CBE 450 Chemical Reactor Fundamentals
Fall, 2009
Homework Assignment #3

1. Numerical Solution of a Single Nonlinear Algebraic Equation

Consider a continuous stirred-tank reactor (CSTR) in which the following dimerization reaction goes from 2A → B with the following mass balance on A at steady state

accumulation = in – out + generation

$$0 = F_{in}C_{A,in} - F_{out}C_A - Vk_{\dim er}C_A^2$$

The inlet flow rate is 1 liter/sec, as is the outlet flow rate. The inlet concentration is 10 mole/liter. The rate constant is 0.5 liter/mol/sec. The volume of the reactor is 1 liter.

(a) Solve this nonlinear equation analytically.
(b) How many roots are there?
(c) Which root is the physically meaningful root? Why?
(d) Solve this nonlinear equation using Goalseek in Excel. Provide a print-out of the spreadsheet.
(e) Solve this nonlinear equation using the Newton-Raphson method with numerical derivatives in Matlab. Note the initial guess you used to converge ot the physically meaningful root.

Solution:

(a) Solve this nonlinear equation analytically.

$$0 = F_{in}C_{A,in} - F_{out}C_A - Vk_{\dim er}C_A^2$$

This is a quadratic equation.

$$ax^2 + bx + c = 0$$

with solution

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

In our case

$$x = \frac{F_{out} \pm \sqrt{F_{out}{}^2 + 4Vk_{\dim er}F_{in}C_{A,in}}}{-2Vk_{\dim er}} = \frac{-1 \pm \sqrt{1+20}}{-1} = -1 \pm \sqrt{21} = 3.58 \ or \ -5.58$$

(b) How many roots are there?

There are two roots to a quadratic equation.

(c) Which root is the physically meaningful root? Why?

3.58 is the physically meaningful root. The root must be positive since it is a concentration. The root must also be less than 10.0, since that is the inlet concentration. 3.58 satisfies both these roots.

(d) Solve this nonlinear equation using Goalseek in Excel. Provide a print-out of the spreadsheet.

a	-0.5	V	1	kdimer	0.5
b	1	Fout	1		
c	10	Fin	1	Cain	10
x	3.582528				
f	0.00022				

(e) Solve this nonlinear equation using the Newton-Raphson method with numerical derivatives in Matlab. Note the initial guess you used to converge ot the physically meaningful root.

I used the newraph_nd.m code.

The input file was:

```
function f = funkeval(x)
CA = x;
Fin = 1;
Fout = 1;
V = 1;
kdimer = 0.50;
CAin = 10;
f = Fin*Cain-Fout*CA-V*kdimer*CA^2;
```

The Matlab output was:

```
» [x0,err] = newraph_nd(5)
icount = 1 xold = 5.000000e+000 f = -7.500000e+000 df = -6.000000e+000 xnew = 3.750000e+000 err = 1.000000e+002
icount = 2 xold = 3.750000e+000 f = -7.812500e-001 df = -4.750000e+000 xnew = 3.585526e+000 err = 4.587156e-002
icount = 3 xold = 3.585526e+000 f = -1.352580e-002 df = -4.585526e+000 xnew = 3.582577e+000 err = 8.233380e-004
icount = 4 xold = 3.582577e+000 f = -4.350281e-006 df = -4.582577e+000 xnew = 3.582576e+000 err = 2.649795e-007
x0 =   3.58257569495594
err =    2.649794554553279e-007
```

2. Numerical Solution of a System of Nonlinear Algebraic Equations

Consider a continuous stirred-tank reactor (CSTR) in which the following isomerization reaction goes from A → B with the following mass balance on A at steady state

accumulation = in – out + generation

$$0 = F_{in}C_{A,in} - F_{out}C_A - Vk_{iso}C_A$$

The inlet flow rate is 1 liter/sec, as is the outlet flow rate. The inlet concentration is 10 mole/liter. The rate constant is

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

where k_o = 1.0 sec^{-1} and E_a = 2500 J/mol/K. The volume of the reactor is 1 liter.

