

ChE 344
Chemical Reaction Engineering
Winter 2000

Exam II

Open Book and Notes

Name SOLUTION

Honor Code _____

Signed _____

1) ____/25 pts

2) ____/10 pts

3) ____/10 pts

4) ____/10 pts

5) ____/20 pts

6) ____/5 pts

7) ____/20 pts

Total 100 pts

(25%) 1) The following reversible, elementary, liquid phase reaction occurs in a CSTR:



The entering flow rate is 10 dm³/s with an entering concentration of 2 M of A and the feed temperature is 300 K. What is the reactor volume necessary to achieve 90% of the equilibrium conversion in a CSTR operated adiabatically?

Additional information:

$$C_{pA} = C_{pB} = 60 \text{ cal/mol/K}$$

$$H_{\text{rxn}}^{\circ} = -10,000 \text{ cal/mol A}$$

Solution:

To begin, you need to use the conversion obtained from the energy balance

$$X_{\text{EB}} = \frac{C_{pA}(T - T_o)}{-H_{\text{rxn}}^{\circ}} = \frac{60 \frac{\text{cal}}{\text{mol K}} (T - 300 \text{ K})}{10000 \frac{\text{cal}}{\text{mol A}}} = X_{\text{EB}}$$

Now, you can plot this line on the X_{eq} versus T curve (see below)

Where the lines intersect is the operating temperature, T, (~ 398 K)

and equilibrium conversion, X_{eq} , (~0.59)

You want 90% of this value (as stated in the problem)

$$X = 0.90 * X_{\text{eq}} = 0.90 * 0.59 = 0.53 = X$$

Now you can use this value in the design equation for a first-order, reversible reaction using a CSTR

$$X = \frac{k}{1+k} \frac{1}{1 + \frac{1}{K_C}}$$

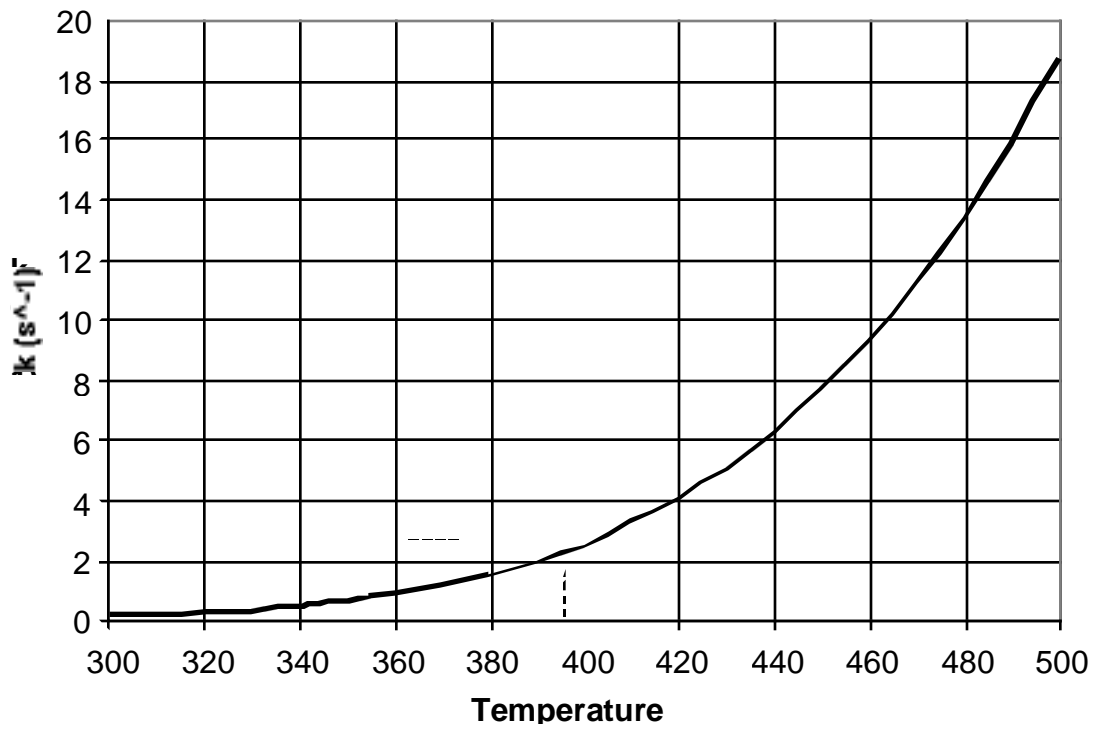
To get values of k and K_C at 398 K, use the plots given (see below)

