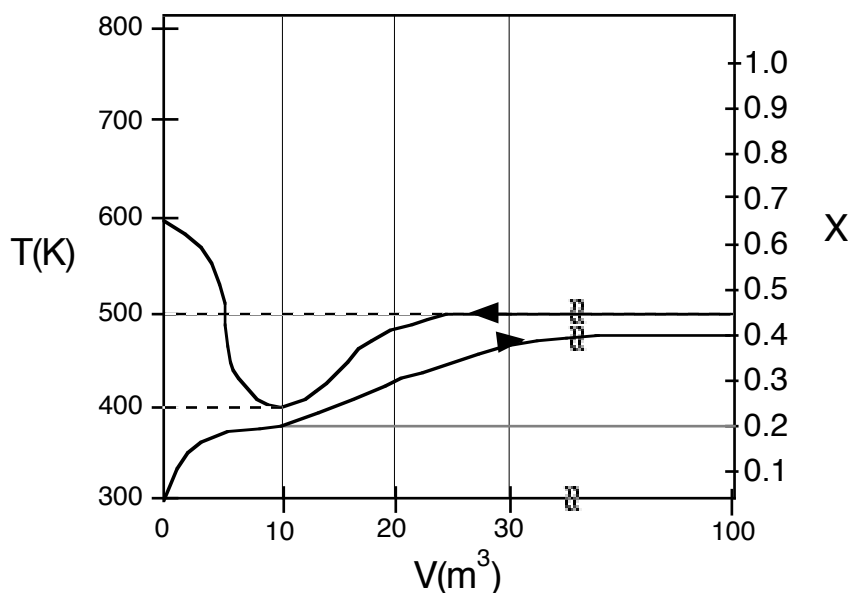
$$F_{A0} = \left(94,600 \text{ dm}^3 \right) \left(0.034 \frac{\text{mg}}{\text{dm}^3 \text{ min}} \right) \times \frac{1 \text{ g}}{1,000 \text{ mg}} \times \left(\frac{60 \text{ min}}{\text{h}} \right) = 195 \frac{\text{g}}{\text{h}}$$

This problem is continued from Problem (6) on MidTerm Exam II (Complete parts (e) and (f))

(10 pts) 11) The temperature and conversion in a virtually infinitely long PFR are shown below as a function of the reactor volume. The reactor is surrounded by a jacket for heat transfer. The value of Ua is $100 \text{ cal}/(\text{sec} \cdot \text{m}^3 \cdot \text{K})$ with T_a being constant. The gas-phase, reversible reaction is



and pure A is fed to the reactor at a concentration $C_{A0} = 1.0 \text{ mol}/\text{m}^3$ and a molar flow rate of $10 \text{ mol}/\text{s}$. The absolute value of the heat of reaction is $5,000 \text{ cal}/\text{mol}$ of A at 500K , and the heat capacities of A, B, and C are each $10 \text{ cal}/\text{mol}/\text{K}$.



(a) Using what is the equilibrium constant at 500 K ?

$K_e(500) = \underline{0.11}$ (From MidTerm Exam II solution)

(b) What is the rate of disappearance of A, $-r_A$, at 10 m^3 ?

$-r_A = \underline{2 \text{ mol}/\text{m}^3 \cdot \text{s}}$ (From MidTerm Exam II solution)

(6 pt) (c) What is the equilibrium constant at 400 K ?

$K_e(400) = \underline{\hspace{2cm}}$

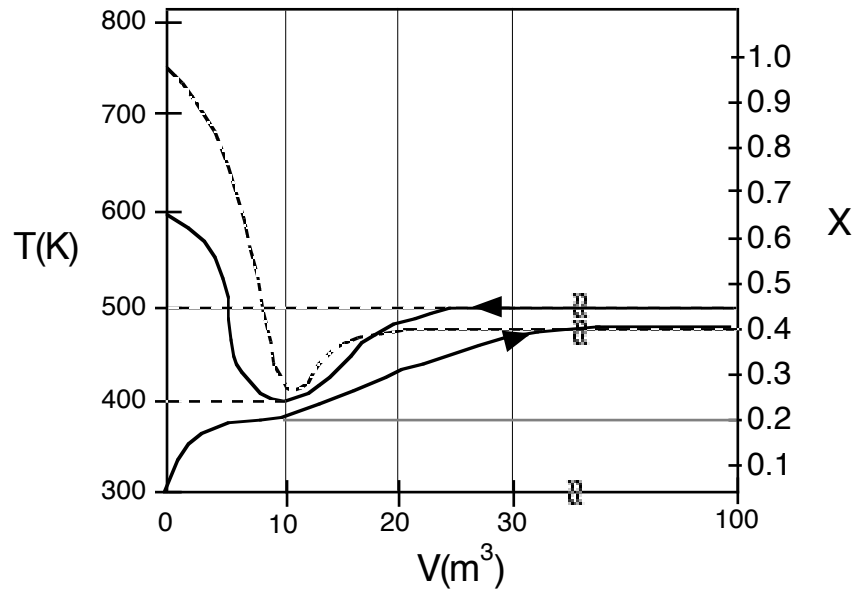
(8 pt) (d) What is the specific reaction rate at $V = 10 \text{ m}^3$?

$k = \underline{\hspace{2cm}}$

(6 pt) (e) What is the total amount of heat added/removed to the entire reactor per mol of A feed? Include proper sign in your numerical answer if possible.

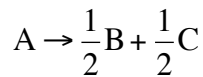
$\frac{\dot{Q}}{F_{A0}} = \underline{\hspace{2cm}}$

Solution



at $V = 10 \text{ m}^3$ $Q_g = Q_r$

(a) $K_e(500) = ?$



$$\delta = 0 \therefore \varepsilon = 0$$

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

$$C_B = C_C = C_{A0} X/2$$

$$\text{at } 500 \text{ K } X = X_e = 0.4 \quad K_e = \frac{C_B C_C}{C_A^2} = \frac{C_{A0}^2 X_e^2}{C_{A0}^2 4(1 - X_e)^2} = \frac{(0.4)^2}{4(1 - 0.4)^2} = \frac{0.16}{4(0.36)} = 0.11$$

$$K_e = 0.11$$

(b) $-r_A = ?$

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

$$\frac{dT}{dV} = \frac{\overbrace{(r_A)(\Delta H_{Rx})}^{Q_g} - \overbrace{Ua(T - T_a)}^{Q_r}}{\sum F_i C_{P_i}}$$

$$\text{At minimum } \frac{dT}{dV} = 0$$

$$Q_g = Q_r$$

At large V no further change in temperature so assume $T = T_a = 500 \text{ K}$ and that T at minimum is 400 K .

