

ChE 344

Fall 2014

Mid Term Exam II

Wednesday, November 19, 2014

*Open Book – Closed Notes (but one 3x5 note card),
Closed Computer, Web, Home Problems and In-class Problems*

Name _____

Honor Code:

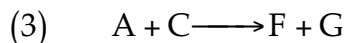
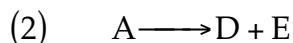
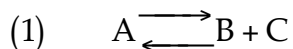
I have neither given nor received unauthorized aid on this examination, nor have I concealed any violations of the Honor Code.

(Sign at the end of exam period)

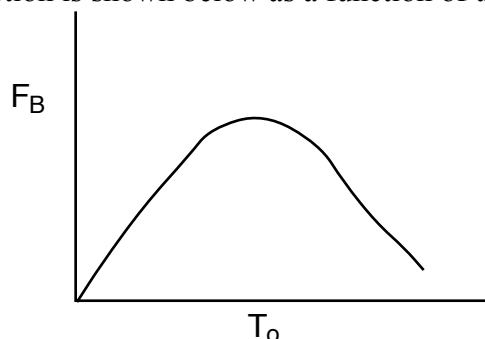
Point Totals

1) ____/ 5 pts
2) ____/10 pts
3) ____/10 pts
4) ____/15 pts
5) ____/15 pts
6) ____/20 pts
7) ____/25 pts
Total ____/100 pts

(5 pts) 1) The reactions



are carried out in a packed bed reactor where B is the desired product. The flow rate of species B exiting the reaction is shown below as a function of the entering temperature, T_o



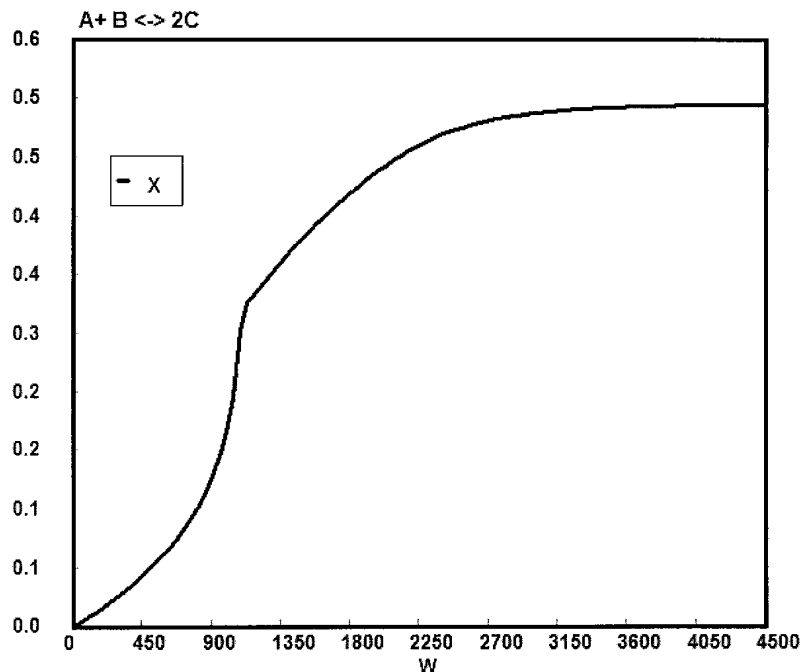
Circle the correct answer, true (T), False (F) or (CT) Can't tell from the information given.

- | | | | |
|---|---|----|--|
| T | F | CT | a) The above figure could represent an adiabatic system where the reaction 1 is adiabatic exothermic and reversible. |
| T | F | CT | b) The above figure could represent an adiabatic system where the reaction 1 is endothermic and reversible. |
| T | F | CT | c) The above figure could represent an adiabatic system where all reactions are endothermic. |
| T | F | CT | d) The above figure could represent a system where the reactions 1 and 3 are endothermic and reaction 2 is exothermic. |
| T | F | CT | e) The above figure could represent a system where the reactions 1 and 2 are endothermic and reaction 3 is exothermic. |

