1. Calculate the conversion for the following cases.

   a) \( N_{A0} = 2.2 \text{ mole}, \quad N_A = 0.05 \text{ mole} \)

   b) \( F_{A0} = 1.2 \frac{\text{ mole}}{\text{ min}}, \quad F_A = 0.4 \frac{\text{ mole}}{\text{ min}} \)

   c) \( C_{A0} = 50 \frac{\text{ mmole}}{\text{ liter}}, \quad C_A = 14 \frac{\text{ mmole}}{\text{ liter}} \)  
      Note: a mmole = millimole = 0.001 mole

\[
N_{A0} = 2.2 \text{ mole}; \quad N_A = 0.05 \text{ mole};
\]

\[
X = \frac{N_{A0} - N_A}{N_{A0}};
\]

(*NumberForm is a function that controls the number of decimals*)

\[
\text{NumberForm}[X, 2]
\]

a) 0.98

b) 0.67

c) 0.72

2. Find the conversion after one hour in a batch reactor for the reaction

\[
A \rightarrow B, \quad -r_A = 3 C_A^{\frac{1}{2}} \frac{\text{ mole}}{\text{ liter hr}}, \quad C_{A0} = 1 \frac{\text{ mole}}{\text{ liter}}
\]

Note: \( k = 3 \) and you need to determine the units.

\[
N_{A0} \frac{dX}{dt} = -r_A V \quad C_{A0} \frac{dX}{dt} = -r_A \quad C_{A0} \int_0^X \frac{1}{-r_A} \, dX = \int_0^t \, dt
\]

Substituting and rearranging the last equation

\[
C_{A0} \int_0^X \frac{1}{kC_{A0}^{0.5} (1-X)^{0.5}} \, dX = t \quad \Rightarrow \quad t = \frac{C_{A0}}{kC_{A0}^{0.5}} \int_0^X \frac{1}{(1-X)^{0.5}} \, dX
\]
\[ t = 1; \ Cl = 1; \ k = 3; \]
\[
\text{Clear}[X]
\]
\[
\int_0^x \frac{1}{(1-x)^{\frac{1}{2}}} \, dx;
\]
\[
2 - 2 \sqrt{1-x}
\]
\[
\text{ans} = \text{Solve}[t = \left( \frac{\text{Cl}}{k^{\frac{1}{2}}} \right) \left( 2 - 2 \sqrt{1-x} \right), x]
\]
\[
\{
\}
\]
Since there is no solution to the problem, we need to find a reason.

\[
\text{fx}[x_] := 1/3 \left( 2 - 2 \sqrt{1-x} \right);
\]
\[
\text{Plot}[\text{fx}[i], \{i, 0, 1\}]
\]
- Since 2/3 hours is less than one hour, the reaction goes to completion ($X = 1$) in 2/3 hours.

Note: It is possible to get a real solution by hand, but back substitution shows that it is not correct. Starting with

$$1 = \frac{1}{3} \left( 2 - 2 \sqrt{1-x} \right)$$

and doing some algebra

$$3 = 2 - 2 \sqrt{1-x}$$

$$3 - 2 = -2 \sqrt{1-x}$$

$$1 = -2 \sqrt{1-x}$$

$$\frac{1}{2} = \sqrt{1-x}.$$ This should be your first clue that you have a problem

$$\left( \frac{1}{2} \right)^2 = \left( \sqrt{1-x} \right)^2$$

$$\frac{1}{4} = 1 - x \implies x = 0.75$$

Back substitution to evaluate the term on the right yields

$$1 = \frac{1}{3} \left( 2 - 2 \sqrt{1-0.75} \right)$$ which evaluates to $1 = 0.333$

$\therefore$ the solution is incorrect.

- MATLAB Program to integrate $\frac{1}{(1-x)^{1/2}}$ and evaluate the results.

```matlab
function orderProblem = fhalforder(n)
syms x y
ival=int(1/(1-x)^(1/2),0,y);
ival=subs(ival,x);
fx=@(x) subs(1/3*(ival),x); Note: This builds the function from
output from the integration (int) routine.
orderProblem=fx(n);
```
In general, reactions with $\alpha$ less than 1 can result in a complete conversion ($X = 1$), while reactions with $\alpha$ greater than 1 never go to complete conversion ($X < 1$).