At minimum

$$\dot{Q}_r = Ua (T - T_s) = 100 (400 - 500) = -10,000 \text{ cal/s} \cdot \text{m}^3$$

$$Q_g = (-r_A)(-\Delta H_{Rx})$$

$$(-r_A)(-\Delta H_{Rx}) = (-r_A)(-5,000) = Q_r = -20,000 \frac{\text{cal}}{\text{m}^3 \cdot \text{s}}$$

$$\boxed{-r_A = \frac{-10,000 \frac{\text{cal}}{\text{s} \cdot \text{m}^3}}{-5,000 \frac{\text{cal}}{\text{mol}}} = 2 \frac{\text{mol}}{\text{m}^3 \cdot \text{s}}}$$

(c) $K_e(400) = ?$ _____

$$K_e(400) = K_C(500) \exp \left[\frac{\Delta H_{Rx}}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right) \right]$$

$$K_e(400) = 0.11 \exp \left[\frac{5,000}{1.987} \left(\frac{1}{500} - \frac{1}{400} \right) \right]$$

$$= 0.11 \exp \left[\frac{-100}{(400)(500)} \frac{5,000}{1.987} \right]$$

$$\boxed{K_e = 0.11 \exp(-1.25) = (0.11)(0.28) = 0.031}$$

(d) $k = ?$ _____

$$-r_A = k \left[C_{A0}^2 - \frac{C_B C_C}{K_e} \right]$$

$$A \rightarrow \frac{B}{2} + \frac{C}{2}$$

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

$$C_B = C_C = \frac{C_{A0}X}{2}$$

at $V = 10 \text{ m}^3$, $T = 400$, $X = 0.2$, $K_e = 0.031$

$$\begin{aligned}
 -r_A &= k \left[C_{A0}^2 (1-X)^2 - \frac{C_{A0}^2 X^2}{4K_C} \right] \\
 &= k C_{A0}^2 \left[(1-X)^2 - \frac{X^2}{4K_e} \right] \\
 &= k \cdot 1 \cdot \left[(1-0.2)^2 - \frac{(0.2)^2}{(4)(0.031)} \right] \\
 &= k \left[0.64 - \frac{0.04}{0.124} \right] = k [0.64 - 0.32]
 \end{aligned}$$

$$-r_A = 2 \frac{\text{mol}}{\text{m}^3 \cdot \text{s}} = 0.32 \left(\frac{\text{mol}}{\text{m}^3} \right)^2 k$$

$$\boxed{k = \frac{2}{0.32} = 6.25 \frac{\text{m}^3}{\text{mol} \cdot \text{s}}}$$

(e) $\frac{\dot{Q}}{F_{A0}} = \underline{\hspace{1cm} ? \hspace{1cm}}$

$$\dot{Q} - F_{A0} \sum \Theta_i C_{P_i} (T - T_0) - [\Delta H_{R_x} + \Delta C_P (T - T_a)] F_{A0} X = 0 \quad \text{Eqn. (11-28)}$$

Per Mole A

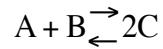
$$\frac{\dot{Q}}{F_{A0}} = C_{P_A} [T - T_0] + [\Delta H_{R_x} + \Delta C_P (T - T_R) X]$$

$$A \xrightarrow{\frac{B}{2}} \frac{C}{2}$$

$$\begin{aligned}
 \Delta C_P &= \frac{C_{P_C}}{2} + \frac{C_{P_B}}{2} - C_{P_A} = \frac{10}{2} + \frac{10}{2} - 10 = 0 \\
 &= 0
 \end{aligned}$$

$$\frac{\dot{Q}}{F_{A0}} = 10(500 - 600) + [+5,000][0.4] = -1,000 + 2,000 = 1,000 \frac{\text{cal}}{\text{mol}}$$

(10 pts) 12) Let's revisit homework Problem P12-3, where the reaction



is carried out in a packed bed reactor. Match the following temperature and conversion profiles for the 4 different heat exchange cases adiabatic, constant T_a , co-current exchange and counter current exchange.

