

Homework Assignment Number Three
Assigned: Thursday, September 23, 1999
Due: Thursday, October 7, 1999 BEGINNING OF CLASS.

Problem (1)

Find an application from your own experience or a classical problem in your own field of research that results in a system of at least 2 linear ODEs.

- (a) Describe the physical problem from which the equation arises. Describe it in sufficient detail that an engineer from a different discipline could understand it.
- (b) Write the ODEs. Write a complete set of reasonable initial conditions.
- (c) If possible, analytically solve for the solution(s).
- (d) Plot the solution.
- (e) Explain the physical significance of the solution(s) and its behavior.

Problem (2)

Consider the initial value problem:

$$\frac{dy}{dx} + a(x)y = b(x)$$

where we have an initial condition of the form:

$$y(x = x_0) = y_0$$

with the specific values given by:

$$a(x) = 2, \quad b(x) = x \sin(3x), \quad y(x = 0) = 1$$

- (a) Analytically solve for $y(x)$ from $x = 0$ to 4.

This is a nonhomogeneous problem with a solution of the form:

$$y_{nh}(x) = y_h(x) + y_p(x)$$

We obtain the homogeneous solution by solving:

$$\frac{dy}{dx} + a(x)y = 0$$

This is easily shown, (using separation of variables) to yield a solution

$$y_h(x) = ce^{-\int a(x)dx} = cy_{id}(x) = ce^{-\int 2dx} = ce^{-2x}$$

The nonhomogeneous solution is given by:

$$y_{nh}(x) = \left[\frac{y_o}{y_{id}(x = x_o)} - \left[\int \frac{b(x)}{y_{id}} dx \right]_{x=x_o} + \int \frac{b(x)}{y_{id}} dx \right] y_{id}(x)$$

where

$$\int \frac{b(x)}{y_{id}} dx = \int \frac{x \sin(3x)}{e^{-2x}} dx = \int x e^{2x} \sin(3x) dx$$

$$\int \frac{b(x)}{y_{id}} dx = \frac{x e^{2x} (2 \sin(3x) - 3 \cos(3x))}{2^2 + 3^2} - \frac{e^{2x} [(2^2 - 3^2) \sin(3x) - 2(2)3 \cos(3x)]}{(2^2 + 3^2)^2}$$

$$\int \frac{b(x)}{y_{id}} dx = \frac{e^{2x}}{169} [(26x + 5) \sin(3x) + (-39x + 12) \cos(3x)]$$

$$\left[\int \frac{b(x)}{y_{id}} dx \right]_{x_o=0} = \frac{e^{2x}}{169} [(26x + 5) \sin(3x) + (-39x + 12) \cos(3x)] = \frac{12}{169}$$

$$y_{id}(x = x_o) = e^{-2x_o} = 1$$

$$y_{nh}(x) = \left[\frac{1}{1} - \frac{12}{169} + \frac{e^{2x}}{169} [(26x + 5) \sin(3x) + (-39x + 12) \cos(3x)] \right] e^{-2x}$$

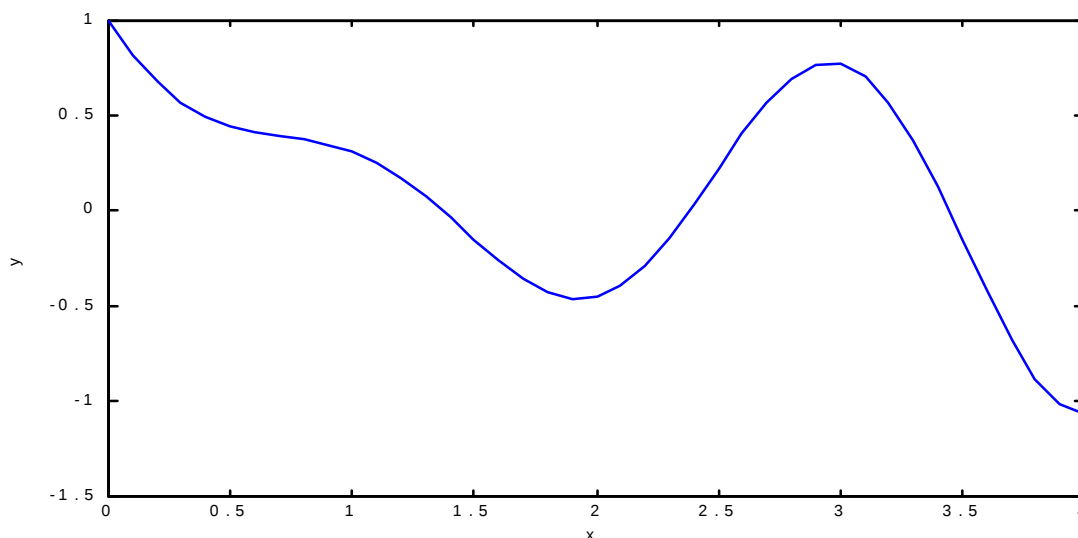
$$y_{nh}(x) = \left[\frac{157e^{-2x}}{169} + \frac{1}{169} [(26x + 5) \sin(3x) + (-39x + 12) \cos(3x)] \right]$$