$$k \sim 2.4 \text{ s}^{-1}$$

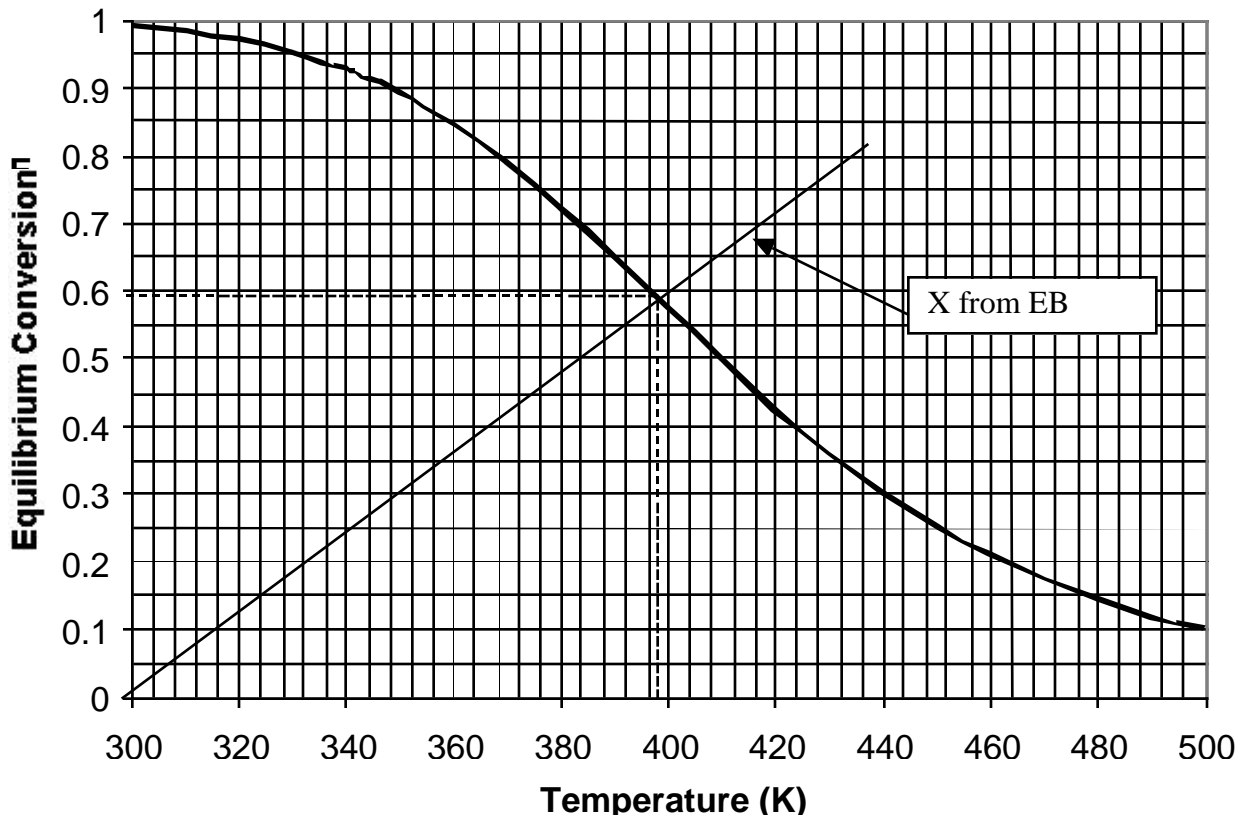
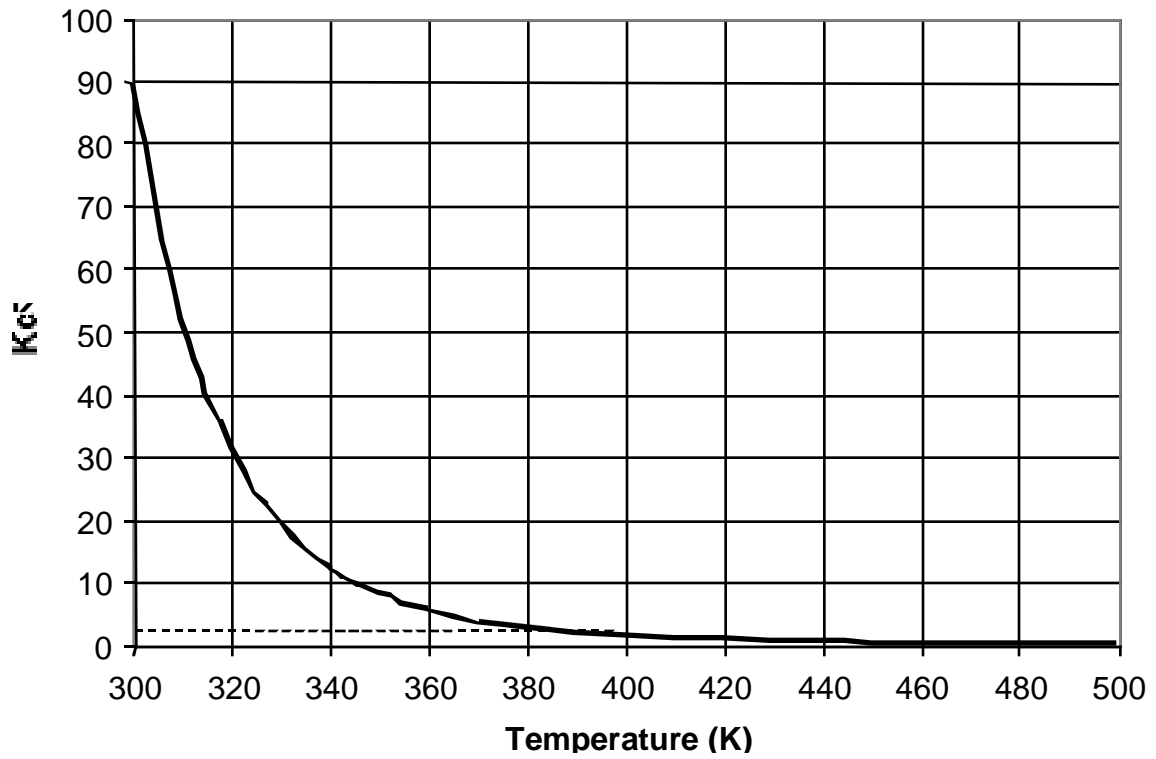
$$K_C \sim 2$$

