CBE 450 Chemical Reactor Fundamentals
Fall, 2009
Homework Assignment #4 Solutions

1. Batch Reactor Analysis via Analytical Expressions

Consider the following isomerization reaction

$$A \rightarrow B$$

with an elementary mechanism such that the rate is

$$r = kC_A$$

where the rate constant is given by

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

The temperature is 300 K. The activation energy is 5000 J/mol. The rate constant prefactor is 10.0 s^{-1}. The initial concentration of A is 10.0 mol/liter.

(a) Provide an analytical expression for the residence time required to achieve a specified conversion for this reaction in a batch reactor.
(b) What residence time is required to reach a conversion of 95%?
(c) What residence time is required to reach a conversion of 95% if the reaction rate prefactor is doubled?
(d) What residence time is required to reach a conversion of 95% if the activation energy is doubled?
(e) What residence time is required to reach a conversion of 95% if the reactor volume is doubled?
(f) What residence time is required to reach a conversion of 95% if the inlet concentration is doubled?
(g) What conversion will one obtain if the residence time is 10 s?
(h) What reactor volume is required to produce 10 mol/s of B at 95% conversion?
(i) What reactor volume is required to produce 10 mol/s of B at 98% conversion?

Solution:

(a) Provide an analytical expression for the residence time required to achieve a specified conversion for this reaction in a batch reactor.

From Fogler page 150

$$t_R = \frac{1}{k}\ln\left(\frac{1}{1-X}\right)$$

(b) What residence time is required to reach a conversion of 95%?

$$k = k_o \exp\left(-\frac{E_a}{RT}\right) = 10\exp\left(-\frac{5000}{8.314*300}\right) = 1.347\, s^{-1}$$

$$t_R = \frac{1}{k}\ln\left(\frac{1}{1-X}\right) = \frac{1}{1.347}\ln\left(\frac{1}{1-0.95}\right) = 2.224\, s$$

(c) What residence time is required to reach a conversion of 95% if the reaction rate prefactor is doubled?

$$k = k_o \exp\left(-\frac{E_a}{RT}\right) = 20\exp\left(-\frac{5000}{8.314*300}\right) = 2.694\, s^{-1}$$

$$t_R = \frac{1}{k}\ln\left(\frac{1}{1-X}\right) = \frac{1}{2.694}\ln\left(\frac{1}{1-0.95}\right) = 1.112\, s$$

(d) What residence time is required to reach a conversion of 95% if the activation energy is doubled?

$$k = k_o \exp\left(-\frac{E_a}{RT}\right) = 10\exp\left(-\frac{10000}{8.314*300}\right) = 0.1815\, s^{-1}$$

$$t_R = \frac{1}{k}\ln\left(\frac{1}{1-X}\right) = \frac{1}{0.1815}\ln\left(\frac{1}{1-0.95}\right) = 16.51 s$$

(e) What residence time is required to reach a conversion of 95% if the reactor volume is doubled?

Residence time doesn’t depend on reactor size for this reaction.

$$t_R = \frac{1}{k}\ln\left(\frac{1}{1-X}\right) = \frac{1}{1.347}\ln\left(\frac{1}{1-0.95}\right) = 2.224\, s$$

(f) What residence time is required to reach a conversion of 95% if the inlet concentration is doubled?

Residence time doesn’t depend on initial concentration for this reaction.

$$t_R = \frac{1}{k}\ln\left(\frac{1}{1-X}\right) = \frac{1}{1.347}\ln\left(\frac{1}{1-0.95}\right) = 2.224\,s$$

(g) What conversion will one obtain if the residence time is 10 s?

$$t_R = \frac{1}{k}\ln\left(\frac{1}{1-X}\right)$$

$$X = 1 - \exp(-kt_R) = 1 - \exp(-1.347 \cdot 10) = 0.9999986$$

(h) What reactor volume is required to produce 10 mol/s of B at 95% conversion?

