ChE 344
Winter 2011
Final Exam

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) <u>Mole Balances, Chapter 1</u>**

The reaction

$$A + B \rightarrow 2C$$

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 <u>all</u> the mole balances are correct

(a)

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

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

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

(b)

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

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

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

(c)

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

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

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

(d)

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

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

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

(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.

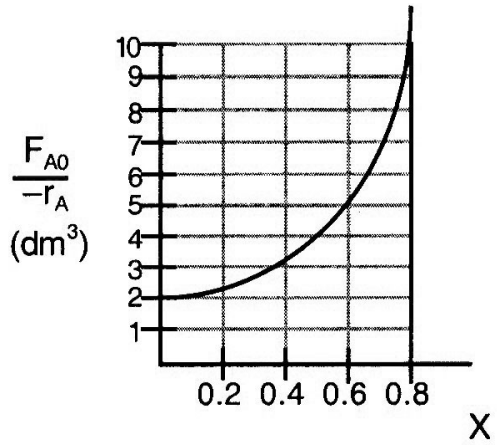
T F CT **(b)** A steady-state CSTR operates at 150°C. The reactor effluent is at the same temperature as the reactor contents. Is the reactor operating isothermally?

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.

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



(1 pt) **(a)** The equilibrium conversion is

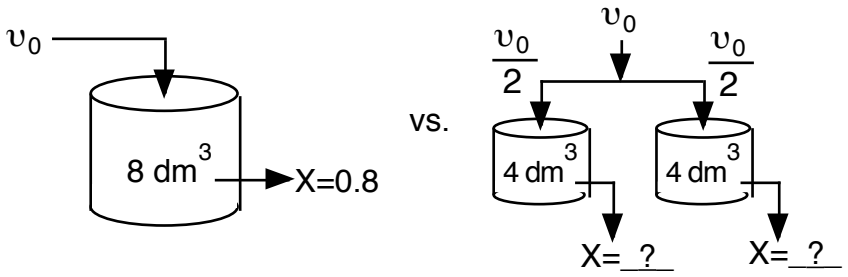
(1) $X_e < 0.6$ (2) $X_e = 0.8$ (3) $X_e > 0.8$ (4) Can't tell from the information given

(1 pt) **(b)** The flow rate to an 8 dm^3 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 dm^3 CSTR is 80%, what would the conversion be if the flow is equally divided into to two CSTRs in parallel with first reactor having a volume of 4 dm^3 each (same total volume).

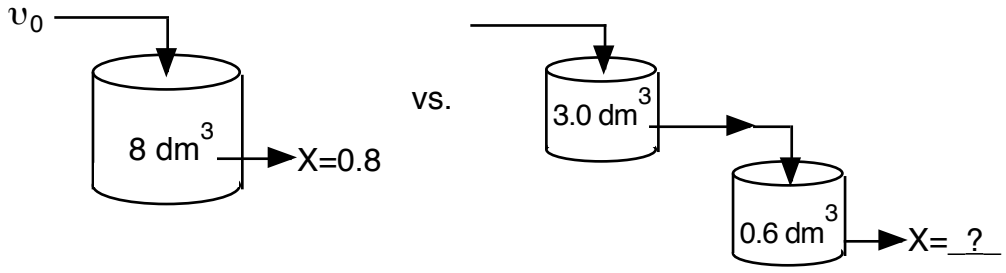


The total reactor volume is constant at 8 dm^3.
The conversion for the two reactors in parallel is

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

Continued

(2 pts) **(d)** If the conversion achieved in a single 8 dm^3 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 dm^3 and the second reactor having a volume of 0.6 dm^3.



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

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

$$2A + B \rightleftarrows C$$

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.

$$-r_A = \_\_\_\_\_$$

(b) The reaction is elementary and reversible

$$-r_A = \_\_\_\_\_$$

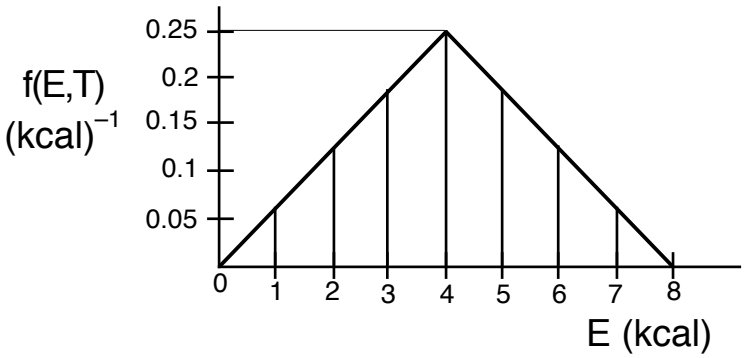
(c) Now consider the case when the reaction is first order in A and first order in B at high concentrations of A and B and is first order in A and second order in B at low concentrations of B. The rate law is

$$-r_A = \_\_\_\_\_$$

(d) What is the rate law for the reaction $CH_3CHO \rightarrow CH_4 + CO$?

$$-r_{CH_3CHO} = \_\_\_\_\_$$

(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?