Plug in values and solving for space time,

$$0.53 = \frac{2.4 \text{ s}^{-1}}{1 + 2.4 \text{ s}^{-1}} \frac{1}{1 + \frac{1}{2}} = 1.1 \text{ s} = \frac{V}{v_o} \quad V = 1.1 \text{ s} * 10 \frac{\text{dm}^3}{\text{s}} = 11 \text{ dm}^3$$



Answer: $V = \underline{\quad 11 \quad} \text{dm}^3$



(10%) 2) Let's revisit Problem 8-20. The heat exchanger in home problem 8-20 is to be replaced by one that has an adjustable heat exchanger area. Assuming everything else remains the same, what is the value of UA needed to obtain the maximum possible conversion in the reactor?

$$UA = \underline{7700} \text{ cal/min} \cdot \text{K}.$$

What is the corresponding conversion?

$$X = \underline{0.91}$$

8-20 The elementary, reversible, liquid phase reaction



takes place in a CSTR with a heat exchanger. Pure A enters the reactor. The heat generated curve (cal/mol) is given below as a function of temperature.

Additional Information:

$$UA = 3,600 \text{ cal/min} \cdot \text{K}, \quad E/R = 20,000 \text{ K}$$

$$C_{pA} = C_{pB} = 40 \text{ cal/mol} \cdot \text{K}, \quad V = 10 \text{ dm}^3$$

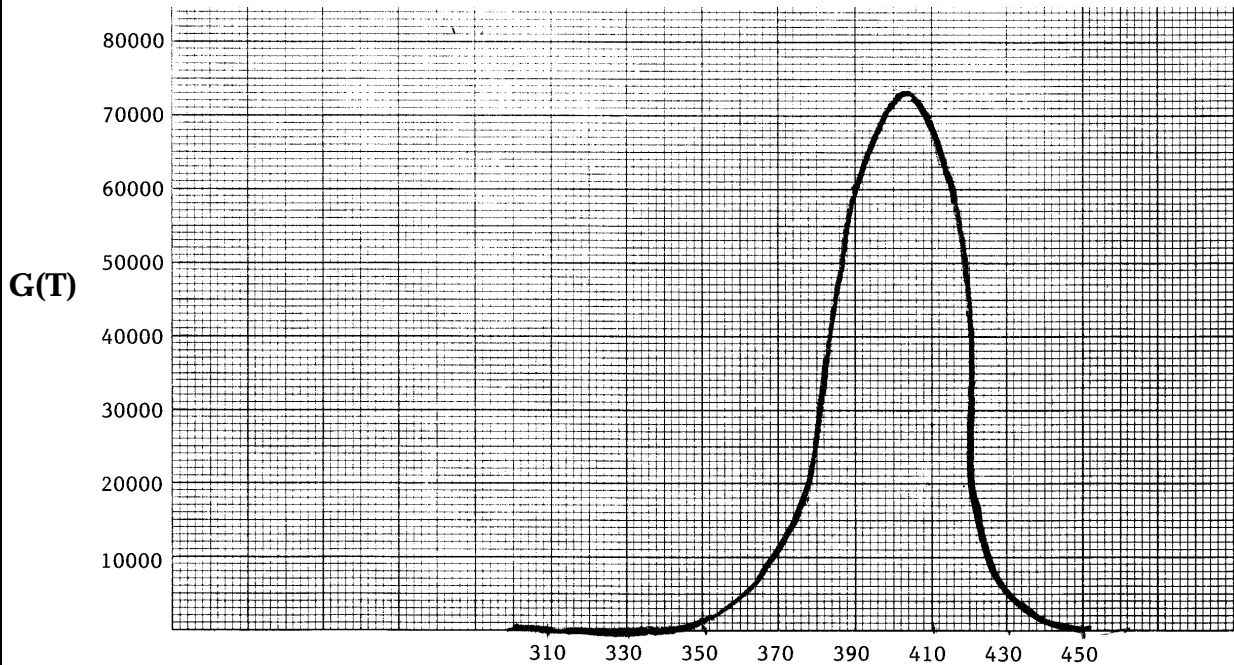
$$H_R = -80,000 \text{ cal/mol A}, \quad v_0 = 1 \text{ dm}^3/\text{min}$$

