

CHME 4500  
Fall 2013

**Chemical Reactor Design**  
**Exam #1(solutions): Chapters 1 – 5**  
**26 September 2013, 12:00-1:50 pm**

Bequette  
26 September 2013

Make sure there are four (4) questions in your exam packet. There is a final page containing some relevant formulas that may be useful on the exam. Only use paper attached to this exam – ask the TAs for more paper if required.

This is a closed-book exam. The only materials allowed are one double-sided, hand-written cribsheet, writing instruments, and a calculator. No laptops are allowed.

This exam is completely self-contained. Please state all assumptions and clearly mark all answers. If you feel you need to define a variable or constant to solve a problem, do so and make it clear.

You have 1 hour and 50 minutes. *Please staple your cribsheet to this exam when you turn it in.*

Good Luck

<b>Problem</b>	<b>Points</b>
<b>#1 (25 pts)</b>	
<b>#2 (25 pts)</b>	
<b>#3 (25 pts)</b>	
<b>#4 (25 pts)</b>	
<b>TOTAL:</b>	

By signing my name below, I am stating that the work contained within this exam is the product of my efforts and my efforts alone; that at no time did I receive or seek out help from anyone while completing the exam.

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(Student's name and signature)

1. (25 points) A Levenspiel plot for an interesting flow system is shown below (note that the units of the y-axis is gallons). This problem has two pages.

a. If a single CSTR of 0.7 gallons is used, what will be the conversion? Show your calculations here and draw appropriate lines on the plot below.

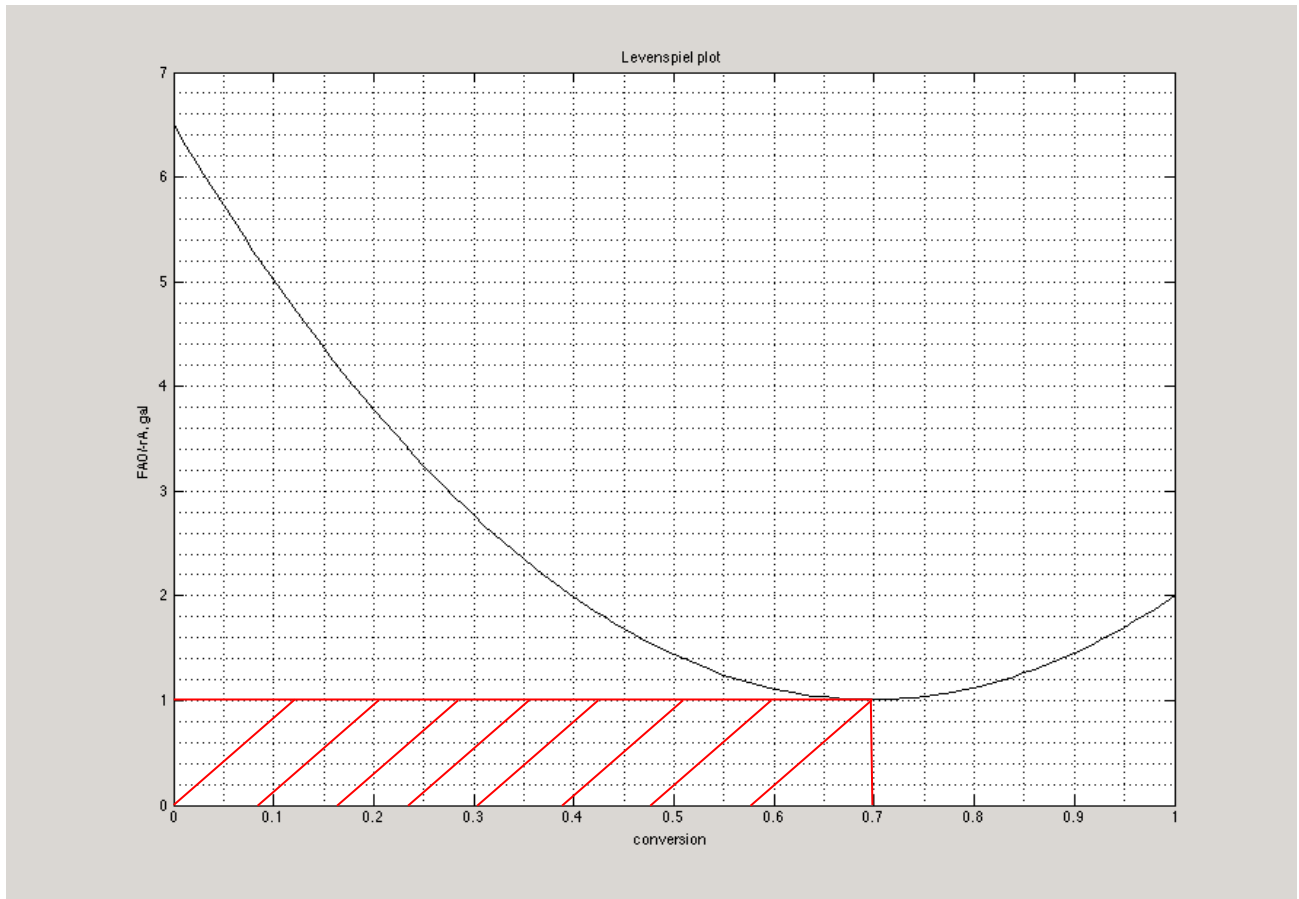
Given volume of a CSTR is 0.7 gallons.

