ChE 344
Winter 2011
Mid Term Exam II + Solution
Wednesday, April 6, 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."

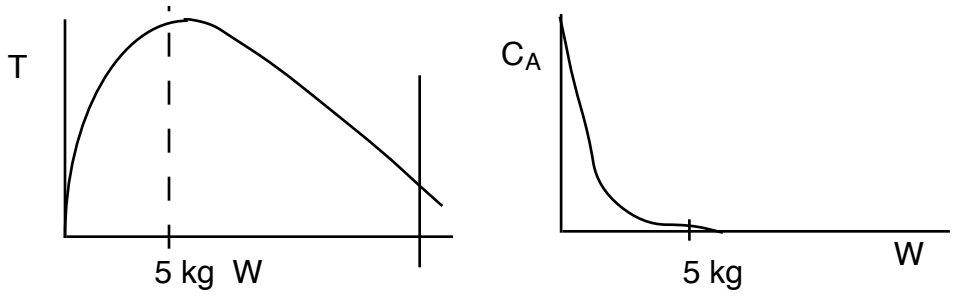
_____
(Signature)

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

(5 pts) 1) The 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 could be 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.

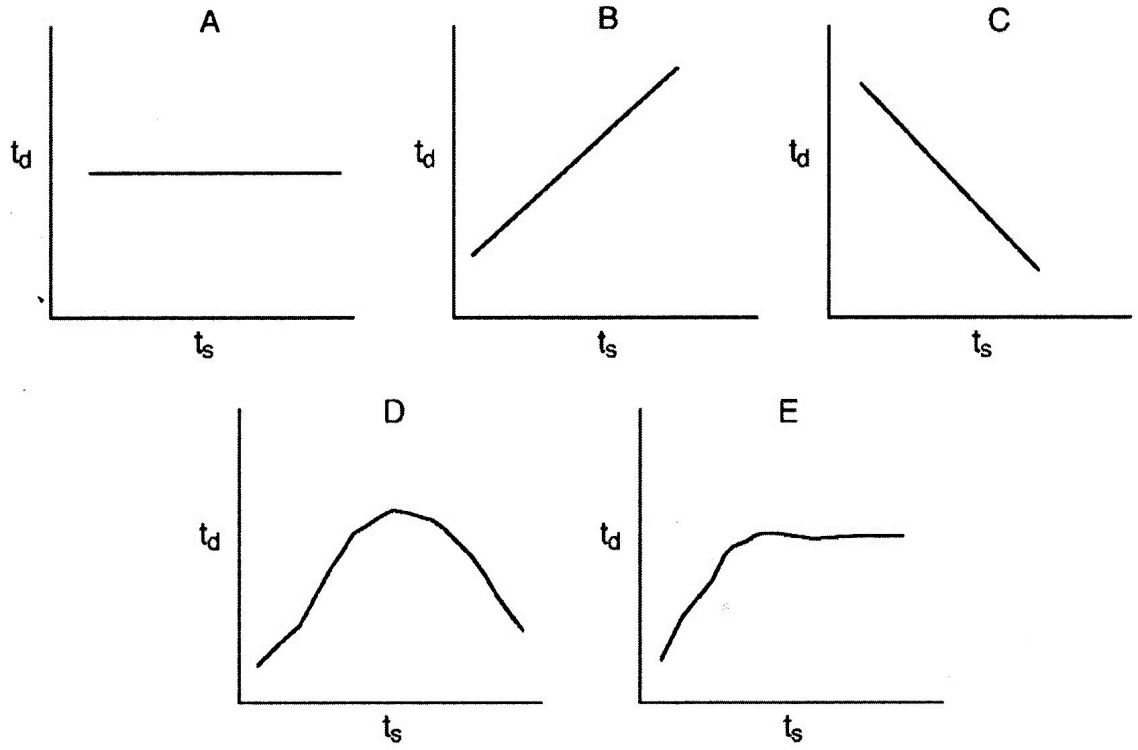
(b) True. Possible when either A → B is exothermic or B → C is endothermic or both.

