CHE 374 Seminar Example: Solving ode's in matlab

ISOTHERMAL Plug Flow Reactor

A plug flow reactor is operated as shown in Figure 1 below.

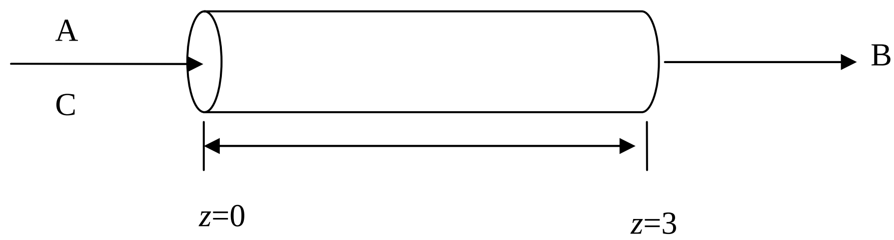

Figure 1: Isothermal plug flow reactor

The components A and C react to form component B.
The mole balance for each component is given by the following differential equations

$$u\frac{dC_A}{dz} = -2kC_A^2 \quad (1)$$

$$u\frac{dC_B}{dz} = 2kC_A^2 \quad (2)$$

$$u\frac{dC_C}{dz} = 0 \quad (3)$$

With the following initial values:

$$C_A(0) = 2\text{kmol/m}^3,\ C_B(0) = 0,\quad C_C(0) = 2\text{kmol/m}^3 \quad (4)$$

If $u = 0.5 m/s, \quad k = 0.3 m^3/kmol\, s, \quad$ and reactor length $z = 3m$. Solve the differential equations and plot the concentration of each species along the reactor length

SOLUTION

This is an initial value problem because all concentrations are given at the same value (z = 0 at the entrance of the reactor)

First, you have to define the problem by means of a function (m-file) and then use matlab to solve the differential equations

Step 1:

Create an m-file which defines the right hand side of the equations. The input parameters to the function are the concentrations of all species, thus we use the following variables:

$$y1 = CA, \quad y2 = CB, \quad y3 = CC$$

The function also needs the velocity, *u*, and the rate constant, *k*.

The distance from the inlet (z) is the independent variable. The rates of reaction are also evaluated, and the function returns the numerical value of the right hand side.

```
% myode1.m
% Isothermal plug flow reactor
% this function provides the function f(z,y) to be integrated
%
function F = myode1( z, y)
% y1 is CA
% y2 is CB
% y3 is CC
% parameters
 k = 0.3 ; u = 0.5;
CA = y(1);
rate = k * CA^2;
F(1) = -2.0 * rate / 0.5;
F(2) = rate / 0.5;
F(3) = 0;

F = F';     % F must be a column vector
end
```

Step 2

You can test this m-file by calling it with specific values for $y_i,\ i = 1,2,3$ to ensure that it is correct. Using y(i) for yi, issue the following commands:

```
>> y(1) = 0.4;     y(2) = 0.6;    y(3) = 0.5;
>> myode1(0.1,y)
```

You should obtain

```
ans =

   -0.1920
    0.0960
         0
```

This agrees with manual calculations. This is a very important step because you need to verify that your function is correct. Matlab will give an answer, whatever equations you give it. The minimum you can do is to ensure that you are solving the right equations.

Step3:

Now we need to write a code which will serve as the program driver. This code must do the following:

(i) set any constants (in this example all constants are set in myode1 for simplicity)
(ii) set the initial conditions and the total reactor length

(iii) call the ode solver. { we are going to use **ode45** from matlab}

```
% run_reaction.m
% this is the driver program to solve the flow reactor problem
%
% set the initial conditions
y0 = [2 0 2];
% set the total span of the independent variable, z.
txspan = [ 0 3];

% call the ode solver

[z , y] = ode45(@myode1, txspan, y0)

% plot the results
plot (z,y)
xlabel ('Length (m)');                  % set the x-axis label
ylabel (' Concentrations (kmol/m^3) '); % set the y-axis label
legend ('A', 'B', 'C');                 % set the legend
```

