ChE 344  
Winter 2013  
Mid Term Exam I + Solution  
Tuesday, February 26, 2013  
Closed Book, Web, and Notes

Name_______________________________

Honor Code___________________________________________________________________
______________________________________________________________________________
______________________________________________________________________________

(Sign at the end of exam period)

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

_____ I have a Laptop with Polymath on it that I can bring to the 2nd Midterm Exam.

_____ I will need to use the computer lab for the 2nd Midterm Exam.
1. Simpson’s Three-eighths rule (4 points)

\[ \int_{x_0}^{x_3} f(x) dx = \frac{3}{8} [f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)] \]

2. \( y = (1 - \alpha W)^{\frac{1}{2}} \)

\[ \frac{dy}{dW} = -\frac{2 \alpha (1 + \varepsilon X) (\frac{T}{T_0})}{2y} \quad \text{where} \quad \alpha = \frac{2 \beta_0}{A_{C} \rho_{C} (1 - \phi) \rho_0}, \quad \text{and} \quad \beta_0 = \frac{C(1 - \phi)}{g_{C} \rho_{C} D_{p} \phi^{3}} \left[ \frac{150(1 - \phi) \mu}{D_{p}} + 1.75G \right] \]

\[ \frac{dy}{dW} = -\frac{2}{2y} \left( \frac{T}{T_0} \right) \left( \frac{T}{T_0} \right) \]

3. Integrals

\[ \int_{0}^{X} \frac{dx}{1 - x} = \ln \frac{1}{1 - x} \]

\[ \int_{0}^{X} \frac{dx}{1 - x} = \frac{1}{x} \ln (1 + \varepsilon X) \]

\[ \int_{0}^{X} \frac{dx}{1 - x} = (1 + \varepsilon) \ln \frac{1}{1 - x} - \varepsilon X \]

\[ \int_{0}^{X} \frac{dx}{ax^{2} + bx + c} = -\frac{2}{2ax + b} + 2 \]

\[ \int_{0}^{X} \frac{dx}{ax^{2} + bx + c} = \frac{1}{a(p - q)} \ln \left( \frac{q}{p} \frac{X - p}{X - q} \right) \]

for \( b^2 > 4ac \) \( \int_{0}^{X} \frac{dx}{1 - x} = \frac{1}{\theta_{B} - 1} \ln \frac{\theta_{B} - X}{\theta_{B}(1 - X)} \quad \text{for} \quad \theta_{B} \neq 1 \)

4. Finite Difference

First Point:

\[ \frac{dC_{A}}{dt} \bigg|_{t_0} = \frac{3 C_{A0} + 4 C_{A1} - C_{A2}}{2 \Delta t} \]

Middle Points:

\[ \frac{dC_{A}}{dt} \bigg|_{t_1} = \frac{C_{A(1+1)} - C_{A(i-1)}}{2 \Delta t} \]

\[ \frac{dC_{A}}{dt} \bigg|_{t_2} = \frac{C_{A(i+1)} - C_{A(i-1)}}{2 \Delta t} \]

e.g.,

\[ \frac{dC_{A}}{dt} \bigg|_{t_3} = \frac{C_{A3} - C_{A4}}{2 \Delta t} = \frac{C_{A4} - C_{A3}}{2 \Delta t} \]

Last Point:

\[ \frac{dC_{A}}{dt} \bigg|_{t_5} = \frac{C_{A4} - 4 C_{A4} + 3 C_{A5}}{2 \Delta t} \]

5. Ideal Gas Constant

\[ R = 8.309 \text{ kPa} \cdot \text{dm}^{3} \text{ mol}^{-1} \text{ K}^{-1} \]

\[ R = 1.987 \text{ BTU} \text{ lb mol}^{-1} \text{ °R}^{-1} \]

\[ R = 0.73 \text{ ft}^{3} \cdot \text{atm} \text{ lb mol}^{-1} \cdot \text{ °R}^{-1} \]

\[ R = 8.3144 \text{ J} \text{ mol}^{-1} \text{ K}^{-1} \]

\[ R = 0.082 \text{ liter} \cdot \text{atm} \text{ mol}^{-1} \cdot \text{ K}^{-1} \]

\[ R = 1.987 \text{ cal} \text{ mol}^{-1} \text{ K}^{-1} \]

Volume of Ideal Gas

1 lb mol of an ideal gas at 32°F and 1 atm occupies 359 ft³.

