Modelling & Simulation of Chemical Engineering Systems

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LECTURE #6

Numerical Solution of Ordinary Differential Equations

ODE Classifications

- Order
- Linearity
- Boundary or Initial

Nonlinear

3rd order

$$\frac{d^3y}{dx^3}+\left(\frac{dy}{dx}\right)^5=kx$$

y: dependent Variable
x: Independent variable

General Form of linear ODE

$$b_o(x)\frac{d^ny}{dx^n}+b_1(x)\frac{d^{n-1}y}{dx^{n-1}}+\ldots\ldots+b_{n-1}(x)\frac{d\ \ y}{dx}+b_n(x)y=R(x)$$

R(x)=0 → Homogeneous ODE

If b_o, b_1,..,b_n don't depend on x and R(x)=0→ autonomous system

- To obtain a unique solution for an nth order ODE we need to specify n values for y or its derivatives at specific value of x → initial or boundary conditions.
- Initial-value problem: y, dy/dx, ….are given at initial value of x
- Boundary-value problem: some of y, dy/dx, ….are given at initial value of x and others at the end value of x

[y (x=0), dy/dx(x=1)]

Canonical Form

ODE of nth order → n simultaneous first order ODEs: Canonical Form

Given:

$$\frac{dz^n}{dx^n} = G\left(z, \frac{dz}{dx}, \frac{d^2z}{dx^2}, \ldots, \frac{d^nz}{dx^n}, x \right)$$

Let

$$z = y_1, \frac{dz}{dx} = y_2, \frac{d^2z}{dx^2} = y_3, \cdots\cdots, \frac{d^{n-1}z}{dx^{n-1}} = y_n$$

Canonical Form

$$\boxed{\begin{aligned} \frac{dy_1}{dx} &= y_2 \\ \frac{dy_2}{dx} &= y_3 \\ &\vdots \\ &\vdots \\ \frac{dy_{n-1}}{dx} &= y_n \\ \frac{dy_n}{dx} &= G\left(y_1, y_2, \cdots, y_{n-1}, x\right) \end{aligned}}$$

If G doesn’t depend on x
→ Autonomous system

Example

$$\frac{d^4z}{dt^4}+5\frac{d^3z}{dt^3}-2\frac{d^2z}{dt^2}-6\frac{dz}{dt}+3z=0$$

$$Let: \quad z=y_1 \quad \frac{dz}{dt}=y_2 \quad \frac{d^2z}{dt^2}=y_3 \quad \frac{d^3z}{dt^3}=y_4 \quad \frac{d^4z}{dt^4}=\frac{dy_4}{dt}$$

$$\frac{dy_1}{dt}=y_2$$

$$\frac{dy_2}{dt}=y_3$$

$$\frac{dy_3}{dt}=y_4$$

$$\frac{dy_4}{dt}=-5y_4+2y_3+6y_2-3y_1$$

Canonical Form

$$\begin{bmatrix}\frac{dy_1}{dt}\\ \frac{dy_2}{dt}\\ \frac{dy_3}{dt}\\ \frac{dy_4}{dt}\end{bmatrix}=\begin{bmatrix}0&1&0&0\\0&0&1&0\\0&0&0&1\\-3&6&2&-5\end{bmatrix}\begin{bmatrix}y_1\\y_2\\y_3\\y_4\end{bmatrix}\Rightarrow\frac{dY}{dt}=AY$$

Solution of Linear ODE

For single ODE:

$$\frac{dy}{dt} = ay, \qquad y(0) = y_o\,, \qquad a:\ \text{constant}$$

$$solution: \qquad y(t) = e^{at} y_o$$

For system of ODE’s (Matrix form)

$$Y' = AY, \qquad Y(0) = Y_o$$

$$Solution: \qquad Y = e^{At} Y_o\,,$$

$$e^{At} = I + At + \frac{A^2t^2}{2!} + \frac{A^3t^3}{3!} + \ldots\ldots$$

Eigenvalue-Eigenvector Method

$$e^{At} = Xe^{\Lambda t} X^{-1}$$

$$e^{\Lambda t} = \begin{bmatrix} e^{\lambda_1 t} & 0 & \cdots & 0 \\ 0 & e^{\lambda_2} t & \cdots & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \cdots & 0 & e^{\lambda_n t} \end{bmatrix}, \qquad X = [x_1, x_2, \cdots x_n]$$