The initial concentration is 10 mol/liter or 10,000 mol/m^3. If we convert 95% of this, then our concentration of B is 9500 mol/m^3. If our residence time is 2.224 seconds, then we can produce

$$9500\frac{mol}{m^3} \cdot \frac{1}{2.224\,\mathrm{s}} = 4271\frac{mol}{m^3 \cdot s}$$

In order to get 10 mol/s,

$$4271\frac{mol}{m^3 \cdot s}V = 10\frac{mol}{s}$$

so the volume is 0.002341 m^3 or 2.341 liters.

(i) What reactor volume is required to produce 10 mol/s of B at 98% conversion?

If we want 98% conversion, the residence time is

$$t_R = \frac{1}{k}\ln\left(\frac{1}{1-X}\right) = \frac{1}{1.347}\ln\left(\frac{1}{1-0.98}\right) = 2.904\,s$$

The initial concentration is 10 mol/liter or 10,000 mol/m^3. If we convert 98% of this, then our concentration of B is 9800 mol/m^3. If our residence time is 2.904 seconds, then we can produce

$$9800\frac{mol}{m^3} \cdot \frac{1}{2.904\,\mathrm{s}} = 3374\frac{mol}{m^3 \cdot s}$$

In order to get 10 mol/s,

$$3374\frac{mol}{m^3 \cdot s}V = 10\frac{mol}{s}$$

so the volume is 0.002963 m^3 or 2.963 liters.

2. Batch Reactor Analysis via Numerical Methods

Consider the following reaction

$$A + B \rightarrow C$$

with an elementary mechanism such that the rate is

$$r = kC_A C_B$$

where the rate constant is given by

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

The temperature is 300 K. The activation energy is 5000 J/mol. The rate constant prefactor is 0.001 s^{-1}. The reactor has a volume of 1 m^3. The initial concentration of A is 10.0 mol/liter. The initial concentration of B is 15.0 mol/liter.

(a) Use Matlab to create a plot of the concentrations of A, B and C as a function of time for the first 7200 s of the reaction. Label A, B and C on the plot. Provide your input file for sysodeinput.m.
(b) Use this plot (or the tabular form of the data in the plot) to determine what residence time is required to reach a conversion of 95%?
(c) What residence time is required to reach a conversion of 95% if the activation energy is doubled?
(d) What conversion will one obtain if the residence time (with the original activation energy) is 1000 s?
(e) What reactor volume is required to produce 10 mol/hr of C at 95% conversion?

Solution:

(a) Use Matlab to create a plot of the concentrations of A, B and C as a function of time for the first 7200 s of the reaction.

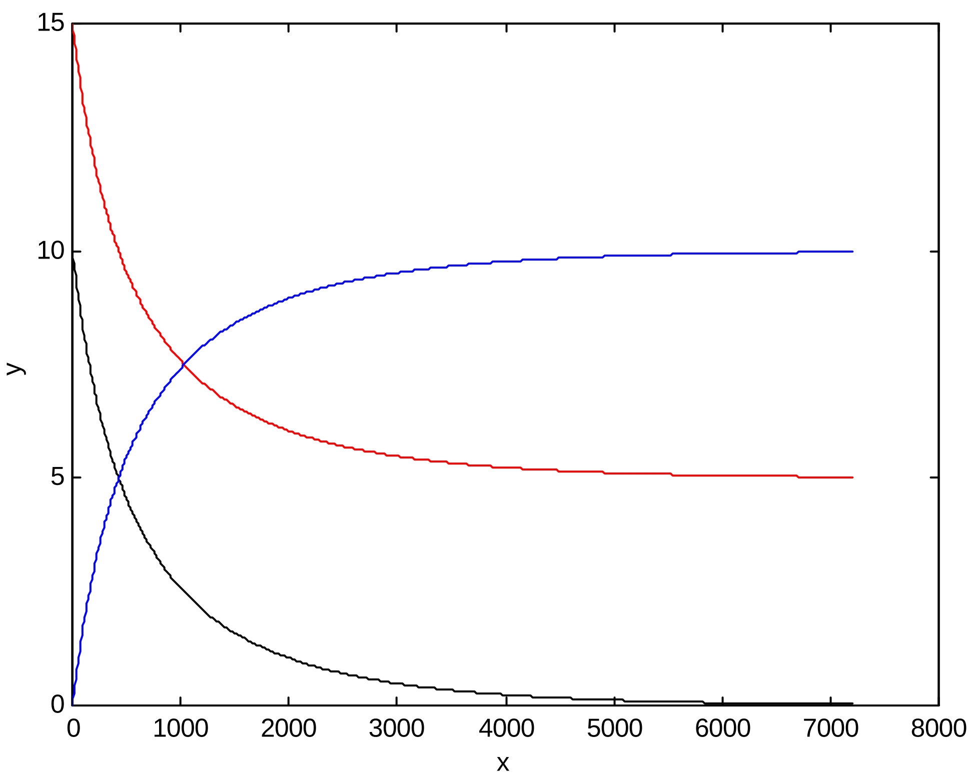
```
function dydt = sysodeinput(x,y,nvec);
%
% homework four problem 2
%
%  A + B --> C
%
nuA = -1;
nuB = -1;
nuC = 1;
CA = y(1);
CB = y(2);
```

```
CC = y(3);
ko = 1.0e-3; % s^-1
Ea = 5000; % J/mol
R = 8.314; % J/mol/K
T = 300; % K
k = ko*exp(-Ea/(R*T));
rate = k*CA*CB;
%  balance on A in terms of conc of A
dydt(1) = nuA*rate;
%  balance on B in terms of conc of B
dydt(2) = nuB*rate;
%  balance on C in terms of conc of C
dydt(3) = nuC*rate;
```

