ChE 344
Winter 2013
Mid Term Exam II + Solution
Tuesday, April 9, 2013

Open Course Textbook Only
Closed everything else (i.e., Notes, In-Class Problems and Home Problems

Name_____

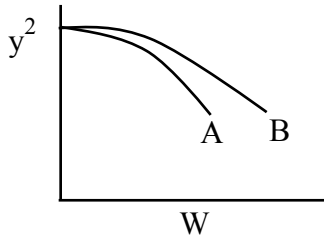
Honor Code (Please sign in the space provided below)

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

_____
(Signature)

1)	____/ 5 pts
2)	____/ 5 pts
3)	____/ 5 pts
4)	____/ 5 pts
5)	____/10 pts
6)	____/10 pts
7)	____/10 pts
8)	____/15 pts
9)	____/15 pts
10)	____/20 pts
Total	____/100 pts

(5 pts) 1) (a) The following plot gives the square pressure drop parameter, y, as a function of catalyst weight, W for an adiabatic endothermic reaction and for an exothermic reaction. The flow is turbulent. The flow properties and catalyst properties are the same in both cases. Assume the absolute magnitude of the heats of reaction and heat capacities are identical as are the feed conditions. Which curve corresponds to the endothemic reaction? _____



Explain:

_____

_____

(b) The Hercules explosion (P13-3_B) could have been prevented by continually increasing the ratio of water to ammonia chloride in the feed to shut the reactor down. Circle the correct answer

True False Insufficent informtion to tell

(c) For an endothermic adiabatic reaction, the addition of inerts up to a certain amount will increase the conversion for a first order reaction when the reactant flow rates, F_{A0}, is held constant

True False Insufficent informtion to tell

(d) For an endothermic adiabatic reaction, the addition of inerts after a certain amount has been added will decrease the converison for a first order reaction when the reactant flow rates, F_{A0}, is held constant

True False Insufficent informtion to tell

(e) In PFR counter-current heat exchange, as one moves down the reactor away from the reactant entrance the ambient temperature will decrease once it falls below the reactor temperature

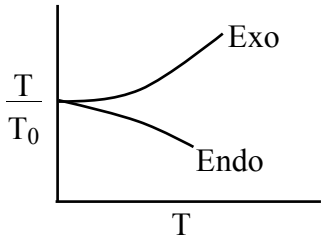
True False Insufficent informtion to tell

Solution

(a) Answer B

$$\frac{dy}{dW} = -\frac{\alpha}{2y}\frac{T}{T_0} \;>\; \frac{dy^2}{dW} = -\overbrace{\alpha\frac{T}{T_0}}^{\text{Slope}}$$

$\alpha =$



$$\Rightarrow \qquad \alpha\frac{T_{exo}}{T_0} \;>\; \alpha\frac{T_{endo}}{T_0}$$

(b) True

(c) True

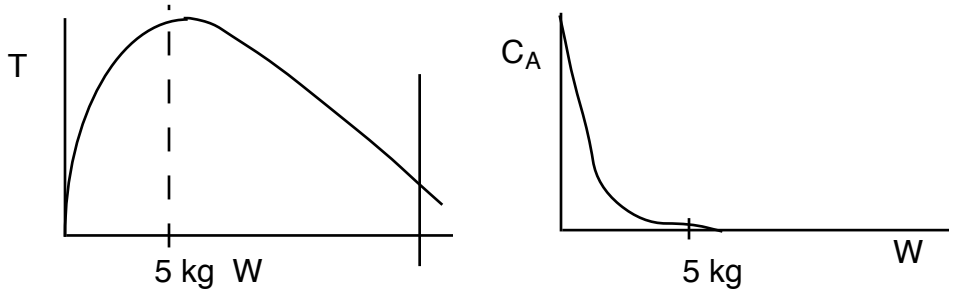
(d) True

(e) True

(5 pts) 2) The elementary series reaction

$$A \longrightarrow B \longrightarrow C$$

is carried out in a packed bed reactor. The following profiles were obtained.



Circle the correct true (T) or False (F) answer for this system

T F (a) The above profiles could represent a system where the reactions are carried out adiabatically.

T F (b) The above profiles could represent a system where there is a heat exchanger attached to the system.

T F (c) The above profiles could represent an adiabatic system where both of the reactions are endothermic.

T F (d) The above profiles could represent an adiabatic system where only one of the reactions is exothermic

T F (e) Assuming the activation energies are virtually the same for both reactions, the above profiles could represent an adiabatic system where increasing the feed temperature will increase the concentration of B in the exit stream.

Solution

(a) True. Possible if A → B is exothermic and B → C is endothermic.

(b) True. Possible when either A → B is exothermic or B → C is endothermic or both.

(c) False. Not possible because the temperature is initially increasing.

(d) True. Same as (a)

(e) False. Increasing the feed temperature will increase the rate of reaction of both A → B and B → C. Hence, exit concentration of B could decrease.

(5 pts) 3) Monsanto Explosion: (Circle the correct answer)

(a) The addition of inerts will decrease the time between the time the heat exchanger came back on line and the time of exposion.

True False Insufficent informtion to tell

(b) If inerts had been added to the reactor it is possible that the explosion would not have occurred.

True False Insufficent informtion to tell

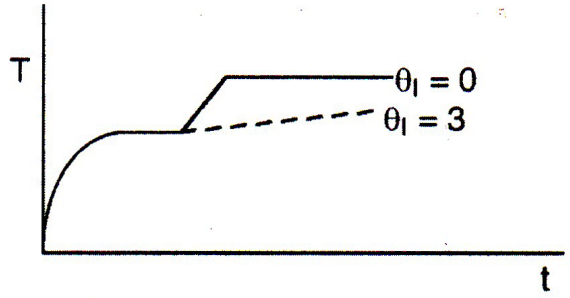
Solution

(a) False
(b) True

Explanation:

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

We see the rate of temperature increase, 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.



(5 pts) 4) (***Reactor selection and operating conditions***) For each of the following sets of reactions, describe your reactor system and conditions to maximize the selectivity to D. Make sketches where necessary to support your choices. The rates are in (mol/dm^3•s), and concentrations are in (mol/dm^3).

(a) (1) $A + B \rightarrow D$ $\quad -r_{1A} = 10\exp(-8{,}000\ K/T)C_A C_B$

(2) $A + B \rightarrow U$ $\quad -r_{2A} = 100\exp(-1{,}000\ K/T)C_A^{1/2} C_B^{3/2}$

Solution

P8-9 (a)

Reactor selection

$A + B \rightarrow D$ $\quad r_D = -r_{1A}$ $\quad r_{1A} = 10\exp(-8000K/T)C_A C_B$

$A + B \rightarrow U$ $\quad r_U = -r_{2A}$ $\quad r_{2A} = 100\exp(-1000K/T)C_A^{1/2} C_B^{3/2}$

$$S_{DU} = \frac{r_D}{r_U} = \frac{10\exp(-8000\text{K}/\text{T})C_A C_B}{100\exp(-1000\text{K}/\text{T})C_A^{1/2}C_B^{3/2}} = \frac{\exp(-8000\text{K}/\text{T})C_A^{1/2}}{10\exp(-1000\text{K}/\text{T})C_B^{1/2}}$$

At T = 300K

$k_1 = 2.62 \times 10^{-11}$ & $k_2 = 3.57$ $\quad S_{D/U} = \dfrac{7.35\times10^{-12}C_A^{1/2}}{C_B^{1/2}}$

At T = 1000K

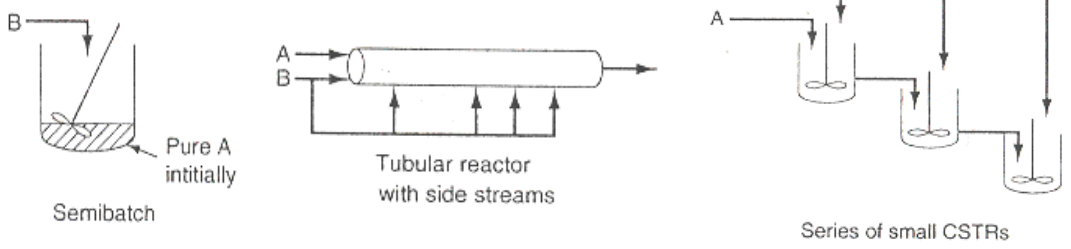
$k_1 = 3.35 \times 10^{-3}$ & $k_2 = 36.78$ $\quad S_{D/U} = \dfrac{9.2\times10^{-5}C_A^{1/2}}{C_B^{1/2}}$

(2 pts) Hence In order to maximize S_{DU}, use higher concentrations of A and lower concentrations of B. This can be achieved using:

1) A semibatch reactor in which B is fed slowly into a large amount of A

2) A tubular reactor with side streams of B continually fed into the reactor

(2 pts) 3) A series of small CSTR's with A fed only to the first reactor and small amounts of B fed to each reactor.