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

$$2A + B \rightleftarrows C$$

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.

$-r_A =$ _____

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

$$A \underset{\text{cat}}{\overset{\longrightarrow}{\longleftarrow}} B$$

is carried out isothermally at 400K in a PBR where the pressure drop occurs with $\alpha = 0.001$ 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

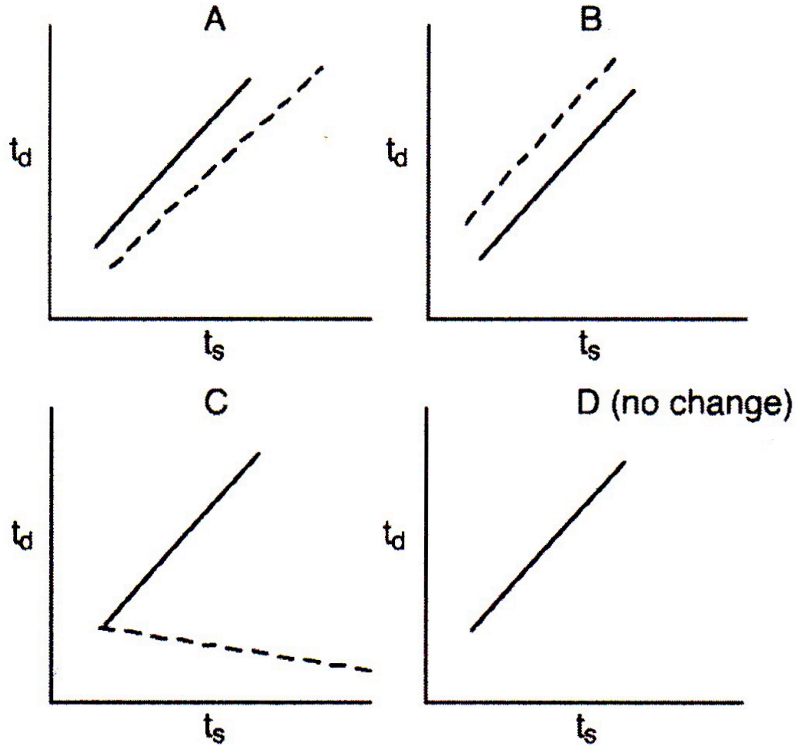
(d) For a fixed mass flow rate $\dot{m}$, if the particle size is increased the equilibrium conversion X_e will

(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

(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_s, and the down time, t_d, would change? The solid line represents the case without inerts?



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

$$H_2 + C_2H_4 \xrightarrow[cat]{} C_2H_6$$

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

$$-r'_E = \frac{kP_EP_H}{1 + K_EP_E}$$

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

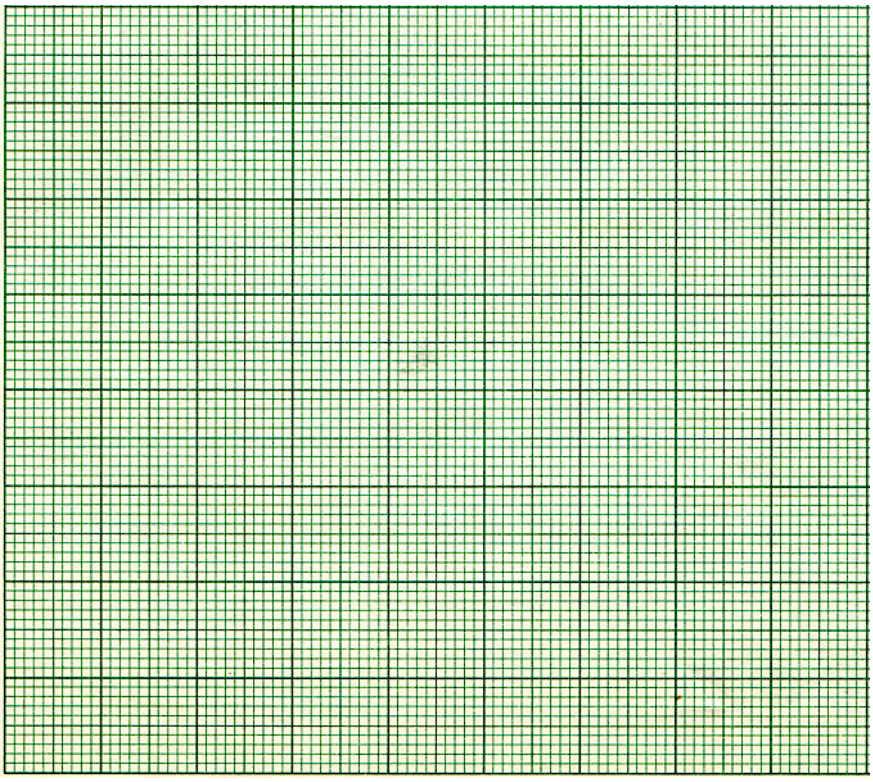
(10 pts) **10) P7-10**$_B$ **Study Problem.** In order to study the photochemical decay of aqueous bromine in bright sunlight, a small quantity of liquid bromine was dissolved in water contained in a glass battery jar and placed in direct sunlight. The following data were obtained at 25°C:

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

(a) 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.)

(b) 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 dm^3) 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.)

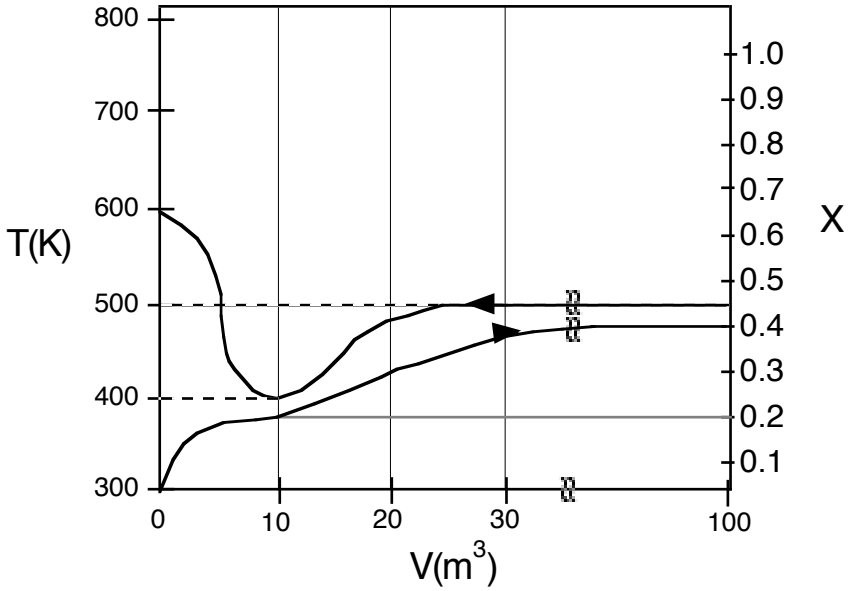


This problem is continued from Problem (6) on MidTerm Exam II (Complete parts (e) and (f))

(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 cal/(sec • m^3 • K) with T_a being constant. The gas-phase, reversible reaction is

$$2\,A \rightleftarrows B + C$$

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



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

K_e (500) = ____0.11____ (From MidTerm Exam II solution)

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

$-r_A$ = __2 mol/m^3•s__ (From MidTerm Exam II solution)

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

K_e (400) = _____

(8 pt) **(d)** What is the specific reaction rate at V = 10 m^3?

k = _____

(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.