The command I used was

```
sysode(2,1000,0,7200,[10,15,0]);
```

which generated this plot:



legend: black = A, red = B, blue = C.

(b) Use this plot (or the tabular form of the data in the plot) to determine what residence time is required to reach a conversion of 95%?

If the initial concentration of A was 10 mol/liter, then after 95% conversion, the concentration of C is 9.5 mol/liter.

From the data file, sysode.out,

```
x              y(1)           y(2)           y(3)
2.9304000e+003 5.1040049e-001 5.5104005e+000 9.4895995e+000
2.9376000e+003 5.0768060e-001 5.5076806e+000 9.4923194e+000
2.9448000e+003 5.0497654e-001 5.5049765e+000 9.4950235e+000
2.9520000e+003 5.0228819e-001 5.5022882e+000 9.4977118e+000
2.9592000e+003 4.9961545e-001 5.4996155e+000 9.5003845e+000
2.9664000e+003 4.9695822e-001 5.4969582e+000 9.5030418e+000
2.9736000e+003 4.9431639e-001 5.4943164e+000 9.5056836e+000
2.9808000e+003 4.9168986e-001 5.4916899e+000 9.5083101e+000
```

So, the residence time is about 2959 sec to reach 95% conversion.

(c) What residence time is required to reach a conversion of 95% if the activation energy is doubled?

```
function dydt = sysodeinput(x,y,nvec);
%
% homework four problem 2
%
%  A + B --> C
%
nuA = -1;
nuB = -1;
nuC = 1;
CA = y(1);
CB = y(2);
CC = y(3);
ko = 1.0e-3; % s^-1
Ea = 10000; % J/mol
R = 8.314; % J/mol/K
T = 300; % K
k = ko*exp(-Ea/(R*T));
rate = k*CA*CB;
%  balance on A in terms of conc of A
dydt(1) = nuA*rate;
%  balance on B in terms of conc of B
dydt(2) = nuB*rate;
%  balance on C in terms of conc of C
dydt(3) = nuC*rate;
```

The command I used was

```
sysode(2,1000,0,30000,[10,15,0]);
```

x	y(1)	y(2)	y(3)
2.1900000e+004	5.0299964e-001	5.5029996e+000	9.4970004e+000
2.1930000e+004	5.0149525e-001	5.5014952e+000	9.4985048e+000
2.1960000e+004	4.9999576e-001	5.4999958e+000	9.5000042e+000
2.1990000e+004	4.9850117e-001	5.4985012e+000	9.5014988e+000
2.2020000e+004	4.9701144e-001	5.4970114e+000	9.5029886e+000

So the residence time for 95% conversion is 21,960 sec.

(d) What conversion will one obtain if the residence time (with the original activation energy) is 1000 s?