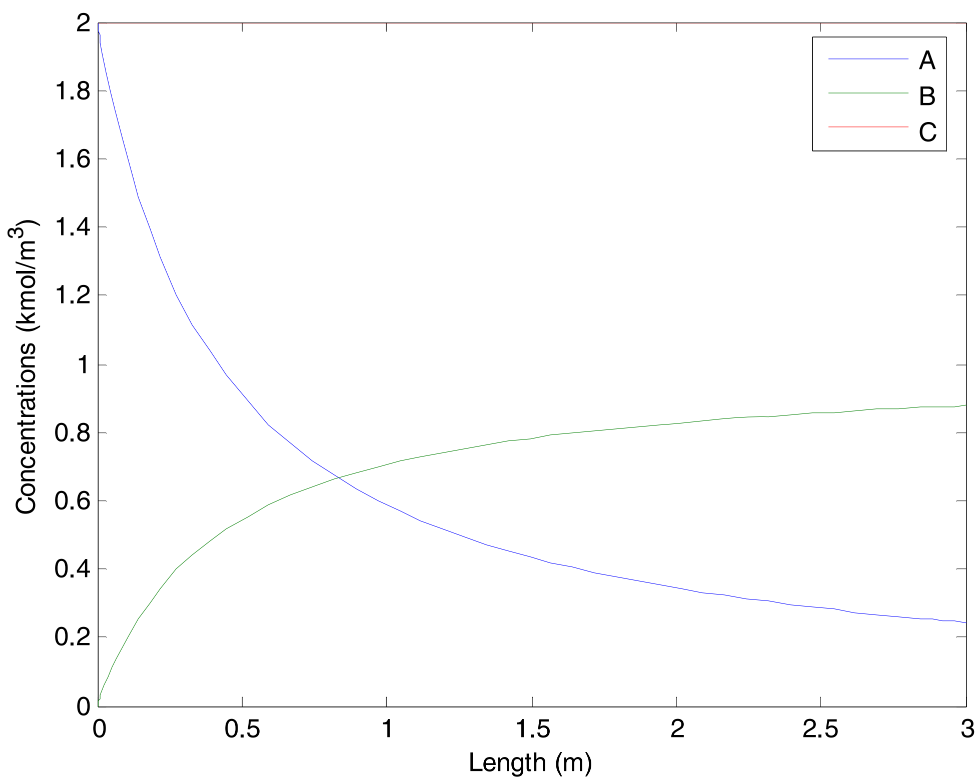

Figure 2: Isothermal pfr solution (solution to equations 1-4)

Step 4 :

Figure 2 shows the plot of results.You can vary the parameters to see their effects.
To obtain Figure 3 with different symbols for each concentration, use the following plot command

```
>> plot (z, y(:,1), '*-', z,y(:,2), '+-', z,y(:,3), 'x-')
```

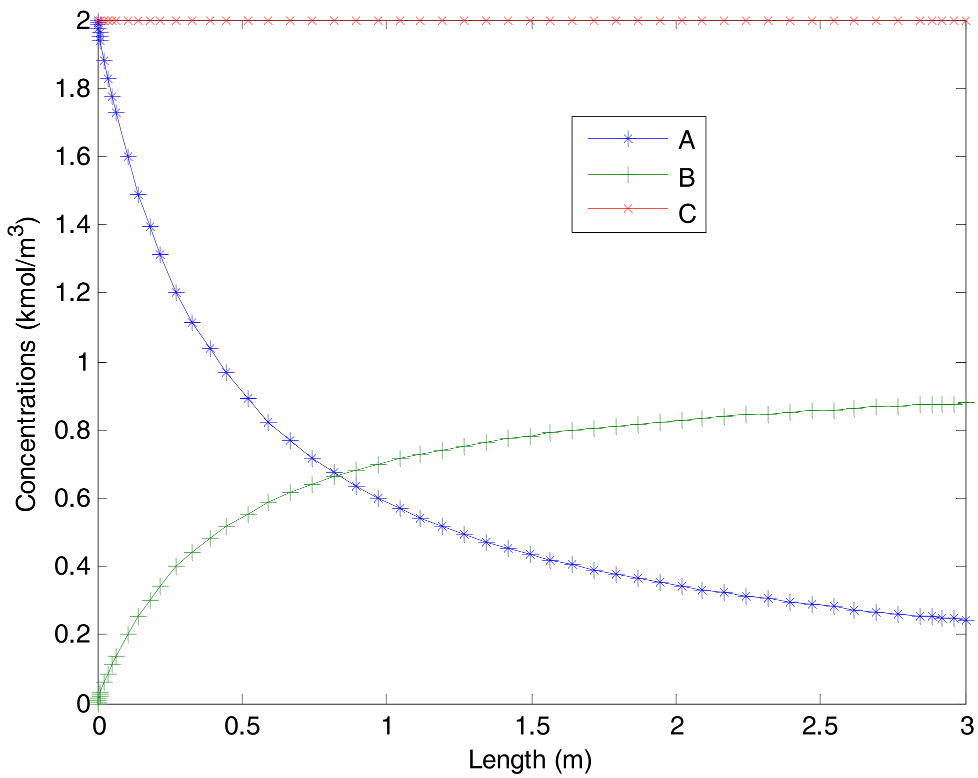

Figure 3: Isothermal pfr solution (solution to equations 1-4) with different symbols