Figure 1

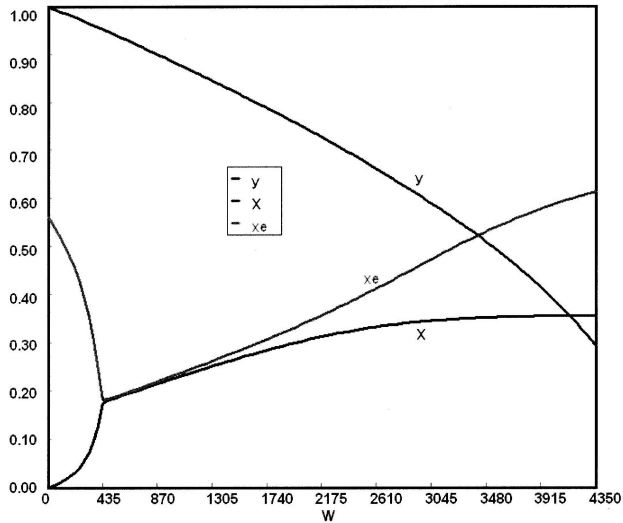


Figure 2

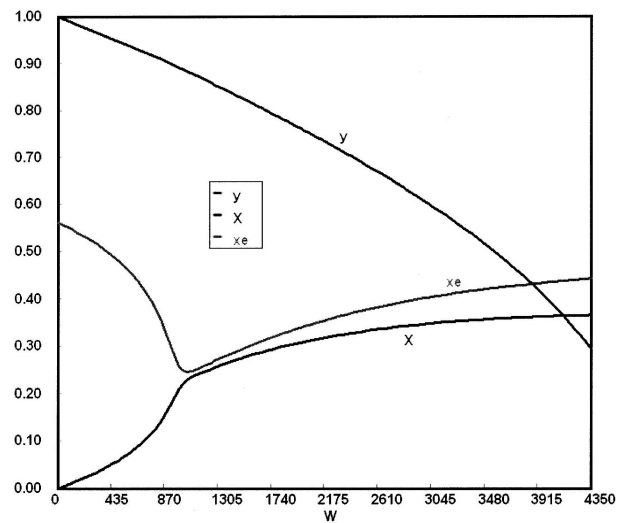


Figure 3

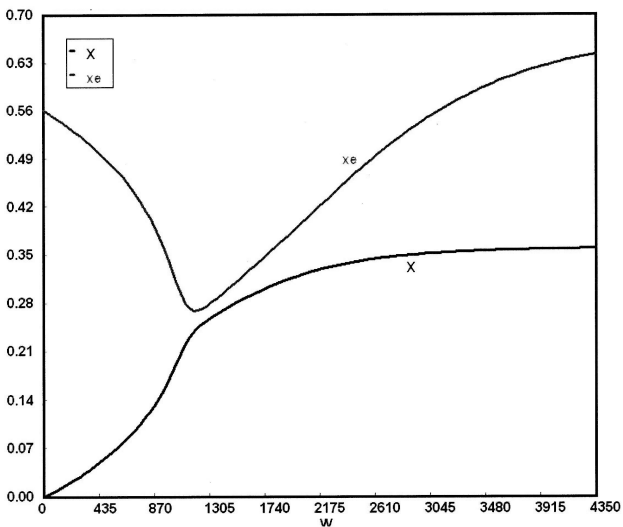


Figure 4

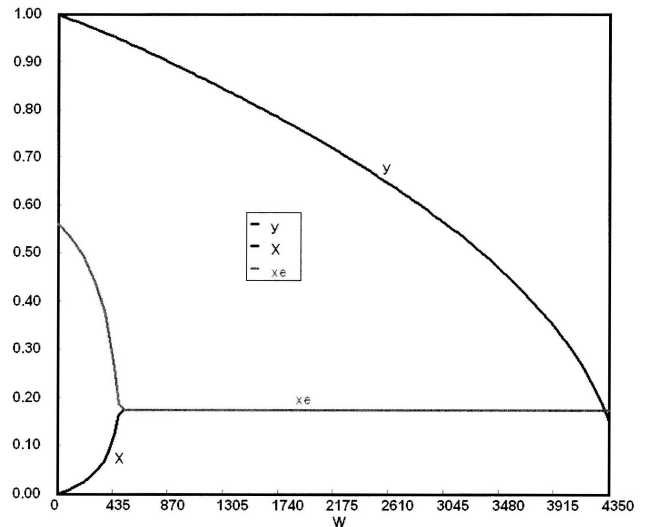


Figure A

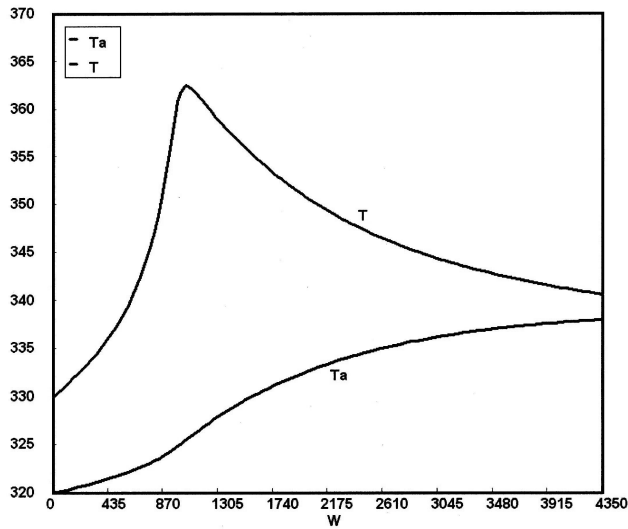


Figure B

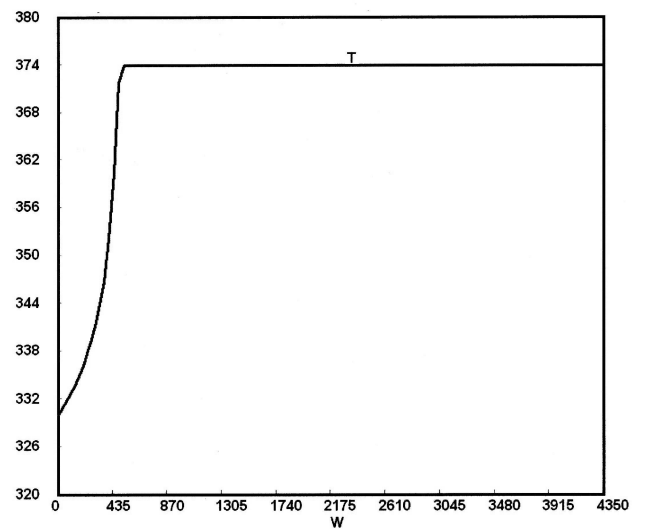


Figure C

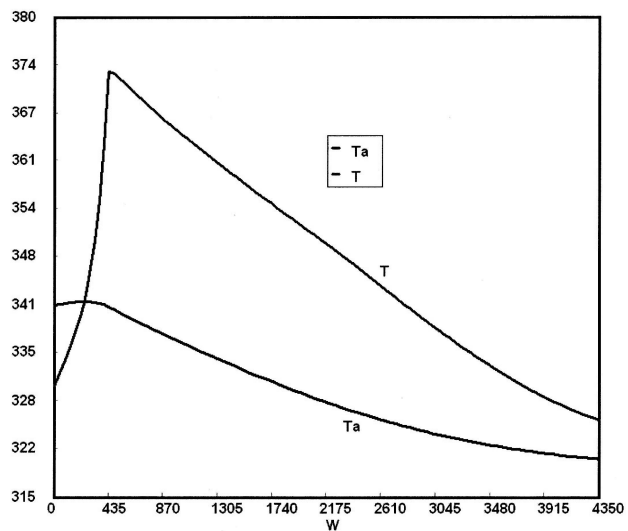
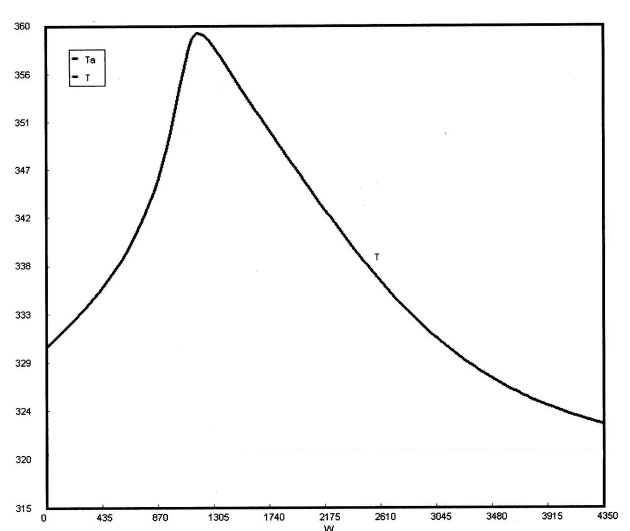


Figure D



- (a) Figure 1 matches Figure ____
 (b) Figure 2 matches Figure ____
 (c) Figure 3 matches Figure ____
 (d) Figure 4 matches Figure ____

Solution

- (a) Figure 1 matches Figure C
 (b) Figure 2 matches Figure A
 (c) Figure 3 matches Figure D
 (d) Figure 4 matches Figure B

In Class Problem 14 Solution

(a) Adiabatic

POLYMATH Report

Ordinary Differential Equations

Calculated values of DEQ variables