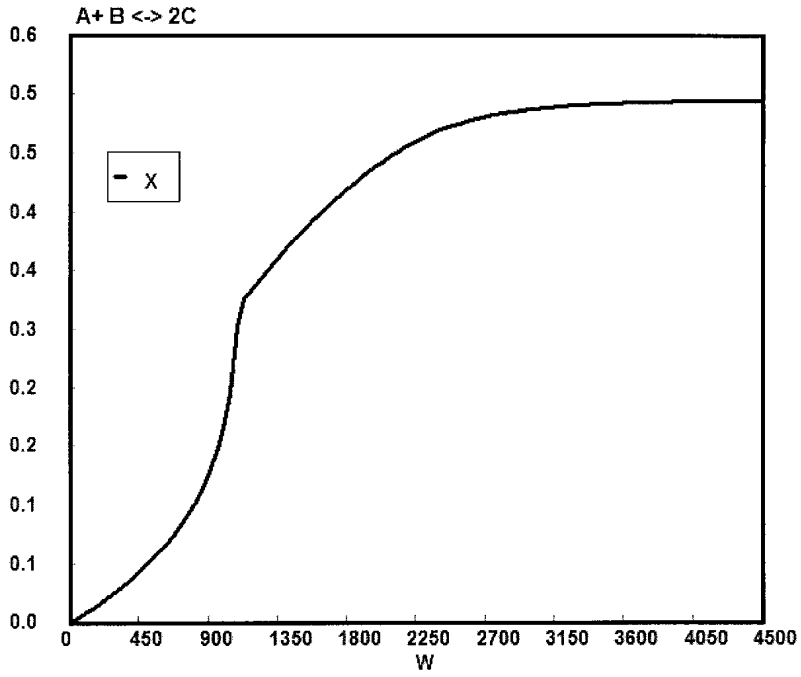


(1 pt) Also, since $E_D > E_U$, so the specific reaction rate for D increases much more rapidly with temperature. Consequently, the reaction system should be operated at highest possible temperature to maximize S_{DU}. Note that the selectivity is extremely low, and the only way to increase it is to keep $\left(\dfrac{C_B}{C_A}\right)^{1/2} < 10^{-6}$ and add B drop by drop.

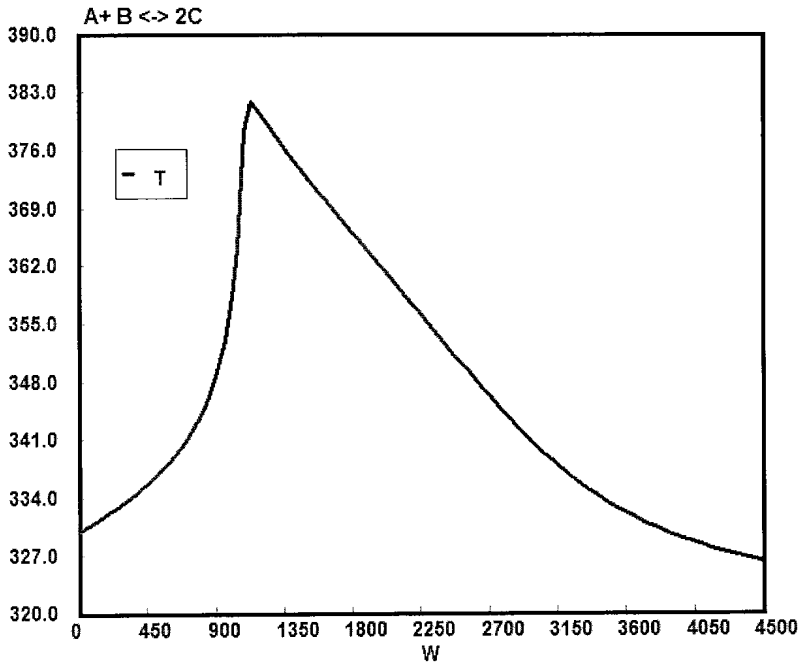
(10 pts) 5) The curves below show the conversion or temperature profiles for the Problem 12-3_B base case. Sketch the requested profiles for the parameters identified. Be sure to label which curve is the maximum and which is the minimum.

(2 pt) (a) Sketch the conversion for the maximum flow rate, i.e., 8 mol/min, and for the minimum flow rate, i.e., 1 mol/min

Flow Rate: Base case shown below for $F_{A0} = 5$

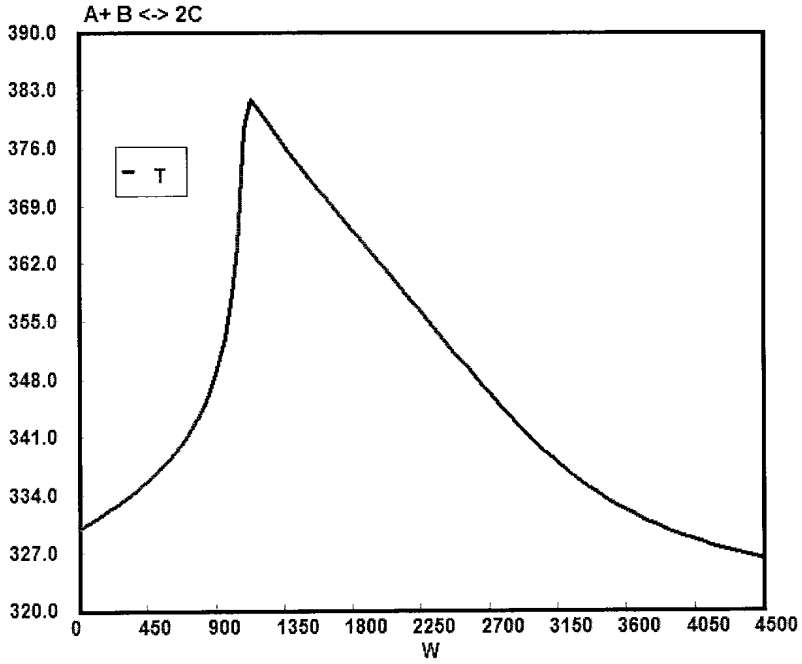


(2 pt) (b) Inert, Θ_I: Sketch the temperature profiles for $\Theta_I = 0.5$ and $\Theta_I = 4$. The base case shown below is for $\Theta_I = 1$

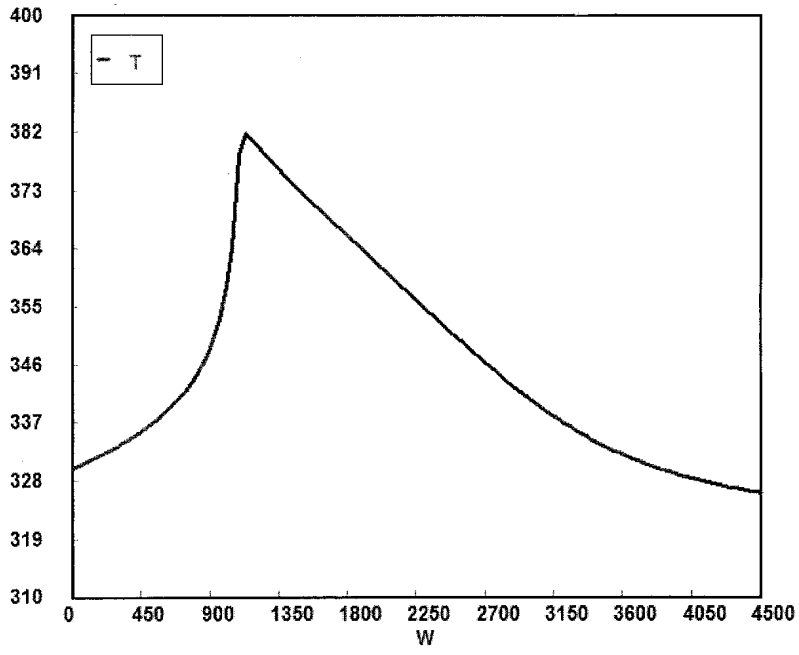


5) (continued)

