Team: Jeremy, Zach, Ryan, Dai

Homework 2 – Due 10/16/20

Jeremy · Hook

1) An irreversible reaction has the stoichiometry:

$$3A + 0.5B \rightarrow 2C + D$$

What is the relationship between r_A, r_B r_C and r_D?

2) You are a Chemical Engineer working at NASA in Houston, Texas. You are part of the team preparing to launch the next space shuttle towards Mars. The goal of the mission is to see if life can occur on Mars. It is critical to have a specific secret compound Z to be able to test life and it must be synthesized immediately prior to testing due to its short lifetime. Therefore, it will be generated directly on the shuttle! The maximum amount of volume in the space shuttle is 84.3 m^3. The reaction to form Z occurs in the liquid phase:

$$A + B + C \rightarrow Z$$

On earth, in your lab you are trying to find the best conditions for your reactor. Your team members carry out the reaction at T = 300 K in a CSTR reactor.

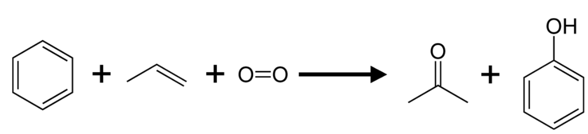
a. Assuming that the reaction is elementary what is the overall order *n* of the reaction and what is the rate law of formation of A?

b. Your team members know that the reaction rate constant is $k(T = 300K) = 0.1\ \mathrm{M}^{1-n}/\mathrm{hr}$. They plan on having a continuous equimolar feed of reactants (same for A, B, and C). Specifically, $C_A = 1.67$ M with a volumetric flow rate $\nu = 400\ \mathrm{L \cdot hr^{-1}}$. You will need at least 80% conversion of reactant A on your space shuttle reactor. Compute the volume that a CSTR would need to reach that conversion.

c. Will it be possible to bring the reactor on the space shuttle given that the seven astronauts on the trip will occupy 7 m^3 ? If not, what would you change as a chemical engineer to reduce the required volume (e.g., changing reactors types and/or operating parameters)?

3) Jonathan van Ness is fed up with his nail polish color and wants to remove it. He is so rich that he has his own chemical engineering plant at home to generate all the materials he desires. He asks you, the team leader, to generate more acetone and to have enough ready for him and his fans to take on his weekend trip to the Superbowl 2021 game. He is willing to purchase both a PFR and CSTR if necessary.

The reaction is



From your first trials in a set of two continuous flow reactors you obtain the following experimental data (B stands for the Benzene):

Conversion X_B	0	0.1	0.2	0.4	0.6	0.8
$F_{B0}/-r_B$ [L]	0.9	1.1	1.8	3.5	4.5	6.5

a. Graphically estimate the overall conversion if the reaction is carried out in a single $V = 2.0\ \mathrm{m}^3$ CSTR?

b. What is the overall conversion if the reaction is carried out in a single $V = 2.0\ \mathrm{m}^3$ PFR? (Suggestion: use the trapezoidal rule to integrate.)

c. What is the overall conversion if the reaction is carried out in a $V_1 = 2.0\ \mathrm{m}^3$ PFR followed by a $V_2 = 2.0\ \mathrm{m}^3$ CSTR?

d. What is the overall conversion if the reaction goes through the CSTR first, then the PFR?

e. What will Jonathan van Ness need to purchase in order get maximum conversion, a PFR, a CSTR, both?

4) You are designing a reactor to carry out an irreversible reaction A → 2B + 2C. You want to determine the optimal type of reactor to use. You decide that you will have an inflow of material F_{A0}= 180 mol/min. You have performed laboratory scale experiments and collected some data on the system:

X_A	0	0.2	0.4	0.5	0.6	0.8	0.9
$-r_A$ [mol L^{-1}min^{-1}]	2.0	4.0	10.0	12.0	8.5	3.5	3.0

a. Create a Jupyter notebook and use Python to construct a Levenspiel plot of the data. For all your plots, be sure to label the axes appropriately (don't forget units!), give it a title, and include a legend.

b. You desire 60% conversion of the reactant. Compute the volume for a CSTR this would require. Compute the volume for a PFR this would require.
Suggestion: Use the `numpy.trapz()` function to find a numerical solution to the integral. (For more information on the function see the documentation available at https://docs.scipy.org/doc/numpy/reference/generated/numpy.trapz.html).

c. For each of the above points, describe what you are coding in Markdown cells and explain why you believe this makes sense.

d. Print out the Jupyter notebook that you used to create your plots and calculate your values.

1) An irreversible reaction has the stoichiometry:

$$3A + 0.5B \rightarrow 2C + D$$

What is the relationship between r_A, r_B r_C and r_D?