1 g mol of an ideal gas at 0°C and 1 atm occupies 22.4 dm³.
Chapter 1 Mole Balances

The reaction

\[ A + B \rightarrow 2C \]

takes place in an unsteady PFR. 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 all the mole balances are correct

(a)

\[
F_A 0 - F_A - \int_A^V r_A dV = \frac{dN_A}{dt}
\]

\[
F_B 0 - F_B - \int_A^V r_A dV = \frac{dN_C}{dt}
\]

\[-F_C + 2 \int_A^V r_A dV = \frac{dN_C}{dt}
\]

Ans: Wrong sign for \( r_A \), should be \( + \int_A^V r_A dV \)

(b)

\[
F_A 0 - F_A + \int_A^V r_A dV = \frac{dN_A}{dt}
\]

\[
F_B 0 - F_B + \int_A^V r_A dV = \frac{dN_B}{dt}
\]

\[
F_C + \int_C dV = \frac{dN_C}{dt}
\]

Ans: Wrong sign for \( F_C \), should be \( -F_C \)

(c)

\[
F_A 0 - F_A + \int_A^V r_A dV = \frac{dN_A}{dt}
\]

\[
F_B 0 - F_B + \int_A^V r_A dV = \frac{dN_B}{dt}
\]

\[-F_C - 2 \int_A^V r_A dV = \frac{dN_C}{dt}
\]

Ans: All are correct.

(d)

\[
F_A 0 - F_A - \int_A^V r_A dV = \frac{dN_A}{dt}
\]

\[
F_B 0 - F_B - \int_A^V r_A dV = \frac{dN_B}{dt}
\]

\[-F_C + \int_C dV = \frac{dN_C}{dt}
\]

Ans: Wrong sign for \( -r_A \), should be \( + \int_A^V r_A dV \)

Solution

Answer is (c).
(5 pts) 2) The reaction

\[ A \rightarrow \text{Product} \]

takes place in the gas phase

You have up to $10,000 to use to purchase a reactor from those given below.

<table>
<thead>
<tr>
<th>Reactor Type</th>
<th>Number</th>
<th>Volume (dm(^3))</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>CSTR</td>
<td>1</td>
<td>2</td>
<td>$1,000</td>
</tr>
<tr>
<td>CSTR</td>
<td>1</td>
<td>4</td>
<td>$2,000</td>
</tr>
<tr>
<td>PFR</td>
<td>1</td>
<td>4</td>
<td>$2,000</td>
</tr>
<tr>
<td>CSTR</td>
<td>1</td>
<td>6</td>
<td>$4,000</td>
</tr>
<tr>
<td>CSTR</td>
<td>1</td>
<td>12</td>
<td>$8,000</td>
</tr>
<tr>
<td>PFR</td>
<td>1</td>
<td>12</td>
<td>$6,000</td>
</tr>
</tbody>
</table>

What reactors do you choose, how do you arrange them and what is the highest conversion you can get for $10,000? Approximately what is the corresponding highest conversion \( X = \) ______ with your arrangement of reactors?

Scheme and Volume

---

W13MidTermExamI.doc
Solution

\( X = 0.8 \)
3) **Chapter 3 Rate Laws**
Write the rate law in terms of concentrations for each of the following

(a) The reaction

\[ 4A + 2B \rightarrow 2C \]

follows an elementary rate law. The feed is equal molar in A and B

\[ -r_A = \] 

(b) The reaction

\[ A \rightarrow B + C \]

is pseudo first order at high concentrations of A and pseudo second order at low concentrations of A

\[ -r_A = \] 

(c) The reaction

\[ A + B \rightarrow C \]

is first order in A and overall zero order.