3. Find the initial concentrations of A in a gas mixture that consists of reactants (A and B) and an inert gas (I).

<table>
<thead>
<tr>
<th>moles A</th>
<th>moles B</th>
<th>moles I</th>
<th>P (atm)</th>
<th>T (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>2</td>
<td>0</td>
<td>10</td>
<td>125</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>2</td>
<td>10</td>
<td>125</td>
</tr>
<tr>
<td>1</td>
<td>5</td>
<td>2</td>
<td>200</td>
<td>200</td>
</tr>
<tr>
<td>0.5</td>
<td>0.3</td>
<td>0.9</td>
<td>20</td>
<td>100</td>
</tr>
</tbody>
</table>

\[ R = \frac{\text{liter atm}}{\text{mole K}}; \]
\[ N_{A0} = 2.0 \text{ mole; } N_{B0} = 2 \text{ mole; } N_{I0} = 0 \text{ mole; } P = 10 \text{ atm; } T = (125 + 273) \text{ K}; \]
\[ Y_{A0} = \frac{N_{A0}}{N_{A0} + N_{B0} + N_{I0}} \]
\[ 0.5 \]
\[ C_{A0} = \frac{Y_{A0} P}{R T}; \text{NumberForm}[C_{A0}, 2] \]

0.15 mole/liter

\[ N_{A0} = 2.0 \text{ mole; } N_{B0} = 2 \text{ mole; } N_{I0} = 2 \text{ mole; } P = 10 \text{ atm; } T = (125 + 273) \text{ K}; \]
\[ Y_{A0} = \frac{N_{A0}}{N_{A0} + N_{B0} + N_{I0}} ; \text{NumberForm}[Y_{A0}, 2] \]
\[ 0.33 \]
\[ C_{A0} = \frac{Y_{A0} P}{R T}; \text{NumberForm}[C_{A0}, 3] \]

0.102 mole/liter
\[ N_{A0} = 1.0 \text{ mole; } N_{B0} = 5 \text{ mole; } N_{I0} = 2 \text{ mole; } P = 200 \text{ atm; } T = (200 + 273) \text{ K}; \]
\[ y_{A0} = \frac{N_{A0}}{N_{A0} + N_{B0} + N_{I0}} \]
\[ 0.125 \]
\[ C_{A0} = \frac{y_{A0} P}{R T}; \text{ NumberForm}[C_{A0}, 2] \]
\[ \frac{0.64 \text{ mole}}{\text{liter}} \]

\[ N_{A0} = 0.5 \text{ mole; } N_{B0} = 0.3 \text{ mole; } N_{I0} = 0.9 \text{ mole; } P = 20 \text{ atm; } T = (100 + 273) \text{ K}; \]
\[ y_{A0} = \frac{N_{A0}}{N_{A0} + N_{B0} + N_{I0}} ; \text{ NumberForm}[y_{A0}, 2] \]
\[ 0.29 \]
\[ C_{A0} = \frac{y_{A0} P}{R T}; \text{ NumberForm}[C_{A0}, 2] \]
\[ \frac{0.19 \text{ mole}}{\text{liter}} \]

4. An aqueous feed containing reactant A (\( \frac{1 \text{ mole}}{\text{liter}} \)) enters a CSTR (mixed flow reactor), \( V = 2 \) liters. Substance A reacts as follows:

\[ 2 A \rightarrow B, \quad -r_A = 0.05 C_A^2 \frac{\text{mole}}{\text{liter}^s}, \quad \text{Note: } k = 0.05 \text{ units = ?} \]

Find what feed rate (\( \frac{\text{liter}}{\text{min}} \)) will give an outlet concentration of \( C_{Af} = 0.5 \frac{\text{mole}}{\text{liter}} \).