$$K_{eq} = 100 \text{ at } 400 \text{ K}, \quad F_{AO} = 10 \text{ mol/min}$$

$$k = 1 \text{ min}^{-1} \text{ at } 400 \text{ K},$$

$$\text{Ambient Temperature } T_A = 37^\circ\text{C}$$

$$\text{Feed Temperature } T_O = 37^\circ\text{C}$$



Using the above information, write a question that involves critical thinking. Explain why the question and answer involve critical thinking. How would you answer this question.

In order to get the maximum conversion, you would want your R(T) curve to intersect the G(T) curve (given below) at the peak of the curve (~7300)
 If the G(T) and R(T) lines were to intersect, you can set them equal to one another, such that R(T) is also equal to 7300

$$R(T) = C_{po} (1 + X) (T - T_C)$$

where $\beta = \frac{UA}{C_{po} F_{Ao}}$ and $T_C = \frac{T_a + T_o}{1 + \beta}$

combining yields

$$R(T) = C_{po} (1 + X) T - \frac{C_{po} (T_a + T_o)}{1 + \beta}$$

substituting in values yields

$$7300 = 40 \frac{\text{cal}}{\text{mol K}} (1 + X) 400 \text{ K} - \frac{310 \text{ K} + 310 \text{ K}}{1 + \beta}$$

now solve for

$$19.275 = \frac{UA}{C_{po} F_{Ao}} \quad UA = 19.275 * 40 \frac{\text{cal}}{\text{mol K}} * 10 \frac{\text{mol}}{\text{min}} = 7700 \frac{\text{cal}}{\text{min K}}$$

Now solve for X

$$G(T) = X * -H_{rx}$$

$$X = \frac{73000}{80000} = 0.91$$

(10%)3) True (T), False (F), Can't tell from information given (CT)

- a) In deriving equation (8-60) page 460 changes in pressure between the inlet and outlet were neglected.

(T) **(F)** (CT)

- b) In deriving equation (9-9) p.536 changes in pressure between the start of the batch and any time t during the batch were neglected.

(T) (F) (CT)

- c) The rate law for the production of a materials for use in sensors that need a sharp-metal-insulation transition is

$$r_{\text{DEP}} = \frac{kP_A^2}{(1 + K_A P_A)^2}$$

(T) (F) (CT)

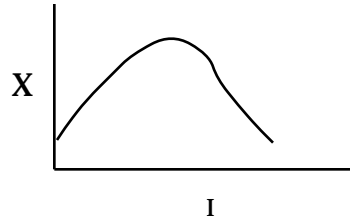
- d) Any species adsorbed on the surface will always cause the rate to decrease as the partial pressure of that species increases.

(T) **(F)** (CT)

- e) The number of temperatures oscillations in returning steady shown in Figure E9-6.1 p. 565 would increase if the gain to the controller were increased.

(T) (F) (CT)

(10%) 4) The following plot shows the exit conversion from a PFR operated adiabatically.



a) This figure could apply to a first order irreversible endothermic reaction.

(T) **(F)** (CT)

b) This figure could apply to a first order reversible endothermic reaction.

(T) **(F)** (CT)

c) This figure could apply to a second order irreversible endothermic reaction.

(T) (F) (CT)

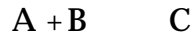
d) This figure could apply to a second order reversible exothermic reaction.