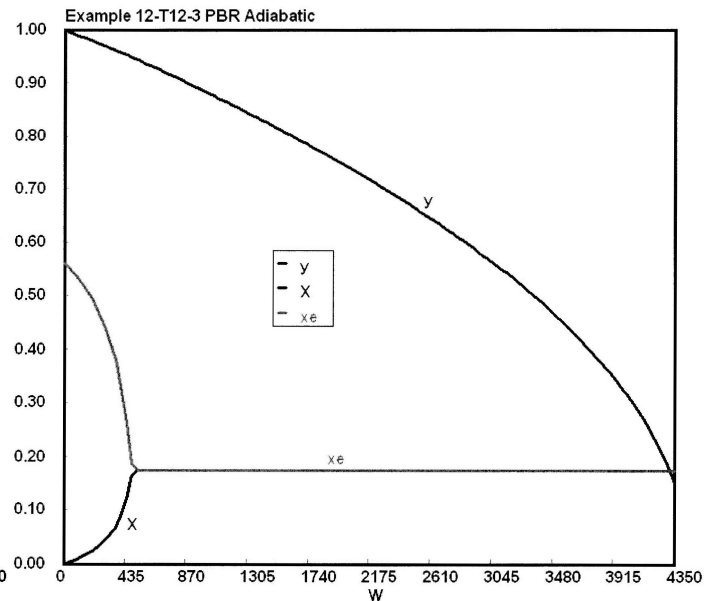
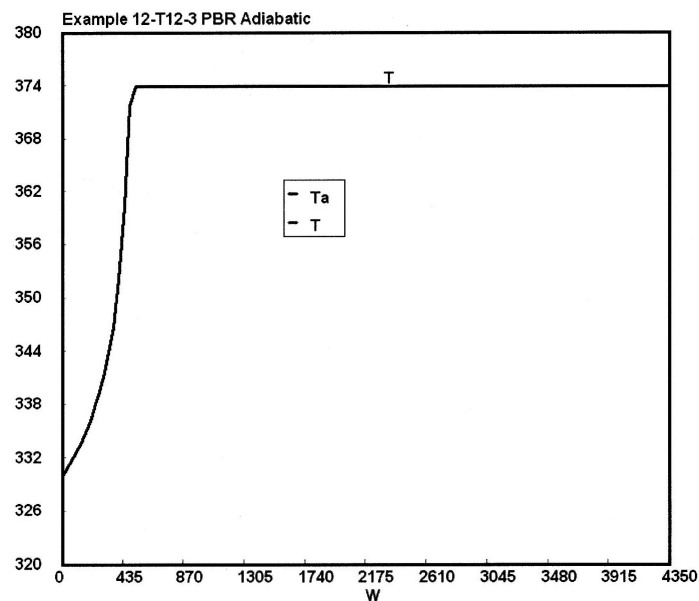
	Variable	Initial value	Final value
1	alpha	0.0002	0.0002
2	Ca	0.1	0.0111573
3	Cao	0.1	0.1
4	Cb	0.1	0.0111573
5	Cc	0	0.0047662
6	CpA	20.	20.
7	CpB	20.	20.
8	CpI	40.	40.
9	Cpmc	18.	18.
10	Cto	0.3	0.3
11	Ea	2.5E+04	2.5E+04
12	Fao	5.	5.
13	Hr	-2.0E+04	-2.0E+04
14	ka	0.046809	4.152669
15	Kc	6.601082	0.1824807
16	Mc	100.	100.
17	ra	-0.0004681	1.126E-19
18	sumcp	80.	80.
19	T	330.	373.9994
20	Ta	320.	320.
21	thetaB	1.	1.
22	thetaI	1.	1.
23	To	330.	330.
24	Uarho	0	0
25	W	0	4350.
26	X	0	0.1759977
27	xe	0.5622921	0.1759977
28	y	1.	0.153458
29	yao	0.3333333	0.3333333

Differential equations

- $d(Ta)/d(W) = Uarho*(T-Ta)/(Mc*Cpmc)$
- $d(y)/d(W) = -alpha/2*(T/To)/y$
- $d(T)/d(W) = (Uarho*(Ta-T)+(-ra)*(-Hr))/(Fao*sumcp)$
- $d(X)/d(W) = -ra/Fao$