\text{CSTR equation: } V = \frac{F_{A0} X}{-r_A} = \frac{C_{A0} v_0 X}{-r_A}

v_0 = . \quad (*\text{use if previous problem leaves a value for } v_0*)

\[ C_{A0} = 1.0 \frac{\text{mole}}{\text{liter}}; \quad V = 2 \text{ liter}; \quad k = 0.05 \frac{\text{liter}}{\text{mole} \cdot \text{min}} \cdot \frac{60 \text{ s}}{60 \text{ s}}; \quad C_{Af} = 0.5 \frac{\text{mole}}{\text{liter}}; \]
\[ C_A [x_] = C_{A0} (1 - x); \quad r_A [x_] = k C_A [x]^2; \]
\[ X = \frac{C_{A0} - C_{Af}}{C_{A0}} \]
\[ 0.5 \]
Solve \[ V = \frac{c_{a0} v_0 X}{r_a[X]} , v_0 \]

\[ \{ [v_0 \rightarrow \frac{3. \text{ liter}}{\text{min}}] \} \]
Data for problem 5 is given in the following table

<table>
<thead>
<tr>
<th>X</th>
<th>(\frac{1}{-x_A})</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.07</td>
</tr>
<tr>
<td>0.07</td>
<td>1.23</td>
</tr>
<tr>
<td>0.158</td>
<td>1.5</td>
</tr>
<tr>
<td>0.23</td>
<td>1.8</td>
</tr>
<tr>
<td>0.31</td>
<td>2.24</td>
</tr>
<tr>
<td>0.389</td>
<td>2.86</td>
</tr>
<tr>
<td>0.452</td>
<td>3.55</td>
</tr>
<tr>
<td>0.52</td>
<td>4.65</td>
</tr>
<tr>
<td>0.6</td>
<td>6.67</td>
</tr>
<tr>
<td>0.67</td>
<td>9.76</td>
</tr>
<tr>
<td>0.74</td>
<td>15.8</td>
</tr>
<tr>
<td>0.79</td>
<td>24.1</td>
</tr>
</tbody>
</table>

5. The \(\frac{1}{-x_A}\) vs X plot below represents the behavior of the reaction \(2A \rightarrow P\).

   (a) What is the size of the CSTR needed to convert \(C_{A0}\) to \(\frac{1}{4} C_{A0}\) if \(F_{A0} = 1000\) mole day^{-1}?

   (b) What is the size of the PFR needed to convert \(C_{A0}\) to \(\frac{1}{3} C_{A0}\) if \(F_{A0} = 500\) mole day^{-1}?

\[
F_{A0} = 1000.0 \text{ mole day}^{-1}, \quad X = \frac{C_{A0} - \frac{1}{4} C_{A0}}{C_{A0}}
\]
\[
\text{ir}_A = \text{irafit}[0.75] \frac{\text{liter min}}{\text{mole}}; \quad (*\text{Note: ir} = \frac{1}{-r_A}*)
\]
\[
V_{\text{CSTR}} = F_{A0} \times \text{ir}_A; \quad \text{NumberForm}[V_{\text{CSTR}}, 2]
\]

9. liter

The problem was a little vague about the units on \(1/(-r_A)\), although it was on the plot so here are the possible other answers. In terms of hours

\[
1000.0 \frac{\text{mole}}{\text{day}} \times \frac{\text{day}}{24 \, \text{hr}} \times \text{irafit}[0.75] \frac{\text{liter hr}}{\text{mole}}
\]

537.605 liter
days

\[
1000.0 \frac{\text{mole}}{\text{day}} \times \text{irafit}[0.75] \frac{\text{liter day}}{\text{mole}}
\]

12902.5 liter

seconds

\[
1000.0 \frac{\text{mole}}{\text{day}} \times \frac{\text{day}}{24 \, \text{hr}} \times \frac{\text{hr}}{60 \, \text{min}} \times \frac{\text{min}}{60 \, \text{s}} \times \text{irafit}[0.75] \frac{\text{liter s}}{\text{mole}}
\]

0.149335 liter

(b) Work using Simpson's rule.