(T) (F) (CT)

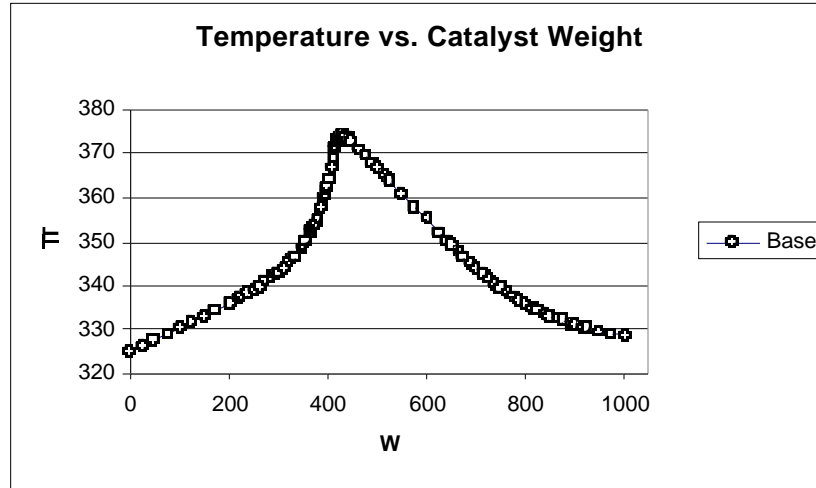
e) This figure could apply to a second order reversible endothermic reaction.

(T) (F) (CT)

(20%) 5) A reversible exothermic reaction

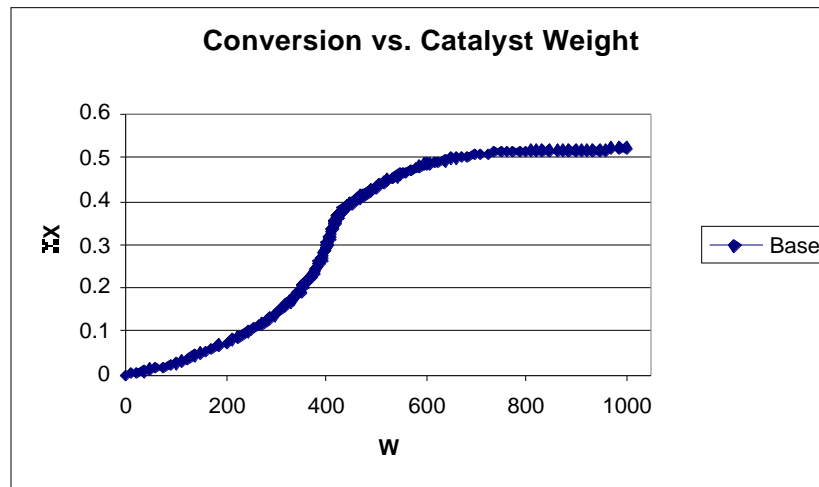


is carried out in a PBR with heat exchange. For a given set of conditions the following temperature profile was obtained



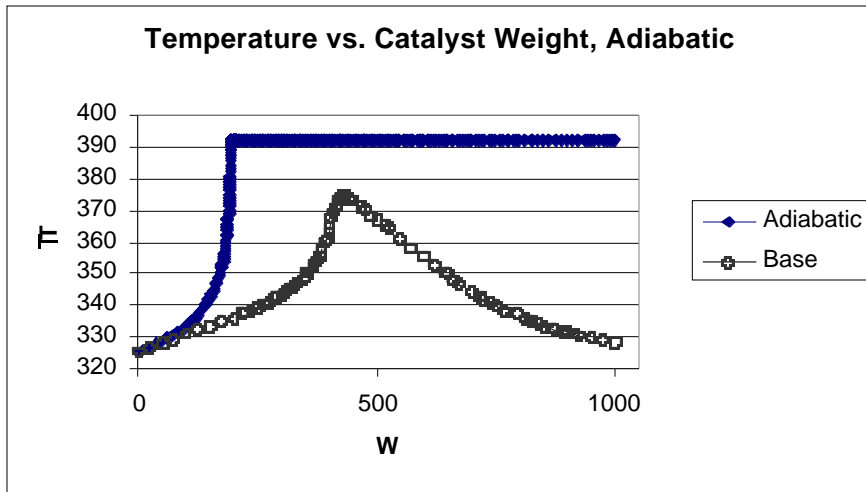
Note that the conversion profile reaches a plateau after the temperature reaches its maximum value.

a) Sketch the corresponding conversion profile



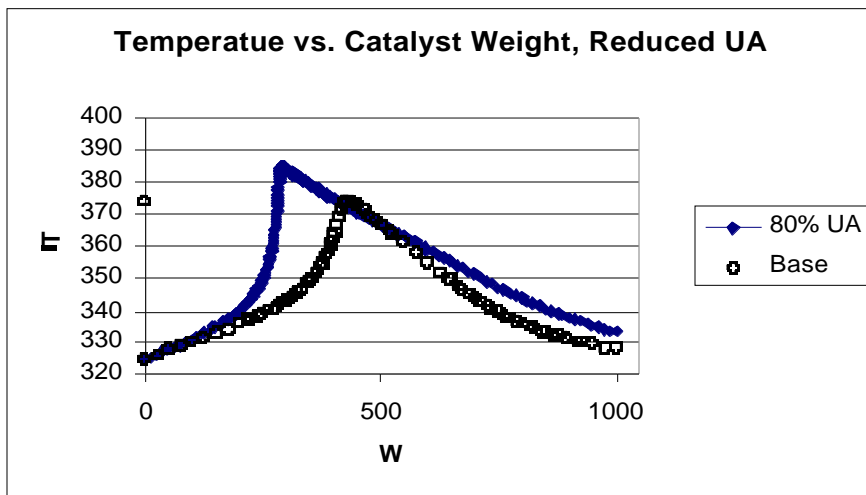
Note that the conversion profile reaches a plateau after the temperature reaches its maximum value.