(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) 2) Let's revisit the explosion in Example 13-2. Suppose that the heating had not failed for 10 minutes down time, t_d, which occurred at 55 minutes after startup, t_s, but instead at a later time, t_s. Which of the following figures relates the down time, t_d, to the time after startup that the heat exchanger failed, t_s, for which the reactor would not explode?



Explain_____

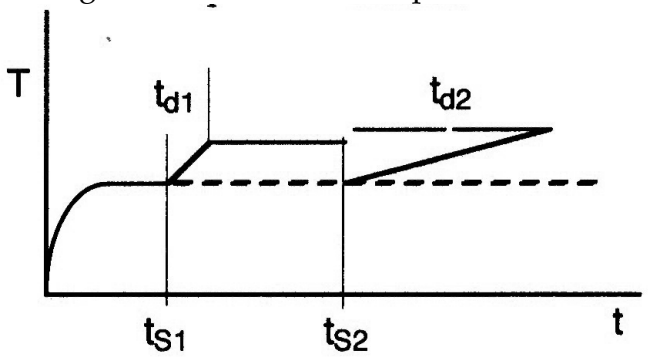
_____

_____

Solution

B

After longer times, t_s, the rate will be slower because reactant will have been consumed. Therefore longer down times will be possible.



(5 pts) 3) The elementary gas phase reaction

$$A \rightleftarrows B + C$$

is carried out in a PFR. The following temperature profile was obtained

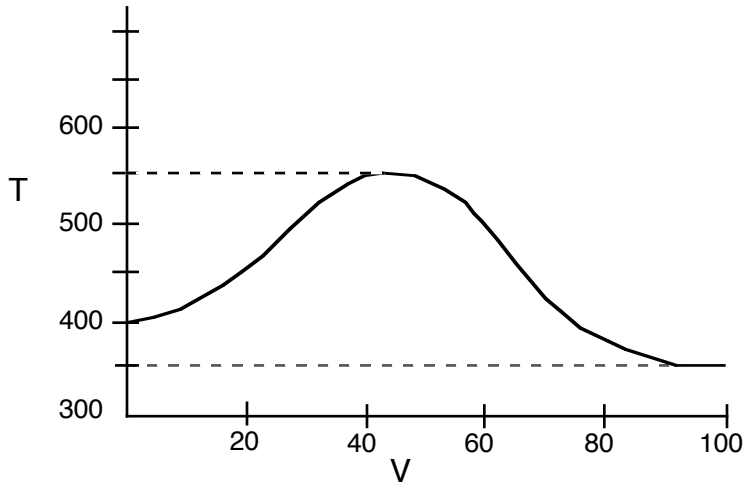


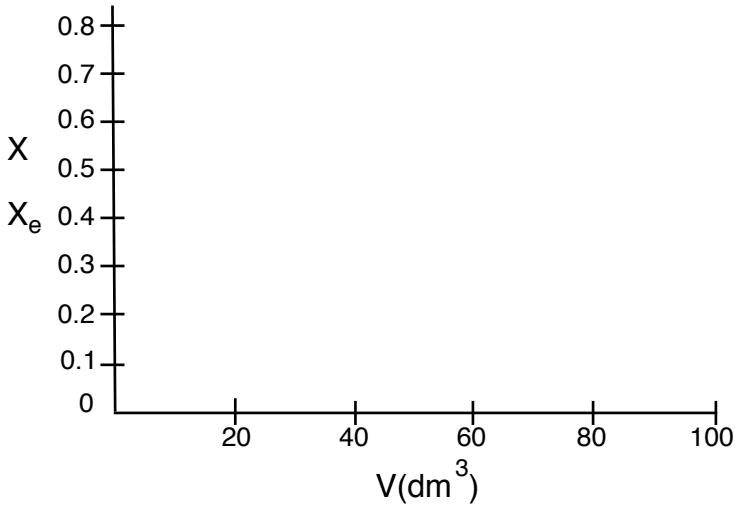
Figure EP5-1

(a) This figure corresponds to which heat exchange case?

