CBE 450 Chemical Reactor Fundamentals
Fall, 2009
Homework Assignment #6 Solutions

1. Reactors in Series

Consider the reaction

$$A + B \rightarrow C$$

with elementary mechanism such that the rate is

$$r = kC_A C_B$$

where the rate constants are given by

$$k = k_o \exp\left(-\frac{E_a}{RT}\right)$$

The temperature is 300 K. The activation energy for the reaction is 5000 J/mol. The rate constant prefactor for the reaction is 0.001 liter/mol/s. The feed flowrate is 2 liters/sec. The concentration of A in the feed stream is 10 mol/liter. The concentration of B in the feed stream is 15 mol/liter. The concentration of C in the feed stream is 0 mol/liter. Consider a CSTR of 100 liters and a PFR of 100 liters total volume.

(a) What is the net conversion of A if the reactors are placed in series with the CSTR first and PFR second?
(b) What is the net conversion of A if the reactors are placed in series with the PFR first and CSTR second?

Solution:

(a) What is the net conversion of A if the reactors are placed in series with the CSTR first and PFR second?

We analyze the CSTR first.

The input file is

```
function dydt = sysodeinput(x,y,nvec);
%
%  one reaction
%  A + B --> C
%
%  example usage:
%  [y,x] = sysode(2,1000,0,1000,[0,0,0]);
%
```

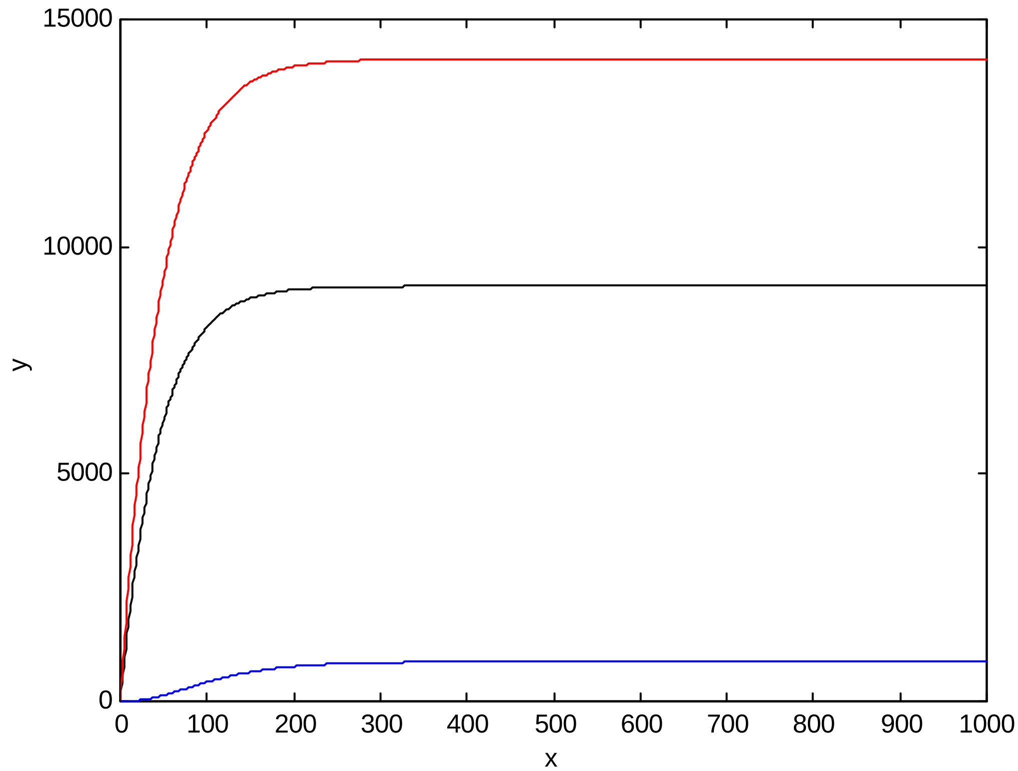
```
CA = y(1);
CB = y(2);
CC = y(3);
%
nuA = -1.0;
nuB = -1.0;
nuC =  1.0;
%
% constant volume;
F = 2.0; % liter/sec
F = 2.0/1000; % m^3/sec
Fin = F;
Fout = F;
CAin = 10.0; % mol/liter
CBin = 15.0; % mol/liter
CCin = 0.0; % mol/liter
CAin = CAin*1000; % mol/m^3
CBin = CBin*1000; % mol/m^3
CCin = CCin*1000; % mol/m^3
%
V = 100; % liter
V = 100/1000; % m^3
R = 8.314; % J/mol/K
T = 300; % K
ko = 1.0e-3; % liter/mol/sec
ko = ko/1000; % m^3/mol/sec
Ea = 5000; % J/mol
k = ko*exp(-Ea/(R*T));
rate = k*CA*CB;
%
%  molar balances
%
dydt(1) = Fin/V*CAin - Fout/V*CA + nuA*rate;
dydt(2) = Fin/V*CBin - Fout/V*CB + nuB*rate;
dydt(3) = Fin/V*CCin - Fout/V*CC + nuC*rate;
```