\[
F_{A0} = 500. \frac{\text{mole}}{\text{day}} \times \frac{\text{day}}{24 \, \text{hr}} \times \frac{\text{hr}}{60 \, \text{min}} \times \text{irafit}[0.75] \frac{\text{liter s}}{\text{mole}}
\]

\[
X = \frac{C_{A0} - \frac{1}{3} C_{A0}}{C_{A0}}; \quad \text{NumberForm}[X, 2]
\]

0.67

\[
h = \frac{X}{3}; \quad \text{NumberForm}[h, 2]
\]

0.22

(*\text{Note: ir} = \frac{1}{-r_A}*)

\[
\text{ir}_{A0} = 1.07 \frac{\text{liter min}}{\text{mole}}; \quad \text{ir}_{A1} = 1.77 \frac{\text{liter min}}{\text{mole}};
\]

\[
\text{ir}_{A2} = 3.41 \frac{\text{liter min}}{\text{mole}}; \quad \text{ir}_{A3} = 9.6 \frac{\text{liter min}}{\text{mole}};
\]

\[
V = F_{A0} \left( \frac{3}{8} h \left( \text{ir}_{A0} + 3 \text{ir}_{A1} + 3 \text{ir}_{A2} + \text{ir}_{A3} \right) \right); \quad \text{NumberForm}[V, 2]
\]

0.76 liter
Check answer using a fit to the curve

\[
\text{eq} = (1.0776 - 1.5155 x + 108.1449 x^2 - 1126.2913 x^3 + 6037.0366 x^4 - 17659.7912 x^5 + 28992.8641 x^6 - 25058.3734 x^7 + 8958.203 x^8) \frac{\text{liter min}}{\text{mole}};
\]

\[
V = F_{a0} \int_0^x \text{eq} \, dx; \quad \text{NumberForm}[V, 2]
\]

0.74 liter

MATLAB Solution

function Problem5
x=[0,0.07,0.158,0.23,0.31,0.389,0.452,0.52,0.6,0.67,0.74,0.79];
y=[1.07,1.23,1.5,1.8,2.24,2.86,3.55,4.65,6.67,9.76,15.8,24.1];
p=polyfit(x,y,6);
plot(x,y,'o',x,polyval(p,x));
xlabel('X')
ylabel('1/r_A')

Fa0=1000*1/24*1/60;
fprintf('Part (a)---------------------')
X=0.75
ira=polyval(p,X)
Vcst=Fa0*X*ira

fprintf('Part (b)---------------------')
Fa0=500*1/24*1/60;
X=2/3
pint=polyint(p);
Vpfr=Fa0*(polyval(pint,X)-polyval(pint,0))
Part (a)-------------------
X=0.7500
ira=17.2034

Vcstr=8.9601

Part (b)-------------------
X=0.6667

Vpfr=0.7393

6. Fogler 2-8 (a, b, c, d) You can download the raw data (X,1/ra) from the Excel file on the web.

The following reads the input file (Excel csv file), fits the data to a 5th order polynomial, and plots the input data and best-fit line.

```mathematica
inputfile = "/Users/peterclark/Desktop/CoursesFall06/ChE354/Homework/HwkWeek2/Fogler2-8.csv"

data0 = Import[inputfile, "CSV"];
```
\[ pfit = \text{PolynomialFit}[\text{data0}, 5]; \]
\[ \text{DisplayTogether}[\text{ListPlot}[\text{data0}, \text{PlotStyle} \to \text{PointSize}[1/55]], \]
\[ \text{AxesLabel} \to \{"X", "\frac{1}{-ra}\}\}, \]
\[ \text{Plot}[pfit[x], \{x, 0, 0.8\}, \text{PlotStyle} \to \{\text{Thickness}[0.007], \text{Red}\}\}]; \]

Assign a value for the constants and rename the fitting function to \( \text{ira} \) (inverse of \( ra \))

\[ F_{N0} = 1 \frac{\text{kg}}{\text{h}} \times 1000 \frac{\text{g}}{\text{kg}}; \]
\[ C_{S0} = 0.25 \frac{\text{g}}{\text{liter}}; \]
\[ \text{ira} = \text{pfit}; \]
\[ \text{ira}[0.4] \]
\[ 0.114141 \]