b) On the figure below sketch the temperature profile that would result if the reaction were carried out adiabatically.



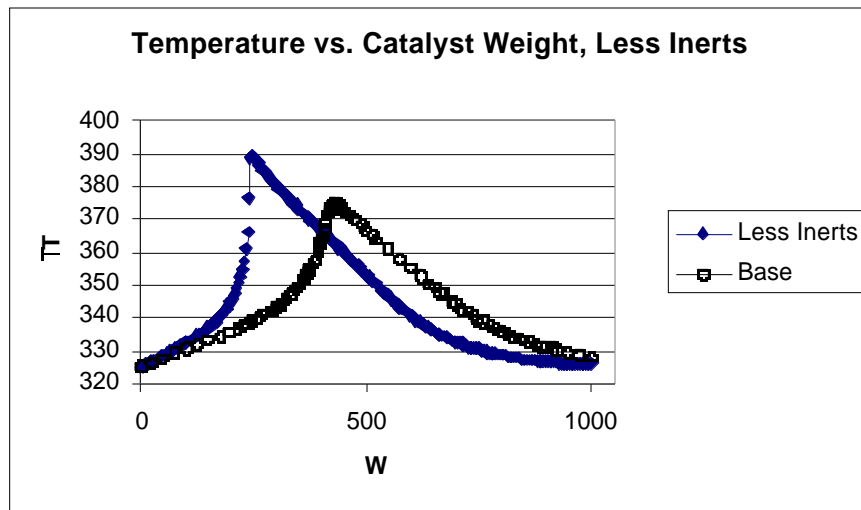
Note that the temperature reaches a plateau at a higher value, and the maximum occurs earlier in the reactor.

c) On the figure below sketch the temperature profile that would result if heat exchange parameter, U_a was reduced by say, approximately 20%



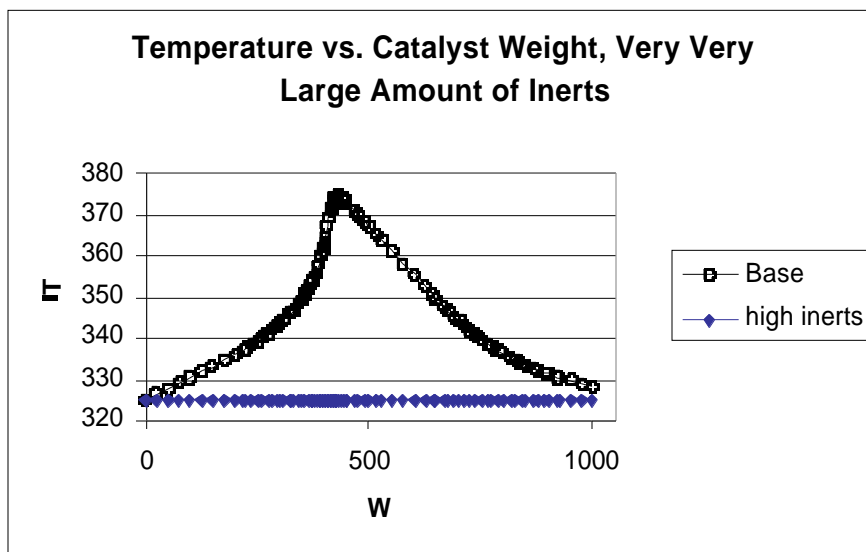
Note that the reaction mixture heats up much faster, and cools down slower.

- d) On the figure below sketch the temperature profile that would result if a somewhat smaller amount of inerts were added to the system.



Note that the reaction mixture heats up much faster, and cools down somewhat faster as well.