The command is

```
[y,x] = sysode(2,1000,0,1000,[0,0,0]);
```

I arbitrarily chose these initial conditions. For this problem, it doesn't matter since the steady state is independent of the initial condition.

The output is



From the tabular output file,

```
9.9600000e+002 9.1309434e+003 1.4130943e+004 8.6905653e+002
9.9700000e+002 9.1309434e+003 1.4130943e+004 8.6905653e+002
9.9800000e+002 9.1309434e+003 1.4130943e+004 8.6905653e+002
9.9900000e+002 9.1309434e+003 1.4130943e+004 8.6905653e+002
1.0000000e+003 9.1309434e+003 1.4130943e+004 8.6905653e+002
```

we find that the steady state concentration of A is 9130.94, B is 14130.94 and C is 869.06 mole/m^3.

We now perform the PFR analysis with the inlet stream given as the output of the CSTR.

The input file is

```
function dydt = sysodeinput(x,y,nvec);
%
%  one reaction
%  A + B --> C
%
%  example usage:
%  [y,x] = sysode(2,1000,0,12.7324,[9.1309434e+003, 1.4130943e+004, 8.6905653e+002]);
%
CA = y(1);
CB = y(2);
CC = y(3);
```

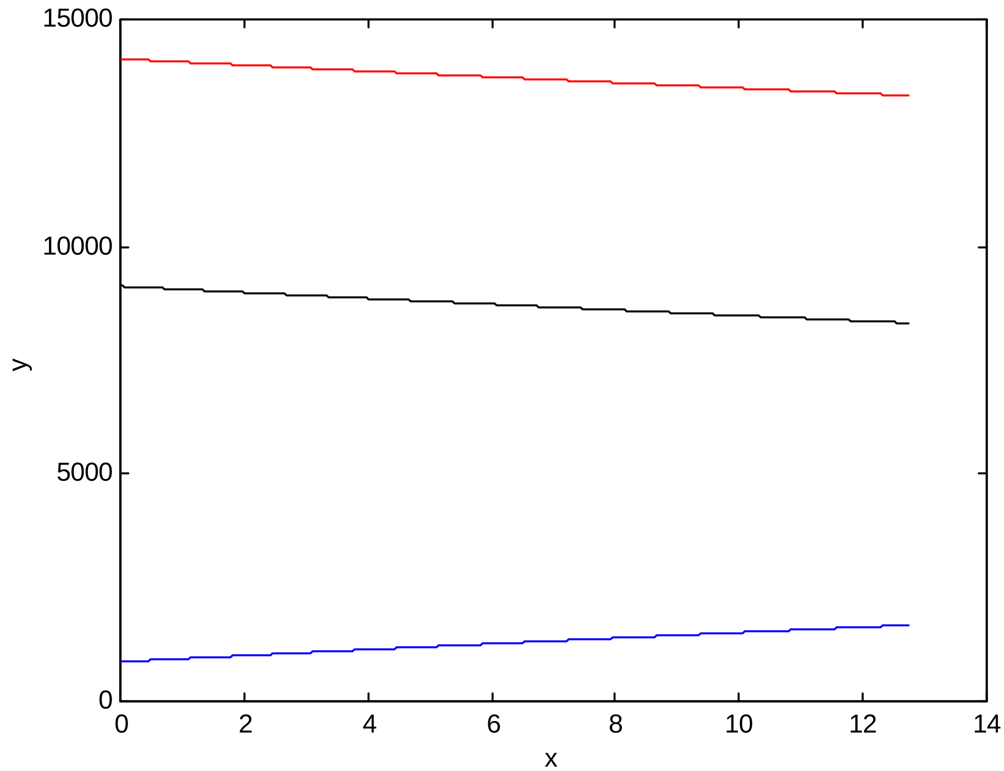
```
%
nuA = -1.0;
nuB = -1.0;
nuC =  1.0;
%
% constant volume;
F = 2.0; % liter/sec
F = 2.0/1000; % m^3/sec
%
%
R = 8.314; % J/mol/K
T = 300; % K
ko = 1.0e-3; % liter/mol/sec
ko = ko/1000; % m^3/mol/sec
Ea = 5000; % J/mol
k = ko*exp(-Ea/(R*T));
rate = k*CA*CB;
%
%  circular pipe
%
Vtot = 100.0; % liters
Vtot = Vtot/1000; % cubic meters
Dp = 0.10; % m
Across = 0.25*pi*Dp*Dp; % m^2
l = Vtot/Across; % m
v = F/Across; % m/s
tr = l/v; % sec
%
%  molar balances
%
% dCAdz = nuA*r/v
dydt(1) = (nuA*rate)/v;
dydt(2) = (nuB*rate)/v;
dydt(3) = (nuC*rate)/v;
```