\[ -r_A = \] 

(d) The reaction

\[ A \rightarrow B + C \]

is carried out in a constant volume batch reactor and where the reciprocal of the concentration of A varies linearly with time.

\[ -r_A = \] 

(e) The reaction

\[ A \rightarrow B + C \]

is carried out in a constant volume batch reactor and where the concentration of A decreases linearly with time.

\[ -r_A = \] 

**Solution**

(a) \[ -r_A = k_A \left[ C_A^4 C_B^2 - \frac{C_C^2}{K_C} \right] \]

(b) \[ -r_A = \frac{k_1 C_A^2}{1 + k_2 C_A} \]

(c) \[ -r_A = \frac{k_1 C_A}{C_B} \]

(d) \[ -r_A = k C_A^2 \]

(e) \[ -r_A = k \]
(5 pts) 4) **What four things are wrong with this solution?**

The gas phase elementary reaction

\[ 2A \rightarrow B + 2C \]

\[ C_{t0} = 0.4 \text{ mol dm}^{-3} \]

\[ F_{A0} = 10 \text{ mol s}^{-1} \]

\[ C_{t0} = 0.4 \text{ mol dm}^{-3} \]

\[ F_{A0} = 10 \text{ mol s}^{-1} \]

is carried out in a membrane reactor in which there is pressure drop with \( \alpha = 0.019 \text{ kg}^{-1} \). An equal molar feed of A and inerts, I, enter the reactor and only species B can exit the membrane. Plot the conversion of A down the membrane reactor containing 50 kg of catalyst. The specific reaction rate is \( k_A = 2.5 \text{ dm}^6/\text{mol/kg/s} \), and the mass transfer coefficient \( k_C = 1.5 \text{ dm}^3/\text{kg} \cdot \text{s} \),

**Solution**

**Differential equations**

1. \( \frac{d(F_A)}{d(W)} = r_a \)
2. \( \frac{d(F_B)}{d(W)} = r_b - r_B \)
3. \( \frac{d(F_C)}{d(W)} = r_c \)

**Explicit equations**

1. \( F_t = F_A + F_B + F_C \)
2. \( k_a = 2.5 \)
3. \( C_{t0} = 0.4 \)
4. \( \alpha = 0.019 \)
5. \( \gamma = (1 - \alpha W)^{0.5} \)
6. \( C_B = C_{t0} F_B \gamma / F_t \)
7. \( C_A = C_{t0} F_A \gamma / F_t \)
8. \( r_B = k_a C_A \)
9. \( r_a = -r_B / 2 \)
10. \( r_c = -r_a \)
11. \( k_C = 1.5 \)
12. \( R_B = k_C C_B \)

Identify 4 things that are incorrect or may not be included with this solution?

<table>
<thead>
<tr>
<th>Reads</th>
<th>Should Read</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Line # ___</td>
<td>__________________________</td>
</tr>
<tr>
<td>2. Line # ___</td>
<td>__________________________</td>
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<tr>
<td>3. Line # ___</td>
<td>__________________________</td>
</tr>
<tr>
<td>4. Line # ___</td>
<td>__________________________</td>
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</tbody>
</table>
Actual Solution

1) $r_B = -kC_A$
   should be $r_A = -kC^2_A$

2) $r_A = -\frac{r_B}{2}$
   should be $r_B = -\frac{r_A}{2}$

3) $F_T = F_A + F_B + F_C$
   should be $F_T = F_A + F_B + F_C + F_I$

4) $y = (1 - \alpha w)^{1/2}$
   should be $\frac{dy}{dW} = -\frac{\alpha}{2y} \frac{F_T}{F_{T0}}$
Problem Statement. The elementary gas phase reaction

\[ A + 2B \rightarrow C \]

is carried out in a packed bed reactor. Calculate the exit conversion from a PBR packed with 800 kg of catalyst. The feed is stoichiometric.