SUMMARY

1. Relative rates of reaction for the generic reaction:

$$A + \frac{b}{a}B \rightarrow \frac{c}{a}C + \frac{d}{a}D \quad \text{(S3-1)}$$

The relative rates of reaction can be written either as

$$\boxed{\frac{-r_A}{a} = \frac{-r_B}{b} = \frac{r_C}{c} = \frac{r_D}{d}} \quad \text{or} \quad \boxed{\frac{r_A}{-a} = \frac{r_B}{-b} = \frac{r_C}{c} = \frac{r_D}{d}} \quad \text{(S3-2)}$$

2. *Reaction order* is determined from experimental observation:

$$A + B \longrightarrow C \quad \text{(S3-3)}$$

$$-r_A = kC_A^{\alpha}C_B^{\beta}$$

The reaction in Equation (S3-3) is α order with respect to species A and β order with respect to species B, whereas the overall order, n, is $(\alpha + \beta)$. If $\alpha = 1$ and $\beta = 2$, we would say that the reaction is first order with respect to A, second order with respect to B, and overall third order. We say a reaction follows an elementary rate law if the reaction orders agree with the stoichiometric coefficients for the reaction as written.

Examples of reactions that follow an elementary rate law:

Irreversible reactions

First order

$$C_2H_6 \longrightarrow C_2H_4 + H_2 \qquad \boxed{-r_{C_2H_6} = kC_{C_2H_6}}$$

Second order

$$CNBr + CH_3NH_2 \longrightarrow CH_3Br + NCNH_2 \qquad \boxed{-r_{CNBr} = kC_{CNBr}C_{CH_3NH_2}}$$

$$\boxed{\frac{-r_A}{3} = \frac{-r_B}{.5} = \frac{r_C}{2} = \frac{r_D}{1}}$$

2) You are a Chemical Engineer working at NASA in Houston, Texas. You are part of the team preparing to launch the next space shuttle towards Mars. The goal of the mission is to see if life can occur on Mars. It is critical to have a specific secret compound Z to be able to test life and it must be synthesized immediately prior to testing due to its short lifetime. Therefore, it will be generated directly on the shuttle! The maximum amount of volume in the space shuttle is 84.3 m^3. The reaction to form Z occurs in the liquid phase:

$$A + B + C \rightarrow Z$$

On earth, in your lab you are trying to find the best conditions for your reactor. Your team members carry out the reaction at T = 300 K in a CSTR reactor.

a. Assuming that the reaction is elementary what is the overall order n of the reaction and what is the rate law of formation of A?

b. Your team members know that the reaction rate constant is $k(T = 300K) = 0.1\ \mathrm{M}^{1-n}/\mathrm{hr}$. They plan on having a continuous equimolar feed of reactants (same for A, B, and C). Specifically, $C_A = 1.67$ M with a volumetric flow rate $v = 400\ \mathrm{L \cdot hr^{-1}}$. You will need at least 80% conversion of reactant A on your space shuttle reactor. Compute the volume that a CSTR would need to reach that conversion.

c. Will it be possible to bring the reactor on the space shuttle given that the seven astronauts on the trip will occupy 7 m^3 ? If not, what would you change as a chemical engineer to reduce the required volume (e.g., changing reactors types and/or operating parameters)?

The dependence of the reaction rate, $-r_A$, on the concentrations of the species present, fn(C_j), is almost without exception determined by experimental observation. Although the functional dependence on concentration may be postulated from theory, experiments are necessary to confirm the proposed form. One of the most common general forms of this dependence is the *power law model*. Here the rate law is the product of concentrations of the individual reacting species, each of which is raised to a power, for example,

$$\boxed{-r_A = k_A C_A^{\alpha} C_B^{\beta}} \quad (3\text{-}3)$$

The exponents of the concentrations in Equation (3-3) lead to the concept of *reaction order*. The **order of a reaction** refers to the powers to which the concentrations are raised in the kinetic rate law.[1] In Equation (3-3), the reaction is *α order with respect to reactant* A, *and β order with respect to reactant* B. The overall order of the reaction, **n**, is

$$n = \alpha + \beta$$

The units of $-r_A$ are always in terms of concentration per unit time, while the units of the specific reaction rate, k_A, will vary with the order of the reaction. Consider a reaction involving only one reactant, such as

$$A \rightarrow \text{Products}$$

with an overall reaction order n. The units of rate, $-r_A$, and the specific reaction rate, k are

$$\{-r_A\} = [\text{concentration/time}]$$

$$\text{and } \{k\} = \frac{[\text{concentration}]^{1-n}}{\text{time}}$$

An *elementary reaction* is one that involves a single reaction step, such as the bimolecular reaction between an oxygen free radical and methanol molecule

$$O\bullet + CH_3OH \rightarrow CH_3O\bullet + OH\bullet$$

The stoichiometric coefficients in this reaction are *identical* to the powers in the rate law. Consequently, the rate law for the disappearance of molecular oxygen is

$$-r_{O\bullet} = kC_{O\bullet}C_{CH_3OH}$$

A)