1) Adiabatic
2) Isothermal
3) Constant ambient temperature co-current heat exchange
4) Variable T_a co-current
5) Variable T_a counter current

(b) On the figure above, sketch the temperature profile if the flow rate were reduced by a factor of 3.

(c) Sketch X and X_e corresponding to Figure EP5-1 with $X_e = 0.6$ where T = 400 K

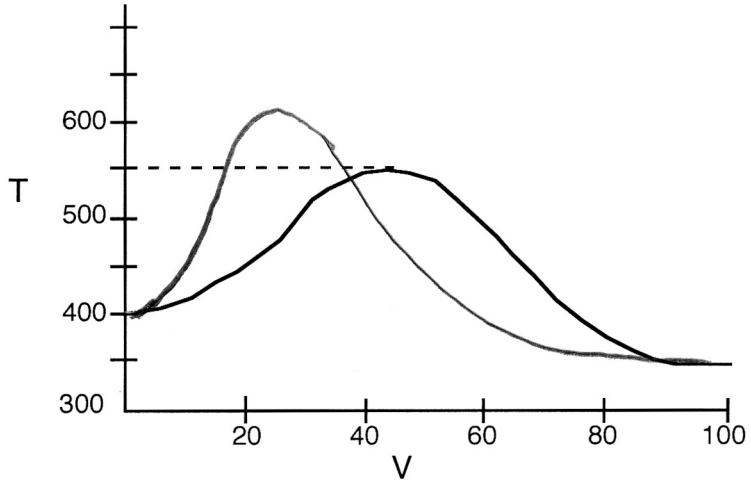


(d) On this same figure, sketch X and X_e when the flow rate is decreased by a factor of 3.

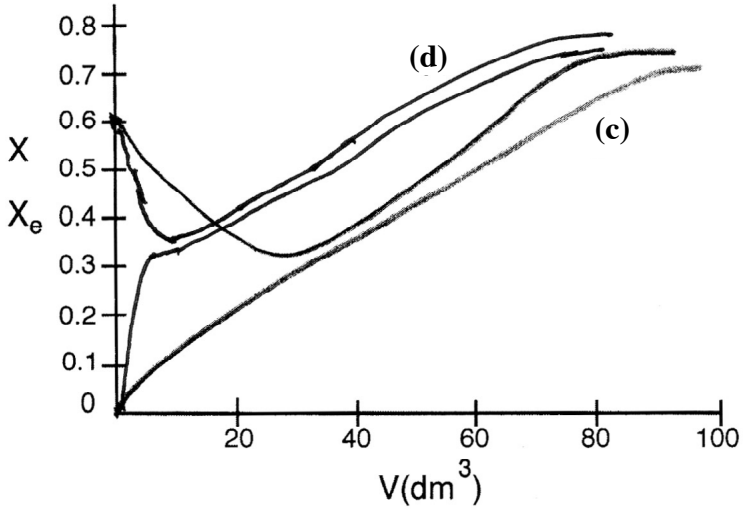
Solution

(a) 3) Constant ambient temperature co-current heat exchange

(b)



(c) & (d)