Additional Information

\[ \alpha = 0.001 \text{ kg}^{-1} \]

\[ C_{A0} = 0.04 \text{ mol/dm}^3 \]

\[ k = 3.0 \text{ dm}^6/\text{mol}^2 \cdot \text{s} \]

\[ v = 20 \text{ dm}^3/\text{s} \]

Solution

1) The rate law is incorrect. It should be:

\[ \frac{d(X)}{d(W)} = -\text{raprime}/Fa_0 \]

Reads

\[ k = 3 \]

Should Read

\[ k = 3 \]

What four things are wrong or may not be included with this solution?

| Line # | Reads                                      | Should Read
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>[ d(X)/d(W) = -\text{raprime}/Fa_0 ]</td>
<td>[ d(X)/d(W) = -\text{raprime}/Fa_0 ]</td>
</tr>
<tr>
<td>2</td>
<td>[ k = 3 ]</td>
<td>[ k = 3 ]</td>
</tr>
<tr>
<td>3</td>
<td>[ C_{A0} = 0.04 ]</td>
<td>[ C_{A0} = 0.04 ]</td>
</tr>
<tr>
<td>4</td>
<td>[ \alpha = 0.001 ]</td>
<td>[ \alpha = 0.001 ]</td>
</tr>
<tr>
<td>5</td>
<td>[ v = 20 ]</td>
<td>[ v = 20 ]</td>
</tr>
</tbody>
</table>

Solution

1) The rate law is incorrect. It should be:
2) The concentrations are incorrect, the feed is stoichiometric.

\[ \dot{Q} = 2 \]

3) The volume change was not included.

\[
\begin{align*}
v &= v_o(1+\varepsilon X)\frac{P}{P_0} \frac{T}{T_0} = v_o(1+\varepsilon X) \\
\varepsilon &= y_A \delta = \frac{1}{3} (1-1-2) = -\frac{2}{3} \\
C_A &= C_{A0} \left[ \frac{(1-X)}{\left( \frac{1}{3} \right)^2} \right] = \frac{2C_{A0}(1-X)}{(1-\frac{2}{3}X)}
\end{align*}
\]

4) The equation for \( y \) is incorrect. There is volume change and \( y = \left( 1 - \alpha \frac{W}{W_0} \right)^{1/2} \) can only be used when \( \varepsilon = 0 \). Therefore, the form of the momentum balance that must be used is

\[
\frac{dy}{dw} = -\frac{\alpha(1+\varepsilon X)}{2y}
\]

Corrected Solution

\[
\begin{align*}
\text{Equations:} \\
d(y)/d(W) &= -\alpha/2/y*(1+\varepsilon*X) \\
d(X)/d(W) &= -\text{raprime}/\text{Fao} \\
\alpha &= 0.001 \\
\varepsilon &= -2/3 \\
k &= 3 \\
C_{A0} &= 0.04 \\
vo &= 20 \\
\text{Fao} &= C_{A0}*vo \\
Ca &= C_{A0}*(1-X)*y/(1+\varepsilon*X) \\
Cb &= C_{A0}*(1-X)*y/(1+\varepsilon*X) \\
\text{raprime} &= -k*C_a*C_b^2 \\
W_0 &= 0, \quad W_f = 800
\end{align*}
\]
(5 pts) 6) **Chapter 7: Analysis of Data**

(2 pts) 6a) From the following plot, what is the reaction order with respect to A?

Circle the correct answer.

A) 0  
B) 0.5  
C) 0.78  
D) 1  
E) 2

Explain

---

**Solution**

D) 1

Slope = 1.01 \approx 1

(3 pts) 6b) The following reaction, batch experiments are conducted to evaluate the reaction kinetics. The slope of a ln (r_B) versus ln (C_B) plot is measured to be 1.02 and the intercept is 0.42 when A is in great excess. What is the *overall* reaction order?

\[ A + 2B \rightarrow \text{Products} \]

Circle the correct answer.