Elementary Reaction

$$-r_A = k_A C_A C_B C_C$$

$$n = 1 + 1 + 1 = 3 = n$$

b. Your team members know that the reaction rate constant is $k(T = 300K) = 0.1\ M^{1-n}/hr$. They plan on having a continuous equimolar feed of reactants (same for A, B, and C). Specifically, $C_A = 1.67\ M$ with a volumetric flow rate $\upsilon = 400\ L \cdot hr^{-1}$. You will need at least 80% conversion of reactant A on your space shuttle reactor. Compute the volume that a CSTR would need to reach that conversion.

Assume:
$T = 300\,K$

4.2.1 Equations for Concentrations in Flow Systems

For a flow system, the concentration C_A at a given point can be determined from the molar flow rate F_A and the volumetric flow rate υ at that point:

$$\boxed{C_A = \frac{F_A}{\upsilon} = \frac{\text{moles/time}}{\text{liters/time}} = \frac{\text{moles}}{\text{liter}}} \tag{4-10}$$

Units of υ are typically given in terms of liters per second, cubic decimeters per second, or cubic feet per minute. We now can write the concentrations of A, B, C, and D for the general reaction given by Equation (2-2) in terms of their respective entering molar flow rates (F_{A0}, F_{B0}, F_{C0}, F_{D0}), the conversion, X, and the volumetric flow rate, υ.

$$C_A = \frac{F_A}{\upsilon} = \frac{F_{A0}}{\upsilon}(1-X) \qquad C_B = \frac{F_B}{\upsilon} = \frac{F_{B0} - (b/a)F_{A0}X}{\upsilon}$$
$$C_C = \frac{F_C}{\upsilon} = \frac{F_{C0} + (c/a)F_{A0}X}{\upsilon} \qquad C_D = \frac{F_D}{\upsilon} = \frac{F_{D0} + (d/a)F_{A0}X}{\upsilon} \tag{4-11}$$

We now focus on determining the volumetric flow rate, υ.

The concentration of A is the number of moles of A per unit volume

$$C_A = \frac{N_A}{V}$$

$$\boxed{C_A = \frac{F_A}{\upsilon} = \frac{\text{moles/time}}{\text{liters/time}} = \frac{\text{moles}}{\text{liter}}} \tag{4-10}$$

$$C_A = C_{A0}(1-X) \tag{4-6}$$

4.1.1 Batch Concentrations for the Generic Reaction, Equation (2-2)

The concentration of A is the number of moles of A per unit volume

$$C_A = \frac{N_A}{V}$$

After writing similar equations for B, C, and D, we use the stoichiometric table to express the concentration of each component in terms of the conversion X:

$$C_A = \frac{N_A}{V} = \frac{N_{A0}(1-X)}{V} \tag{4-2}$$

$$C_B = \frac{N_B}{V} = \frac{N_{B0} - (b/a)N_{A0}X}{V} \tag{4-3}$$

$$C_C = \frac{N_C}{V} = \frac{N_{C0} + (c/a)N_{A0}X}{V} \tag{4-4}$$

$$C_D = \frac{N_D}{V} = \frac{N_{D0} + (d/a)N_{A0}X}{V} \tag{4-5}$$

Because almost all batch reactors are solid vessels, the reactor volume is constant, so we can take $V = V_0$, then

$$C_A = \frac{N_A}{V_0} = \frac{N_{A0}(1-X)}{V_0}$$

$$C_A = C_{A0}(1-X) \tag{4-6}$$

We will soon see that Equation (4-6) for constant volume batch reactors also applies to continuous-flow *liquid-phase* systems.

4.2.2 Liquid-Phase Concentrations

For liquids, the fluid volume change with reaction is negligible when no phase changes are taking place. Consequently, we can take

$$\upsilon = \upsilon_0$$

Then

$$C_A = \frac{F_{A0}}{\upsilon_0}(1-X) = C_{A0}(1-X) \tag{4-12}$$

$$C_B = C_{A0}\left(\Theta_B - \frac{b}{a}X\right) \tag{4-13}$$

and so forth for C_C and C_D.