The command is

```
[y,x] = sysode(2,1000,0,12.7324,[9.1309434e+003, 1.4130943e+004, 8.6905653e+002]);
```

I chose the length arbitrarily but the length and diameter must be chosen to maintain the proper total volume of the reactor.

The output is



From the tabular output file,

1.2732400e+001 8.3250921e+003 1.3325092e+004 1.6749079e+003

we find that the final steady state concentration of A leaving the reactor is 8325 mole/m^3.

The conversion of A

$$X_A = 1 - \frac{C_A}{C_{A,in}} = 1 - \frac{8325}{10000} = 0.1675$$

(b) What is the net conversion of A if the reactors are placed in series with the PFR first and CSTR second?

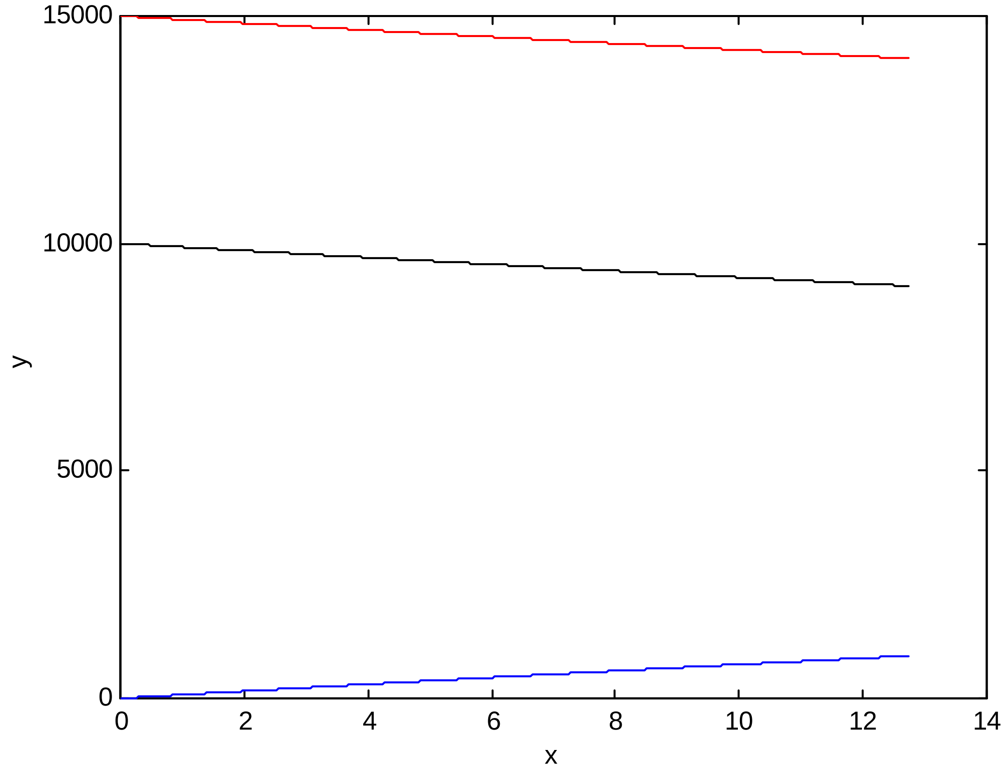
The input file for the PFR does not change.