A) 0.42  
B) 1.02  
C) 1.44  
D) Can’t tell on the basis of this experiment

Explain

---
Solution

D) Can’t tell on the basis of this experiment

\[-r_A = \frac{-r_B}{2} = kC_A^\alpha C_B^\beta = \ln\left(\frac{-r_B}{2}\right) = \ln k + \alpha \ln C_A + \beta \ln C_B\]

Both \(C_A\) and \(C_B\) vary, need to find \(\alpha\) by varying \(C_A\)
Chapter 4 Stoichiometry

The reversible reaction

\[ 2A \rightleftharpoons B \]

is carried out in a flow reactor where pure A is fed at a concentration of 4.0 mol/dm\(^3\). If the equilibrium conversion is found to be 60%

(a) What is the equilibrium constant, \(K_C\) if the reaction is a gas phase reaction?

Gas \( K_C = \) ____________

(b) What is the \(K_C\) if the reaction is a liquid phase reaction?

Liquid \( K_C = \) ____________

**Solution**

(a) Gas

\[-r_A = k \left( C_A^2 - \frac{C_B}{K_C} \right) \]

At equilibrium, \(-r_A = 0\)

\[ K_{Ce} = \frac{C_{Be}}{C_{Ae}^2} \]

\[ \delta = \frac{1}{2}-1 = -\frac{1}{2}, y_{A0} = 1, \varepsilon = -\frac{1}{2} \]

\[ C_A = C_{A0} \left[ \frac{(1 - X_e)}{(1 + \varepsilon X_e)} \right] \]

\[ C_B = C_{B0} \left[ \frac{\frac{1}{2}X_e}{(1 + \varepsilon X_e)} \right] \]

\[ K_{Ce} = \frac{C_{A0}^2 \left[ \frac{\frac{1}{2}X_e}{(1 + \varepsilon X_e)} \right]}{C_{A0}^2 \left[ \frac{(1 - X_e)}{(1 + \varepsilon X_e)} \right]^2} = \frac{X_e (1 + \varepsilon X_e)}{2C_{A0} (1 - X_e)^2} \]

\[ = \frac{X_e (1 - 0.5X_e)}{2C_{A0} (1 - X_e)^2} = \frac{0.6(0.7)}{8(0.4)^2} = 0.328 \text{ dm}^3 / \text{mol} \]

(b) Liquid

\[-r_A = k \left( C_A^2 - \frac{C_B}{K_C} \right) \]

At equilibrium, \(-r_A = 0\)

\[ K_{Ce} = \frac{C_{Be}}{C_{Ae}^2} \]
\[ C_A = C_{A0} \left( 1 - X \right) \]
\[ C_B = C_{A0} \frac{1}{2} X \]
\[ K = \frac{C_{A0} \left[ \frac{1}{2} X_e \right]^3}{C_{A0} \left( 1 - X_e \right)^3} \]
\[ = \frac{X_e}{2C_{A0}} \left( 1 - X_e \right)^3 \]
\[ = \frac{0.6}{8(0.4)^3} \]
\[ = 0.469 \text{ dm}^3 / \text{mol} \]
8) **Multiple Choice (15 points)**

(3 pts) 8a) A reversible, liquid-phase reaction that is first order in both directions proceeds to 50% conversion in a PFR operating isothermally, isobarically, and at steady state. What conversion would be obtained in a CSTR with the same volume and feed stream and operating at exactly the same temperature and pressure?

(A) X > 50%  
(B) X < 50%  
(C) 50%  
(D) insufficient information to answer definitively

Reason: __________________________________________________________

__________________________

**Solution**

8a) Answer: (B) X < 50%

(3 pts) 8b) The gas reaction A + B → C is carried out in a packed bed where there is pressure drop. Currently 40% conversion is achieved. If the catalyst weight remains the same, but the particle size is increased, then the conversion would

(A) increase  
(B) decrease  
(C) remain the same  
(D) insufficient information to tell. You don’t know which part of the curve you are on.

Reason: __________________________________________________________

__________________________

**Solution**

8b) Answer: (D) insufficient information to tell. You don’t know which part of the curve you are on.