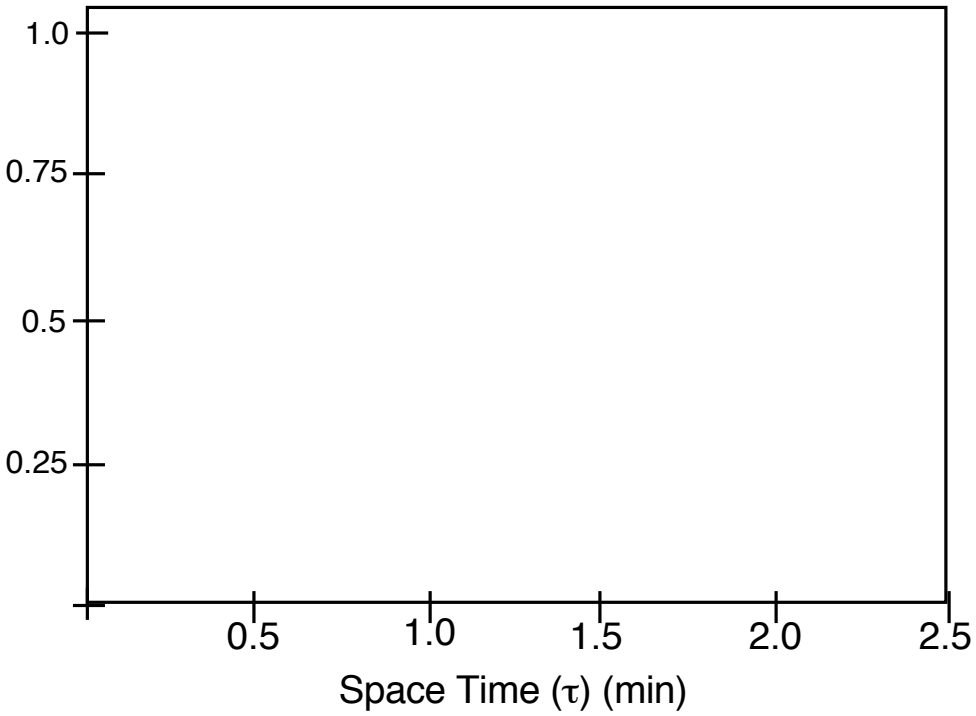


(10 pts) 4) Consider the reaction

$$A \xrightarrow{k_1} D \xrightarrow{k_2} U$$

Pure A is fed to a 1.0 dm^3 CSTR where it reacts to form a desired product (D), which can then react further to produce an undesired product (U); both reactions are elementary and irreversible and everything is liquid phase. The entering concentration of A is 1 mole/dm^3 at a molar flow rate of 1 mol/min.

(a) Sketch graphs of the conversion of A, X, the instantaneous selectivity of D to U, $S_{D/U}$, and the instantaneous yield of D, Y_D, as a function of space time (make sure to label them on the plot). You may want to write a sentence or two of reasoning for partial credit purposes.



If at τ = 1.0 minutes the instantaneous selectivity, $S_{D/U}$, is (1/2) and the conversion of A is (0.5) what are the specific reactions rates k_1 and k_2?

(b) k_1 = _____

(c) k_2 = _____

Explain_____

_____

_____

Solution

(a)

$$A \rightarrow D \rightarrow U$$

Let B = D and C = U

$$A \rightarrow B \rightarrow C$$

Balance on A

$$\upsilon_0 C_{A0} - \upsilon_0 C_A - k_1 C_A V = 0$$

Balance on B

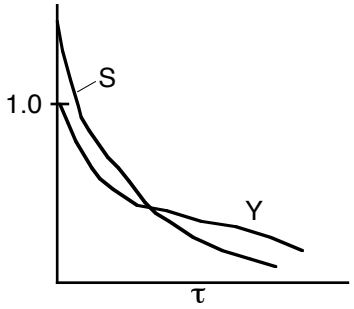
$$0 - \upsilon_0 C_B + (k_1 C_A - k_2 C_B)\upsilon = 0$$

$$C_A = \frac{C_{A0}}{1+\tau k_1} \qquad C_B = \frac{k_1 \tau C_A}{1+k_2\tau} = \frac{\tau k_1 C_{A0}}{(1+k_1\tau)(1+k_2\tau)}$$