$$\frac{\dot{Q}}{F_{A0}} = \_\_\_\_\_$$

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

$$A + B \rightleftarrows 2C$$

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

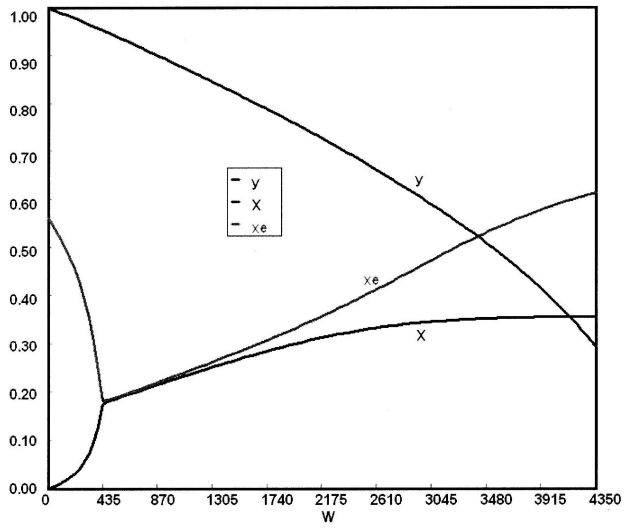


Figure 2

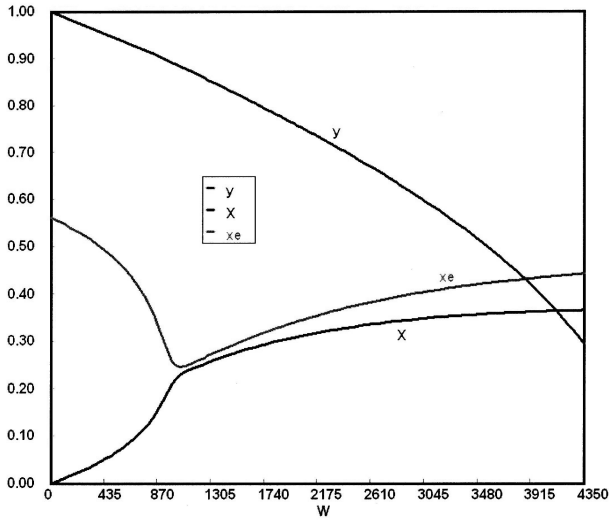


Figure 3

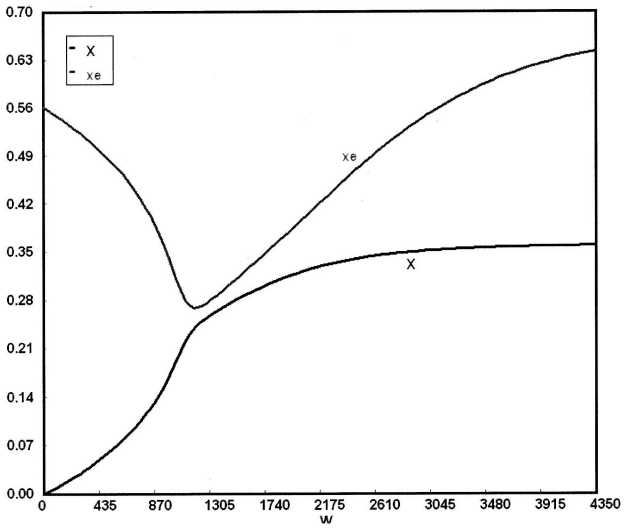


Figure 4

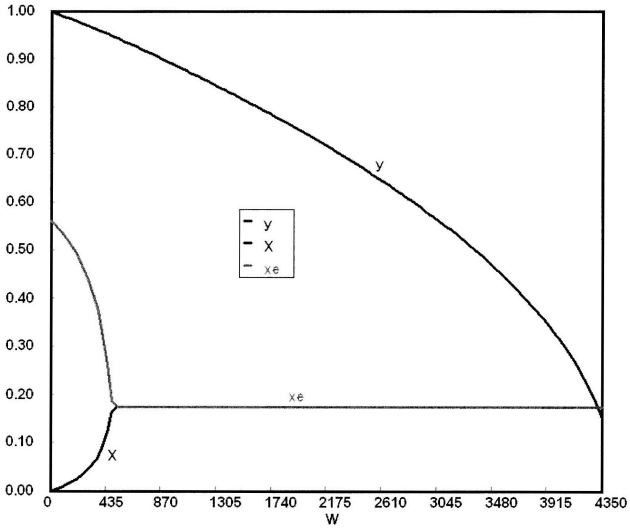


Figure A

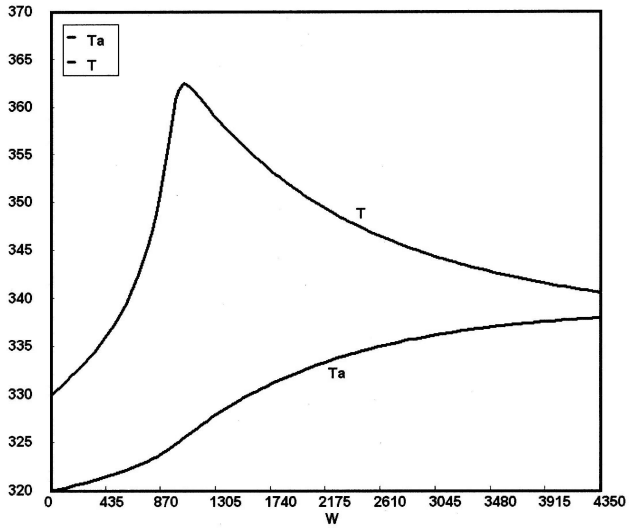


Figure B

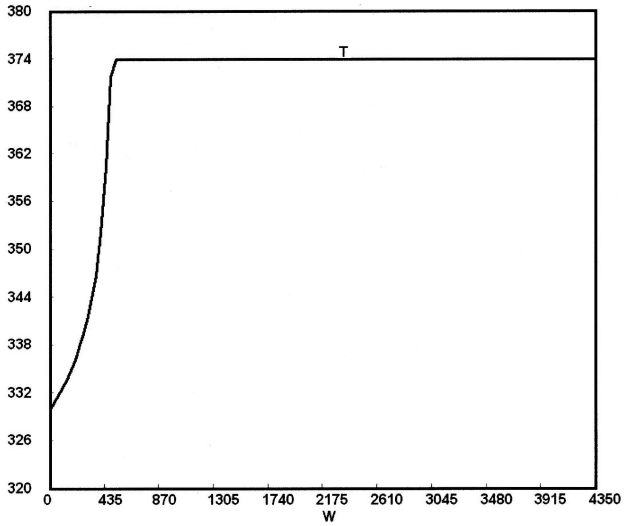


Figure C

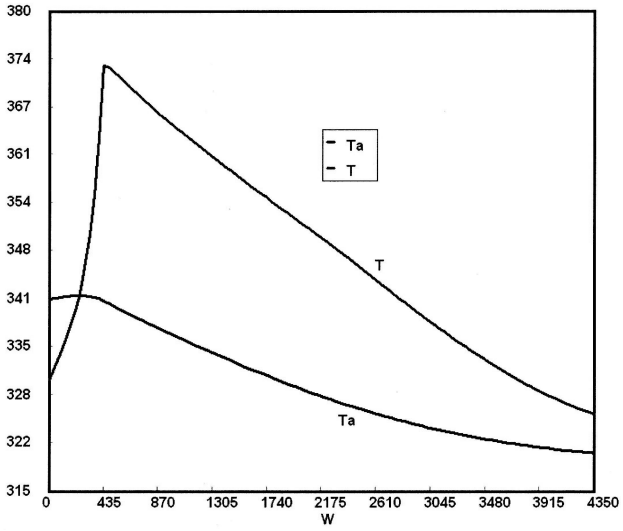
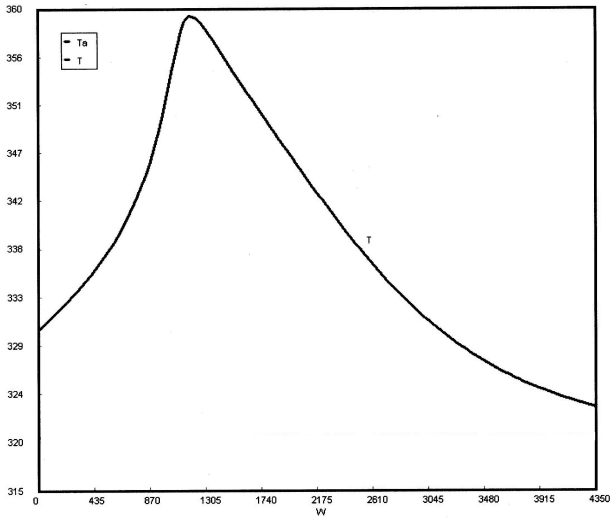


Figure D



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

(20 pts) **13)** The following reactions are taking place in a 2,000 dm^3 liquid phase batch reactor under a pressure of 400 psig

$$A + 2B \xrightarrow{k_{1A}} C \qquad \Delta H_{Rx1B} = -5{,}000 \text{ cal/mol} \qquad -r_{1A} = k_{1A} C_A C_B^2$$

$$3C + 2A \xrightarrow{k_{2A}} D \qquad \Delta H_{Rx2C} = +10{,}000 \text{ cal/mol} \qquad -r_{2A} = k_{2A} C_A C_C$$

$$B + 3C \xrightarrow{k_{3C}} E \qquad \Delta H_{Rx3B} = -50{,}000 \text{ cal/mol} \qquad -r_{3C} = k_{3C} C_B C_C$$

The initial temperture is 450 K and the initial concentrations of A, B and C are 1.0, 0.5 and 0.2 mol/dm^3 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 cal/s•K.

(a) What is Q_r at t = 0?

(b) What is Q_g at t = 0?

(c) If $Q_r > Q_g$ 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?

$\frac{dT}{dt} =$ _____

(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?

$\frac{dT}{dt} =$ _____

(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 $(\Delta C_P \cong 0)$

Specific reaction rates at 450 K are

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

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

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

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

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

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