(2 pt) (c) Sketch the temperature profiles for $\frac{Ua}{\rho_b} = 0.1\ \text{cal/kg} \bullet \text{s} \bullet \text{K}$ and for $\frac{Ua}{\rho_b} = 0.8 \text{cal/kg} \bullet \text{s} \bullet \text{K}$. The base case profile $\left(\frac{Ua}{\rho_b} = 0.5 \text{cal/kg} \bullet \text{s} \bullet \text{K}\right)$ is shown below

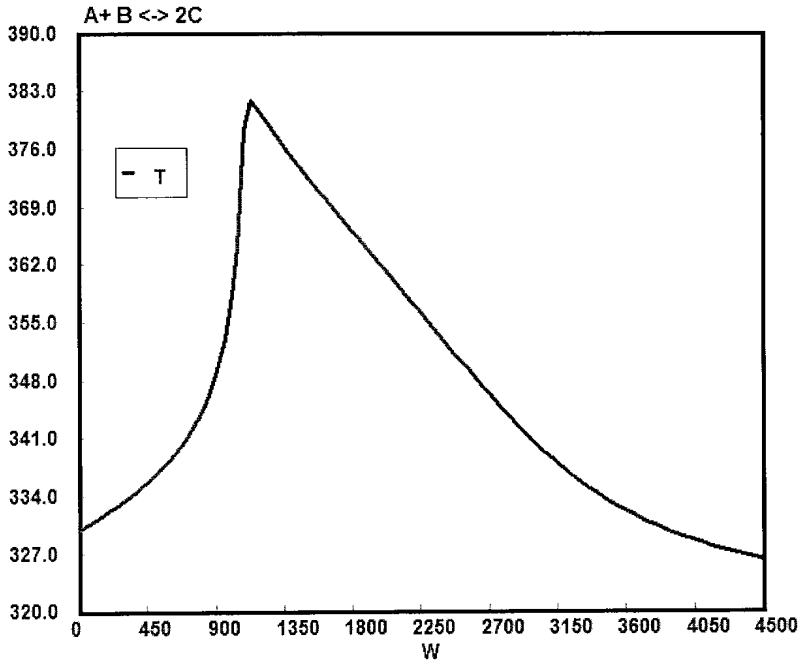


(2 pt) (d) Sketch the temperature profiles for an inlet temperature $T_0 = 310$ and for $T_0 = 350$ on the base case profile shown below for $T_0 = 330K$



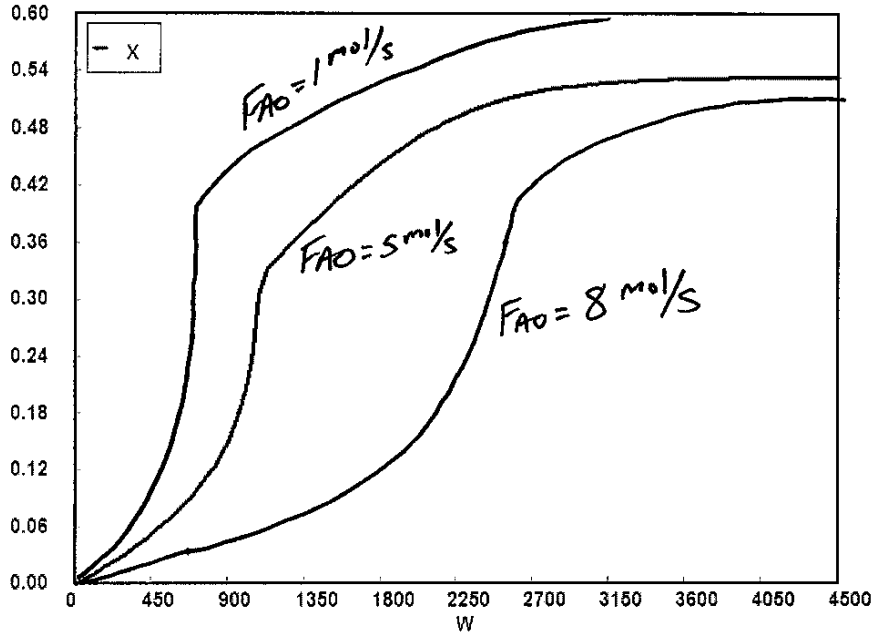
5) (continued)

(2 pt) (e) Sketch the temperature profiles for constant coolant temperatures of T_a = 300K and for T_a = 340K on the base case profile shown below for T_a = 320K

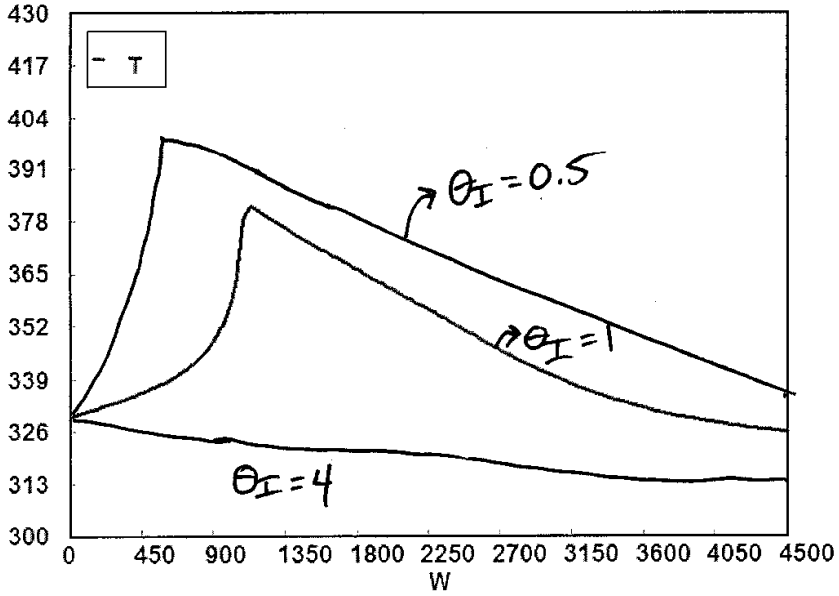


Solution

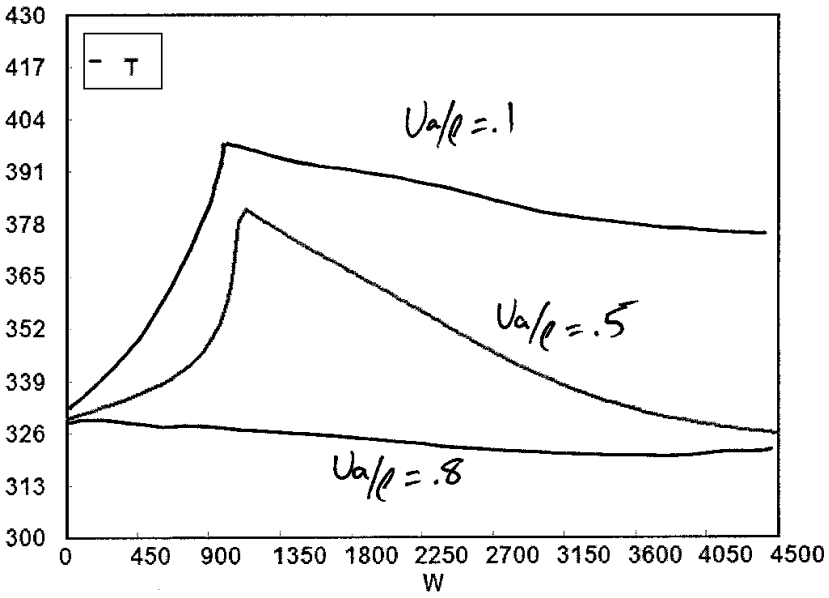
a) MIN : F_{A0} = 1 mol/s
BASE : F_{A0} = 5 mol/s
MAX : F_{A0} = 8 mol/s