Explicit equations

- alpha = .0002
- To = 330
- Uarho = 0.5*0
- Mc = 100
- Cpmc = 18
- Hr = -20000
- Fao = 5
- thetaI = 1
- CpI = 40
- CpA = 20
- thetaB = 1
- CpB = 20
- Cto = 0.3
- Ea = 25000
- $Kc = 100*(exp(Hr/1.987*(1/303-1/T)))$
- $ka = .004*exp(Ea/1.987*(1/310-1/T))$
- $yao = 1/(1+thetaB+thetaI)$
- $xe = Kc^{0.5}/(2+Kc^{0.5})$
- Cao = yao*Cto
- sumcp = (thetaI*CpI+CpA+thetaB*CpB)
- $Ca = Cao*(1-X)*y*To/T$
- $Cb = Cao*(1-X)*y*To/T$
- $Cc = Cao*2*X*y*To/T$
- $ra = -ka*(Ca*Cb-Cc^2/Kc)$



In Class Problem 14 Solution

(b) Constant T_c Heat Exchange

POLYMATH Report

Ordinary Differential Equations

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	alpha	0.0002	0.0002	0.0002	0.0002
2	Ca	0.1	0.0216333	0.1	0.0216333
3	Cao	0.1	0.1	0.1	0.1
4	Cb	0.1	0.0216333	0.1	0.0216333
5	Cc	0	0	0.0467561	0.0243159
6	CpA	20.	20.	20.	20.
7	CpB	20.	20.	20.	20.
8	CpI	40.	40.	40.	40.
9	Cpmc	18.	18.	18.	18.
10	Cto	0.3	0.3	0.3	0.3
11	Ea	2.5E+04	2.5E+04	2.5E+04	2.5E+04
12	Fao	5.	5.	5.	5.
13	Hr	-2.0E+04	-2.0E+04	-2.0E+04	-2.0E+04
14	ka	0.046809	0.0200561	1.05569	0.0200561
15	Kc	6.601082	0.5458201	13.00416	13.00416
16	Mc	100.	100.	100.	100.
17	ra	-0.0004681	-0.0020396	-8.474E-06	-8.474E-06
18	sumcp	80.	80.	80.	80.
19	T	330.	322.8237	359.3692	322.8237
20	Ta	320.	320.	320.	320.
21	thetaB	1.	1.	1.	1.
22	thetaI	1.	1.	1.	1.
23	To	330.	330.	330.	330.
24	Uarho	0.5	0.5	0.5	0.5
25	W	0	0	4350.	4350.
26	X	0	0	0.3597967	0.3597967
27	xe	0.5622921	0.2697522	0.6432475	0.6432475
28	y	1.	0.3305639	1.	0.3305639
29	yao	0.3333333	0.3333333	0.3333333	0.3333333

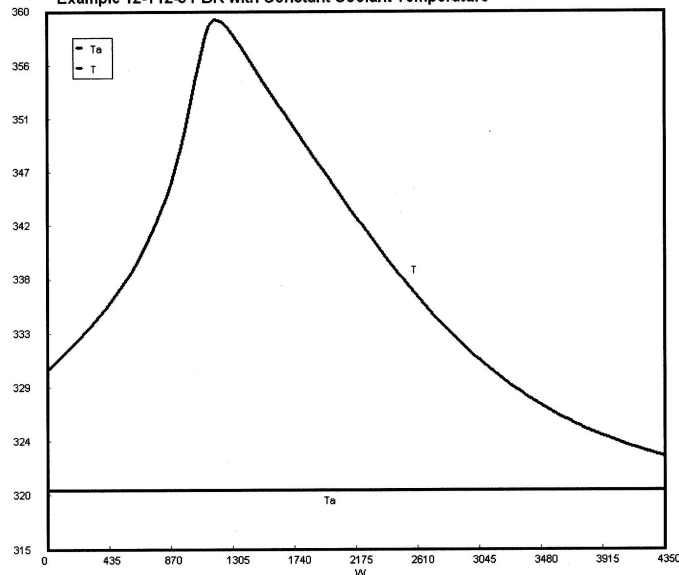
Differential equations

- $d(Ta)/d(W) = Uarho*(T-Ta)/(Mc*Cpmc)*0$
- $d(y)/d(W) = -alpha/2*(T/To)/y$
- $d(T)/d(W) = (Uarho*(Ta-T)+(-ra)*(-Hr))/(Fao*sumcp)$
- $d(X)/d(W) = -ra/Fao$

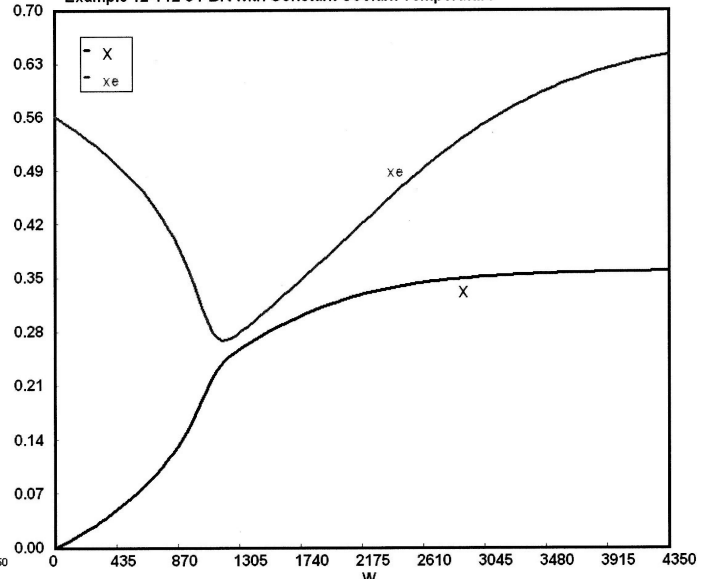
Explicit equations

- alpha = .0002
- To = 330
- Uarho = 0.5
- Mc = 100
- Cpmc = 18
- Hr = -20000
- Fao = 5
- thetaI = 1
- CpI = 40
- CpA = 20
- thetaB = 1
- CpB = 20
- Cto = 0.3
- Ea = 25000
- $Kc = 100*(exp(Hr/1.987*(1/303-1/T)))$
- $ka = .004*exp(Ea/1.987*(1/310-1/T))$
- $yao = 1/(1+thetaB+thetaI)$
- $xe = Kc^{0.5}/(2+Kc^{0.5})$
- Cao = yao*Cto
- sumcp = (thetaI*CpI+CpA+thetaB*CpB)
- Ca = Cao*(1-X)*y*To/T
- Cb = Cao*(1-X)*y*To/T
- Cc = Cao*2*X*y*To/T
- $ra = -ka*(Ca*Cb-Cc^2/Kc)$