Balance on C

$$0 - C_C \upsilon_0 + k_2 C_B V = 0$$

$$C_C = \tau k_2 C_B = \frac{\tau k_2 C_{A0} \tau k_1}{(1+\tau k_1)(1+\tau k_2)}$$



$$\boxed{S_{B/C} = \frac{C_B}{C_C} = \frac{\dfrac{\tau k_1 C_{A0}}{(1+\tau k_1)(1+\tau k_2)}}{\dfrac{\tau k_1 \tau k_2 C_{A0}}{(1+\tau k_1)(1+\tau k_2)}} = \frac{1}{\tau k_2}}$$

$$Y_B = \frac{C_B}{C_{A0} - C_A} = \frac{\dfrac{\tau k_1 C_{A0}}{(1+\tau k_1)(1+\tau k_2)}}{\underbrace{C_{A0}\left(1 - \dfrac{1}{(1+\tau k_1)}\right)}_{1+\tau k_1 - 1}} = \frac{\dfrac{\tau k_1}{(1+\tau k_1)(1+\tau k_2)}}{\dfrac{\tau k_1}{1+\tau k_1}}$$

$$\boxed{Y_B = \frac{1}{(1+\tau k_2)}}$$

(b) $k_1 = \underline{1\ \text{min}^{-1}}$

$$V = \frac{F_{A0}X}{kC_{A0}(1-X)} = \frac{\upsilon_0 C_{A0} X}{kC_{A0}(1-X)}$$

$$\tau = \frac{X}{k_1(1-X)} = \frac{0.5}{(1-0.5)k}$$

$$\tau k_1 = 1$$

$$k_1 = 1$$

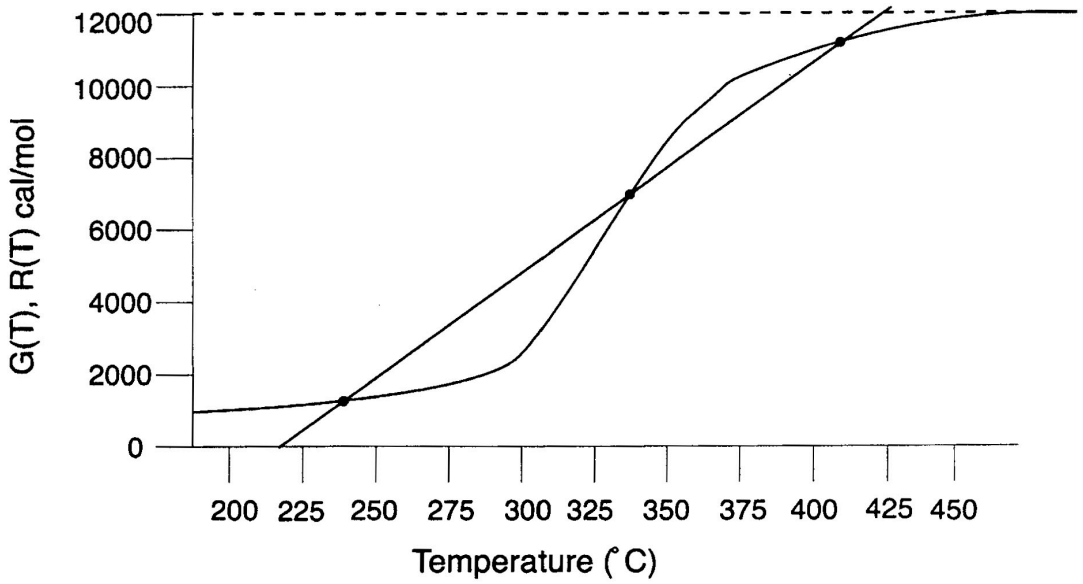
(c) $k_2 = \underline{2\ \text{min}^{-1}}$

At $\tau = 1.0$ $S_{B/C} = 0.5 = \dfrac{1}{1 \cdot k_2}$, $k_2 = 2$

(15 pts) 5) 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 conversions corresponding to at the ignition and extinction temperatures?