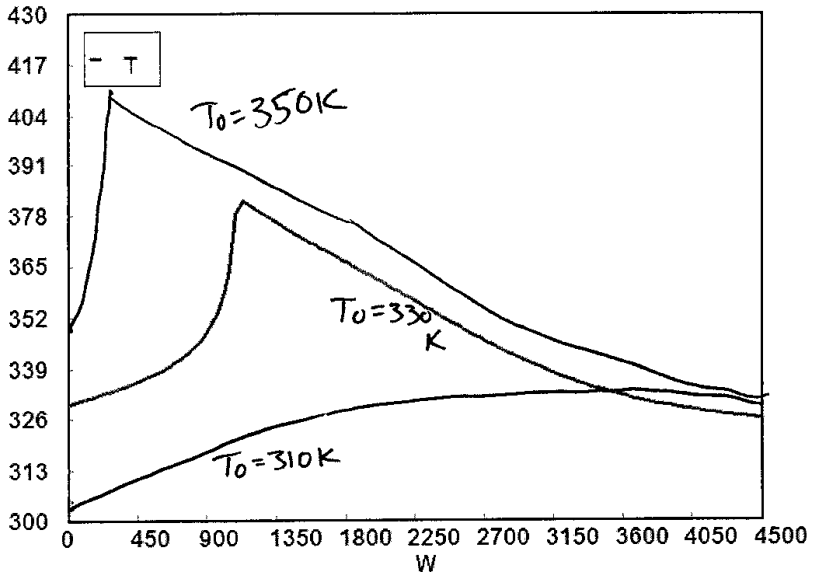
b) MIN: $\theta_I = 0.5$
BASE: $\theta_I = 1$
MAX: $\theta_I = 4$



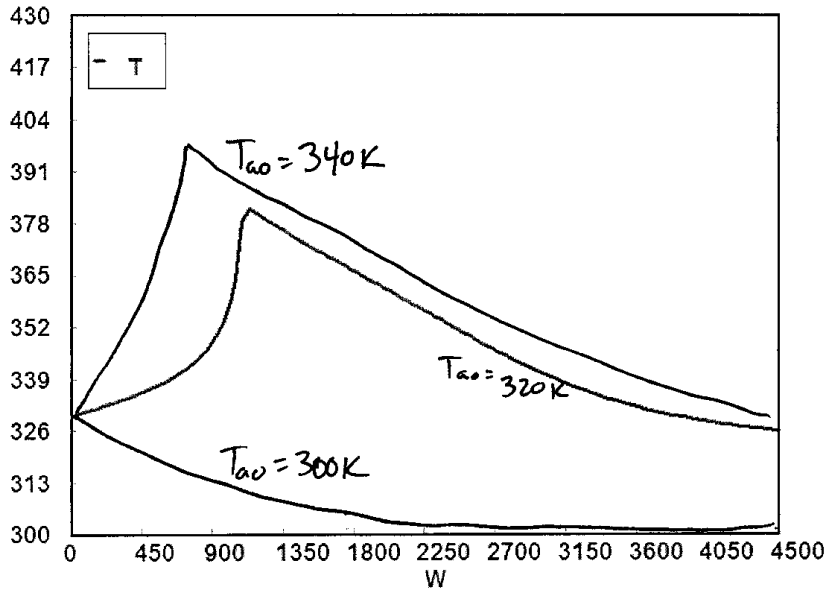
c) MIN: $U_a/\ell = .1$
BASE $U_a/\ell = .5$
MAX $U_a/\ell = .8$



d) MIN: $T_o = 310$ K
BASE: $T_o = 330$ K
MAX: $T_o = 350$ K



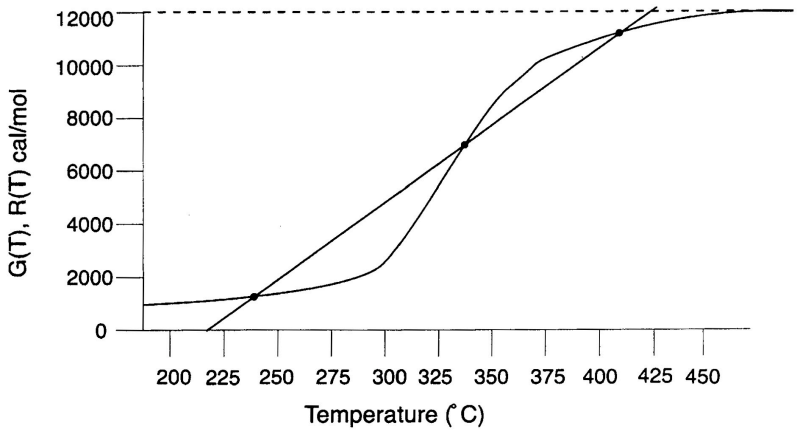
e) MIN: $T_{ao} = 300$K
BASE: $T_{ao} = 320$K
MAX: $T_{ao} = 340$K



(10 pts) 6) The irreversible reaction

$$A + B \longrightarrow C + D$$

is carried out adiabatically in a CSTR. The "heat generated" [G(T)] and the "heat removed" [R(T)] curves are shown below



(a) What is the ΔH_{Rx} of the reaction?

ΔH_{Rx} = _____ cal/mol

(b) What are the inlet temperatures for ignition and extinction?

Ignition = _____ °C

Extinction = _____ °C

(c) What are all the corresponding temperatures in the reactor corresponding to the inlet ignition and extinction temperature?

Ignition

T = _____°C, _____°C

Extinction

T = _____°C, _____°C

(d) What are the upper and lower conversions corresponding to at the ignition and extinction temperatures?

X (Ignition) = _____, _____

X (Extinction) = _____, _____

(e) In the above figure, what is the conversion at the unstable steady state?