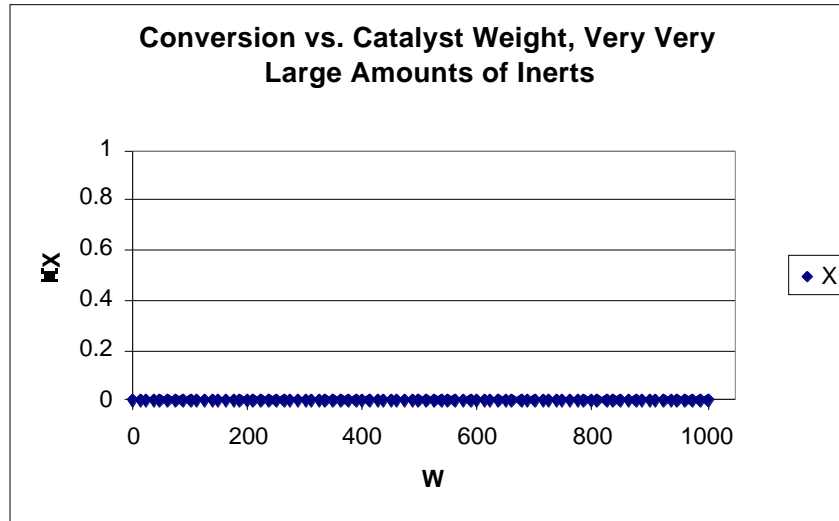
- e) On the figure below sketch the temperature profile that would result if a very very large amount of inerts were added to the system.



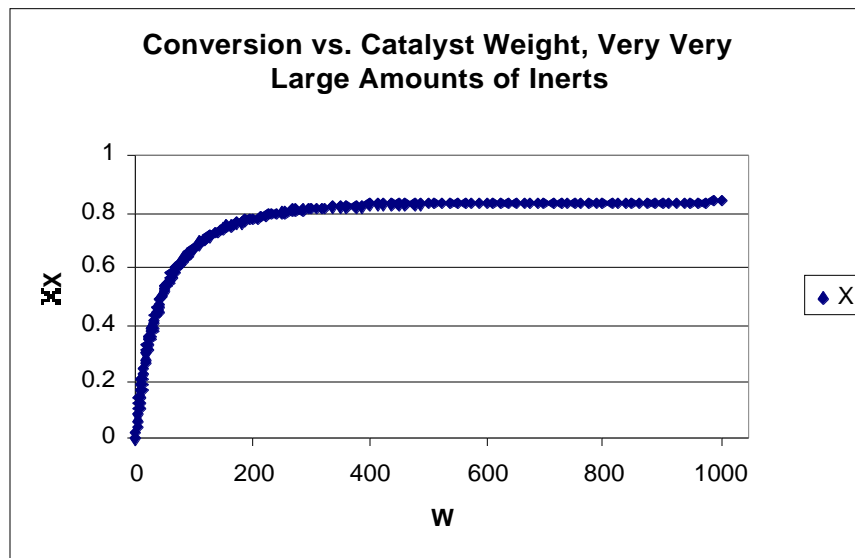
Note that the temperature profile becomes flat (isothermal conditions).

f) For part (e) above sketch two possible conversion profiles that could result.

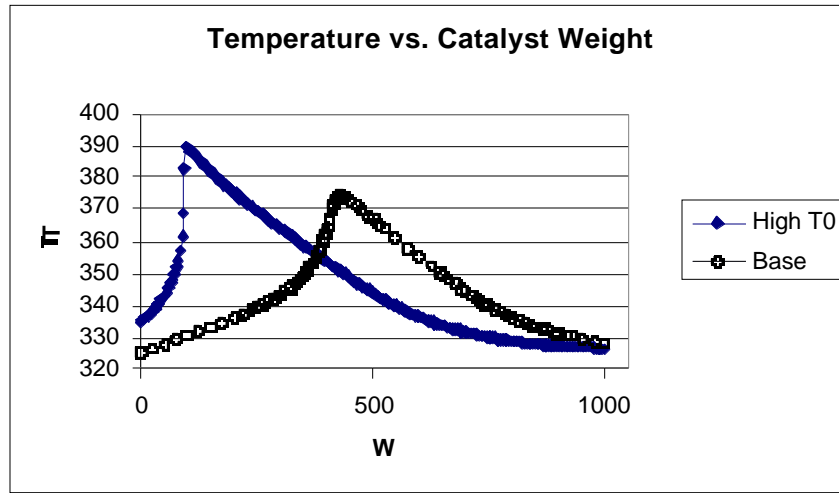
Case 1) Very low value of k , reaction practically does not occur, unless the temperature were to increase owing to the heat of reaction.



Case 2) Very large value of k , reaction reaches the equilibrium conversion corresponding to the inlet temperature very fast.



- g) On the figure below sketch the temperature profile that would result if the entering temperature were increased.