(a) For \( X = 0.4 \)
\[ X = 0.4; \]
\[ V_{\text{CSTR}} = F_{N0} X \text{ira}[X] \frac{\text{liter h}}{\text{g}} \]

45.6563 liter

(b) \( X = 0.8 \)
\[ X = 0.8; \]
\[ V_{\text{CSTR}} = F_{N0} X \text{ira}[X] \frac{\text{liter h}}{\text{g}} \]

636.465 liter
(c) $V_{\text{CSTR}} = 80$ liter

$$V_{\text{CSTR}} = 80; \quad \text{FindRoot} [V_{\text{CSTR}} = F_{N0}[[1]] x \, \text{ira}[x], \{x, 0.1\}]$$

$$\{x \to 0.505374\}$$

$$V_{\text{PFR}} = 80; \quad \text{ans} = \text{FindRoot} [V_{\text{PFR}} = F_{N0}[[1]] \int_0^x \text{ira}[x] \, dx, \{x, 0.1\}] ; \text{Chop}[\text{ans}]$$

$$\{x \to 0.143502\}$$

(d) Minimum volume for CSTR followed by a PFR

$$\text{fmin} = \text{FindMinimum} [\text{ira}[x], \{x, 0.8\}]$$

$$\{0.11414, \{x \to 0.39949\}\}$$

$$\text{XMin} = \text{fmin}[[2, 1, 2]]$$

$$0.39949$$

$$V_{\text{Total}} = F_{N0} \, \text{XMin} \, \text{ira}[\text{XMin}] \, \frac{\text{liter} \, h}{g} + F_{N0} \left( \int_{\text{XMin}}^{0.8} \text{ira}[x] \, dx \right) \, \frac{\text{liter} \, h}{g}$$

$$180.454 \, \text{liter}$$

Volume for two CSTRs
MATLAB Solution

function Fogler2_8
filename='Fogler2-8.xls'
data=xlsread(filename);
x=data(:,1);
y=data(:,2);
pfit=polyfit(x,y,8);

plot(x,y,'o',x,polyval(pfit,x))
xlabel('X')
ylabel('1/(r_A)')

fprintf('Part (a)---------------------')
Fn0=1000;
Cs0=0.25;
X=0.4
Vcstr=Fn0*X*polyval(pfit,X)

fprintf('Part (b)---------------------')
X=0.8
Vcstr=Fn0*X*polyval(pfit,X)

fprintf('Part (c)---------------------')
Vcstr=80
Vpfr=80

fx=@(xx) Fn0*xx*polyval(pfit,xx)-Vcstr
X=fzero(fx,0.5)
pint=polyint(pfit);
fx=@(xx) Fn0*(polyval(pint,xx)-polyval(pint,0))-Vpfr
X=fzero(fx,0.01)

fprintf('Part (d)---------------------')
fx=@(xx) polyval(pfit,xx)
xmin=fminbnd(fx,0,0.7)

fprintf('CSTR first---PFR second')
Vtotal=Fn0*xmin*polyval(pfit,xmin)+Fn0*(polyval(pint,0.8)-polyval(pint,xmin))

fprintf('PFR first---CSTR second')
Vtotal=Fn0*(polyval(pint,xmin)-polyval(pint,0))+Fn0*0.8*polyval(pfit,0.8)
■ Answers

Part (a)----------------------
X=0.4000

Vcstr=45.2496

Part (b)----------------------
X=0.8000

Vcstr=638.5573

Part (c)----------------------
Vcstr=80

Vpfr=80

fx=
   @(xx) Fn0*xx*polyval(pfit,xx)-Vcstr

X=0.5050

fx=
   @(xx) Fn0*(polyval(pint,xx)-polyval(pint,0))-Vpfr

X=0.1439

Part (d)----------------------
fx=
   @(xx) polyval(pfit,xx)

xmin=0.3981

CSTR first---PFR second
Vtotal1=180.0579

PFR first---CSTR second
Vtotal=768.9466