X = _____

Solution

Assume Adiabatic

(a) –12,000 cal/mol

(b) Ignition = 260°C
Extinction = 190°C

(c) Ignition, T = 300°C, 475°C
Extinction, T = 215°C, 375°C

(d) X (Ignition) = 0.281

X (Extinction) = 0.86

(e) $X = \frac{G}{\Delta H_{Rx}} = \frac{7{,}000}{12{,}000} = 0.583$

(10 pts) 7) The reaction

$$A + B \rightleftarrows 2C$$

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

Figure 1

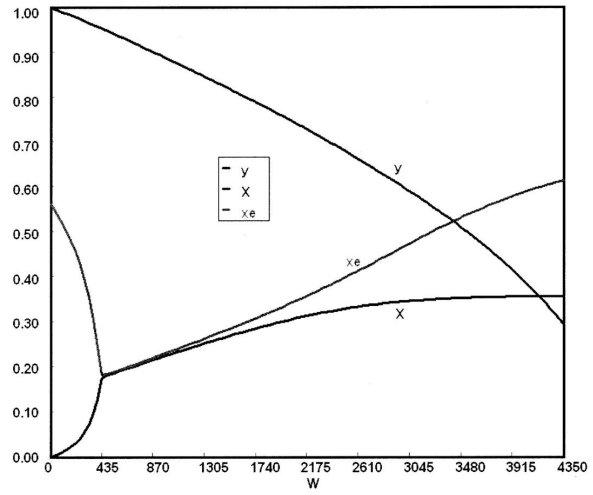


Figure 2

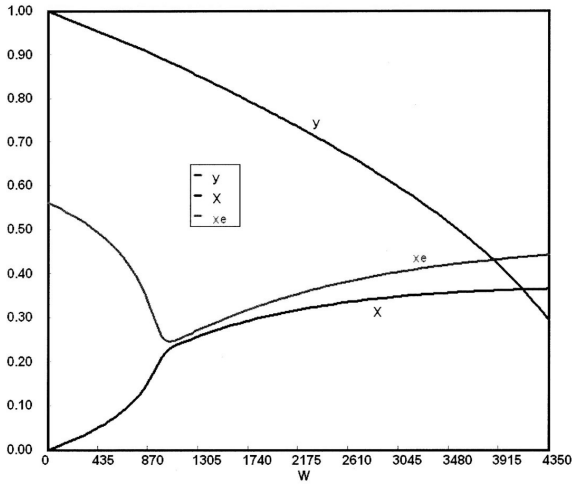


Figure 3

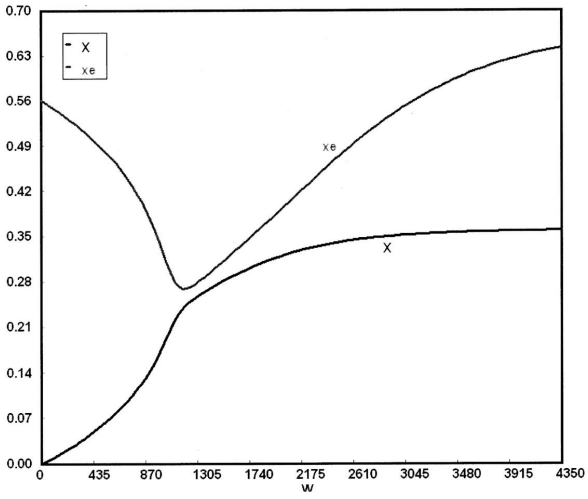
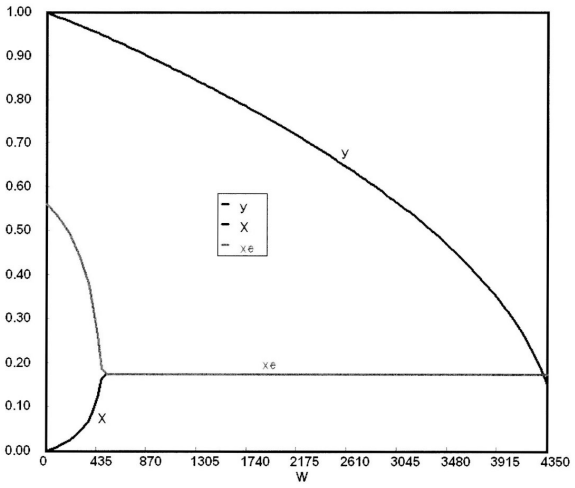


Figure 4



7) (continued)

Figure A

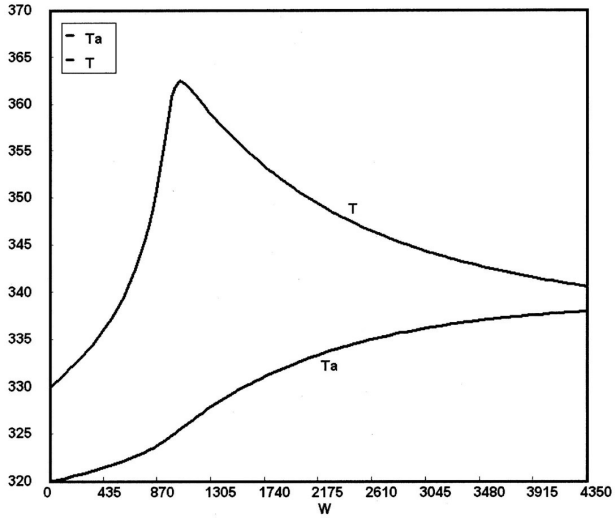


Figure B

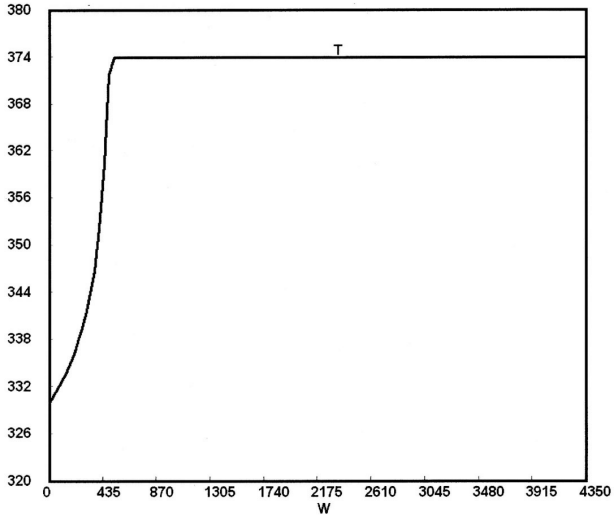


Figure C

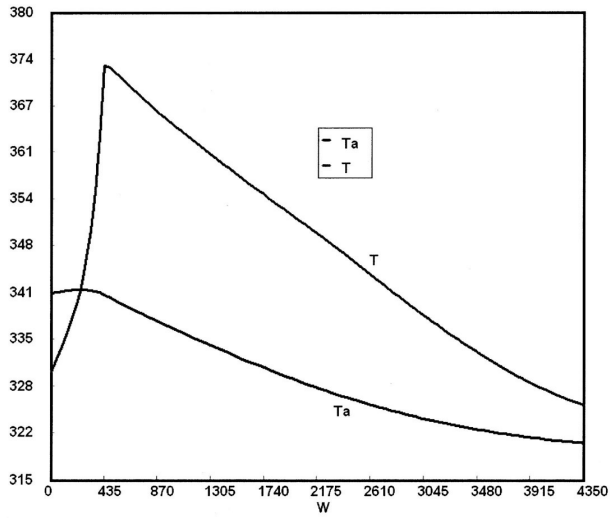
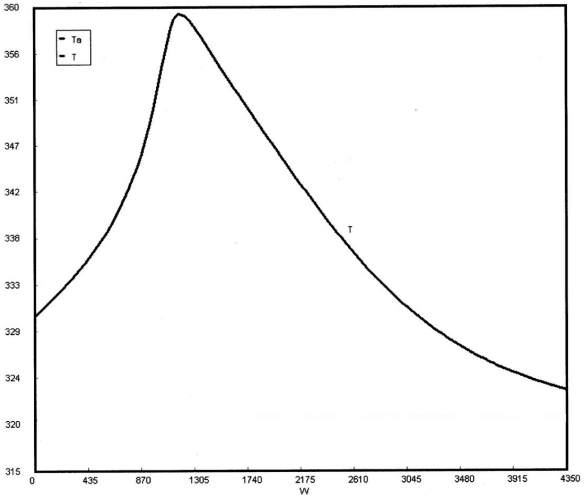


Figure D



(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_

(a) Adiabatic

POLYMATH Report

Ordinary Differential Equations

Calculated values of DEQ variables

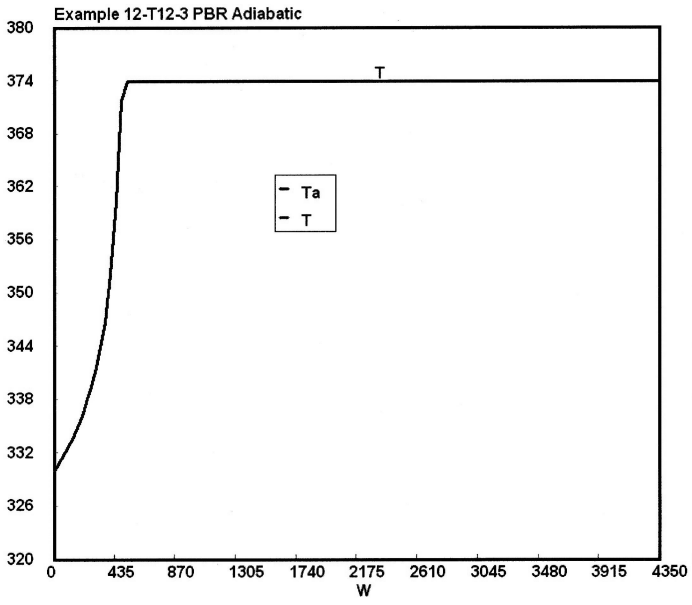
	Variable	Initial value	Final value
1	alpha	0.0002	0.0002
2	Ca	0.1	0.0111573
3	Cao	0.1	0.1
4	Cb	0.1	0.0111573
5	Cc	0	0.0047662
6	CpA	20.	20.
7	CpB	20.	20.
8	CpI	40.	40.
9	Cpmc	18.	18.
10	Cto	0.3	0.3
11	Ea	2.5E+04	2.5E+04
12	Fao	5.	5.
13	Hr	-2.0E+04	-2.0E+04
14	ka	0.046809	4.152669
15	Kc	6.601082	0.1824807
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