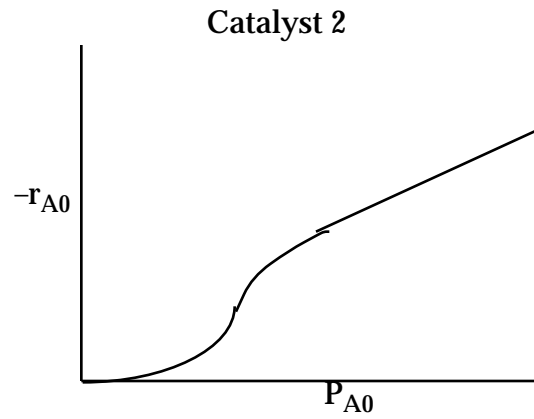
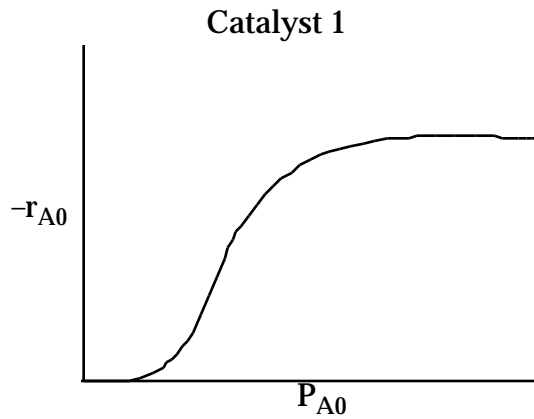


Note that the inlet temperature is higher (at $w=0$) than that of the base case, reaction rate is higher, reaction mixture heats up much faster and the temperature reaches a higher maximum, and the maximum occurs earlier in the reactor.

(5%) 6) The following reaction occurs in the presence of catalyst:



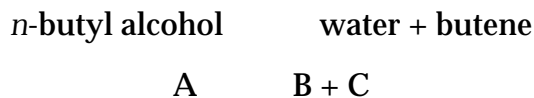
Two catalysts are experimentally evaluated and the results are plotted below. From this information, which type of mechanism occurs for each case?



- a) Single site binding for reaction step
- b) Dual site binding for reaction step**
- c) Eley-Rideal mechanism
- d) Can't tell
- e) None of the above
- f) All of the above

- a) Single site binding for reaction step
- b) Dual site binding for reaction step
- c) Eley-Rideal mechanism**
- d) Can't tell
- e) None of the above
- f) All of the above

(20%) 7) The dehydration of *n*-butyl alcohol over an alumina-silica catalyst was investigated.



The following data were obtained using a modified differential reactor operated at 750°F.

$-r'_{A0}$ (lb mol/h/lb catalyst)	P_{A0} (atm)	P_{B0} (atm)	P_{C0} (atm)
0.3	25	0	30
0.6	25	0	0
0.7	50	0	0
0.2	10	2	0
0.7	150	0	0
0.6	25	30	0
0.3	25	30	30
0.75	100	50	0
0.6	200	0	0
0.2	10	0	0
0.6	25	15	0

Suggest a rate law that is consistent with the experimental data

- P_B has no effect on the rate, therefore not in rate law or weakly adsorbed
- P_C has a negative effect on the rate, therefore it must adsorb on the surface and be found in the denominator
- P_A has a positive effect on the rate until a point and then has a negative effect, therefore, P_A must be in the numerator, but squared in the denominator (suggesting a dual site mechanism)

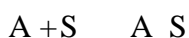
Putting 1-3 together, we get the following rate law

$$-r_A = \frac{k_A P_A}{(1 + k_A P_A + k_C P_C)^2}$$

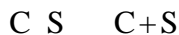
Suggest a mechanism and rate-controlling step that are consistent with the proposed rate law.

A corresponding mechanism to the above rate law is as follows

If B is not adsorbed



or if B is weakly adsorbed



How would you linearize the rate law to evaluate the rate law parameters? What would you plot against what? (Do not make any calculations).

To linearize the rate law

$$-r_A = \frac{k_A P_A}{(1 + k_A P_A + k_C P_C)^2}$$

$$\frac{-r_A}{P_A} = \frac{k_A}{(1 + k_A P_A + k_C P_C)^2}$$

$$\frac{P_A}{-r_A} = \frac{(1 + k_A P_A + k_C P_C)^2}{k_A}$$

$$\sqrt{\frac{P_A}{-r_A}} = \frac{1}{\sqrt{k_A}} + \frac{1}{k_A P_A} + \frac{1}{k_C P_C}$$

Now plot $\sqrt{\frac{P_A}{-r_A}}$ versus $\frac{1}{P_A}$ for the trials where P_C is held constant

Now plot $\sqrt{\frac{P_A}{-r_A}}$ versus $\frac{1}{P_C}$ for the trials where P_A is held constant

This way, you will get all of the rate law parameters

How would the initial rate law change if the feed contained an inert compound that could reversibly bind to catalyst sites?

Any inerts would most likely adsorb onto the surface, thus taking up sites and reducing the reaction rate

$$-r_A = \frac{k_A P_A}{(1 + k_A P_A + k_C P_C + k_I P_I)^2}$$