λ_i : eigenvalues of A (scalar)

x_i : Eigenvactor of A (vector)

$$Ax_i = \lambda_i x_i$$

Example: Solve the following ODEs system:

$$\frac{dY}{dt}=\begin{bmatrix}2 & 1\\ 3 & 0\end{bmatrix}Y, \qquad Y_o=\begin{bmatrix}1\\ 0\end{bmatrix}$$

Solution : $Y = Xe^{\Lambda t}X^{-1}Y_o$

First determine the eignevalues and eignevectors of A

$$AX=\lambda X \Rightarrow (A-\lambda I)X=0$$

$$\left(\begin{bmatrix}2 & 1\\ 3 & 0\end{bmatrix}-\begin{bmatrix}\lambda & 0\\ 0 & \lambda\end{bmatrix}\right)X=0$$

$$\det\begin{bmatrix}2-\lambda & 1\\ 3 & -\lambda\end{bmatrix}=0 \qquad \Rightarrow (2-\lambda)(-\lambda)-(3)(1)=0$$

$$\lambda^2-2\lambda-3=0 \qquad \Rightarrow \lambda_1=3 \qquad \lambda_2=-1$$

Eigenvector x_1 for λ_1

$$Ax_1=3x_1$$

$$\begin{bmatrix}2 & 1\\ 3 & 0\end{bmatrix}\begin{bmatrix}x_{11}\\ x_{12}\end{bmatrix}=3\begin{bmatrix}x_{11}\\ x_{12}\end{bmatrix}$$

$$2x_{11}+x_{12}=3x_{11}\rightarrow x_{11}=x_{12}\rightarrow x_1=\begin{bmatrix}1\\ 1\end{bmatrix}$$

Eigenvector x_2 for λ_2

$$Ax_2=-x_2$$

$$\begin{bmatrix}2 & 1\\ 3 & 0\end{bmatrix}\begin{bmatrix}x_{21}\\ x_{22}\end{bmatrix}=-\begin{bmatrix}x_{21}\\ x_{22}\end{bmatrix}$$

$$2x_{21}+x_{22}=-x_{21}\rightarrow x_{22}=-3x_{21}\rightarrow x_2=\begin{bmatrix}-1\\ 3\end{bmatrix}$$

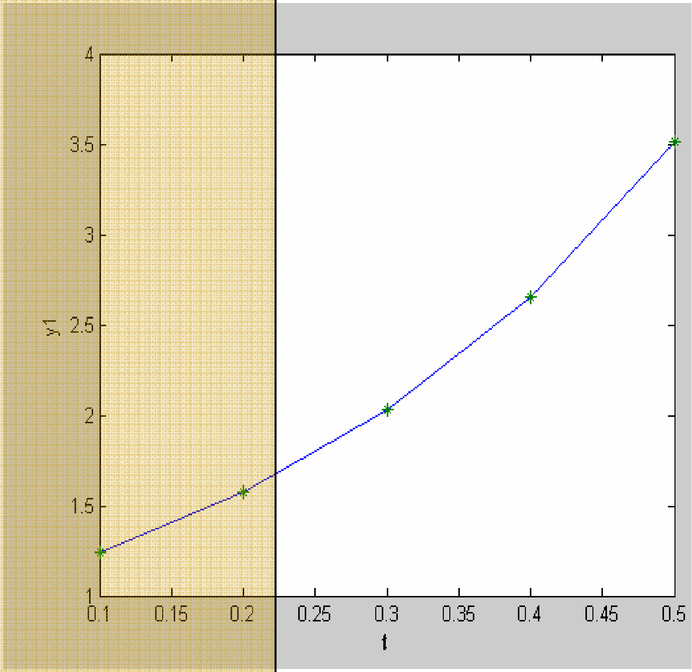
$$Y=Xe^{\Lambda t}X^{-1}Y_o=\begin{bmatrix}1 & -1\\ 1 & 3\end{bmatrix}\begin{bmatrix}e^{3t} & 0\\ 0 & e^{-t}\end{bmatrix}\begin{bmatrix}1 & -1\\ 1 & 3\end{bmatrix}^{-1}\begin{bmatrix}1\\ 0\end{bmatrix}$$

$$Y=\begin{bmatrix}y_1(t)\\ y_2(t)\end{bmatrix}=\begin{bmatrix}0.75e^{3t}+0.25e^{-t}\\ 0.75e^{3t}-0.75e^{-t}\end{bmatrix}$$