The command is

[y,x] = sysode(2,1000,0,12.7324,[10000, 15000, 0]);

which provides the appropriate inlet concentrations.

The output looks as follows



The last line of the output file is

1.2732400e+001 9.0682304e+003 1.4068230e+004 9.3176962e+002

from which we find that the steady state concentration leaving the PFRof A is 9068.23, B is 14068.23 and C is 931.77 mole/m^3.

We now put this into the inlet concentration for the CSTR, which does require a change in the input file.

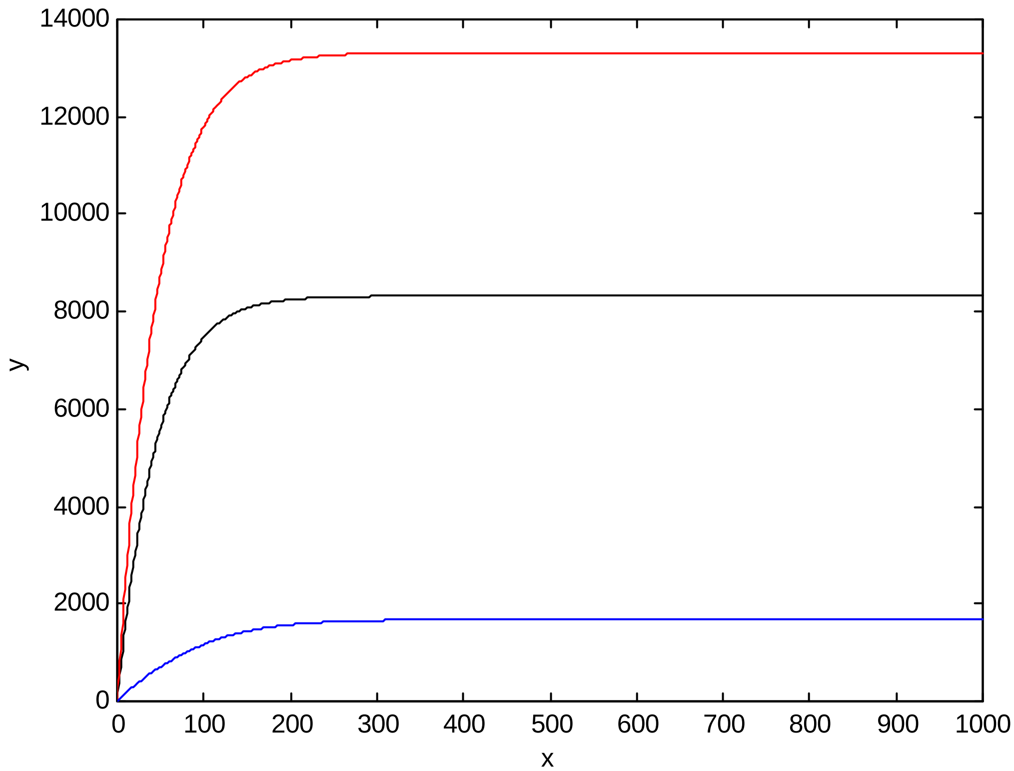
```
function dydt = sysodeinput(x,y,nvec);
%
%  one reaction
%  A + B --> C
%
%  example usage:
%  [y,x] = sysode(2,1000,0,1000,[0,0,0]);
%
CA = y(1);
CB = y(2);
CC = y(3);
%
nuA = -1.0;
```

```
nuB = -1.0;
nuC =  1.0;
%
% constant volume;
F = 2.0; % liter/sec
F = 2.0/1000; % m^3/sec
Fin = F;
Fout = F;
CAin =  9.0682304; % mol/liter
CBin = 14.068230; % mol/liter
CCin = 0.93176962; % mol/liter
CAin = CAin*1000; % mol/m^3
CBin = CBin*1000; % mol/m^3
CCin = CCin*1000; % mol/m^3
%
V = 100; % liter
V = 100/1000; % m^3
R = 8.314; % J/mol/K
T = 300; % K
ko = 1.0e-3; % liter/mol/sec
ko = ko/1000; % m^3/mol/sec
Ea = 5000; % J/mol
k = ko*exp(-Ea/(R*T));
rate = k*CA*CB;
%
%  molar balances
%
dydt(1) = Fin/V*CAin - Fout/V*CA + nuA*rate;
dydt(2) = Fin/V*CBin - Fout/V*CB + nuB*rate;
dydt(3) = Fin/V*CCin - Fout/V*CC + nuC*rate;
```