Consequently, using any one of the rate laws in Chapter 3, we can now find $-r_A = f(X)$ for liquid-phase reactions. **However**, for gas-phase reactions the volumetric flow

rate most often changes during the course of the reaction because of a change in the total number of moles or a change in temperature or pressure. Hence, one cannot always use Equation (4-13) to express concentration as a function of conversion for gas-phase reactions.

$$V = F_{A0}X\left(\frac{1}{-r_A}\right)_{X=0.4}$$

$$-r_A = k_A C_A C_B C_C = k_A (C_A)^3, \quad C_A = C_B = C_C$$

$$V = \frac{F_{A0} \cdot x}{-r_A} = \frac{F_{A0} \cdot x}{(k_A C_A C_B C_C)} = \frac{F_{A0} \cdot x}{k_A C_A^3} = \frac{(C_A \cdot \upsilon) \cdot x}{k_A C_A^3} = \frac{C_A \cdot \upsilon \cdot x}{k_A (C_{A0}(1-x))^3}$$

$$V = \frac{C_A \cdot \upsilon \cdot x}{k_A (C_{A0}(1-x))^3} = \frac{(1.67)(400)(.8)}{(.1)(1.67(0.2))^3} = \frac{534.4}{0.0037259704}$$

$$\left[\frac{[\cancel{M}][L/\cancel{hr}]}{[M^{-2}/\cancel{hr}][\cancel{M^3}]}\right]$$

$$\boxed{\begin{aligned} V &= 143{,}426\ L \\ &= 143.4\ m^3 \end{aligned}}$$

B)

c. Will it be possible to bring the reactor on the space shuttle given that the seven astronauts on the trip will occupy 7 m^3 ? If not, what would you change as a chemical engineer to reduce the required volume (e.g., changing reactors types and/or operating parameters)?

2) You are a Chemical Engineer working at NASA in Houston, Texas. You are part of the team preparing to launch the next space shuttle towards Mars. The goal of the mission is to see if life can occur on Mars. It is critical to have a specific secret compound Z to be able to test life and it must be synthesized immediately prior to testing due to its short lifetime. Therefore, it will be generated directly on the shuttle! The maximum amount of volume in the space shuttle is 84.3 m^3. The reaction to form Z occurs in the liquid phase:

$$A + B + C \rightarrow Z$$

On earth, in your lab you are trying to find the best conditions for your reactor. Your team members carry out the reaction at T = 300 K in a CSTR reactor.

max volume on Space Shuttle = 84.3 m^3

volume of reactor + astronauts

$(143.4\,m^3) + (7\,m^3) = 150.4\,m^3 \approx 150\,m^3$

$\boxed{150\,m^3 > 84.3\,m^3 \text{ (Not Possible)}}$ c)

(Operating Parameters)

Since we want to keep reaction at 80% conversion we could find a way to increase our k (ex: increasing Temp.)

we could also increase our C_{A0} value

(Changing Reactors Types)

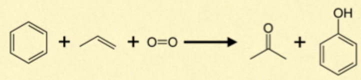
(A PFR Reactor would be a good Choice as it does not depend on the shape but Total volume)

(Running a CSTR in Series Could reduce space as well)

(research could be done to see if a Solid Catalyst would aid in this reaction ($\uparrow k$) in which case a PBR would work well)

3) Jonathan van Ness is fed up with his nail polish color and wants to remove it. He is so rich that he has his own chemical engineering plant at home to generate all the materials he desires. He asks you, the team leader, to generate more acetone and to have enough ready for him and his fans to take on his weekend trip to the Superbowl 2021 game. He is willing to purchase both a PFR and CSTR if necessary.

The reaction is



From your first trials in a set of two continuous flow reactors you obtain the following experimental data (B stands for the Benzene):

Conversion X_B	0	0.1	0.2	0.4	0.6	0.8
$F_{B0}/-r_B$ [L]	0.9	1.1	1.8	3.5	4.5	6.5

$$V = F_{A0}X\left(\frac{1}{-r_A}\right)$$

a. Graphically estimate the overall conversion if the reaction is carried out in a single $V = 2.0\ m^3$ CSTR?

b. What is the overall conversion if the reaction is carried out in a single $V = 2.0\ m^3$ PFR? (Suggestion: use the trapezoidal rule to integrate.)

c. What is the overall conversion if the reaction is carried out in a $V_1 = 2.0\ m^3$ PFR followed by a $V_2 = 2.0\ m^3$ CSTR?

d. What is the overall conversion if the reaction goes through the CSTR first, then the PFR?