Check initial condition.

$$y_{nh}(x = 0) = \left[\frac{157e^{-2(0)}}{169} + \frac{1}{169} [(26(0) + 5) \sin(3(0)) + (-39(0) + 12) \cos(3(0))] \right] = 1$$

(b) Plot the analytical solution.

In MATLAB: » x=[0:0.1:4];
 » nx = max(size(x));
 » for i =1:1:nx
 t=x(i);
 y(i)=157*exp(-2*t)/169 +((26*t+5)*sin(3*t) + (-39*t+12)*cos(3*t))/169;
 end
 » plot(x,y); xlabel('x'); ylabel('y')

**Problem (3)**

Given the eigenvectors and eigenvalues of the acetylene in the solution to homework #1, solve for the trajectories of each atom as a function of time, given the initial conditions,

$$\underline{x}(t=0) = \begin{bmatrix} -0.1 \\ 0 \\ 0.25 \\ 0.5 \end{bmatrix} \text{ and initial velocities } \dot{\underline{x}}(t=0) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Solve and plot the trajectories for $t = 0$ to 2 sec, using the following values for the masses and the spring constants.

$$m_H = 1.0, \quad m_C = 12.0, \quad k_{HC} = 1.0, \quad k_{CC} = 10.0$$

Reminder: the eigenvalues are

$$\lambda_1 = 0$$

$$\lambda_2 = -\frac{k_{HC}(m_H + m_C)}{m_H m_C}$$

$$\lambda_3 = \frac{-k_{HC}m_H - 2k_{CC}m_H - k_{HC}m_C + K}{2m_H m_C}$$

$$\lambda_4 = \frac{-k_{HC}m_H - 2k_{CC}m_H - k_{HC}m_C - K}{2m_H m_C}$$

where

$$K = \sqrt{k_{HC}^2 m_H^2 + 4k_{HC}k_{CC}m_H^2 + 2k_{HC}^2 m_H m_C + 4k_{CC}^2 m_H^2 - 4k_{HC}k_{CC}m_H m_C + k_{HC}^2 m_C^2}$$

The eigenvectors are:

$$\underline{w}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \quad \underline{w}_2 = \begin{bmatrix} \frac{1}{m_H} \\ -\frac{m_C}{m_H} \\ -\frac{m_H}{m_C} \\ 1 \end{bmatrix} \quad \underline{w}_3 = \begin{bmatrix} -1 \\ -b_+ \\ b_+ \\ 1 \end{bmatrix} \quad \underline{w}_4 = \begin{bmatrix} -1 \\ -b_- \\ b_- \\ 1 \end{bmatrix}$$