Example 12-T12-3 PBR with Constant Coolant Temperature



Example 12-T12-3 PBR with Constant Coolant Temperature



In Class Problem 14 Solution

(c) Variable T, Co-Current Heat Exchange

POLYMATH Report

Ordinary Differential Equations

Calculated values of DEQ variables

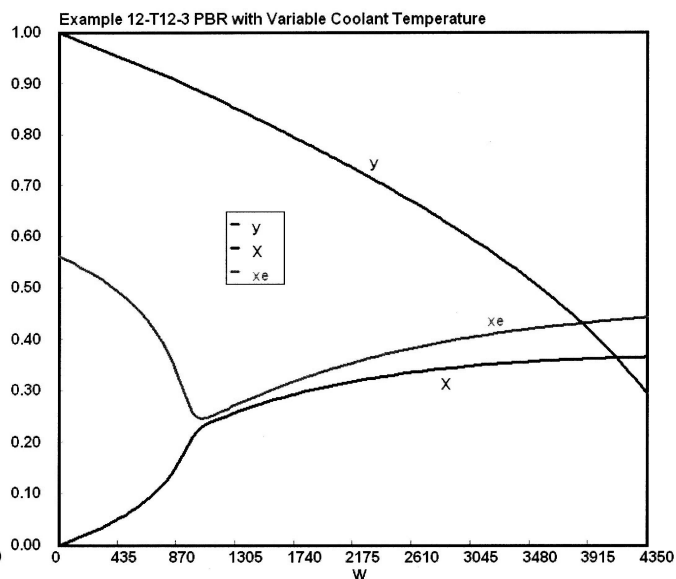
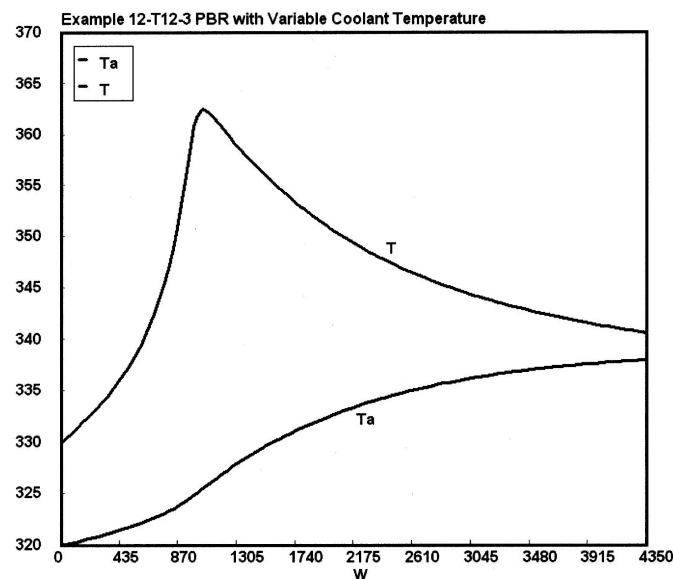
	Variable	Initial value	Maximal value	Final value
1	alpha	0.0002	0.0002	0.0002
2	Ca	0.1	0.1	0.0181239
3	Cao	0.1	0.1	0.1
4	Cb	0.1	0.1	0.0181239
5	Cc	0	0.0443144	0.0210077
6	CpA	20.	20.	20.
7	CpB	20.	20.	20.
8	CpI	40.	40.	40.
9	Cpmc	18.	18.	18.
10	Cto	0.3	0.3	0.3
11	Ea	2.5E+04	2.5E+04	2.5E+04
12	Fao	5.	5.	5.
13	Hr	-2.0E+04	-2.0E+04	-2.0E+04
14	ka	0.046809	1.441253	0.1538474
15	Kc	6.601082	6.601082	2.548041
16	Mc	100.	100.	100.
17	ra	-0.0004681	-2.389E-05	-2.389E-05
18	sumcp	80.	80.	80.
19	T	330.	362.5934	340.6307
20	Ta	320.	338.0216	338.0216
21	thetaB	1.	1.	1.
22	thetaI	1.	1.	1.
23	To	330.	330.	330.
24	Uarho	0.5	0.5	0.5
25	W	0	4350.	4350.
26	X	0	0.3669116	0.3669116
27	xe	0.5622921	0.5622921	0.4438665
28	y	1.	1.	0.2954995
29	yao	0.3333333	0.3333333	0.3333333

Differential equations

- $d(Ta)/d(W) = Uarho*(T-Ta)/(Mc*Cpmc)$
- $d(y)/d(W) = -alpha/2*(T/To)/y$
- $d(T)/d(W) = (Uarho*(Ta-T)+(-ra)*(-Hr))/(Fao*sumcp)$
- $d(X)/d(W) = -ra/Fao$

Explicit equations

- alpha = .0002
- To = 330
- Uarho = 0.5
- Mc = 100
- Cpmc = 18
- Hr = -20000
- Fao = 5
- thetaI = 1
- CpI = 40
- CpA = 20
- thetaB = 1
- CpB = 20
- Cto = 0.3
- Ea = 25000
- $Kc = 100*(exp(Hr/1.987*(1/303-1/T)))$
- $ka = .004*exp(Ea/1.987*(1/310-1/T))$
- $yao = 1/(1+thetaB+thetaI)$
- $xe = Kc^{0.5}/(2+Kc^{0.5})$
- Cao = yao*Cto
- sumcp = (thetaI*CpI+CpA+thetaB*CpB)
- Ca = Cao*(1-X)*y*To/T
- Cb = Cao*(1-X)*y*To/T
- Cc = Cao*2*X*y*To/T
- ra = -ka*(Ca*Cb-Cc^2/Kc)