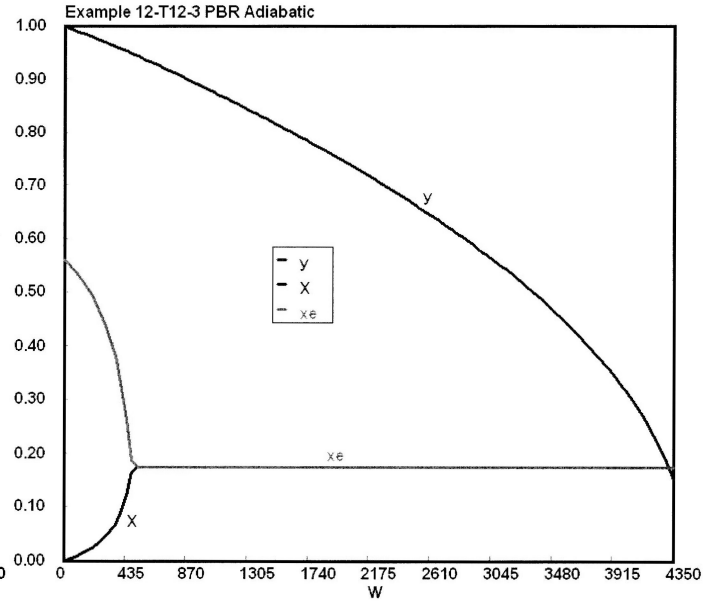
Differential equations

1 d(Ta)/d(W) = Uarho*(T-Ta)/(Mc*Cpmc)
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*0
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
23 Cc = Cao*2*X*y*To/T
24 ra = -ka*(Ca*Cb-Cc^2/Kc)





(b) Constant T_a 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

1 d(Ta)/d(W) = Uarho*(T-Ta)/(Mc*Cpmc)*0 ← **Constant T_a**

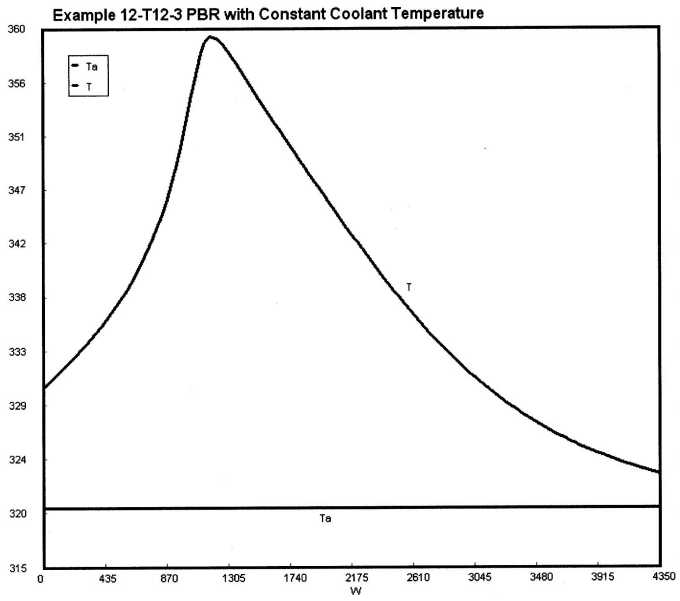
2 d(y)/d(W) = -alpha/2*(T/To)/y

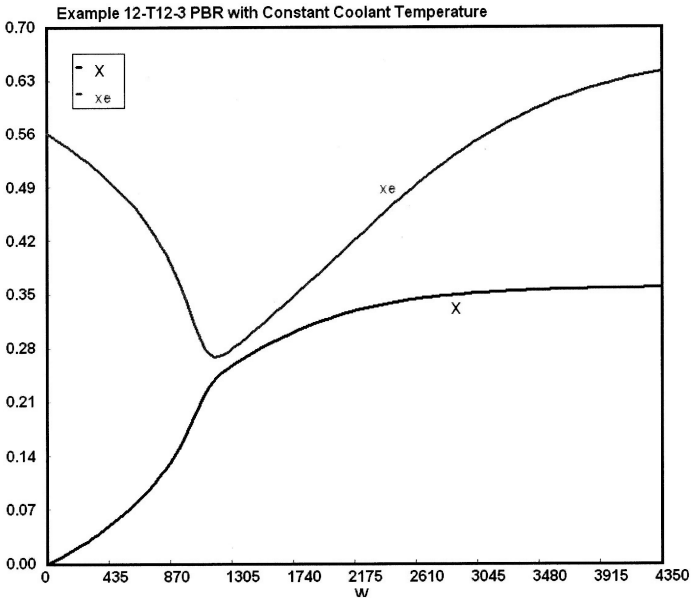
3 d(T)/d(W) = (Uarho*(Ta-T)+(-ra)*(-Hr))/(Fao*sumcp)

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
23 Cc = Cao*2*X*y*To/T
24 ra = -ka*(Ca*Cb-Cc^2/Kc)





(c) Variable T_a Co-Current Heat Exchange

POLYMATH Report
Ordinary Differential Equations

Calculated values of DEQ variables

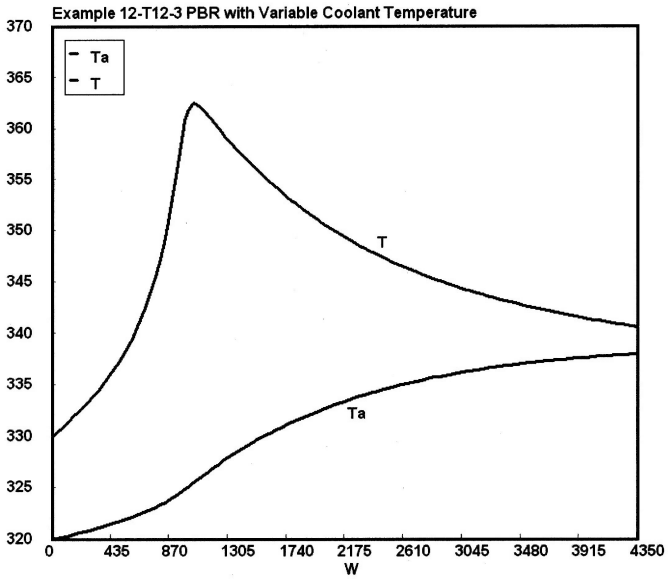
	Variable	Initial value	Maximal value	Final value
1	alpha	0.0002	0.0002	0.0002
2	Ca	0.1	0.1	0.0181239
3	Cao	0.1	0.1	0.1
4	Cb	0.1	0.1	0.0181239
5	Cc	0	0.0443144	0.0210077
6	CpA	20.	20.	20.
7	CpB	20.	20.	20.
8	CpI	40.	40.	40.
9	Cpmc	18.	18.	18.
10	Cto	0.3	0.3	0.3
11	Ea	2.5E+04	2.5E+04	2.5E+04
12	Fao	5.	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

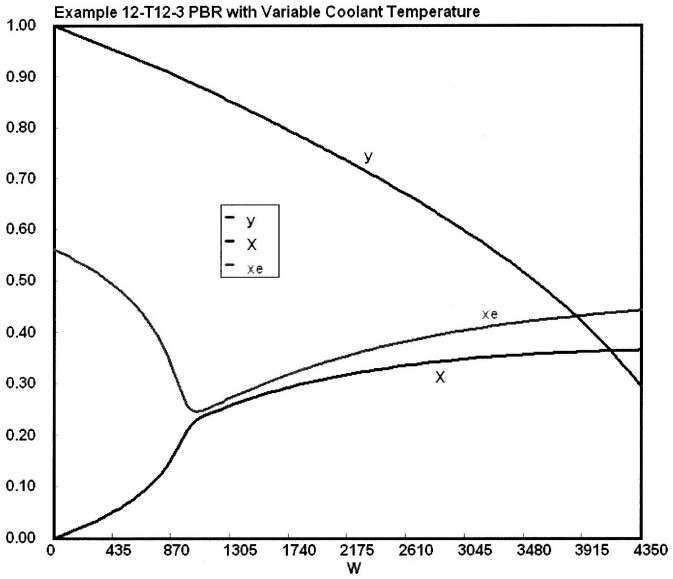
Differential equations

1 d(Ta)/d(W) = Uarho*(T-Ta)/(Mc*Cpmc)
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
23 Cc = Cao*2*X*y*To/T
24 ra = -ka*(Ca*Cb-Cc^2/Kc)