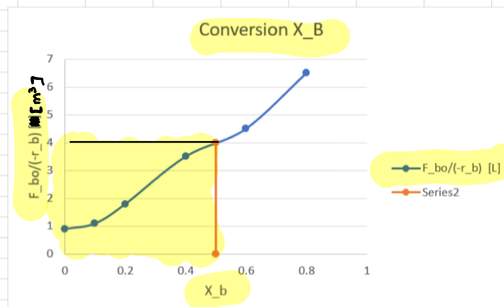
e. What will Jonathan van Ness need to purchase in order get maximum conversion, a PFR, a CSTR, both?

$V = 2.0 m^3$

$\frac{F_{B0}}{-r_B} = 4, \quad X_B = .5$

$(4 \times .5) = 2.0 m^3$

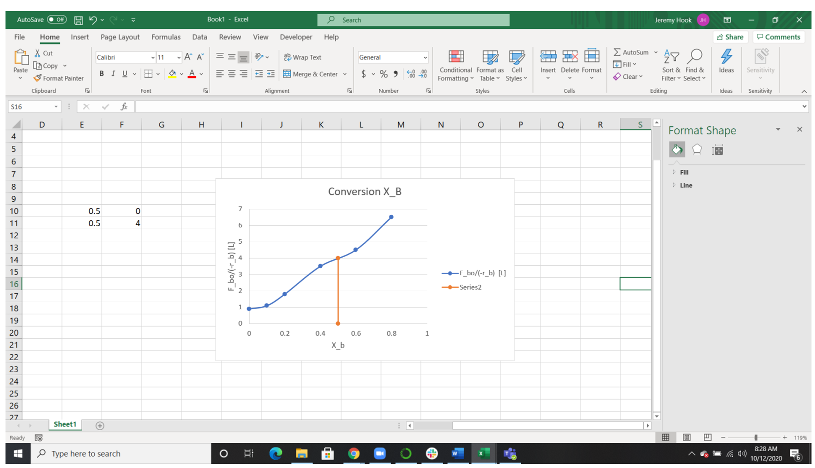
0.5	0
0.5	4



★ CSTR ★

$X_B = 0.5$

$\frac{F_{B0}}{-r} = 4 m^3$



b. What is the overall conversion if the reaction is carried out in a single $V = 2.0\ m^3$ PFR? (Suggestion: use the trapezoidal rule to integrate.)

(Trapezoidal Rule)

$V = 2.0\ m^3$ PFR:

Conversion X_B	0	0.1	0.2	0.4	0.6	0.8
$F_{B0}/-r_B$ [L]	0.9	1.1	1.8	3.5	4.5	6.5

$$V = \left(.1\left(\frac{.9+1.1}{2}\right)\right) + \left(.1\left(\frac{1.1+1.8}{2}\right)\right) + \left(.2\left(\frac{1.8+3.5}{2}\right)\right) + \left(.2\left(\frac{3.5+4.5}{2}\right)\right) + (x-.6)\left(\frac{4.5+(F_{B0}/-r)}{2}\right) = 2$$

$$= 0.1 + 0.145 + 0.53 + 0.8 + (x-.6)(2.25(F_{B0}/-r))$$

$$\frac{F_{B0}}{-r} = f(x) = mx + b \qquad m = \frac{6.5-3.5}{.8-.4} = \frac{3}{.4} = 7.5$$

when $f(0.8) = (7.5)(.8) + b = 6.5 = 6 + b$, $b = .5$

$$\longrightarrow 1.575 + (x-.6)(1.75[7.5(x)+.5]) = 2\ m^3$$

(Wolfram Alpha)

$$X = .669 \approx .67$$

(Redo with slope between .6 - .8 for more accurate results)

$$\frac{F_{B0}}{-r} = f(x) = mx+b;\quad m = \left(\frac{6.5-4.5}{.8-.6}\right) = 10;\quad f(.8) = (10)(.8) + b = 6.5;\quad 8 + b = 6.5;\quad b = -1.5$$

$$= 1.575 + (x-.6)(2.25(10(x)-1.5)) = 0.686$$

$$\approx 0.686$$

$$\boxed{X = .686}$$

c. What is the overall conversion if the reaction is carried out in a $V_1 = 2.0\ m^3$ PFR followed by a $V_2 = 2.0\ m^3$ CSTR?

$$V = \left(\frac{F_{B0}}{-r_B}\right)(X_{CSTR} - X_{PFR})$$

$$2 = ((10x-1.5))(x-.685)$$

$$2 = 10x^2 - 6.85x - 1.5x + 1.0275$$

$$2 = 10x^2 - 8.35x + 1.0275$$

(Wolfram Alpha)

$$x = 0.938611$$

(Assume actual point is between .6 - .8 X_B)

$$\left(\frac{F_{B0}}{-r} = (10(X)) - 1.5\right)$$

$$10X - 1.5$$

$$\boxed{X = 0.939}$$

d. What is the overall conversion if the reaction goes through the CSTR first, then the PFR?