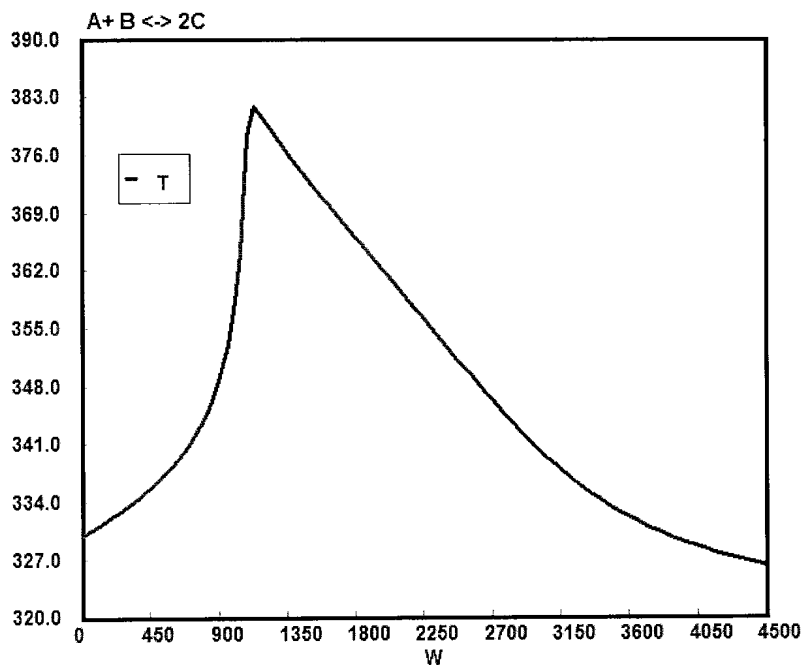
(10 pts) 2) The curves below show the conversion or temperature profiles for the Problem 12-3_B base case. Sketch the requested profiles for the parameters identified. Be sure to label which curve is the maximum and which is the minimum.

(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 $F_{A0} = 5$



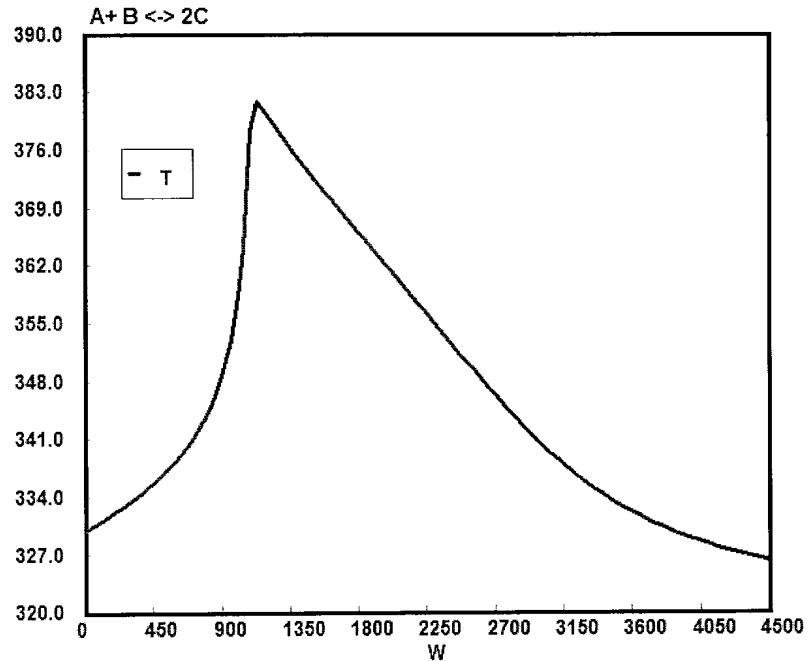
(2 pt) (b) Inert, Θ_I : Sketch the temperature profiles for $\Theta_I = 0.5$ and $\Theta_I = 4$. The base case shown below is for $\Theta_I = 1$