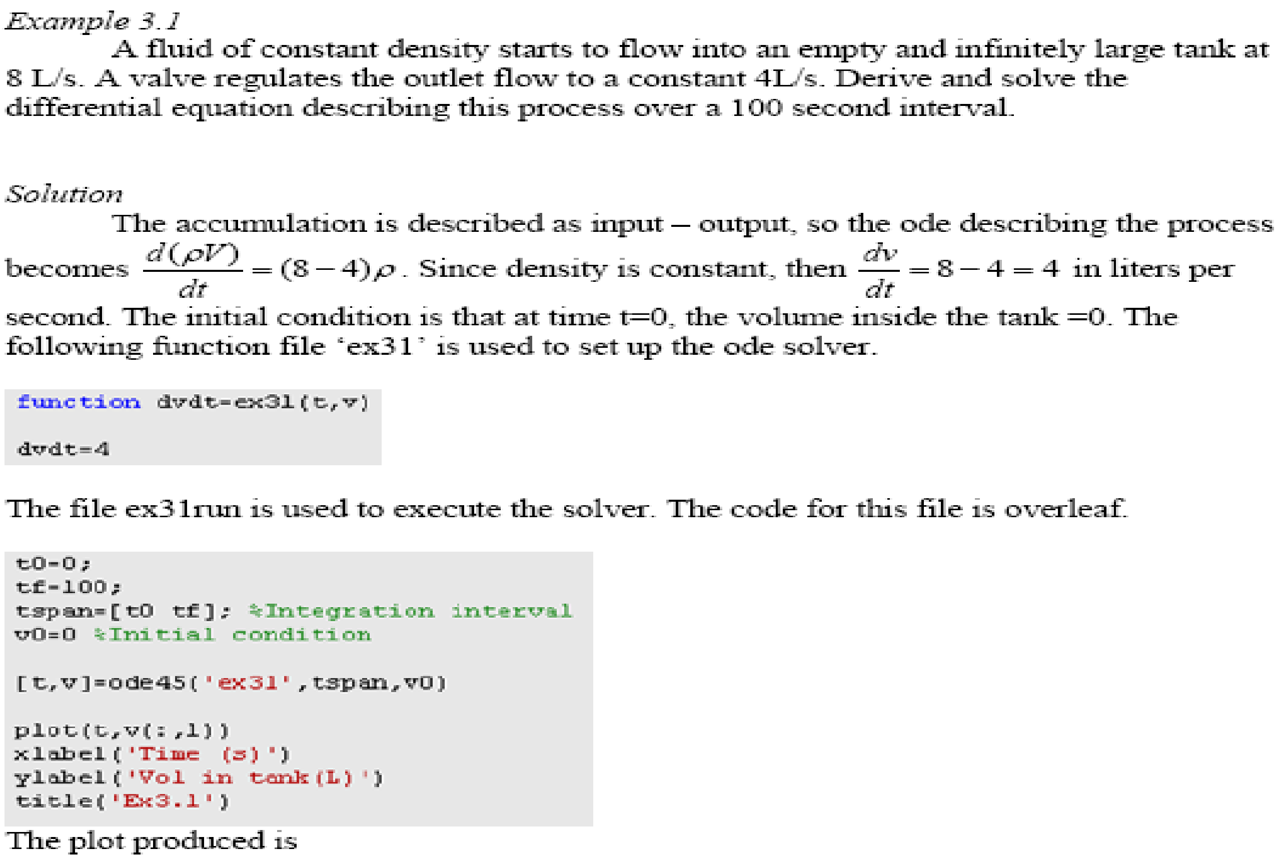
Eigenvalue-Eigenvactor Method using MATLAB

```
% Eignevalue-Eigenvector method Linear ODE system
% dY/dt=AY , Y(t=0)=Y0 ==> Y(t)=exp(At)Y0
% exp(At)=X exp(lambda*t) inv(X)

%[V,D] = EIG(X) produces a diagonal matrix D of eigenvalues and a
%   full matrix V whose columns are the corresponding eigenvectors so
%    that X*V = V*D.
Y0=[1 0]'
A=[2 1; 3 0]
[X,lambda]=eig(A)
for n=1:5
t(n)=.1*n
AL=[exp(lambda(1,1)*t(n)) 0; 0 exp(lambda(2,2)*t(n))]
Y(:,n)=X*AL*inv(X)*Y0
end
for n=1:5
    t(n)=.1*n
y1(n)=0.75*exp(3*t(n))+0.25*exp(-t(n))
y2(n)=0.75*exp(3*t(n))-0.75*exp(-t(n))
end
plot(t,Y(1,:),t,y1,'*')
```



ODE MATLAB Solver



Example 3.1

A fluid of constant density starts to flow into an empty and infinitely large tank at 8 L/s. A valve regulates the outlet flow to a constant 4L/s. Derive and solve the differential equation describing this process over a 100 second interval.