The command is

```
[y,x] = sysode(2,1000,0,1000,[0,0,0]);
```

The output is



From the output file

9.9500000e+002	8.3215718e+003	1.3321571e+004	1.6784282e+003
9.9600000e+002	8.3215718e+003	1.3321571e+004	1.6784282e+003
9.9700000e+002	8.3215718e+003	1.3321571e+004	1.6784282e+003
9.9800000e+002	8.3215718e+003	1.3321571e+004	1.6784282e+003
9.9900000e+002	8.3215718e+003	1.3321571e+004	1.6784282e+003
1.0000000e+003	8.3215718e+003	1.3321571e+004	1.6784282e+003

We find that the final steady state concentration of A leaving the reactor is 8322 mole/m^3.

The conversion of A

$$X_A = 1 - \frac{C_A}{C_{A,in}} = 1 - \frac{8322}{10000} = 0.1678$$

It's just about the same conversion.

2. Gas-Phase Batch Reactor

Consider the gas-phase reaction

A + B → C

with elementary mechanism such that the rate is

$$r = kC_A C_B$$

where the rate constants are given by

$$k = k_o \exp\left(-\frac{E_a}{RT}\right)$$

The temperature is 500 K. The pressure is constant at 10 atm. The activation energy for the reaction is 5000 J/mol. The rate constant prefactor for the reaction is 0.001 m^3/mol/s.. Consider a batch reactor of variable volume . The initial mole fraction of A is 0.6 and B is 0.4. The initial volume of the reactor is 10 m^3.

(a) Generate a plot of the concentration of A, B and C as a function of time.
(b) What is the concentration of C after 100 sec?
(c) What is the conversion of A after 100 sec?
(d) What is the volume of the reactor after 100 sec?

Solution:

(a) Generate a plot of the concentration of A, B and C as a function of time.

The input file is

```
function dydt = sysodeinput(x,y,nvec);
%
% gas-phase batch reactor with variable volume
%
%
%  sample usage:
% [y,x] = sysode(2,1000,0,2000,[146.2473,97.4982,0,10]);
% total initial concentration
%CTin = p/(R*T) = 243.7455 mol/m^3
% initial concentrations of A and B
%CAin = 0.6*CTin = 146.2473 mol/m^3
%CBin = 0.4*CTin = 97.4982 mol/m^3
%
CA = y(1);
CB = y(2);
CC = y(3);
V = y(4);
%
%  A + B --> C
%
nuA = -1;
nuB = -1;
nuC = 1;
sumnu = nuA + nuB + nuC;
```