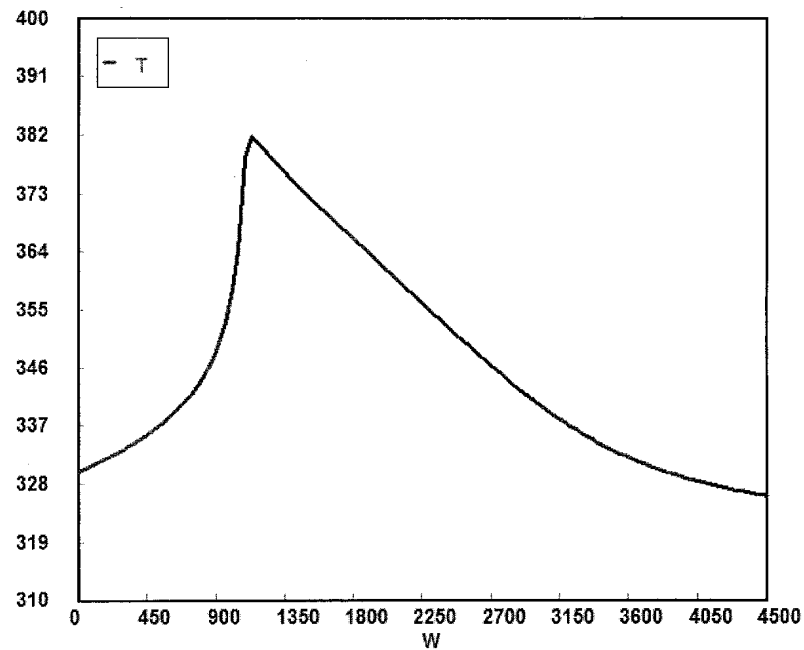
2) (continued)

(2 pt) (c) Sketch the temperature profiles for $\frac{U_a}{\rho_b} = 0.1 \text{ cal/kg} \cdot \text{s} \cdot \text{K}$ and for

$\frac{U_a}{\rho_b} = 0.8 \text{ cal/kg} \cdot \text{s} \cdot \text{K}$. The base case profile $\left(\frac{U_a}{\rho_b} = 0.5 \text{ cal/kg} \cdot \text{s} \cdot \text{K} \right)$ is shown below

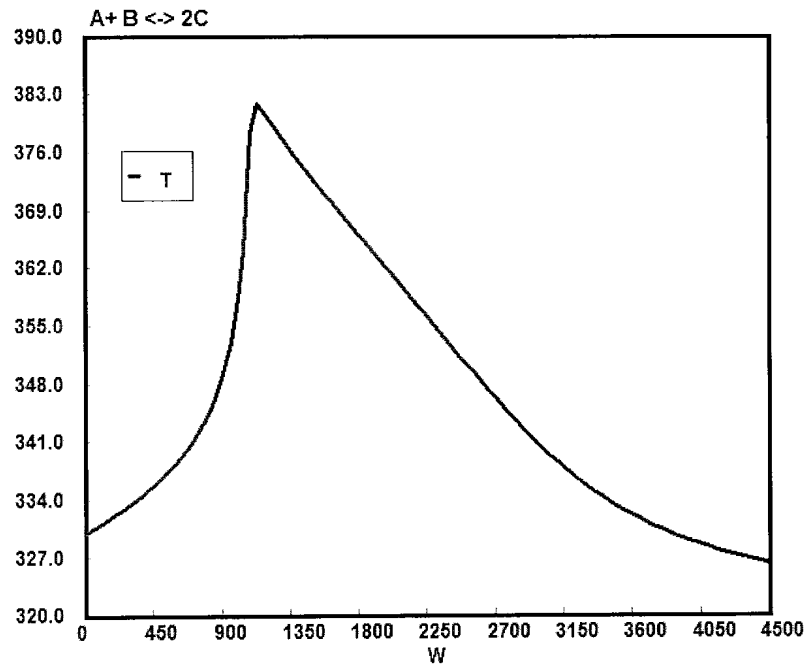


(2 pt) (d) Sketch the temperature profiles for an inlet temperature $T_0 = 310$ and for $T_0 = 350$ on the base case profile shown below for $T_0 = 330\text{K}$