Hence, from the plot, area of the rectangle should be 0.7 gallons ( $-F_{AO}/r_A \times X$ )

Clearly, for  $X = 0.7$ ,  $-F_{AO}/r_A$  from the y-axis is 1 gallon.

The area of the rectangle shown in the graph below is:  $0.7 \times 1.4 = 0.7$ , which is the volume of the CSTR.

Thus, the conversion from a 0.7 gallons CSTR is 70 %



part (b) on the next page.

**b.** If a single plug flow reactor is used, what volume is required to achieve a conversion of 0.7? Show your calculations here and your work on the Levenspiel plot below.

The volume of PFR required for a 70% conversion is equal to the area under the curve of a Levenspiel plot, from  $X = 0$  to  $X = 0.7$ . The required area is marked in the plot below.

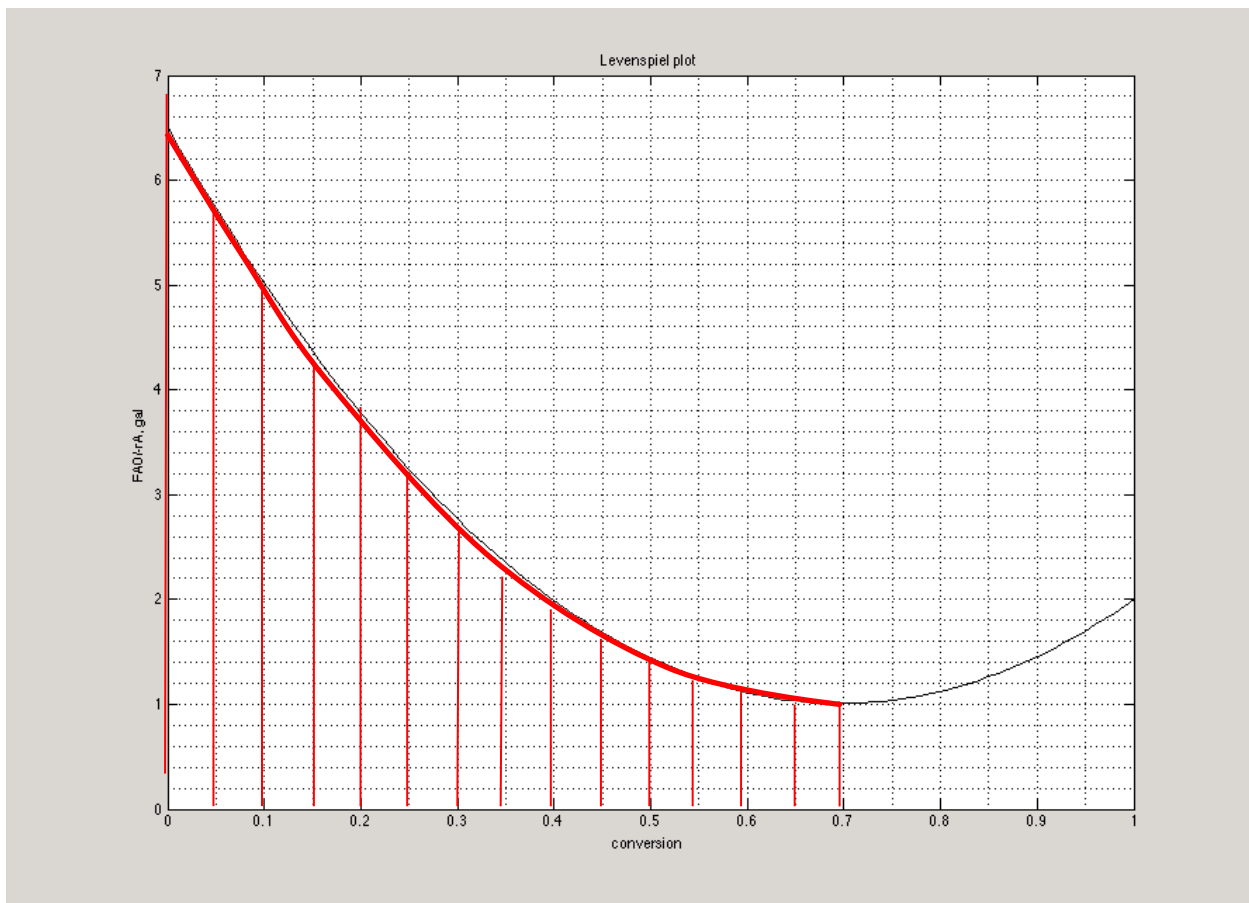
For calculating the area, Simpson's 1/3<sup>rd</sup> rule is used:

$$X_1 = 0; \quad X_3 = 0.7; \quad h = (X_2 - X_1)/2 = 0.35; \quad X_2 = X_1 + h = 0.35$$

$$\text{Area} = h/3 [(-F_{AO}/r_A)_{X_1} + 4(-F_{AO}/r_A)_{X_2} + (-F_{AO}/r_A)_{X_3}] = 0.35/3 [6.5 + 4 \times 2.3 + 1] = 1.95$$

(Values taken from the plot)

Hence the volume of PFR required is 1.95 gallons



2. (25 pts) You are responsible for the design of a gas-phase packed-bed reactor and are concerned about the pressure drop across the reactor. Neglecting the effect of conversion, and using (where  $y = P/P_0$ ), a known value of  $\alpha = 0.01 \text{ kg}^{-1}$

$$\frac{dy}{dW} = -\frac{\alpha}{2y}$$

a. What is the absolute maximum amount of catalyst that could be used? State your assumptions analyze and show your work.

The absolute maximum amount of catalyst can be found for a hypothetical situation where the outlet pressure is zero ( $P = 0$ ).

$$\text{Or } y = P/P_0 = 0$$

From the appendix, the analytical solution is:  $y = (1 - \alpha W)^{1/2}$

$$\text{Or } W = (1/\alpha)(1 - y^2)$$

Thus, the absolute maximum catalyst weight is  $W = (1/0.01)(1-0^2) = 100 \text{ kg}$

b. If the dimensionless pressure ratio at the reactor outlet is 0.2, what is the maximum amount of catalyst that can be used?