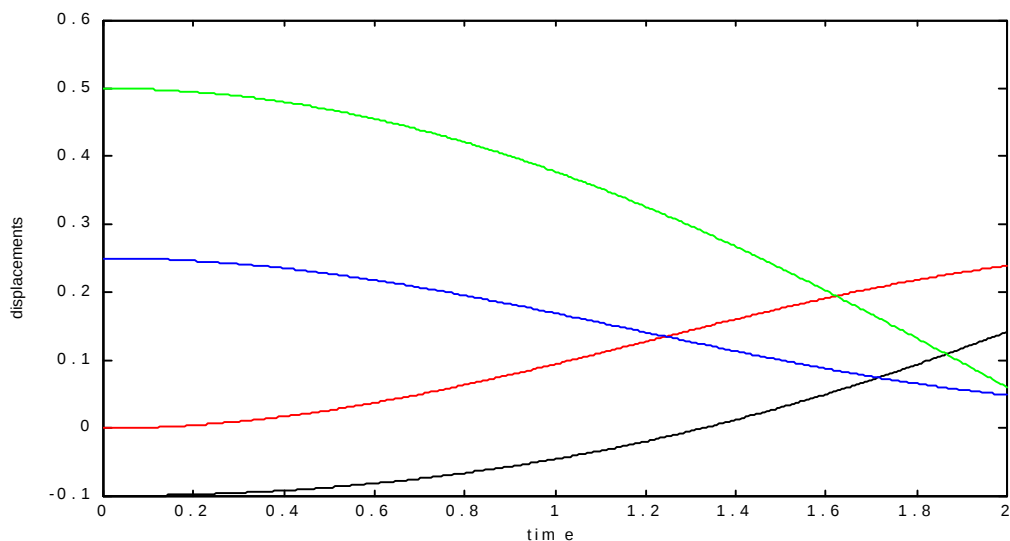
where

$$b_+ = \frac{-k_{HC}m_H - 2k_{CC}m_H - k_{HC}m_C + K}{2k_{HC}m_C} + 1 = \frac{m_H\lambda_3}{k_{HC}} + 1$$

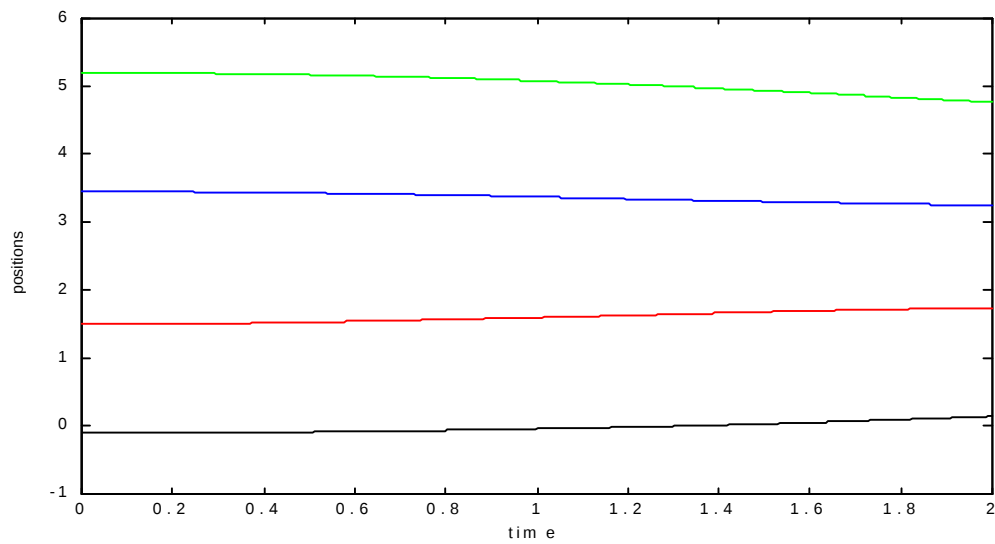
$$b_- = \frac{-k_{HC}m_H - 2k_{CC}m_H - k_{HC}m_C - K}{2k_{HC}m_C} + 1 = \frac{m_H\lambda_4}{k_{HC}} + 1$$

Solution:

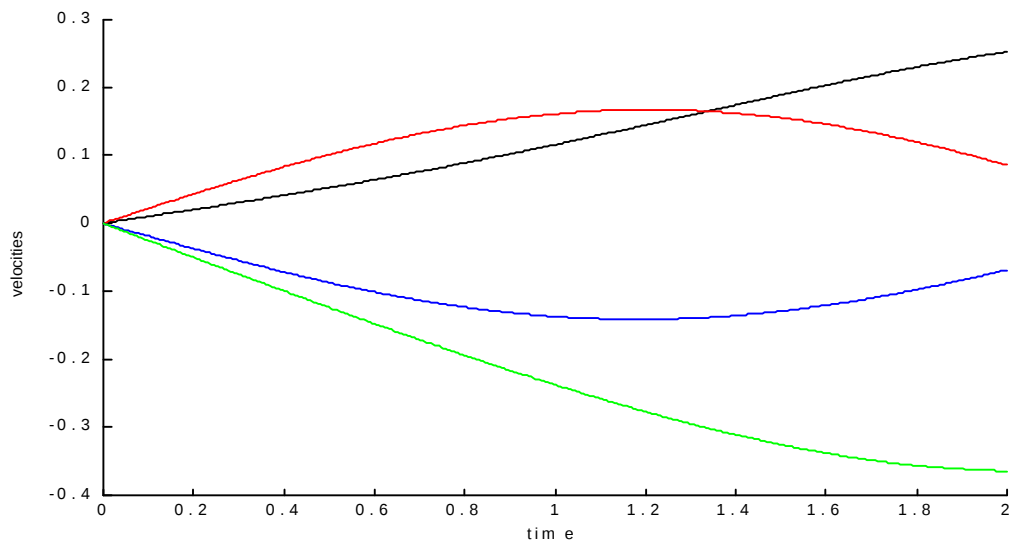
Here are the displacements of the 4 molecules. (black = H1, red=C1, blue=C2, green=H2)