Conversion X_B	0	0.1	0.2	0.4	0.6	0.8
$F_{B0}/-r_B$ [L]	0.9	1.1	1.8	3.5	4.5	6.5

$X_{CSTR} = 0.5$; $V = \int_{X_{CSTR}}^{X_{PFR}} \frac{F_{B0}}{-r_B} dx$

CSTR :

$f(x) = mx + b$; $m = \frac{4.5-4}{.6-.5} = \frac{.5}{.1} = 5$; $4 = f(.5) = 5(.5) + b$; $b = 1.5$

$f(x) = 5(x) + 1.5$

PFR:

$\frac{F_{B0}}{-r} = f(x) = mx + b$; $m = \left(\frac{6.5-4.5}{.8-.6}\right) = 10$; $f(.8) = (10)(.8) + b = 6.5$; $8 + b = 6.5$; $b = -1.5$

$f(x) = 10x - 1.5$

$2 m^3 = \int_{.5}^{.6} 5x + 1.5\, dx + \int_{.6}^{x} 10x - 1.5\, dx$ (Wolfram Alpha)

$x = 0.869375 \approx 0.87$

$\boxed{x = 0.87}$

e. What will Jonathan van Ness need to purchase in order get maximum conversion, a PFR, a CSTR, both?

In order to get the maximum conversion, Jonathan Van Ness should use a PFR that has a volume of 4 m^3 Alternatively we could also use both a PFR and a CSTR each with a volume of 2 m^3

4) You are designing a reactor to carry out an irreversible reaction $A \rightarrow 2B + 2C$. You want to determine the optimal type of reactor to use. You decide that you will have an inflow of material F_{A0}= 180 mol/min. You have performed laboratory scale experiments and collected some data on the system:

X_A	0	0.2	0.4	0.5	0.6	0.8	0.9
$-r_A$ [mol $L^{-1}min^{-1}$]	2.0	4.0	10.0	12.0	8.5	3.5	3.0

a. Create a Jupyter notebook and use Python to construct a Levenspiel plot of the data. For all your plots, be sure to label the axes appropriately (don't forget units!), give it a title, and include a legend.

b. You desire 60% conversion of the reactant. Compute the volume for a CSTR this would require. Compute the volume for a PFR this would require.
Suggestion: Use the `numpy.trapz()` function to find a numerical solution to the integral. (For more information on the function see the documentation available at https://docs.scipy.org/doc/numpy/reference/generated/numpy.trapz.html).

c. For each of the above points, describe what you are coding in Markdown cells and explain why you believe this makes sense.

d. Print out the Jupyter notebook that you used to create your plots and calculate your values.

In [44]:
```
#CHEME 465 Fall 2020
#HW2
#Question#4
```

In [45]:
```
import numpy as np
from scipy.misc import derivative
import matplotlib.pyplot as plt
```

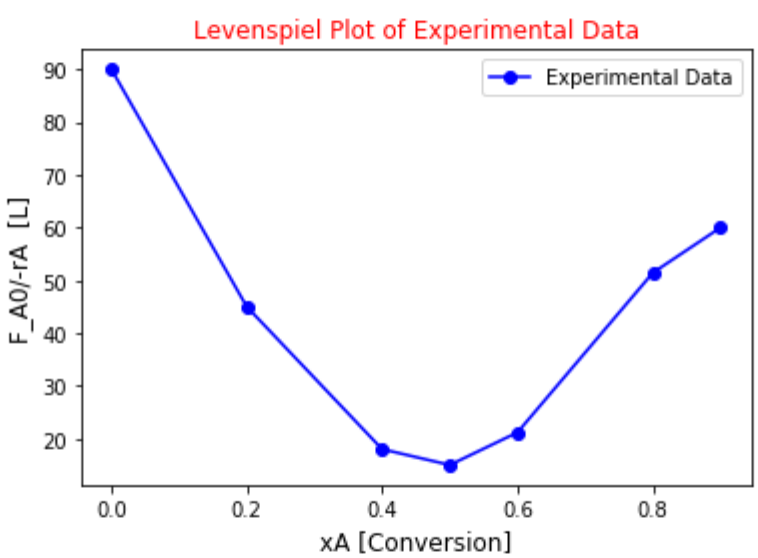
In [46]:
```
#Reaction given in the problem statement: A -> 2B + 2C #Reaction given in the
 problem statement
# Data given
F_A0 = 180 #molar flow rate per unit time of the entering reactant A given in
 mol/min
xA = np.array([0.0, 0.2, 0.4, 0.5, 0.6, 0.8, 0.9]) #conversion of A (nA reacte
d)/(nA fed)
negative_rA = np.array([2.0, 4.0, 10.0, 12.0, 8.5, 3.5, 3.0]) #rate of disappe
arance of reactant A in units of mol/(L*min)
print(negative_rA)
```

```
[ 2.   4.  10.  12.   8.5  3.5  3. ]
```