Given that  $y = 0.2$

The maximum amount of catalyst that can be used is  $W = (1/\alpha)(1 - y^2)$  (from part (a))

$$\text{Or } W = (1/0.01)(1-0.2^2) = 96 \text{ kg}$$

c. Now consider each of the following stoichiometric reactions. For each one, indicate whether you expect the actual pressure drop to be greater than, equal to, or less than the analytical solution, and discuss why.

i.  $A \rightarrow B$

The stoichiometric coefficients suggest that 1 mol of a gaseous reactant yields 1 mol of a gaseous product. Hence the pressure *drop* is not expected to change. For the given reaction,

$$\delta = 1-1 = 0 \text{ and hence } \varepsilon = 0 \quad (\text{assuming a feed of pure A})$$

The actual system is expected to have a pressure *drop* equal to the analytical solution, which assumes  $\varepsilon = 0$ .

ii.  $A \rightarrow 2B$

The stoichiometric coefficients suggest that 1 mol of a gaseous reactant yields 2 mols of a gaseous product. Hence the pressure drop is expected to increase compared to the analytical solution. . For the given reaction,

$$\delta = 2 - 1 = 1 \text{ and hence } \varepsilon = 1 \text{ (positive } \varepsilon) \quad (\text{assuming a feed of pure A})$$

The analytical solution, that assumes  $\varepsilon = 0$ , would thereby yield a pressure drop less than what the actual pressure drop should be.

iii.  $A \rightarrow 1/2 B$

The stoichiometric coefficients suggest that 1 mol of a gaseous reactant yields 0.5 mols of a gaseous product. Hence the pressure *drop* is expected to decrease compared to the analytical solution. For the given reaction,

$$\delta = 1/2 - 1 = -1/2 \text{ and hence } \varepsilon = -1/2 \text{ (negative } \varepsilon \text{)} \quad \text{(assuming a feed of pure A)}$$

The actual pressure *drop* will then be less than that predicted by the analytical solution, which assumes  $\varepsilon = 0$ .

3. (25 pts) Consider an irreversible **second-order** reaction,  $2A \rightarrow B$  (with rate,  $-r_A = kC_A^2$ ) that has been carried out in a batch reactor. The initial concentration is 1 mol/liter, and after 30 minutes the concentration is 0.25 mol/liter.

What is the value of the second-order rate constant? Show units.

Given: Irreversible second-order reaction:  $-r_A = kC_A^2$

Batch reactor;  $C_{A0} = 1$  mol/liter;  $C_A = 0.25$  mol/liter after time(t) = 30 min

Now, for a batch reactor, the rate equation is written as:

$$\frac{dC_A}{dt} = -kC_A^2 \quad \text{or} \quad \frac{dC_A}{C_A^2} = -kdt$$

Integrating within limits ( $C_{A0}$  for  $t=0$  and  $C_A$  for  $t=t$ )

$$\int_{C_{A0}}^{C_A} \frac{dC_A}{C_A^2} = \int_0^t -k dt$$

$$\left[ \frac{1}{C_{A0}} - \frac{1}{C_A} \right] = -kt$$

$$k = \frac{1}{t} \left[ \frac{1}{C_A} - \frac{1}{C_{A0}} \right]$$

Plugging in the values,

$$k = 0.1 \text{ liter mol}^{-1}\text{min}^{-1}$$

Now, the reaction is to be conducted in a plug flow reactor, with a feed concentration of 1 mol/liter and a flowrate of 2 liters/minute. To achieve an outlet concentration of 0.25 mol/liter, what should be the volume of the PFR? Show your work.

Given: Irreversible second-order reaction:  $-r_A = kC_A^2$

PFR;  $C_{A0} = 1$  mol/liter;  $C_A = 0.25$  mol/liter at reactor outlet;  $v_0 = 2$  liters/min

The PFR design equation is:

$$\frac{dF_A}{dV} = r_A = -kC_A^2$$

Assuming a liquid phase reaction,  $v_0$  remains constant.