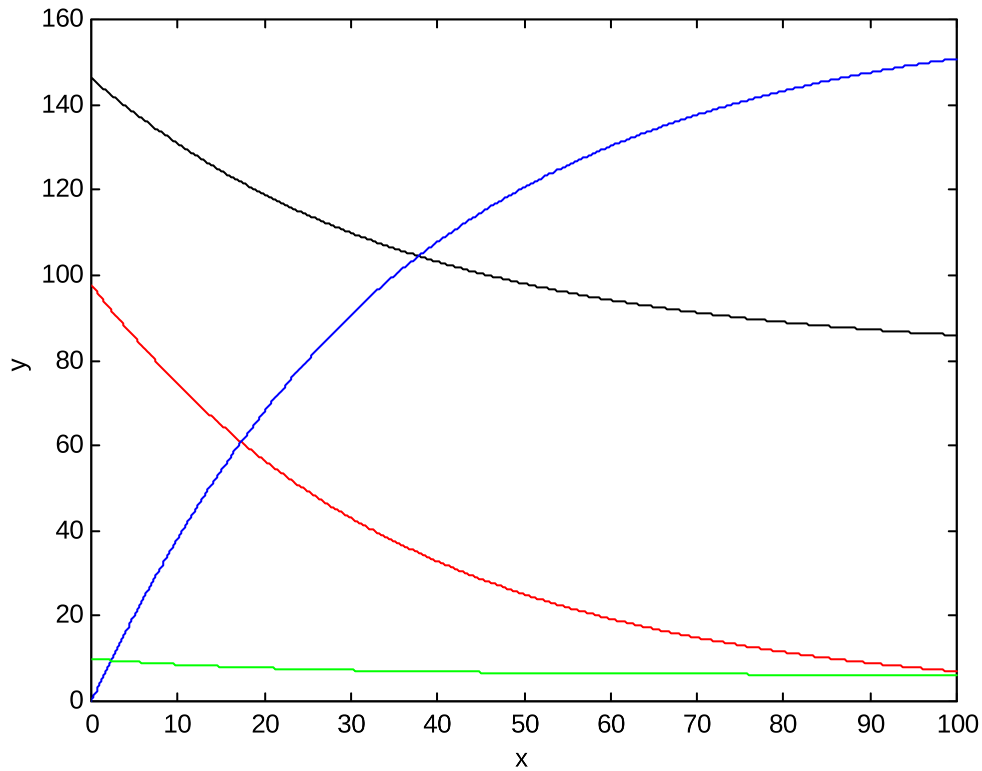
```
%
%
%
p = 1013250.0; % Pa
R = 8.314; % J/mol/K
T = 500; % K
%
dVR = sumnu*R*T/p; % m^3
ko = 1.0e-3; % m^3/mol/sec
Ea = 5000; % J/mol
k = ko*exp(-Ea/(R*T));
rate = k*CA*CB;
%  balance on A in terms of conc of A
dydt(1) = (nuA - CA*dVR)*rate;
%  balance on B in terms of conc of B
dydt(2) = (nuB - CB*dVR)*rate;
%  balance on C in terms of conc of C
dydt(3) = (nuC - CC*dVR)*rate;
%  volume balance
dydt(4) = dVR*rate*V;
```

The command is

```
[y,x] = sysode(2,1000,0,100,[146.2473,97.4982,0,10]);
```

where the initial concentrations are calculated using 60% and 40% of the total concentration at the given temperature and pressure, using the ideal gas law.

The output is



(b) What is the concentration of C after 100 sec?

From sysode.out, the values at 100 secs are

1.0000000e+002 8.5912877e+001 6.9965617e+000 1.5083607e+002 6.1773158e+000

So the concentration of C is 150.83 moles/m^3.

(c) What is the conversion of A after 100 sec?

The initial moles of A are

$$N_{A,in} = C_{A,in} V_{in} = 146.2473 \cdot 10 = 1462.473 \text{ moles}$$

The final number of moles is

$$N_{A,f} = C_{A,f} V_f = 85.91 \cdot 6.18 = 530.9 \text{ moles}$$

$$X_A = 1 - \frac{C_A}{C_{A,in}} = 1 - \frac{530.9}{1462.473} = 0.6370$$

(d) What is the volume of the reactor after 100 sec?

From the output, the final volume is 6.18 m^3.

3. Constant-Volume CSTRs with variable exit flowrate

Consider the gas-phase reaction

$$A + B \rightarrow C$$

with elementary mechanism such that the rate is

$$r = kC_A C_B$$

where the rate constants are given by

$$k = k_o \exp\left(-\frac{E_a}{RT}\right)$$

The temperature is 500 K and the pressure is 10 atm. The activation energy for the reaction is 5000 J/mol. The rate constant prefactor for the reaction is1.0 m^3/mol/s. The feed flowrate is 1.0 m^3/sec. The inlet feed stream is 60% A and 40% B.