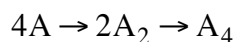


2) (continued)

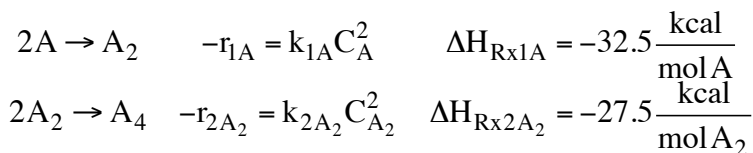
- (2 pt) (e) Sketch the temperature profiles for constant coolant temperatures of $T_a = 300\text{K}$ and for $T_a = 340\text{K}$ on the base case profile shown below for $T_a = 320\text{K}$



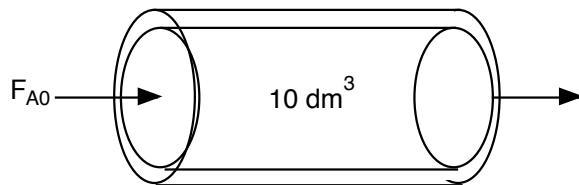
(10 pts) 3) **What's wrong with this solution?** The liquid phase dimer-quadmer series addition reaction



can be written as

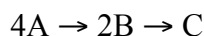


and is carried out in a 10 dm³ PFR.



The mass flow rate through the heat exchanger surrounding the reactor is sufficiently large that the temperature of the coolant in the exchanger is constant at $T_a = 315\text{K}$ and the entering temperature T_0 is 300K. Pure A is fed to the reactor at a volumetric flow rate of 50 dm³/s and a concentration of 2 mol/dm³.

[Hint: to avoid any confusion in the subscripts let $B = A_2$, $C = A_4$.]



Plot F_A , F_B , F_C , T , Q_g and Q_r as a function of reactor volume V .

Additional Information

$$k_{1A} = 0.6 \frac{\text{dm}^3}{\text{mol s}} \text{ at } 300 \text{ K with } E_1 = 4,000 \frac{\text{cal}}{\text{mol}}$$

$$k_{2A_2} = 0.35 \frac{\text{dm}^3}{\text{mol} \cdot \text{s}} \text{ at } 320 \text{ K with } E_2 = 5,000 \frac{\text{cal}}{\text{mol}}$$

$$C_{PA} = 25 \frac{\text{cal}}{\text{mol A K}}, C_{PA_2} = 50 \frac{\text{cal}}{\text{mol A}_2 \text{ K}}, C_{PA_4} = 100 \frac{\text{cal}}{\text{mol A}_4 \text{ K}}$$

$$Ua = 1,000 \frac{\text{cal}}{\text{dm}^3 \text{ s K}}$$

What 5 things (lines of code) are wrong with the solution? See next page.

	Line Number	Is	Should be
1			
2			
3			
4			
5			

3) (continued)