In Class Problem 14 Solution

(d) Variable T, Counter Current Heat Exchange

POLYMATH Report

Ordinary Differential Equations

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	alpha	0.0002	0.0002	0.0002	0.0002
2	Ca	0.1	0.019166	0.1	0.019166
3	Cao	0.1	0.1	0.1	0.1
4	Cb	0.1	0.019166	0.1	0.019166
5	Cc	0	0	0.0430954	0.0213071
6	CpA	20.	20.	20.	20.
7	CpB	20.	20.	20.	20.
8	CpI	40.	40.	40.	40.
9	Cpmc	18.	18.	18.	18.
10	Cto	0.3	0.3	0.3	0.3
11	Ea	2.5E+04	2.5E+04	2.5E+04	2.5E+04
12	Fao	5.	5.	5.	5.
13	Hr	-2.0E+04	-2.0E+04	-2.0E+04	-2.0E+04
14	ka	0.046809	0.027341	3.66453	0.027341
15	Kc	6.601082	0.2016806	10.1491	10.1491
16	Mc	100.	100.	100.	100.
17	ra	-0.0004681	-0.0066177	-8.82E-06	-8.82E-06
18	sumcp	80.	80.	80.	80.
19	T	330.	325.4108	372.6143	325.4108
20	Ta	341.	320.132	341.4065	320.132
21	thetaB	1.	1.	1.	1.
22	thetaI	1.	1.	1.	1.
23	To	330.	330.	330.	330.
24	Uarho	0.5	0.5	0.5	0.5
25	W	0	0	4350.	4350.
26	X	0	0	0.3572674	0.3572674
27	xe	0.5622921	0.1833697	0.6143288	0.6143288
28	y	1.	0.2940479	1.	0.2940479
29	yao	0.3333333	0.3333333	0.3333333	0.3333333

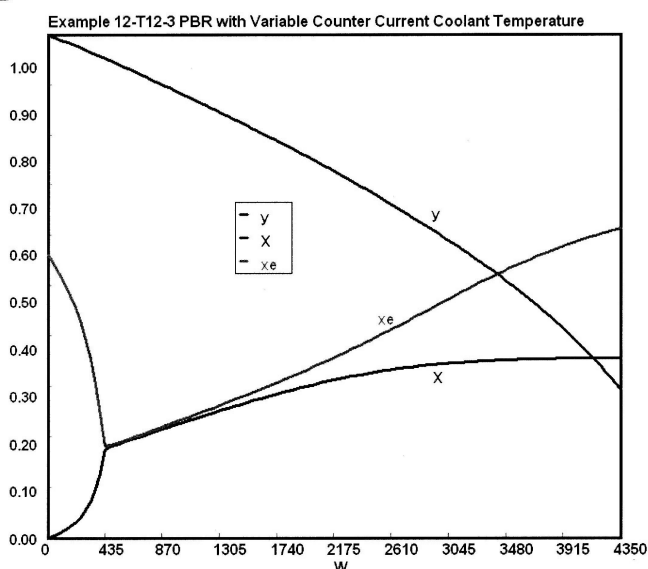
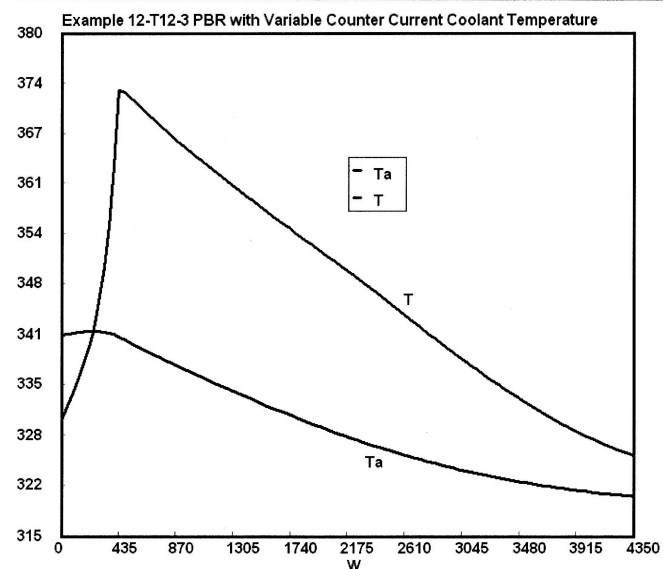
Differential equations

- 1 $d(Ta)/d(W) = Uarho*(T-Ta)/(Mc*Cpmc)*(-1)$
- 2 $d(y)/d(W) = -alpha/2*(T/To)/y$
- 3 $d(T)/d(W) = (Uarho*(Ta-T)+(-ra)*(-Hr))/(Fao*sumcp)$
- 4 $d(X)/d(W) = -ra/Fao$

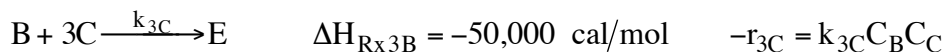
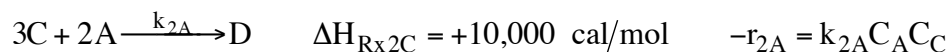
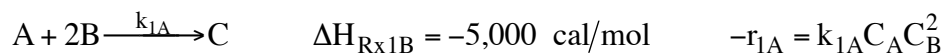
Explicit equations

- 1 alpha = .0002
- 2 To = 330
- 3 Uarho = 0.5
- 4 Mc = 100
- 5 Cpmc = 18
- 6 Hr = -20000
- 7 Fao = 5
- 8 thetaI = 1
- 9 CpI = 40
- 10 CpA = 20
- 11 thetaB = 1
- 12 CpB = 20
- 13 Cto = 0.3
- 14 Ea = 25000
- 15 $Kc = 100*(exp(Hr/1.987*(1/303-1/T)))$
- 16 $ka = .004*exp(Ea/1.987*(1/310-1/T))$
- 17 $yao = 1/(1+thetaB+thetaI)$
- 18 $xe = Kc^{0.5}/(2+Kc^{0.5})$
- 19 $Cao = yao*Cto$
- 20 $sumcp = (thetaI*CpI+CpA+thetaB*CpB)$
- 21 $Ca = Cao*(1-X)*y*To/T$
- 22 $Cb = Cao*(1-X)*y*To/T$

Matches



(20 pts) **13)** The following reactions are taking place in a 2,000 dm³ liquid phase batch reactor under a pressure of 400 psig



The initial temperature is 450 K and the initial concentrations of A, B and C are 1.0, 0.5 and 0.2 mol/dm³ respectively. The coolant flow rate was at it's maximum value so that $T_{a1} = T_{a2} = T_a = 400$ K so that the product the exchange area and overall heat transfer coefficient, UA, is $UA = 100 \text{ cal/s} \cdot \text{K}$.