If the displacements look confusing, you can add bond lengths to the displacements to get the positions, which then look like:



The velocities looked like:



The MATLAB code used to generate the solution and the three plots is given below. This code also first performs the eigenanalysis of the modes of motion (which is not necessary to the solution of this problem.)

```

clear
mh = 1;
mc = 12;
khc = 1;
kcc = 10;

K = sqrt(khc^2*mh^2 + 4*khc*kcc*mh^2 +
2*khc^2*mh*mc+4*kcc^2*mh^2 - 4*khc*kcc*mh*mc + khc^2*mc^2)

%
% define eigenvalues and eigenvectors from analytical solution
%
lam(1) = 0;
lam(2) = -khc*(mh+mc)/(mh*mc);
lam(3) = (-khc*mh-2*kcc*mh-khc*mc+K)/(2*mh*mc);
lam(4) = (-khc*mh-2*kcc*mh-khc*mc-K)/(2*mh*mc);

a = -mh/mc;
bp = mh*lam(3)/khc + 1;
bn = mh*lam(4)/khc + 1;
w = [ 1 1 -1 -1
      1 a -bp -bn
      1 a bp bn
      1 1 1 1];

fprintf(1,'here are eigenvalues from analytical solution: \n
')
lam
fprintf(1,'here are eigenvectors from analytical solution: \n
')
w
%
% now plot analytical solution
%
fprintf(1,'\nhere we are working on the transient analytical
solution: \n ')

A = zeros(8,8);
A(1,:) = [0 0 0 0 1 0 0 0];
A(2,:) = [0 0 0 0 0 1 0 0];
A(3,:) = [0 0 0 0 0 0 1 0];
A(4,:) = [0 0 0 0 0 0 0 1];
A(5,:) = [-khc/mh khc/mh 0 0 0 0 0 0];
A(6,:) = [-khc/mc -(khc+kcc)/mc kcc/mc 0 0 0 0 0];
A(7,:) = [0 kcc/mc -(khc+kcc)/mc khc/mc 0 0 0 0];
A(8,:) = [0 0 khc/mh -khc/mh 0 0 0 0];

yo = [-0.1 0 0.25 0.5 0.0 0.0 0.0 0.0];
to = 0.0;
tf = 2.0;
n = max(size(A));
% compute eigenvalues and eigenvectors
[wcov, lambdac] = eig(A);
wcovinv = inv(wcov);

```

```

% set up discretized solution grid
npnts = 1000;
dt = (tf-to)/npnts;
for i = 1:1:npnts+1
    tp(i) = (i-1)*dt + to;
end
% calculate solution
explambda = zeros(n,n);
yp = zeros(n,npnts);
for i = 1:1:npnts+1
    for j = 1:n
        explambda(j,j) = exp(lambdac(j,j)*(tp(i) - to));
    end
    yp(:,i) = wcov*explambda*wcovinv*yo;
end
%
% remove spurious imaginary components due round-off
truncation errors
%
for j = 1:1:n
    for i = 1:1:npnts
        if (abs(imag(yp(j,i))) < 1.0e-15)
            yp(j,i) = real(yp(j,i));
        end
    end
end
%plot
figure(1)
clf
for j = 1:1:n
    if (j==1)
        plot (tp,yp(j,:), 'k-'), xlabel( 't' ), ylabel ( 'y' )
    elseif (j==2)
        plot (tp,yp(j,:), 'r-'), xlabel( 't' ), ylabel ( 'y' )
    elseif (j==3)
        plot (tp,yp(j,:), 'b-'), xlabel( 't' ), ylabel ( 'y' )
    elseif (j==4)
        plot (tp,yp(j,:), 'g-'), xlabel( 't' ), ylabel ( 'y' )
    end
    hold on
end
ylabel('displacements')
xlabel('time')
hold off
figure(2)
clf
bondhco = 1.5;
bondcco = 1.7;
for j = 1:1:n
    if (j==1)
        plot (tp,yp(j,:), 'k-'), xlabel( 't' ), ylabel ( 'y' )
    elseif (j==2)
        plot (tp,yp(j,:)+bondhco, 'r-'), xlabel( 't' ), ylabel (
'y' )