POLYMATH Report Ordinary Differential Equations

Calculated values of DEQ variables

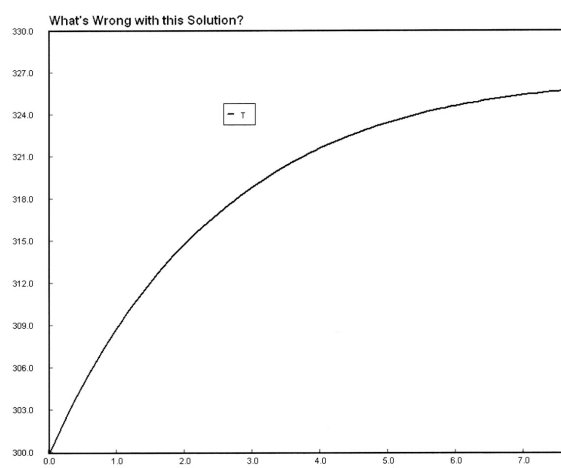
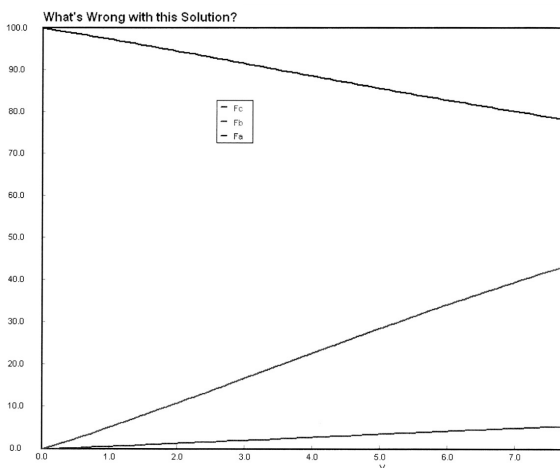
	Variable	Initial value	Minimal value	Maximal value	Final value
1	Ca	2.	1.459847	2.	1.459847
2	Cb	0	0	1.080307	1.080307
3	Cpa	25.	25.	25.	25.
4	Cpb	50.	50.	50.	50.
5	Cpc	100.	100.	100.	100.
6	DH1a	-3.25E+04	-3.25E+04	-3.25E+04	-3.25E+04
7	DH2b	-2.75E+04	-2.75E+04	-2.75E+04	-2.75E+04
8	E1	4000.	4000.	4000.	4000.
9	E2	5000.	5000.	5000.	5000.
10	Fa	100.	72.99233	100.	72.99233
11	Fb	0	0	54.01534	54.01534
12	Fc	0	0	6.751918	6.751918
13	k1	0.6	0.6	0.6	0.6
14	k1a	0.6	0.6	1.026949	1.026864
15	k2	0.35	0.35	0.35	0.35
16	k2b	0.35	0.35	0.6851962	0.6851254
17	Qg	1.2E+04	1.094E+04	1.497E+04	1.094E+04
18	Qr	-1.5E+04	-1.5E+04	1.112E+04	1.111E+04
19	r1a	-2.4	-2.994262	-2.188403	-2.188403
20	r1b	2.4	2.188403	2.994262	2.188403
21	r2b	0	-0.7995845	0	-0.7995845
22	ra	-2.4	-2.994262	-2.188403	-2.188403
23	rb	2.4	2.188403	2.994262	2.188403
24	rc	0.6	0.5471007	0.7485654	0.5471007
25	sumCp	2500.	2500.	5200.767	5200.767
26	T	300.	300.	326.1184	326.114
27	T1	300.	300.	300.	300.
28	T2	320.	320.	320.	320.
29	Ta	315.	315.	315.	315.
30	Ua	1000.	1000.	1000.	1000.
31	V	0	0	10.	10.
32	vo	50.	50.	50.	50.

Differential equations

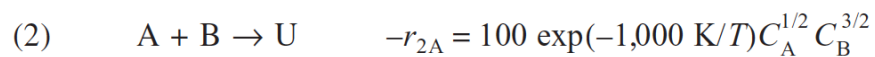
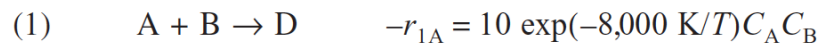
- $d(T)/d(V) = (Qg - Qr)/\text{sumCp}$
- $d(Fc)/d(V) = rc$
- $d(Fb)/d(V) = rb - ra$
- $d(Fa)/d(V) = ra$

Explicit equations

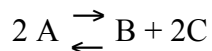
- $Cpc = 100$
- $Cpb = 50$
- $Cpa = 25$
- $k2 = .35$
- $Ta = 315$
- $Ua = 1000$
- $DH2b = -27500$
- $DH1a = -32500$
- $T1 = 300$
- $E1 = 4000$
- $k1 = .60$
- $T2 = 320$
- $E2 = 5000$
- $k2b = k2 \cdot \exp((E2/1.987) \cdot (1/300 - 1/T))$
- $vo = 50$
- $Cb = Fb/vo$
- $Ca = Fa/vo$
- $\text{sumCp} = (Fa \cdot Cpa + Fb \cdot Cpb + Fc \cdot Cpc)$
- $k1a = k1 \cdot \exp((E1/1.987) \cdot (1/300 - 1/T))$
- $r1a = -k1a \cdot Ca^2$
- $r2b = -k2b \cdot Cb^2$
- $r1b = -r1a$
- $rc = -r1a/4$
- $rb = r1b$
- $ra = r1a$
- $Qg = ra \cdot DH1a + rb \cdot DH2b$
- $Qr = Ua \cdot (T - Ta)$