(d) Variable T_a 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

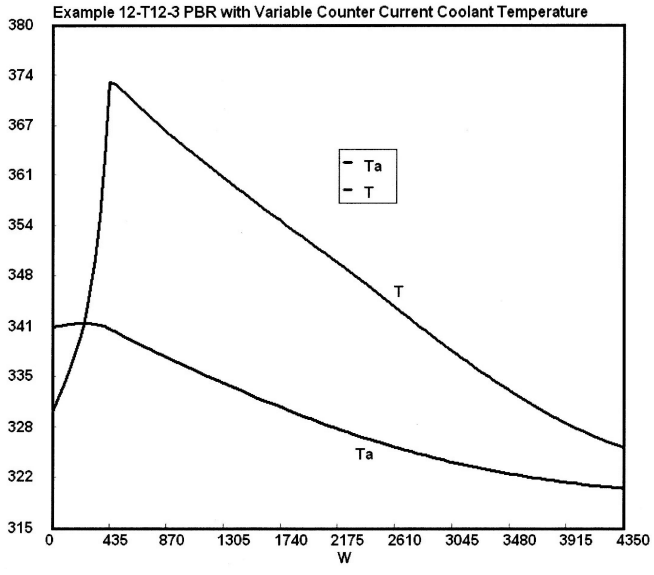
Differential equations

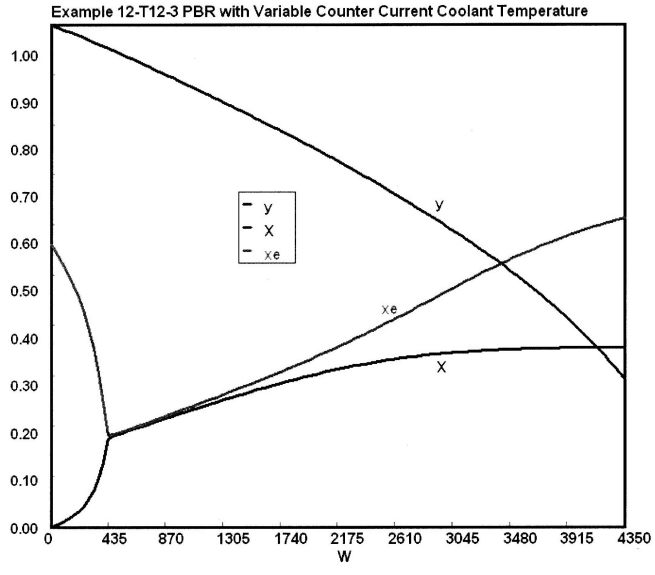
1 d(Ta)/d(W) = Uarho*(T-Ta)/(Mc*Cpmc)*(-1)
2 d(y)/d(W) = -alpha/2*(T/To)/y
3 d(T)/d(W) = (Uarho*(Ta-T)+(-ra)*(-Hr))/(Fao*sumcp)
4 d(X)/d(W) = -ra/Fao

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

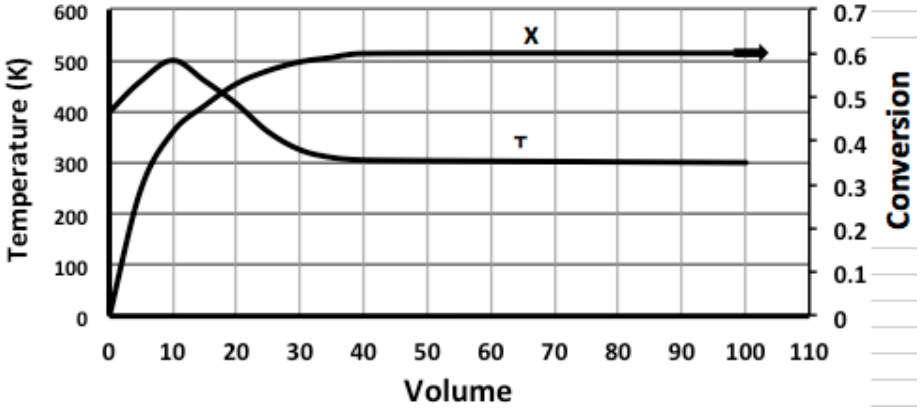




(15 pts) 8) The temperature and conversion in a very long (i.e., virtually infinite) PFR are shown below as a function of the reactor volume. The reactor is surrounded by a jacket for heat transfer. The value of Ua is 100 cal/(sec • m^3 • K) with T_a being constant. The elementary gas-phase, reversible reaction is

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

and pure A is fed to the reactor at 0.05 mol/dm^3. The absolute value of the heat of reaction is 20,000 cal/mol of A at 500K, and the heat capacities of A, B, and C are 10, 10, and 5 cal/mol/K, respectively.



(7 pt) (a) What is the rate of disappearance of A at V = 10 m^3?

$-r_A$ = _____ mol/m^3•s

(7 pt) (b) What is the total amount of heat removed (in cal/mol) from the entire reactor per mol of A fed in cal/mol?

Q = _____ cal/mol A

(1 pt) (c) What is the equilibrium conversion at 300 K

X_e = _____

Solution

(a) $-r_A$ = _____

At maximum

$Q_g = Q_r$

$\dot{Q}_r = Ua\,(T - T_a) = 100\,(500 - 300) = 20{,}000$ cal/s•m^3

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

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

$$-r_A = \frac{20{,}000\,\dfrac{\text{cal}}{\text{s}\bullet\text{m}^3}}{20{,}000\,\dfrac{\text{cal}}{\text{mol}}} = 1\,\frac{\text{mol}}{\text{m}^3\bullet\text{s}}$$

(b) $\dot{Q} - F_{A0}\sum\Theta_i C_{P_i}\left(T - T_0\right) - \left[\Delta H^\circ_{Rx} + \Delta C_P\left(T - T_a\right)\right]F_{A0}X = 0$ Eqn. (8-28)

Per Mole A

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

$$A \underset{\leftarrow}{\overset{\rightarrow}{}} \frac{B}{2} + C$$

$$\Delta C_P = C_{P_C} + \frac{C_{P_B}}{2} - C_{P_A} = 5 + \frac{10}{2} - 10 = 0$$

$$= 0$$

$$\frac{\dot{Q}}{F_{A0}} = 10\left(300 - 400\right) + \left[-20{,}000\right]\left[0.6\right] = -1000 - 12{,}000 = -13{,}000\,\frac{\text{cal}}{\text{mol}}$$

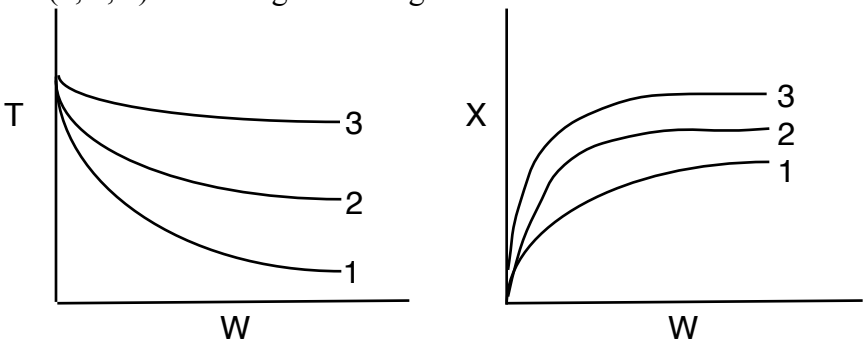
(c) At ∞ reactor length $X_e = 0.6$

(15 pts) 9) Circle the correct answer

(3 pt) (a) The reaction A → D is carried out adiabatically. The heat capacities of A and D are approximately equal at 20 J/mol-K. When a conversion of 50% is achieved in a PFR, the outlet temperature is 50 K higher than the inlet. What the heat of reaction?

A) $\Delta H_{Rx} = 0.5$ kJ/mol
B) $\Delta H_{Rx} = -0.5$ kJ/mol
C) $\Delta H_{Rx} = 2$ kJ/mol
D) $\Delta H_{Rx} = -2$ kJ/mol

(4 pt) (b) The conversion and temperature are shown below as a function of catalyst weight for three sets (1, 2, 3) of cooling or heating rates



Circle the correct answer.

A) One of the curves could correspond to an exothermic irreversible reaction with too high of a cooling rate.