```

```

elseif (j==3)
    plot (tp,yp(j,:)+bondhco+bondcco,'b-'), xlabel( 't' ),
    ylabel ( 'y' )
elseif (j==4)
    plot (tp,yp(j,:)+bondhco+bondcco+bondhco,'g-'), xlabel(
't' ), ylabel ( 'y' )
end
hold on
end
ylabel('positions')
xlabel('time')
hold off
figure(3)
clf
for j = 1:1:n
    if (j==5)
        plot (tp,yp(j,:), 'k-'), xlabel( 't' ), ylabel ( 'y' )
    elseif (j==6)
        plot (tp,yp(j,:), 'r-'), xlabel( 't' ), ylabel ( 'y' )
    elseif (j==7)
        plot (tp,yp(j,:), 'b-'), xlabel( 't' ), ylabel ( 'y' )
    elseif (j==8)
        plot (tp,yp(j,:), 'g-'), xlabel( 't' ), ylabel ( 'y' )
    end
    hold on
end
ylabel('velocities')
xlabel('time')
hold off

```

Problem (4)

Perform a stability analysis on the linear ODE model you created in Problem (1).

- Find the eigenvalues and eigenvectors.
- Describe the type of critical point.
- Describe the stability of the critical point.
- Give a physical description of the eigenvectors.
- Show a phase plot with the critical point, eigenvectors, and a couple representative trajectories plotted on it.

Problem (5)

In the notes on ODE stability, there is the example of a first order reaction occurring in an adiabatic CSTR. Repeat the problem when the reaction is second order. Use all of the same parameters as are used in the example in the notes, except make the reactor volume 10 liters.

For those students who are not chemical engineers, I give the parameters and ODEs below. For those students who are chemical engineers, you should be able to derive these ODEs.

```

x = y(1);           % extent of reaction
T = y(2);           % Temperature K
Cin = 3.0;           % inlet concentration mol/l
C = Cin*(1-x);       % concentration
Q = 60e-3;           % volumetric flowrate l/s
R = 8.314;           % gas constant J/mol/K
Ea = 62800;          % activation energy J/mol
ko = 4.48e+6;         % reaction rate prefactor 1/s
k = ko*exp(-Ea/(R*T)); % reaction rate constant 1/s
V = 10;              % reactor volume l
Cp = 4.19e3;          % heat capacity J/kg/K
Tin = 298;           % inlet feed temperature K
Tref = 298;          % thermodynamic reference temperature K
DHR = -2.09e5;        % heat of rxn J/mol
rho = 1.0;           % density kg/l
dydt(1) = 1/V*(Q*Cin - Q*C - k*C*C*V); % mass balance mol/s
dydt(2) = 1/(Cp*rho*V)*(Q*Cp*rho*Tin - Q*Cp*rho*T -
DHR*k*C*C*V);        % NRG balance J/s
dydt(1) = -1/Cin*dydt(1); % convert conc. to extent

```

- Find the critical points.
- Determine the type and stability of the critical point by plotting a few trajectories in the phase plane.

Solution to Problem (5)

The critical points are located at:

yc1 =	yc2 =	yc3 =
0.0302	0.3025	0.8648
302.5164	343.2630	427.4140

These critical points were obtained by using the routine syseqn.m as it appears on the website and input file syseqninput.m with the following content:

```
function [f] = syseqninput(x0)
    x = x0(1);           % extent of reaction
    T = x0(2);           % Temperature K
    Cin = 3.0;           % inlet concentration mol/l
    C = Cin*(1-x);       % concentration
    Q = 60e-3;           % volumetric flowrate l/s
    R = 8.314;           % gas constant J/mol/K
    Ea = 62800;          % activation energy J/mol
    ko = 4.48e+6;         % reaction rate prefactor 1/s
    k = ko*exp(-Ea/(R*T)); % reaction rate constant 1/s
    V = 10;              % reactor volume l
    Cp = 4.19e3;          % heat capacity J/kg/K
    Tin = 298;           % inlet feed temperature K
    Tref = 298;          % thermodynamic reference temperature K
    DHr = -2.09e5;        % heat of rxn J/mol
    rho = 1.0;           % density kg/l
    f(1) = 1/V*(Q*Cin - Q*C - k*C*C*V); % mass balance mol/s
    f(2) = 1/(Cp*rho*V)*(Q*Cp*rho*Tin - Q*Cp*rho*T -
    DHr*k*C*C*V); % NRG balance J/s
```