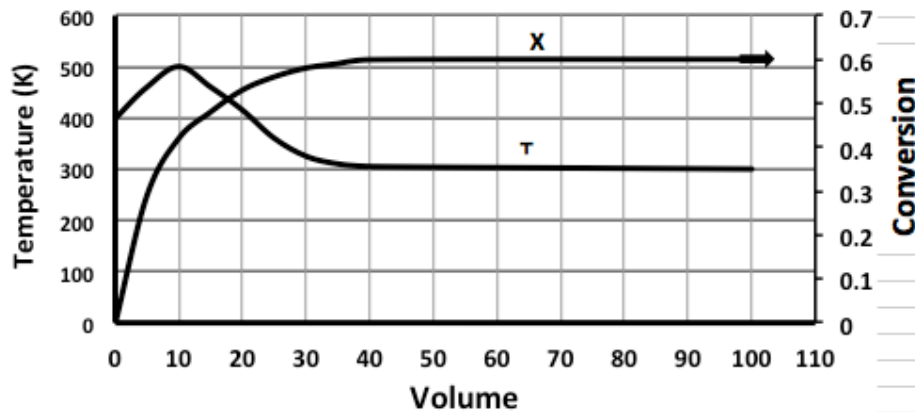
(15 pts) 4) (**Reactor selection and operating conditions**) For the following set of liquid reactions, describe all possible reactor systems and conditions to maximize the selectivity to D. Make sketches where necessary to support your choices. The rates are in (mol/dm³ • s), and concentrations are in (mol/dm³).



- (15 pts) 5) 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 $100 \text{ cal}/(\text{sec} \cdot \text{m}^3 \cdot \text{K})$ with T_a being constant. The elementary gas-phase, reversible reaction is

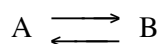


and pure A is fed to the reactor at $0.05 \text{ mol}/\text{dm}^3$. The absolute value of the heat of reaction is $20,000 \text{ cal}/\text{mol}$ of A at 500K , and the heat capacities of A, B, and C are 10, 10, and 5 $\text{cal}/\text{mol}/\text{K}$, respectively.



- (7 pt) (a) What is the rate of disappearance of A at $V = 10 \text{ m}^3$?
- $-r_A = \underline{\hspace{2cm}} \text{ mol}/\text{m}^3 \cdot \text{s}$
- (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 ?
- $Q = \underline{\hspace{2cm}} \text{ cal}/\text{mol A}$
- (1 pt) (c) What is the equilibrium conversion at 300 K
- $X_e = \underline{\hspace{2cm}}$

(20 pts) 6) The reversible liquid phase reaction



is carried out in a 12 dm³ CSTR with heat exchange. Both the entering temperature, T_0 , and the heat exchange fluid, T_a , are at 330 K. An equal molar mixture of inerts and A enter the reactor.

- Choose a temperature, T , and carry out a calculation to find $G(T)$ to show that your calculation agrees with the corresponding $G(T)$ value on curve shown below at the temperature you choose.
- Find the exit conversion and temperature from the CSTR. $X = \underline{\hspace{2cm}}$ $T = \underline{\hspace{2cm}}$.
- What entering temperature T_0 would give you the maximum conversion?
 $T_0 = \underline{\hspace{2cm}}$ $X = \underline{\hspace{2cm}}$
- What would the exit conversion and temperature be if the heat exchange system failed (i.e., $UA = 0$)?