Solution

The accumulation is described as input – output, so the ode describing the process becomes $\frac{d(\rho V)}{dt} = (8-4)\rho$. Since density is constant, then $\frac{dv}{dt} = 8-4=4$ in liters per second. The initial condition is that at time t=0, the volume inside the tank =0. The following function file ‘ex31’ is used to set up the ode solver.

```
function dvdt=ex31(t,v)

dvdt=4
```

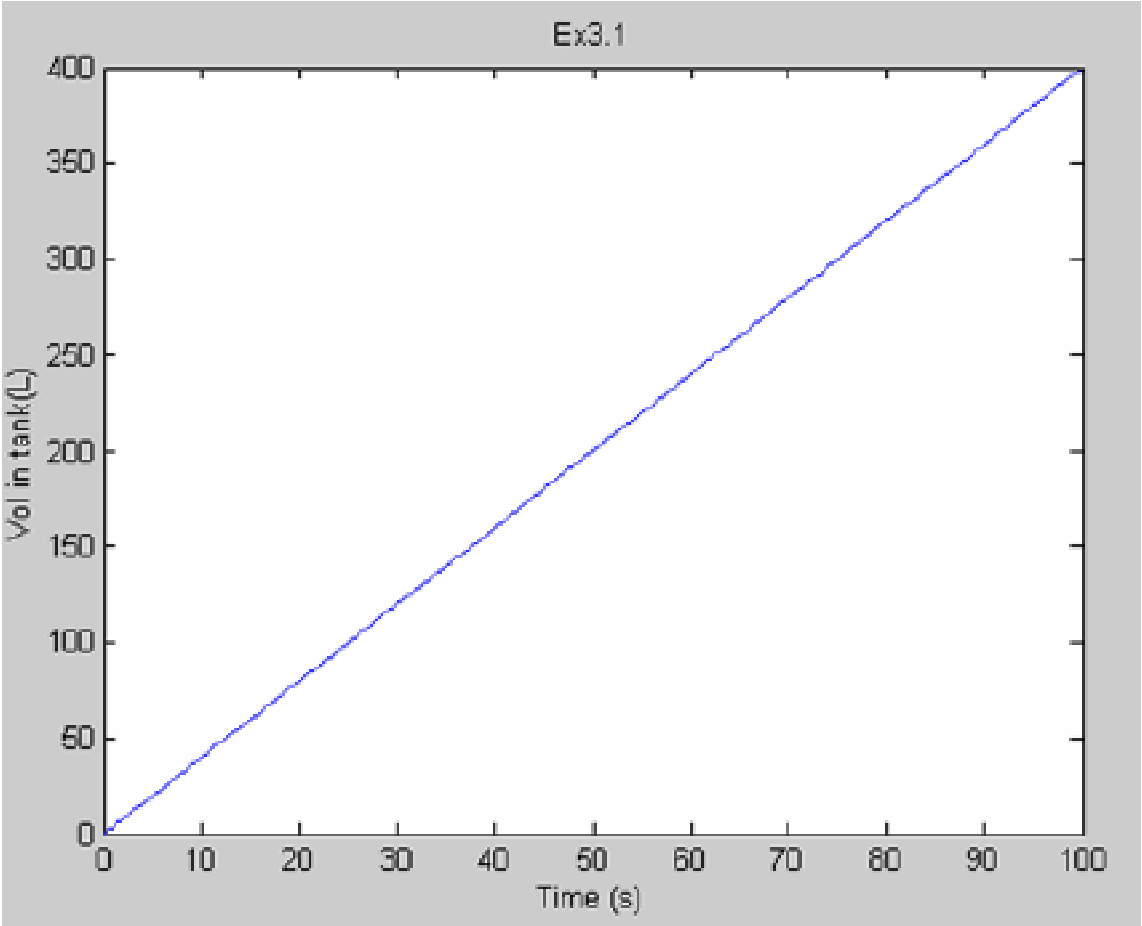
The file ex31run is used to execute the solver. The code for this file is overleaf.