The initial guesses I used to converge to each solution are given below:

```
» syseqn(1,[0,300])
```

Attempting solution with MATLABs fsolve function

VARIABLE	INPUT	OUTPUT
1	0.0000000e+000	3.0181616e-002
2	3.0000000e+002	3.0251644e+002

```
syseqn(1,[0.5,350])
```

Attempting solution with MATLABs fsolve function

VARIABLE	INPUT	OUTPUT
1	5.0000000e-001	3.0247541e-001
2	3.5000000e+002	3.4326303e+002

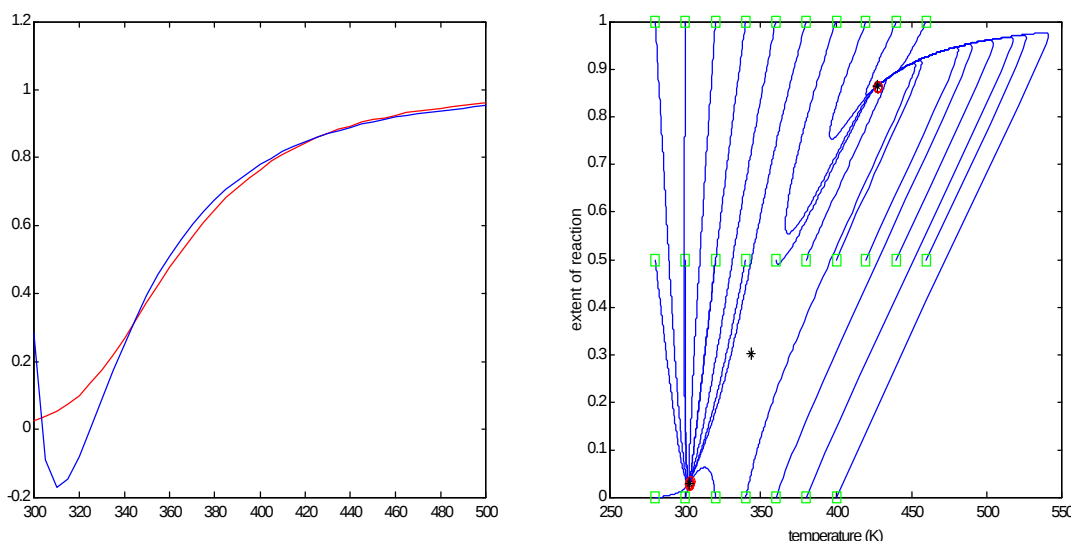
```
syseqn(1,[0.9,460])
```

Attempting solution with MATLABs fsolve function

VARIABLE	INPUT	OUTPUT
1	9.0000000e-001	8.6482379e-001
2	4.6000000e+002	4.2741397e+002

(b)

The mass and energy balances are plotted below, as a function of extent and temperature. Where they intersect, we have a critical point. A phase plane with critical points and trajectories is also shown.



From the trajectory plots given above we can determine the nature of the critical points (steady state solutions in this example). The low-conversion/low-temperature and the high-conversion/high-temperature solutions are stable, node-like attractors. The intermediate solution is an unstable node. The eigenvalues of this systems are purely real. The eigenvalues associated with the attractors are less than zero. At least one eigenvalue associated with the unstable node is negative.

We can also see some qualitative information about the system. We can define roughly the basins of attraction for the two attractors. For the coarse grid we used, any initial temperature of 400 K or higher converged to the high critical point. Any initial temperature of 320 K or lower converged to the low critical point. For initial temperatures of 340, 360 and 380 K, those with high initial extents of reaction proceeded to the low root; those with low initial extents of reaction converged to the high root.

Some initial conditions with low initial extent of reaction and low temperature, proceeded through temperatures higher than the high root on their way to the high root. This is because the reactor is full of unreacted product. It reacts initially, which, since the reaction is exothermic, heats up the reactor. It then takes some time for new feed to enter and cool the reactor to its steady state temperature.

The trajectories were generated using the sysode.m program as it appears on the website and a sysodeinput.m file analogous to that given for syseqninput.m above.