X (Ignition) = _____, _____ X (Extinction) = _____, _____

(e) For the figure above 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) = $\frac{2,500}{12,000} = 0.21$

X (Extinction) = $\frac{10,000}{12,000} = 0.83$

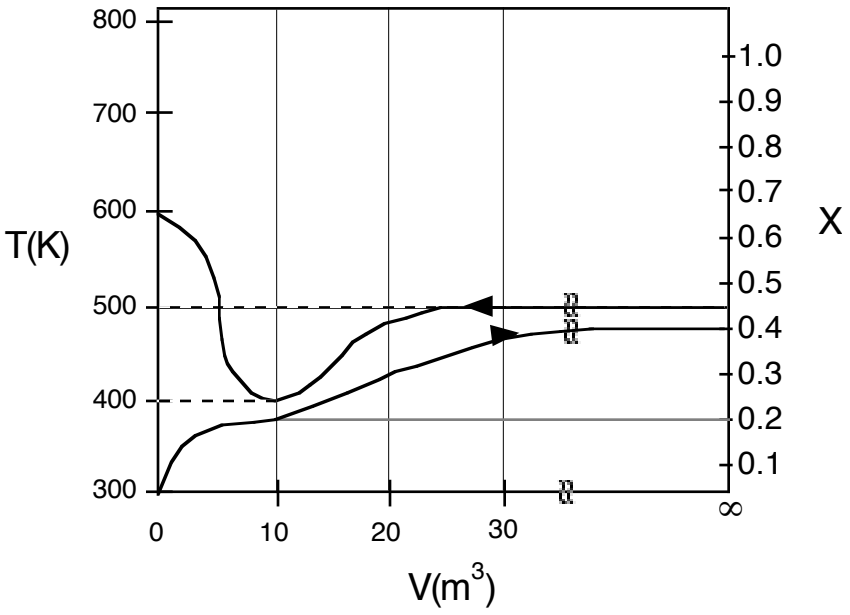
(e) X = $\frac{7,000}{12,000} = 0.58$

All conversions are
±0.3 depending how one reads the graph

(20 pts) 6) 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

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

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.



(5 pt) (a) Sketch X_e versus V on the above figure.

(5 pt) (b) Using what is the equilibrium constant at 500 K?

K_e (500) = _____

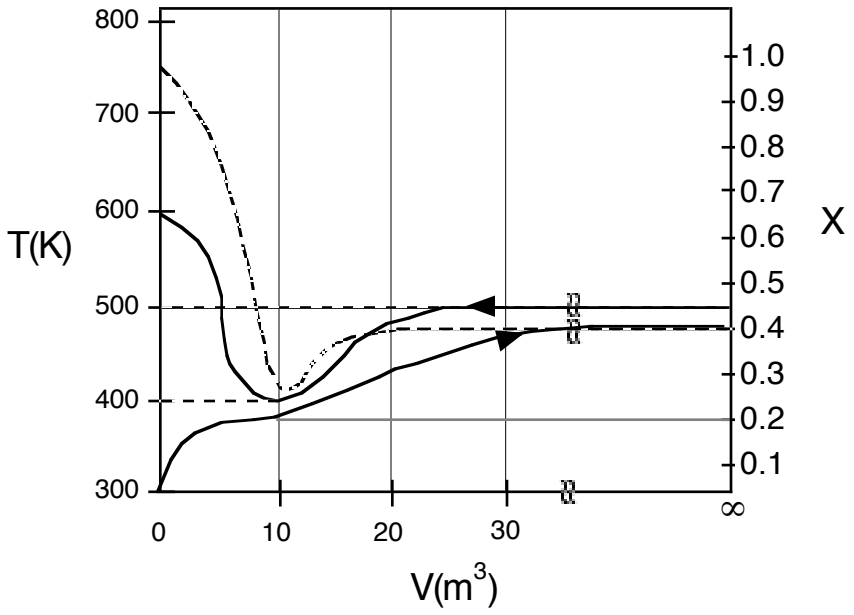
(10 pt) (c) What is the rate of disappearance of A, $-r_A$, at 10 m^3?

$-r_A$ = _____

Note: You may want to bring your answers to parts (a) – (c) to the Final Exam as you may see a continuation of this problem, i.e., parts (d) – (f) on the Final Exam.