In [47]:
```
#Part A
#Making a Levenspiel Plot
np.set_printoptions(precision=3)
x1 = xA
y1 = (F_A0)/(negative_rA) #F_A0/-rA = (mol/min)/(mol/(min*L)) = L

plt.title("Levenspiel Plot of Experimental Data", color='r')
plt.xlabel("xA [Conversion]", fontsize = 12)
plt.ylabel("F_A0/-rA  [L]", fontsize = 12)
plt.plot(x1, y1, 'b-o', label = "Experimental Data")
plt.legend()
```

Out[47]: <matplotlib.legend.Legend at 0x22bcf36b108>



In [48]:
```
#Part b:
#Compute the volume for a CSTR this would require + Compute the volume for a P
FR this would require.

xA_desired = 60/100 #Desired condition

#From Data
diff = xA[4] - xA_desired
print("The difference between xA[4] and xA_desired =", diff, ", xA[4]) = xA_de
sired")

#According to CTSR formula volume you can find the change through this equatio
n:
V_CTSR = F_A0*xA[4]/negative_rA[4]
print("Volume for a CSTR with ", str(xA_desired), "conversion is:", V_CTSR,
"L")

#PFR measures the volume according to the area under the curve of the Levenspi
el plot
#To use numpy.trap(), we must define:
x1_PFR = x1[0:5]
y1_PFR = y1[0:5]
# Check: print(x1_PFR)
#Integral of d/dxA [F_A0/neg_rA]:
integral = np.trapz(y1_PFR, x1_PFR) #integrate along the given axis using the
 composite trapezoidal rule
#According to PFR formula, the volume to achieve the desired condition is:
V_PFR = integral
print("Volume for a PFR with ", str(xA_desired), "conversion is:", V_PFR, "L")
```

```
The difference between xA[4] and xA_desired = 0.0 , xA[4]) = xA_desired
Volume for a CSTR with  0.6 conversion is: 12.705882352941176 L
Volume for a PFR with  0.6 conversion is: 23.258823529411764 L
```

Part c:

In part a, I used the Levenspiel Plot in Figure 2-2B at page 43 (textbook) as a referrence for the formula of y- and x-axis. We can see that the x-axis is the conversion of A with no units just the conversion. The y-axis is initial molar flow rate over the rate of A disappearance. I calculated the units to be in L (liters). 4 In part b, the problem wants calculation for the volume of the reactor given its conversion is 60 percent

Similar to example 2-1 in the textbook page 44, using equation (2-13) to calculate the volume for CSTR reactor. From the 0.6 conversion (xA), we can look up the data for neg_rA on the table to be 8.5. Use the position of xA and neg_rA to link to the wanted values.

For PFR reactor, the volume formula requires an integral. Using recommendation from the problem, I looked up np.trapz and its required values. its function defined "integrate along the given axis using the composite trapezoidal rule." The required values are: np.trapz(y_array_like, x_arraylike) yarray_like: Input array to integrate. xarray_like: The sample points corresponding to the y values. Given our plot in part a, we integrate along the y-axis of our plot, and define new arrays of x and y until x reaches 0.6.

With 0.6 conversion, the final solutions for part b volume of a CSTR is 12.7 L, volume for a PFR is 23.3 L. The volume of PFR reactor is twice the volume of a CSTR reactor. From the graphs below, the area for PFR volume is bigger than the area of CSTR volume. Which would be consistent with what we have learned