(a) What is the steady state conversion of A?
(b) Provide a plot of the exit flow-rate as a function of time from your initial conditions to steady state.
(c) What is the steady state exit flow-rate?

Solution:

(a) What is the steady state conversion of A?

I used the following input file:

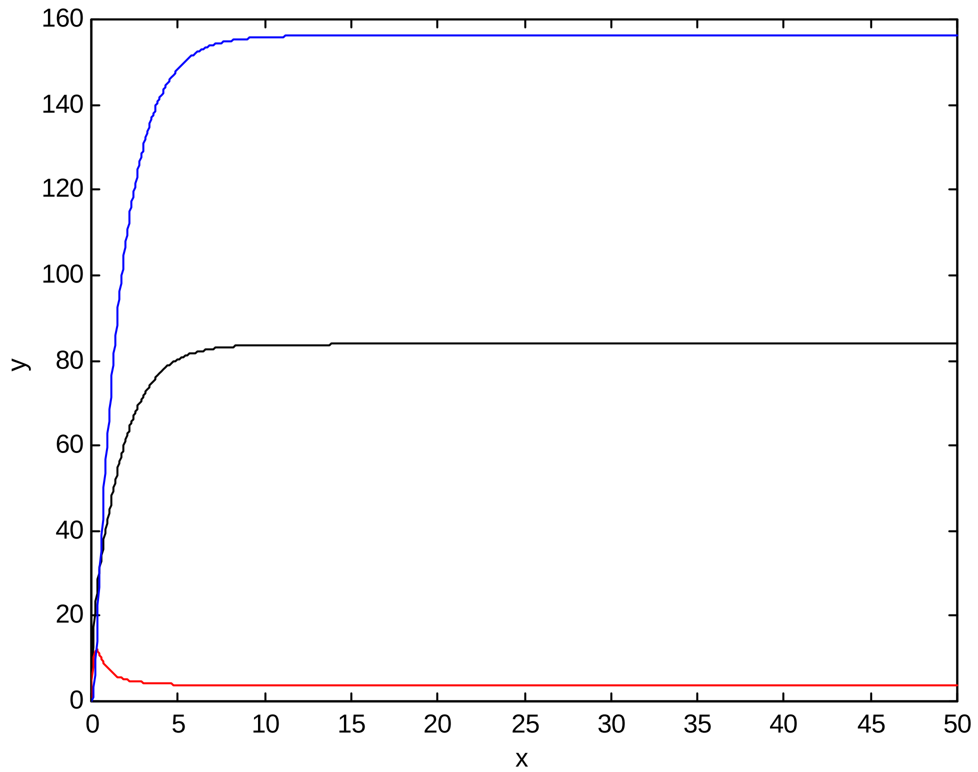
```
function dydt = sysodeinput(x,y,nvec);
%
% gas-phase CSTR with variable exit flow-rate
%
%
%  sample usage:
% [y,x] = sysode(2,1000,0,100,[0,0,0]);
% initially tank is filled with A at one atm.
%
CA = y(1);
CB = y(2);
CC = y(3);
%
```

```
%  A + B --> C
%
nuA = -1;
nuB = -1;
nuC = 1;
sumnu = nuA + nuB + nuC;
%
%
%
p = 1013250.0; % Pa
R = 8.314; % J/mol/K
T = 500; % K
CTin = p/(R*T); % mol/m^3
% initial concentrations of A and B
CAin = 0.6*CTin; % mol/m^3
CBin = 0.4*CTin; % mol/m^3
CCin = 0.0;
%
dVR = sumnu*R*T/p; % m^3
ko = 1.0; % m^3/mol/sec
Ea = 5000; % J/mol
k = ko*exp(-Ea/(R*T));
rate = k*CA*CB;
%
Fin = 1.0; % m^3/sec
V = 1.0; % m^3;
Fout = Fin + dVR*rate*V;
%
%  molar balances
%
dydt(1) = Fin/V*CAin - Fout/V*CA + nuA*rate;
dydt(2) = Fin/V*CBin - Fout/V*CB + nuB*rate;
dydt(3) = Fin/V*CCin - Fout/V*CC + nuC*rate;
```