(3 pts) 8c) For an irreversible second order reaction 50% conversion is currently achieved in one PFR of 1,000 dm³. It is proposed to use two 500 dm³ PFRs placed in series. The exit conversion for the two PFRs will be

(1) > 50%  
(2) 50%  
(3) 50% <  
(4) Can’t tell without the rate law
Solution

8c) Answer: (2) 50%

![Diagram of 1 PFR and 2 PFRs]

(3 pts) 8d) The rate constant for an irreversible, heterogeneously catalyzed, gas-phase, second order reaction, A → Product(s), was determined to be 0.234 from experimental data in a packed-bed reactor. The person analyzing the experimental failed to include the large pressure drop in the reactor in his analysis. If the pressure drop were properly accounted for, the rate constant would be

(1) >0.234  (2) < 0.234  (3) 0.234  (4) insufficient information to answer definitively

Solution

8d) Answer: (1) >0.234

\[-r_A = kC_{A0}^2 \left(1 - X \right)^2 y^2\]

\[-r_A \propto ky^2\]

\[y^2 < 1\]

\[k^{true} y^2 = k = 0.234\]

\[k^{true} = \frac{0.234}{y^2} > 0.234\]
(3 pts) 8e) Consider the reaction

\[ A \rightarrow B \]

If the diameter of a PBR is doubled while keeping the turbulent flow mass flow rate, \( \dot{m} \), constant, what can be said about that factor by which the rate of pressure drop (dy/dW) will be lowered?

Circle the correct answer.

A) It will be lowered by a factor of 4  
B) It will be lowered by a factor of 16  
C) It will be lowered by a factor of 32  
D) It will be lowered by a factor of 48 or more

Explain

\[ \alpha \sim \frac{\dot{m}}{AC} \sim \frac{\pi}{D^2} \]

\[ \alpha_{2} = \alpha \left( \frac{D_1}{D_2} \right)^6 = \alpha_1 \left( \frac{1}{2} \right)^6 = \frac{\alpha_1}{64} \]

Solution

8e) Answer: D  
It will be lowered by more than a factor of 48.
Study Problem P5-20\textsubscript{B}, Modified California Problem

The elementary gas phase reaction

\[ A + B \rightarrow C + D \]

takes place isobarically and isothermally in a PFR where 50% conversion is achieved. The feed is equimolar in A and B. It is proposed to put a CSTR of equal volume upstream, i.e., of the PFR. What will be the intermediate and exit conversions \( X_1 \) and \( X_2 \) respectively? The entering flow rates and all other variables remain the same as that for the single PFR.

\[
X_1 = \boxed{\text{_______}}
\]

\[
X_2 = \boxed{\text{_______}}
\]

Solution

Case 1

Mole Balance

\[
\frac{dX}{dV} = -r_A
\]

Rate Law

\[-r_A = kC_A C_B\]

Stoichiometry

Gas \( \delta = 0, \ \Theta_B = 1 \)

\[
C_A = C_{A0}(1 - X)
\]

\[
C_B = C_{A0}(1 - X)
\]

Combine

\[-r_A = kC_{A0}^2(1 - X)^2\]

\[
\frac{dX}{dV} = \frac{kC_{A0}^2 (1 - X)^2}{F_{A0}}
\]

\[
\frac{dX}{(1 - X)^2} = \frac{kC_{A0}^2}{F_{A0}} dV
\]

\[
V = 0, \ X = 0
\]

\[
V = V, \ X = 0.5
\]
\[
\int_{0}^{X} \frac{dX}{(1-X)^2} = \frac{X}{1-X} = \frac{kC_{A0}^2 V}{F_{A0}}
\]

\[
kC_{A0}^2 V = \frac{0.5}{1-0.5} = 1
\]

Case 2

(1) \( V_{\text{CSTR}} = \frac{F_{A0}X}{-r_A} \)