$$\text{Also, } F_A = C_A v_0$$

Thus, the differential equation becomes,

$$\frac{dC_A}{dV} = -\frac{kC_A^2}{v_0}$$

or 
$$\frac{dC_A}{C_A^2} = -\frac{k}{v_0} dV$$

Integrating within limits ( $C_{A0}$  for  $V=0$  and  $C_A$  for  $V=V$ )

$$\int_{C_{A0}}^{C_A} \frac{dC_A}{C_A^2} = \int_0^V -\frac{k}{v_0} dV$$

$$\left[ \frac{1}{C_{A0}} - \frac{1}{C_A} \right] = -\frac{k}{v_0} V$$

$$V = \frac{v_0}{k} \left[ \frac{1}{C_A} - \frac{1}{C_{A0}} \right]$$

Plugging in the value of  $k$  from the previous part and the values of  $v_0$ ,  $C_{A0}$  and  $C_A$

$V = 60 \text{ liters}$
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4. (25 pts) You are a manager of a process engineering group and you have asked one of your young process engineers to determine the conversion in a CSTR, for a reaction system that is expected to be irreversible with first order kinetics  $A \rightarrow B$ . The value of the rate constant is  $1 \text{ hr}^{-1}$ . The engineer has determined that, at steady-state, with a residence time of 1 hour, the conversion will be 50%.

a. Confirm this result. Show all of your work.

Given: CSTR; Irreversible reaction; First order kinetics ( $-r_A = kC_A$ );  $k = 1 \text{ hr}^{-1}$ ;  $\tau = 1 \text{ hour}$ ;  $X = 0.5$  (50%)

Design equation for a CSTR in terms of conversion:

$$\frac{F_{A0}X}{-r_A} = V = \frac{F_{A0}X}{kC_A} \dots\dots\dots(1)$$

Assuming a liquid phase reaction,

$$F_{A0} = C_{A0} v_0 \text{ and } C_A = C_{A0}(1-X)$$

Making the substitutions, Eq (1) reduces to:

$$\frac{X}{1-X} = \frac{V}{v_0} k = \tau k = 1$$

Solving for X, we get, X = 0.5 or 50% conversion thereby confirming the result.

b. It turns out that the rate constant and irreversible assumption is only true for low conversions. An experimental CSTR, with a residence time of 1 hour results in a conversion of only 25%. Assuming that the first-order rate constant is correct, but that **the reaction is reversible**, what is the value of the reaction equilibrium constant  $K_C$ ? Show your work.

Given: CSTR;  $\tau = 1$  hour;  $X = 0.25$  (25%);  $k = 1 \text{ hr}^{-1}$ ; Reaction is reversible  
To find:  $K_C$  the equilibrium constant

For the reversible reaction, the rate expression can be written as:

$$-r_A = k\left[C_A - \frac{C_B}{K_C}\right]$$

Design equation for a CSTR in terms of conversion:

$$\frac{F_{AO}X}{-r_A} = V = \frac{F_{AO}X}{k\left[C_A - \frac{C_B}{K_C}\right]} \dots \dots \dots (2)$$

Assuming a liquid phase reaction, with a feed of pure A ( $\Theta_B = 0$ )

$$F_{AO} = C_{AO} v_0 ; C_A = C_{AO}(1-X) \text{ and } C_B = C_{AO}X$$

Making the substitutions, Eq (2) reduces to:

$$\frac{X}{k\left[(1-X) - \frac{X}{K_C}\right]} = \frac{V}{v_0} = \tau$$

Putting  $X = 0.25$  and solving for  $K_C$ ,

$K_C = 0.5$
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## Appendix

Gas phase pressure drop across packed bed reactors. Recall that the differential equation for dimensionless pressure,  $y = P/P_0$ , as a function of conversion (X) and catalyst mass (W) is

$$\frac{dy}{dW} = -\frac{\alpha}{2y}(1 + \varepsilon X)$$

$$\varepsilon = \delta y_{A0}$$

$$\delta = \frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1 \quad \text{for the stoichiometry, } aA + bB \rightarrow cC + dD$$

If the  $\varepsilon X$  term can be neglected, the simplified expression is

$$\frac{dy}{dW} = -\frac{\alpha}{2y}$$

which has the analytical solution

$$y = (1 - \alpha W)^{1/2}$$