From the output file, sysode.out, of the first run, we have

x	y(1)	y(2)	y(3)
9.8640000e+002	2.6110780e+000	7.6110780e+000	7.3889220e+000
9.9360000e+002	2.5918983e+000	7.5918983e+000	7.4081017e+000
1.0008000e+003	2.5729072e+000	7.5729072e+000	7.4270928e+000
1.0080000e+003	2.5541020e+000	7.5541020e+000	7.4458980e+000
1.0152000e+003	2.5354802e+000	7.5354802e+000	7.4645198e+000

So at 1000 s, the conversion is about 74.3%.

(e) What reactor volume is required to produce 10 mol/hr of C at 95% conversion?

At 95% conversion of C, we obtain 9.5 mol/liter of C after 2959 sec.

$$9.5\frac{mol}{l}\cdot\frac{1}{2959\mathrm{s}}=0.003211\frac{mol}{l\cdot s}=0.003211\frac{mol}{l\cdot s}=11.56\frac{mol}{l\cdot hr}$$

In order to get 10 mol/hr,

$$11.56\frac{mol}{l\cdot hr}V=10\frac{mol}{hr}$$

so the volume is 0.865 liters.

3. CSTR Analysis via Analytical Expressions

Consider the following isomerization reaction

$$A \rightarrow B$$

with an elementary mechanism such that the rate is

$$r=kC_A$$

where the rate constant is given by

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

The temperature is 300 K. The activation energy is 5000 J/mol. The rate constant prefactor is 10.0 s^{-1}. The inlet flowrate is 2 liters/sec. The concentration of A in the inlet stream is 10 mol/liter.

(a) Provide an analytical expression for the residence time required to achieve a specified conversion for this reaction in a batch reactor.
(b) What is the Damköhler number for 95% conversion?
(c) What residence time is required to reach a conversion of 95%?
(d) If the volume of the reactor is 1 liter, what is the volumetric flowrate of the inlet stream?
(e) If the inlet flowrate is 2 liter/sec, what volume is required to obtain a 95% conversion?
(f) If the reactor is operating at 95% conversion and you want to produce 10,000 mol/hr of B, determine the volume of the reactor and the volumetric flowrate required.

Solution:

(a) Provide an analytical expression for the residence time required to achieve a specified conversion for this reaction in a batch reactor.

$$X_A = \frac{Da}{1+Da} = \frac{\tau_R k}{1+\tau_R k}$$

Rearranging this for the residence time yields

$$\tau_R = \frac{1}{k}\frac{X_A}{1-X_A}$$

(b) What is the Damköhler number for 95% conversion?

Rearrange the above expression.

$$Da = \frac{X_A}{(1-X_A)} = \frac{0.95}{(1-0.95)} = 19$$

(c) What residence time is required to reach a conversion of 95%?

$$k = k_o \exp\left(-\frac{E_a}{RT}\right) = 10 \exp\left(-\frac{5000}{8.314*300}\right) = 1.347\, s^{-1}$$

$$Da = kt_R$$

$$t_R = \frac{Da}{k} = \frac{19}{1.347} = 14.1\,s$$

(d) If the volume of the reactor is 1 liter, what is the volumetric flowrate of the inlet stream?

$$t_R = \frac{V}{F}$$

$$F = \frac{V}{t_R} = \frac{1}{14.1} = 0.07089\frac{l}{s}$$

(e) If the inlet flowrate is 2 liter/sec, what volume is required to obtain a 95% conversion?

The residence time for 95% conversion is 14.1 s.

$$V = t_R F = 14.1 \cdot 2 = 28.2\,liters$$

(f) If the reactor is operating at 95% conversion and you want to produce 10,000 mol/hr of B, determine the volume of the reactor and the volumetric flowrate required.

We want 10,000 mol/hr of B, which at 95% conversion requires 10526 mol/hr of A. A comes in at 10 mol/liter. So we need

$$FC_A = \dot{N}_A$$

$$F = \frac{\dot{N}_A}{C_A}$$

$$F = 10526\frac{mol}{hr} \cdot \frac{liter}{10\,mol} = 1053\frac{liter}{hr}$$

The residence time for 95% conversion is 14.1 s or 0.003917 hr.

$$V = t_R F = 0.003917 \cdot 1053 = 4.124\,liters$$