Additional information

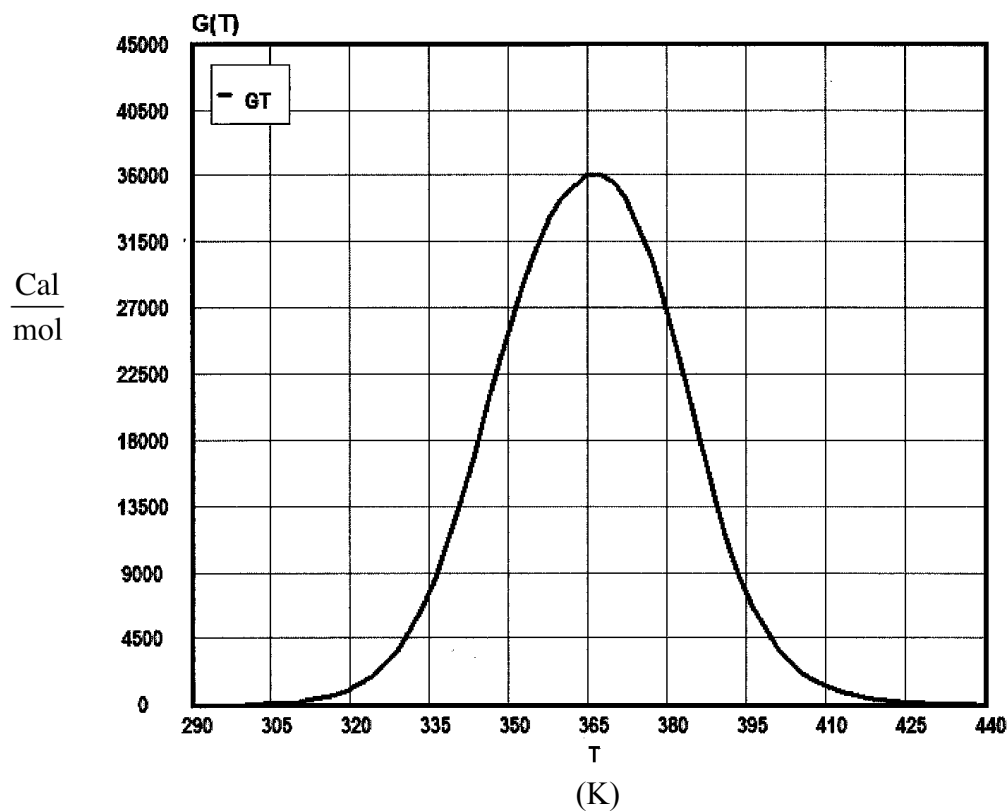
The $G(T)$ curve for this reaction is shown below

$$C_{pA} = C_{pB} = 100 \text{ cal/mol/K}, C_{pI} = 150 \text{ cal/mol/K} \quad UA = 5,000 \text{ cal/h/K}$$

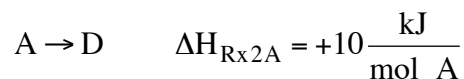
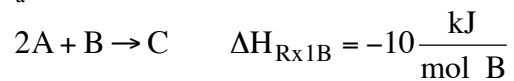
$$F_{A0} = 10 \text{ mol/h}, C_{A0} = 1 \text{ mol/dm}^3, v_0 = 10 \text{ dm}^3/\text{h} \quad k = 0.001 \text{ h}^{-1} \text{ at } 300 \text{ K with } E = 30,000 \text{ cal/mol}$$

$$\Delta H_{Rx} = -42,000 \text{ cal/mol}$$

$$K_C = 5,000,000 \text{ at } 300 \text{ K}$$



(25 pts) 7) The following elementary reactions are to be carried out in a PFR with a co-current heat exchange with constant T_a



The reactants all enter at 400 K. Only A and B enter the reactor. The entering concentration of A is 3 molar and that of B is 1 molar at a volumetric flow rate of $10 \text{ dm}^3/\text{s}$

Additional information

$$U_a = 1,000 \text{ J/dm}^3/\text{s/K}$$

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

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

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

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

$$C_{P_C} = 30 \text{ J/mol/K}$$

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

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

$$C_{P_E} = 80 \text{ J/mol/K}$$

What coolant temperature T_a is necessary such that at the reactor entrance, i.e., $V = 0$, that

$$\frac{dT}{dV} = 0$$

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