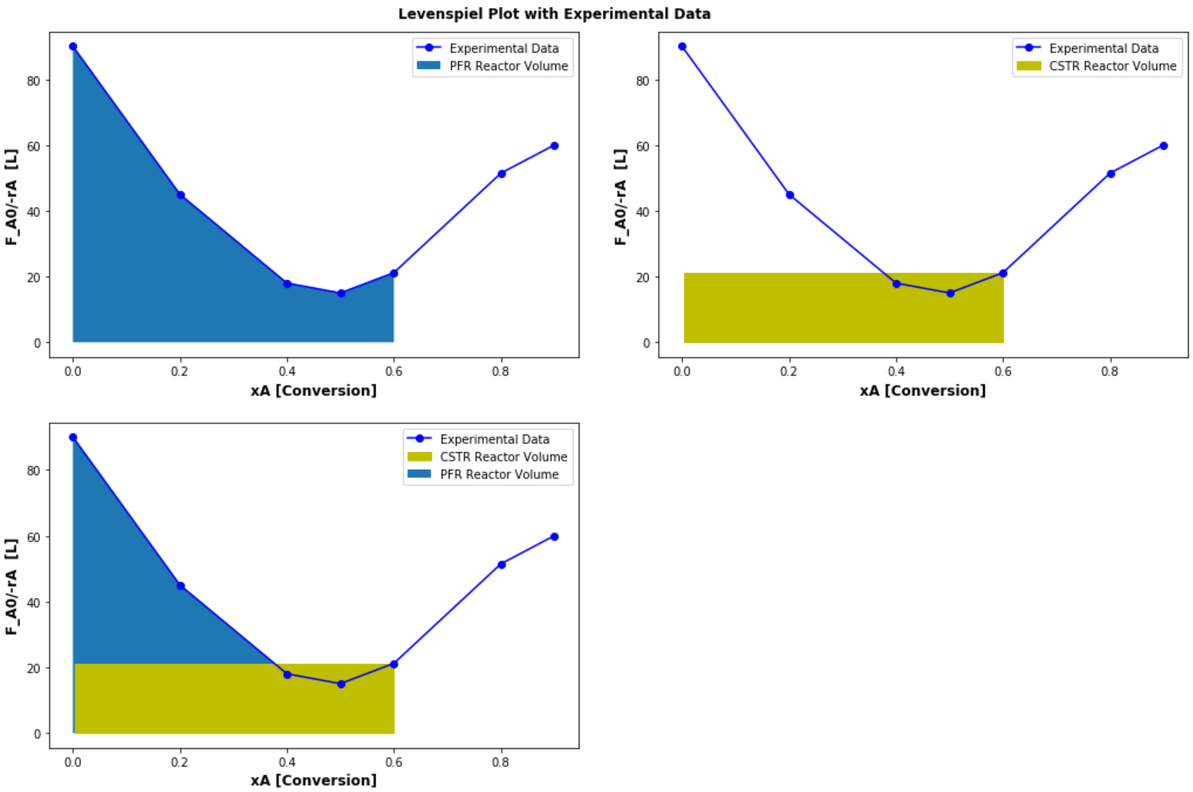
For this problem, if we want to design a reactor at 60 percent conversion with a smaller volume, we should choose the CSTR reactor.

In [49]:
```
#Part C
plt.figure(figsize=(15, 10))
plt.suptitle("Levenspiel Plot with Experimental Data", fontweight = 'bold') #m
ake plot for all the graphs to go into
plt.subplot(221) #Find prf reactor volume
plt.xlabel("xA [Conversion]", fontweight = 'bold', fontsize = 12)
plt.ylabel("F_A0/-rA  [L]", fontweight = 'bold', fontsize = 12)
plt.plot(x1, y1, 'b-o', label = "Experimental Data")
plt.fill_between(x1[0:5], y1[0:5], label = 'PFR Reactor Volume')# highlight th
e area under the curve
plt.legend()

plt.subplot(222) #Find CSTR Reactor Volume
plt.xlabel("xA [Conversion]", fontweight = 'bold', fontsize = 12)
plt.ylabel("F_A0/-rA  [L]", fontweight = 'bold', fontsize = 12)
plt.plot(x1, y1, 'b-o', label = "Experimental Data")
plt.axhspan(0, 21, xmin = 0.05, xmax = 0.65, color = 'y', label ='CSTR Reactor
Volume')# highlight the area under the curve
plt.legend()

plt.subplot(223) #find combined PFR, and CSTR Reactor
plt.xlabel("xA [Conversion]", fontweight = 'bold', fontsize = 12)
plt.ylabel("F_A0/-rA  [L]", fontweight = 'bold', fontsize = 12)
plt.plot(x1, y1, 'b-o', label = "Experimental Data")
plt.fill_between(x1[0:5], y1[0:5], label = 'PFR Reactor Volume')
plt.legend()
plt.axhspan(0, 21, xmin = 0.05, xmax = 0.65, color = 'y', label ='CSTR Reactor
Volume')# highlight the area under the curve
plt.legend()

plt.subplots_adjust(top=.95, bottom=0.1, left=0.10, right=1, hspace=0.2,
                    wspace=0.15) # adjust plots to make look nice
```


Levenspiel Plot with Experimental Data
Experimental Data
PFR Reactor Volume
CSTR Reactor Volume
F_A0/-rA [L]
xA [Conversion]
0
20
40
60
80
0.0
0.2
0.4
0.6
0.8

```
In [ ]:
```

```
In [ ]:
```

```
In [ ]:
```