- (a) What is Q_r at $t = 0$?
 (b) What is Q_s at $t = 0$?
 (c) If $Q_r > Q_s$ at time $t = 0$, and there is no failure of the heat exchange system, is there any possibility that reactor will run away? Explain_____

- (d) What is the initial rate of increase in temperature, (dT/dt) at $t = 0$?

$$\frac{dT}{dt} = \underline{\hspace{2cm}}$$

- (e) Suppose that the ambient temperature T_a is lowered from 400 K to 350 K, what is the initial rate of reactor temperature change?

$$\frac{dT}{dt} = \underline{\hspace{2cm}}$$

- (f) A suggestion was made to add 50 mole of inerts at a temperature of 450 K. Will the addition of the inerts make runaway more likely or less likely? How? Show quantitatively.

Additional information

As a first approximation, assume all heats of reaction are constant ($\Delta C_p \approx 0$)

Specific reaction rates at 450 K are

$$k_{1A} = 1 \times 10^{-3} \left(\text{dm}^3/\text{mol} \right)^2 / \text{s}$$

$$k_{2A} = \frac{1}{3} \times 10^{-3} \left(\text{dm}^3/\text{mol} \right)^2 / \text{s}$$

$$k_{3C} = 0.6 \times 10^{-3} \left(\text{dm}^3/\text{mol} \right)^2 / \text{s}$$

$$C_{P_A} = 10 \text{ cal/mol/K} \quad C_{P_D} = 80 \text{ cal/mol/K}$$

$$C_{P_B} = 10 \text{ cal/mol/K} \quad C_{P_E} = 50 \text{ cal/mol/K}$$

$$C_{P_C} = 50 \text{ cal/mol/K}$$

Solution

Part (a)

$$Q_r = UA(T - T_a) = 100 \frac{\text{cal}}{5 \cdot \text{K}} [450 - 400] \text{K} = 5,000 \frac{\text{cal}}{\text{s}}$$

Part (b)

$$Q_g = V[r_{1B}\Delta H_{R_{X1B}} + r_{2C}\Delta H_{R_{X2C}} + r_{3B}\Delta H_{R_{X3B}}]$$

Initially $T = 350 \text{ K}$

$$\text{Reaction 1:} \quad \frac{r_{1A}}{-1} = \frac{r_{1B}}{-2} = \frac{r_{1C}}{1} \quad r_{1B} = 2r_{1A}$$

$$\text{Reaction 2:} \quad \frac{r_{2A}}{-2} = \frac{r_{2C}}{-3} = \frac{r_{2D}}{1} \quad r_{2C} = \frac{3}{2}r_{2A}$$

$$\text{Reaction 3:} \quad \frac{r_{3B}}{-1} = \frac{r_{3C}}{-3} = \frac{r_{3E}}{1} \quad -r_{3B} = \frac{1}{3}r_{3C}$$

$$Q_g = V\left[2k_{1A}C_A C_B^2\right] \left[-\Delta H_{R_{X1B}}\right] + V\left[\frac{3}{2}k_{2A}C_A C_C\right] \left[-\Delta H_{R_{X2C}}\right] + V\left[\frac{1}{3}k_{3C}C_B C_C\right] \left[-\Delta H_{R_{X3C}}\right]$$

$$\begin{aligned} &= (2,000) \left[\underbrace{(2)(10^{-3})(1)(0.5)^2 5,000}_{5,000} \right] + 2,000 \left[\underbrace{\frac{3}{2} \left(\frac{1}{3} \times 10^{-3} \right) (1)(0.2) [10,000]}_{-2,000} \right] + \\ &+ 2,000 \left[\underbrace{\frac{1}{3} (0.6 \times 10^{-3}) (0.5)(0.2)}_{+2,000} \right] \cdot [50,000] = 5,000 \end{aligned}$$

$$Q_g = 5,000 \text{ cal/s}$$

$$\frac{dT}{dt} = \frac{Q_r - Q_g}{N_{A0}C_{P_A} + N_{B0}C_{P_B} + N_{C0}C_{P_C}} = \frac{5,000 - 5,000}{N_{A0}C_{P_A} + N_{B0}C_{P_B} + N_{C0}C_{P_C}} = 0$$

Part (c)

$$\frac{dT}{dt} = \frac{Q_g - Q_r}{N_A C_{P_A} + N_B C_{P_B} + N_C C_{P_C}}$$

If $Q_r > Q_g$ then the temperature can only decrease causing the specific reaction rates k_i to decrease, hence runaway is unlikely.

Part (d)

$$N_{A0}C_{P_A} = C_{A0}VC_{P_A} = (1)(2,000)(10) = 20,000$$

$$N_{B0}C_{P_B} = C_{B0}VC_{P_B} = (0.5)(2,000)(10) = 10,000$$

$$N_{C0}C_{P_C} = C_{C0}VC_{P_C} = (0.2)(2,000)(50) = 20,000$$

$$\frac{dT}{dt} = \frac{Q_g - Q_r}{50,000}$$

Part (e)

Drop T_a by 50

$$Q_r = UA(T - T_a) = 100(450 - 350) = 10,000$$

$$\frac{dT}{dt} = \frac{5,000 - 10,000}{50,000} = -0.1$$

Part (f)

$$\frac{dT}{dt} = \frac{Q_g - Q_r}{\sum N_i C_{P_i}} = \frac{[r_{1B}V\Delta H_{Rx1B} + r_{2C}V\Delta H_{Rx2C} + r_{3A}V\Delta H_{Rx3A}] - UA(T - T_a)}{N_A C_{P_A} + N_B C_{P_B} + N_C C_{P_C} + N_D C_{P_D} + N_E C_{P_E} + N_{Inerts} C_{P_{Inerts}}}$$

Inerts (N_{Inerts}) will not change Q_g or Q_r , they will only show the rate of temperature increase or decrease.

Blank sheet

Blank sheet