The steady state energy balance is

accumulation = in – out + generation

$$0 = F_{in}H_{in} - F_{out}H - \Delta H_R V k_{iso} C_A$$

where the inlet enthalpy, $H_{in} = C_p T_{in}$, where the heat capacity is 4.0 kJ/liter/K and the inlet temperature is 300 K, where the enthalpy of the reactor is $H = C_p T$, and where the heat of reaction, ΔH_R , is -30 kJ/mol.

Find the steady state concentration of A and temperature. Provide Matlab equation input file and screen output. (You do not have to provide the entire Newton Raphson code provided in class.)

Solution:

I used the NRNDN.m code with the syseqninput.m input file.

The input file was:

```
function f = syseqninput(x);
CA = x(1); % mol/liter
T = x(2); % K
ko = 1.0; % 1/sec
Ea = 2500; % J/mol/K
R = 8.314; % J/mol/K
Tin = 300; % K
k = ko*exp(-Ea/(R*T));
Fin = 1.0; % liter/sec
Fout = 1.0; % liter/sec
V = 1.0; % liter
```

```
Cain = 10.0; % mol/liter
Cp = 4000; % J/liter/K
Hin = Cp*Tin; % J/liter
H = Cp*T; % J/liter
deltaHR = -30000.0; % J/mol
f(1) = Fin*Cain - Fout*CA - V*k*CA;
f(2) = Fin*Hin - Fout*H - deltaHR*V*k*CA;
```

The Matlab output was

```
» [f,x] = NRNDN([5,300],1.0e-6,1)
iter =    1, err = 1.48e+001
 iter =    2, err = 2.03e-001
 iter =    3, err = 5.43e-005
 iter =    4, err = 3.85e-012

f =  2.034285145325335e-008
x = 1.0e+002 *
   0.07183711607372   3.21122162944709
```

The outlet concentration is 7.18 mol/liter and the reactor temperature is 321 K.

3. Numerical Solution of a System of Nonlinear Ordinary Differential Equations

Consider a continuous stirred-tank reactor (CSTR) in which the following isomerization reaction goes from A → B with the following mass balance on A

accumulation = in – out + generation

$$V\frac{dC_A}{dt} = F_{in}C_{A,in} - F_{out}C_A - Vk_{iso}C_A$$

The inlet flow rate is 1 liter/sec, as is the outlet flow rate. The inlet concentration is 10 mole/liter. The rate constant is

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

where k_o = 1.0 sec^{-1} and E_a = 2500 J/mol/K. The volume of the reactor is 1 liter.

The steady state energy balance is

accumulation = in – out + generation

$$VC_p\frac{dT}{dt} = F_{in}H_{in} - F_{out}H - \Delta H_R V k_{iso}C_A$$

where the inlet enthalpy, $H_{in} = C_p T_{in}$, where the heat capacity is 4.0 kJ/liter/K and the inlet temperature is 300 K, where the enthalpy of the reactor is $H = C_p T$, and where the heat of reaction, ΔH_R, is -30 kJ/mol.

The initial conditions within the reactor are T(t=0) = 300 K and C_A(t=0) = 0.0 mol/liter.

(a) Find the transient behavior of the concentration and temperature. Provide Matlab equation input file and graphical output. (You do not have to provide the entire Runge-Kutta code provided in class.)
(b) What are the long-time (steady state values) of the concentration of A and the temperature?
(c) How do the values in (b) compare with the steady state solutions obtained in problem 2?

Solution:

(a) Find the transient behavior of the concentration and temperature. Provide Matlab equation input file and graphical output. (You do not have to provide the entire Runge-Kutta code provided in class.)

I used the sysode.m code with the sysodeinput.m input file.