(2) & (3) Rate Law, Stoichiometry same as Case 1

\[
V_{\text{CSTR}} = \frac{F_{A0}X_1}{kC_{A0}^2(1-X_1)^2}
\]

\[
VkC_{A0}^2 = 1 = \frac{X_1}{1-2X_1 + X_1^2}
\]

\[
1 - 2X_1 + X_1^2 = X_1
\]

\[
X_1^2 - 3X_1 + 1 = 0
\]

\[
X_1 = \frac{3 \pm \sqrt{9 - 4}}{2} = \frac{3 - \sqrt{5}}{2} = \frac{3 - 2.24}{2} = 0.38
\]

PFR \( X_1 = 0.38 \)

\[
\frac{dX}{dV} = \frac{kC_{A0}^2(1-X)^2}{F_{A0}}, \quad \int_{X_1}^{X_2} \frac{dX}{(1-X)^2} = \frac{kC_{A0}^2 V}{F_{A0}}
\]

\[
V = 0 \quad X = X_1 = 0.38
\]

\[
V = V \quad X = X_2
\]

\[
kC_{A0}^2 V = 1 = \frac{1}{1-X_2} - \frac{1}{1-X_1}
\]

\[
\frac{1}{1-X_2} = 1 + \frac{1}{1-X_1} = 1 + \frac{1}{0.62} = 2.62
\]

\[
1 - X_2 = 0.38
\]

\[
X_2 = 0.62
\]
(25 pts) 10) Study problem P5-9b. The gas phase reaction
\[
A \rightarrow B + C
\]
follows an elementary rate law and is to be carried out first in a PFR and then in a separate experiment in a CSTR. When Pure A is fed to a 10 dm³ PFR at 300K and a volumetric flow rate of 5 dm³/s the conversion is 80%.

When a mixture of 50% A and 50% inert (I) is fed to a 10 dm³ CSTR at 320K and a volumetric flow rate of 5 dm³/s the conversion is 80%.

What is the activation energy in cal/mol?
\[
E = \underline{\text{__________________}}
\]

Solution
PFR
\[
\frac{dX}{dV} = - \frac{r_A}{F_{A0}} = \frac{kC_{A0}(1-X)}{C_{A0}v_0(1+\varepsilon X)} = \frac{k(1-X)}{v_0(1+\varepsilon X)}
\]

\[
\int X \frac{(1+\varepsilon X)}{(1-X)} \, dX = \int k \frac{dV}{v_0} = k\tau
\]

\[
k = \frac{1}{\tau} \left[ \left(1+\varepsilon\right) \ln \frac{1}{1-\varepsilon X} \right]^{-\varepsilon X}
\]

\[
\tau = \frac{10\text{dm}^3}{5\text{dm}^3/\text{s}} = 2\text{s}
\]

\[
\varepsilon = y_{A0}\delta = 1(1+1-1) = 1
\]

\[
k = \frac{1}{2} \left[ \left(1+1\right) \ln \left(\frac{1}{1-0.8}\right) - 0.8 \right]
\]

\[
k = \frac{1}{2}[2 \times 1.61 - 0.8] = 1.209 \text{ at 300K}
\]

CSTR
\[
V = - \frac{r_A}{r_A} = \frac{v_0C_{A0}X}{kC_{A0}(1-X) = \frac{v_0X(1+\varepsilon X)}{k(1-X)}}
\]

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\[ \varepsilon = \frac{1}{2}(1+1-1) \]

\[ \varepsilon = 0.5 \]

\[ k = \frac{1}{\tau} \frac{X(1 + \varepsilon X)}{(1 - X)} = \frac{1}{2} \left( \frac{0.8(1 + 0.5(0.8))}{0.2} \right) \]

\[ = 2.8 \]

\[ \ln \frac{k_2}{k_1} = \frac{E}{R} \left[ \frac{1}{T_1} - \frac{1}{T_2} \right] \]

\[ \ln \frac{2.8}{1.21} = \frac{E}{R} \left[ \frac{1}{300} - \frac{1}{320} \right] = \frac{20}{R \cdot (320)(300)} \]

\[ E = R \left( \frac{300)(320)}{20} \right) \ln \frac{2.8}{1.21}, \quad R = 1.987 \text{ cal/mol}^\circ \text{K} \]

\[ E = 8010 \text{ cal/mol} \]