True False Insufficent informtion to tell

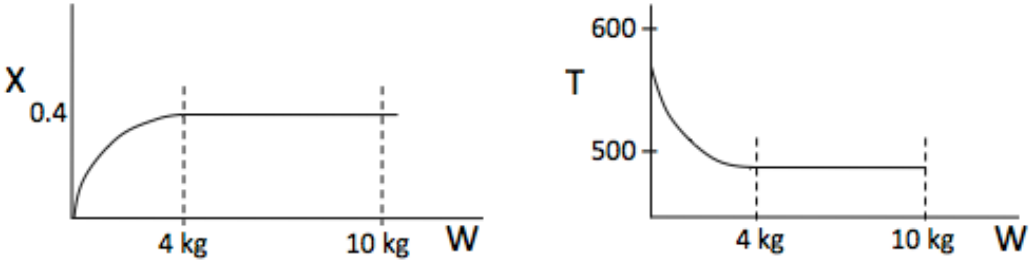
B) One of the curves could correspond to an endothermic reversible reaction with too high of a heating rate.

True False Insufficent informtion to tell

C) The reaction could be second order exothermic and carried out adiabatically.

True False Insufficent informtion to tell

(4 pt) (c) The elementary isomerization of A to B was carried out in a packed bed reactor. The following profiles were obtained

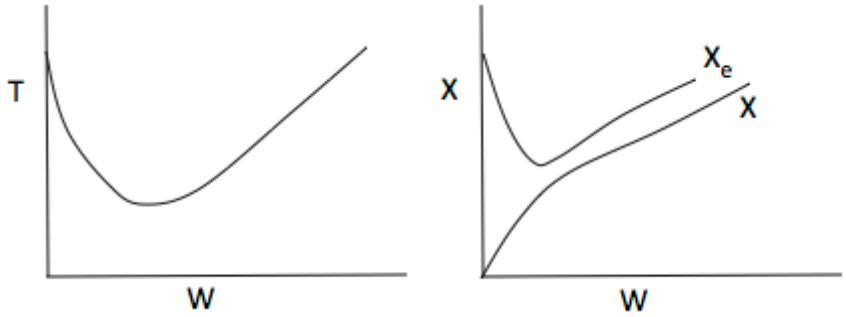


If the total entering volumetric remains constant the addition of inerts to the feed stream will most likely

A) Increase conversion.
B) Decrease conversion.
C) Have no effect.
D) Insufficient information to tell

9) (continued)

(4 pt) (d)



Which of the following statements are true?

A) The above reaction could be adiabatic.
B) The above reaction could be exothermic with constant cooling temperature.
C) The above reaction could be endothermic with constant heating temperature.
D) The above reaction could be second order.

Solution

(a) D) $\Delta H_{Rx} = -2$ kJ/mol

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

$(-\Delta H_{Rx})\ 0.5 = (20)(50)$

(b) A) True. k(T) smaller ∴ X smaller

$$\frac{dX}{dV} = \frac{k}{v_0}(1-X)$$

$v_0 = \text{constant}$

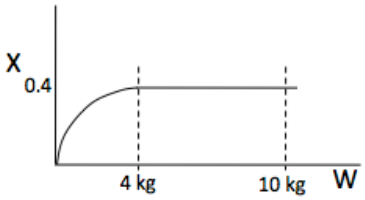
B) False. For endothermic reactions conversion always increases with heating rate up to isothermal conditions.

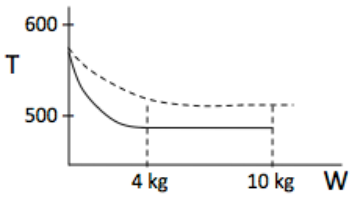
C) False. For exothermic adiabatic reaction T always increases with increasing W.

(c) A) Increase conversion.

$$\frac{dX}{dV} = \frac{k}{v_0}(1-X)$$

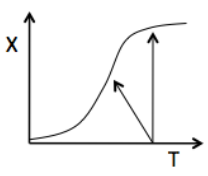
$$-\Delta H_{Rx} = \frac{C_{P_A}(T-T_0)}{X} = \frac{(20)(50)}{0.5} = \frac{2\text{kJ}}{\text{mol}},\ \Delta H_{Rx} = -\frac{2\text{kJ}}{\text{mol}}$$





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

If it is an adiabatic system, then it has to be endothermic, because the temperature decreases and the heat of reaction is positive. Increasing inerts increases the temperature, increasing k, increasing the rate and hence increasing conversion.



(d) Answer: C and D

A) The above reaction could be adiabatic. False.
X_e could not increase if adiabatic.

B) The above reaction could be exothermic with constant cooling temperature. False.
T would increase then decrease follow slope temperature curve.

C) The above reaction could be endothermic with constant heating temperature. True.

D) The above reaction could be second order. True.

(20 pts) 10) The following elementary reactions are to be carried out in a PFR with a heat exchange with constant T_a

$$2A + B \rightarrow C \qquad \Delta H_{Rx1B} = -10 \frac{kJ}{mol\ B}$$

$$A \rightarrow D \qquad \Delta H_{Rx2A} = +10 \frac{kJ}{mol\ A}$$

$$B + 2C \rightarrow E \qquad \Delta H_{Rx3C} = -20 \frac{kJ}{mol\ C}$$

The reactants all enter at 400 K. Only A and B enter the reactor. The entering concentration of A and B are 3 molar and 1 molar at a volumetric flow rate of 10 dm^3/s

Additional information

$Ua = 100\ \ J/dm^3/s/K$

$k_{1A}(400\ \ K) = 1\left(\frac{dm^3}{mol}\right)^2 \Big/ s$

$k_{2A}(400\ \ K) = 0.5\ \ s^{-1}$

$k_{3B}(400\ \ K) = 2\left(\frac{dm^3}{mol}\right)^2 \Big/ s$

$C_{P_A} = 10\ J/mol/K$

$C_{P_B} = 20\ J/mol/K$

$C_{P_C} = 40\ J/mol/K$

$C_{P_D} = 20\ J/mol/K$

$C_{P_E} = 100\ J/mol/K$

(15 pt) (a) What coolant temperature is necessary such that at the reactor entrance, i.e., V = 0, that $\frac{dT}{dV} = 0$?

T_a = _____K

(5 pt) (b) Repeat part (a) when an inert stream with a molar flow rate of 20 mol/s with C_{P_I} = 100 J/mol/s is added to the feed stream.

T_a = _____K

Solution

(a) $$\frac{dT}{dV} = \frac{r_{1B}\Delta H_{Rx1B} + r_{2A}\Delta H_{Rx2B} + r_{3C}\Delta H_{Rx3C} - Ua(T - T_a)}{F_A C_{P_A} + F_B C_{P_B} + F_C C_{P_C} + F_D C_{P_D} + F_E C_{P_E}}$$

at V = 0, T = T_0 = 400 K for $\frac{dT}{dV} = 0$

$$T_a = T - \left[\frac{r_{1B}\Delta H_{Rx1B} + r_{2A}\Delta H_{Rx2A} + r_{3C}\Delta H_{Rx3C}}{Ua}\right]$$

$$-r_{1A} = k_{1A} C_A^2 C_B$$

$$-r_{2A} = k_{2A} C_A$$

$$-r_{3B} = k_{3B} C_B C_C^2$$

(1)

$$\frac{r_{1B}}{1} = \frac{r_{1A}}{2}$$

$$\Delta H_{Rx1B} r_{1B} = \Delta H_{Rx1B} \frac{r_{1A}}{2} = (-10{,}000)\left(-\frac{1}{2} k_{1A} C_{A0}^2 C_{B0}\right)$$

$$= (5{,}000)(1)(3)^2(1) = 45{,}000$$

(2)

$$\Delta H_{Rx2A} r_{2A} = (-\Delta H_{Rx2A})(-r_{2A})$$

$$= (-10{,}000) k_{2A} C_{A0} = (-10{,}000)(0.5)(3)$$

$$= -15{,}000$$

(3)

$$\Delta H_{Rx3C} r_{3C}$$

$$\frac{r_{3B}}{1} = \frac{r_{3C}}{2}$$

$$\Delta H_{Rx3C} r_{3C} = \Delta H_{Rx3C} 2 r_{3B} = (-20{,}000)\left(-2 k_{3B} C_{B0} C_{C0}^{\ 2}\right) = 0$$

$$T_a = 400 - \left[\frac{45{,}000 - 15{,}000}{Ua}\right] = 400 - \frac{30{,}000}{100}$$

$$\boxed{T_a = 100 \text{ K}}$$

(b) No change, $\frac{dT}{dV} = 0$

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