I used the following command:

```
[y,x] = sysode(2,1000,0,50,[0,0,0]);
```

The output plot was



The last lines of the output file are:

```
4.9700000e+001 8.3770723e+001 3.7833393e+000 1.5619143e+002
4.9750000e+001 8.3770723e+001 3.7833393e+000 1.5619143e+002
4.9800000e+001 8.3770723e+001 3.7833393e+000 1.5619143e+002
4.9850000e+001 8.3770723e+001 3.7833393e+000 1.5619143e+002
4.9900000e+001 8.3770723e+001 3.7833393e+000 1.5619143e+002
4.9950000e+001 8.3770723e+001 3.7833393e+000 1.5619143e+002
5.0000000e+001 8.3770723e+001 3.7833393e+000 1.5619143e+002
```

The steady steady state concentration of A is 83.77 moles/m^3.

The steady state conversion is

$$X_A = 1 - \frac{C_A}{C_{A,in}} = 1 - \frac{83.77}{146.2473} = 0.4272$$

where I used the ideal gas law to determine CA,in.

$$C_{A,in} = \frac{N}{V} = \frac{p}{RT} = 146.2473 \frac{\text{mol}}{\text{m}^3}$$

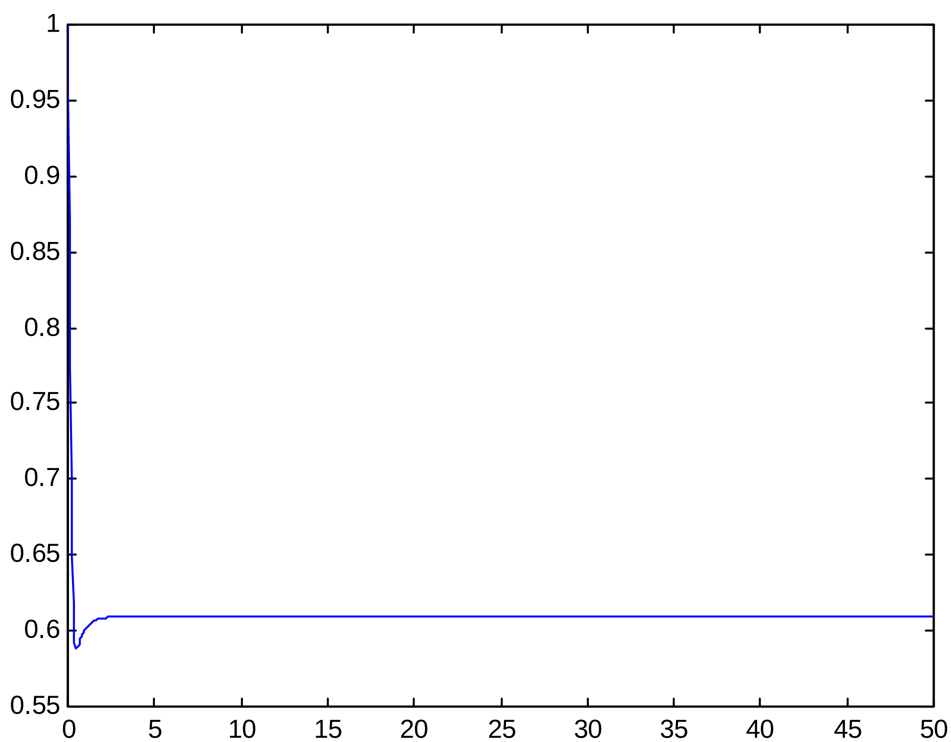
(b) Provide a plot of the exit flow-rate as a function of time from your initial conditions to steady state.

I typed the following commands in matlab

After I ran part A, I have the concentrations stored in the y matrix and time stored in the x vector.

I then ran

```
k = 0.30035;
rate = k*y(:,1).*y(:,2);
dVR = -0.00410264001974;
Fin = 1.0; % m^3/sec
V = 1.0; % m^3;
Fout = Fin + dVR*rate*V;
plot(x,Fout)
```



(c) What is the steady state exit flow-rate?

Fout(1001) = 0.60945984012260 m^3/sec
The steady state outlet flowrate is 0.61 m^3/sec.