Solution

(a)



at V = 10 m³ $Q_g = Q_r$

(b) K_e (500) = _?_____

$$A \rightarrow \frac{1}{2}B + \frac{1}{2}C$$

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

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

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

K_e = <u>0.11</u>

(c) $-r_A$ = _?_____

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

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

At minimum $\dfrac{dT}{dV} = 0$ T = 400 K, T_a = 500 K

$Q_g = Q_r$

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

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

$$\left(-r_A\right)\left(-\Delta H_{Rx}\right) = \left(-r_A\right)\left(-5{,}000\right) = Q_r = -10{,}000\,\frac{cal}{m^3 \cdot s}$$

$$-r_A = \frac{-10{,}000\,\dfrac{cal}{s \bullet m^3}}{-5{,}000\,\dfrac{cal}{mol}} = 2\,\frac{mol}{m^3 \bullet s}$$

(20 pts) 7) 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

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

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

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

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

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

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

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

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

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

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

T_a = _____

Solution

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

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)

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

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

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

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

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

(20 pts) 8) **Study Problem (Modified)**

P12-6$_B$ The endothermic liquid-phase elementary reaction

$$A + B \rightarrow 2C$$

proceeds, substantially, to completion in a single steam-jacketed, continuous-stirred reactor (Table P12-6$_B$). From the following data, calculate the steady-state reactor temperature:

Reactor volume: 16 ft^3
Steam jacket heat transfer area: 10 ft^2
Jacket steam: 150 psig (365.9°F saturation temperature)
Overall heat-transfer coefficient of jacket, *U*: 150 Btu/h•ft^2•°F
Agitator shaft horsepower: 63,525 Btu/h
Heat of reaction, ΔH°_{Rx} = 20,000 Btu/lb-mol of A (independent of temperature)

TABLE P12-6$_B$ FEED CONDITIONS AND PROPERTIES

	Component		
	A	*B*	*C*
Feed (lb-mol/hr)	10.0	10.0	0
Feed temperature (°F)	80	80	—
Specific heat (Btu/lb-mol · °F	51.0	44.0	47.5
Molecular weight	128	94	111
Density (lb$_m$/ft^3	63.0	67.2	65.0

(Courtesy of the California Board of Registration for Professional & Land Surveyors.)

Solution

P12-6

$$A + B \rightarrow 2C$$

	A	B	C
$F_{io}\left(\frac{lb-mole}{hr}\right)$	10	10	0.0
T_{io}(F)	80	80	-
$C_{Pio}\left(\frac{\tilde{Btu}}{lb\ mole°F}\right)$	51	44	47.5
$MW,\left(\frac{lb}{lb\ mol}\right)$	128	94	222
$\rho_{i,}\left(\frac{lb}{ft^3}\right)$	63	67.2	65

$$\Delta H_R = 20,000 \frac{Btu}{lb\ mol\ A},$$

Energy balance with work term included is:

$$\frac{\dot{Q} - \dot{W}_S}{F_{A0}} - X_A \Delta H_R = \sum \theta_i \tilde{C}_{Pi} \left[T - T_o \right]$$

$$\theta_A = 1, \theta_B = \frac{F_{B0}}{F_{A0}} = \frac{10}{10} = 1, X_{AF} = 1$$

$$\dot{Q} = UA(Ts - T)$$

Substituting into energy balance,

$$UA\left(T_S - T\right) - W_S - F_{A0} \Delta H_R X_{AF} = F_{A0} \left[C_{pA} + C_{pB} \right] \left[T - T_0 \right]$$

$$\Rightarrow UA\left(T_S - T_0\right) - W_S - F_{A0} \Delta H_R = \left\{ F_{A0} \left[C_{pA} + C_{pB} \right] + UA \right\} \left[T - T_0 \right]$$

$$T = T_0 + \left(-UA\left(T_S - T_0\right) - W_S - F_{A0} \Delta H_R \right) \Big/ \left(F_{A0} \left[C_{pA} + C_{pB} \right] + UA \right)$$

$$-W_S = 63525 \text{ Btu/hr}$$

$$T = 199°\text{F}$$