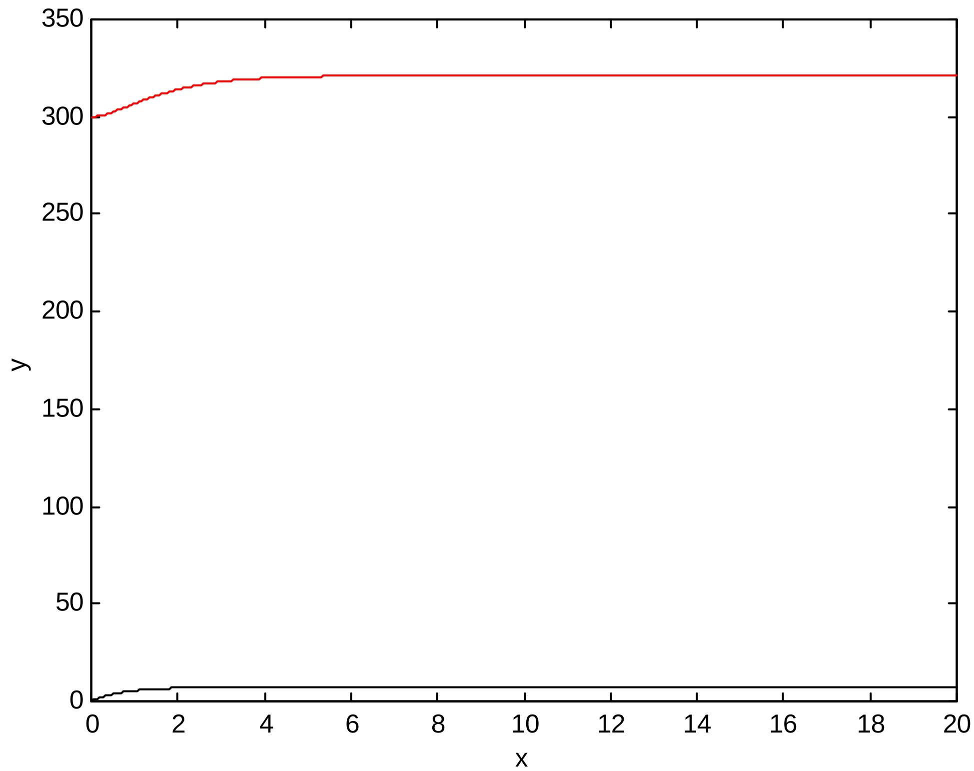
The input file was:

```
function dydt = sysodeinput(x,y,nvec);
CA = y(1); % mol/liter
T = y(2); % K
ko = 1.0; % 1/sec
Ea = 2500; % J/mol/K
R = 8.314; % J/mol/K
Tin = 300; % K
k = ko*exp(-Ea/(R*T));
Fin = 1.0; % liter/sec
Fout = 1.0; % liter/sec
V = 1.0; % liter
Cain = 10.0; % mol/liter
Cp = 4000; % J/liter/K
Hin = Cp*Tin; % J/liter
H = Cp*T; % J/liter
deltaHR = -30000.0; % J/mol
dydt(1) = (Fin*Cain - Fout*CA - V*k*CA)/V;
dydt(2) = (Fin*Hin - Fout*H - deltaHR*V*k*CA)/(V*Cp);
```

The command at the command-line prompt was:

```
[y,x] = sysode(2,1000,0,20,[0,300]);
```

The plot looked as follows:



The black line is the concentration of A. The red line is the temperature. You can see that the system is already at steady state at t = 20 sec.

(b) What are the long-time (steady state values) of the concentration of A and the temperature?

An examination of the output file gives the concentration and temperature at t = 20 sec.

2.0000000e+001 7.1837116e+000 3.2112216e+002

The final concentration is 7.18 mol/liter. The temperature is 321 K.

(c) How do the values in (b) compare with the steady state solutions obtained in problem 2?

These values agree to about 8 significant figures with the steady state values obtained in problem 2.