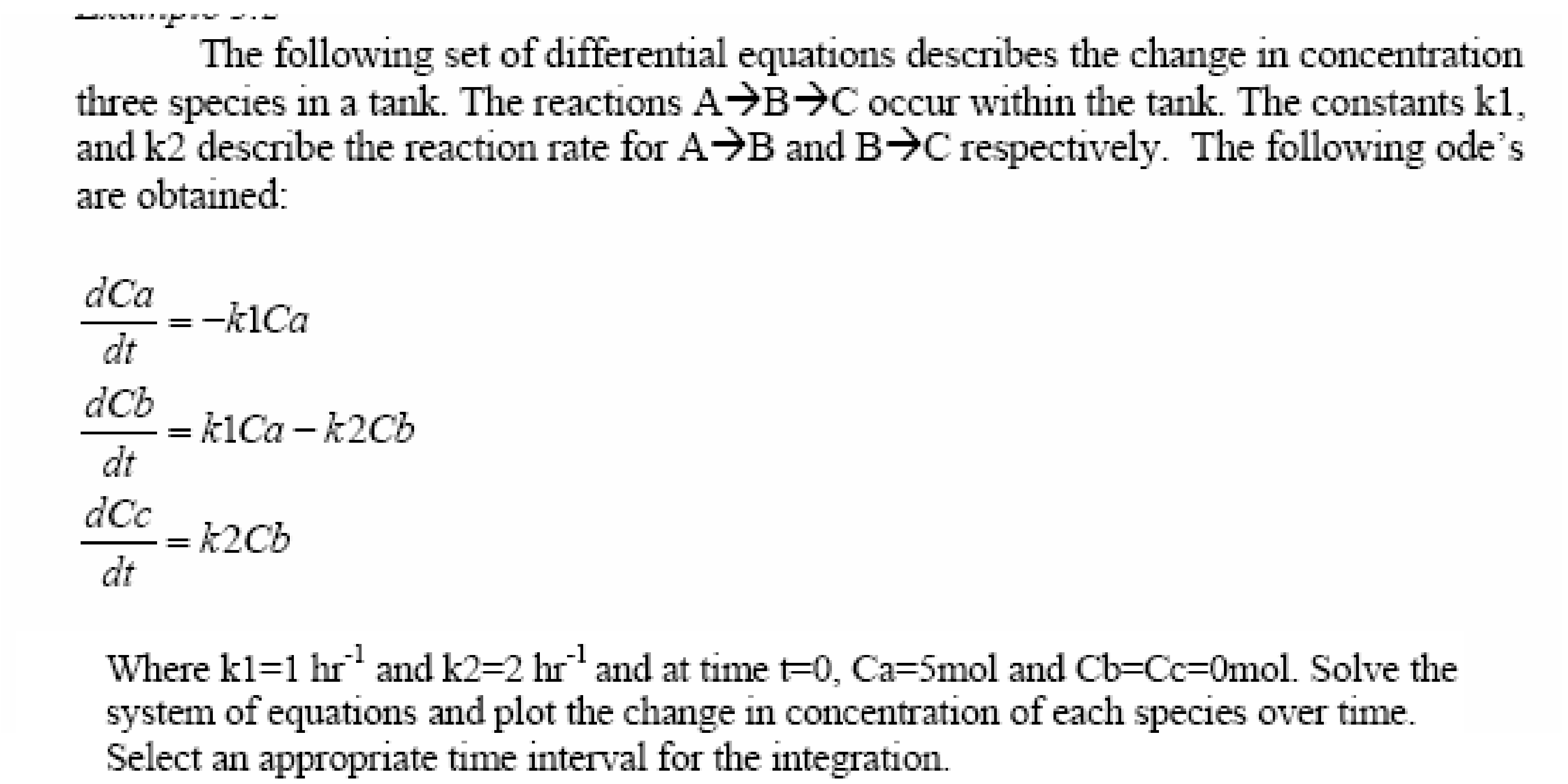
```
t0=0;
tf=100;
tspan=[t0 tf]; %Integration interval
v0=0 %Initial condition

[t,v]=ode45('ex31',tspan,v0)

plot(t,v(:,1))
xlabel('Time (s)')
ylabel('Vol in tank(L)')
title('Ex3.1')
```

The plot produced is


Ex3.1
Vol in tank(L)
0
50
100
150
200
250
300
350
400
0
10
20
30
40
50
60
70
80
90
100
Time (s)



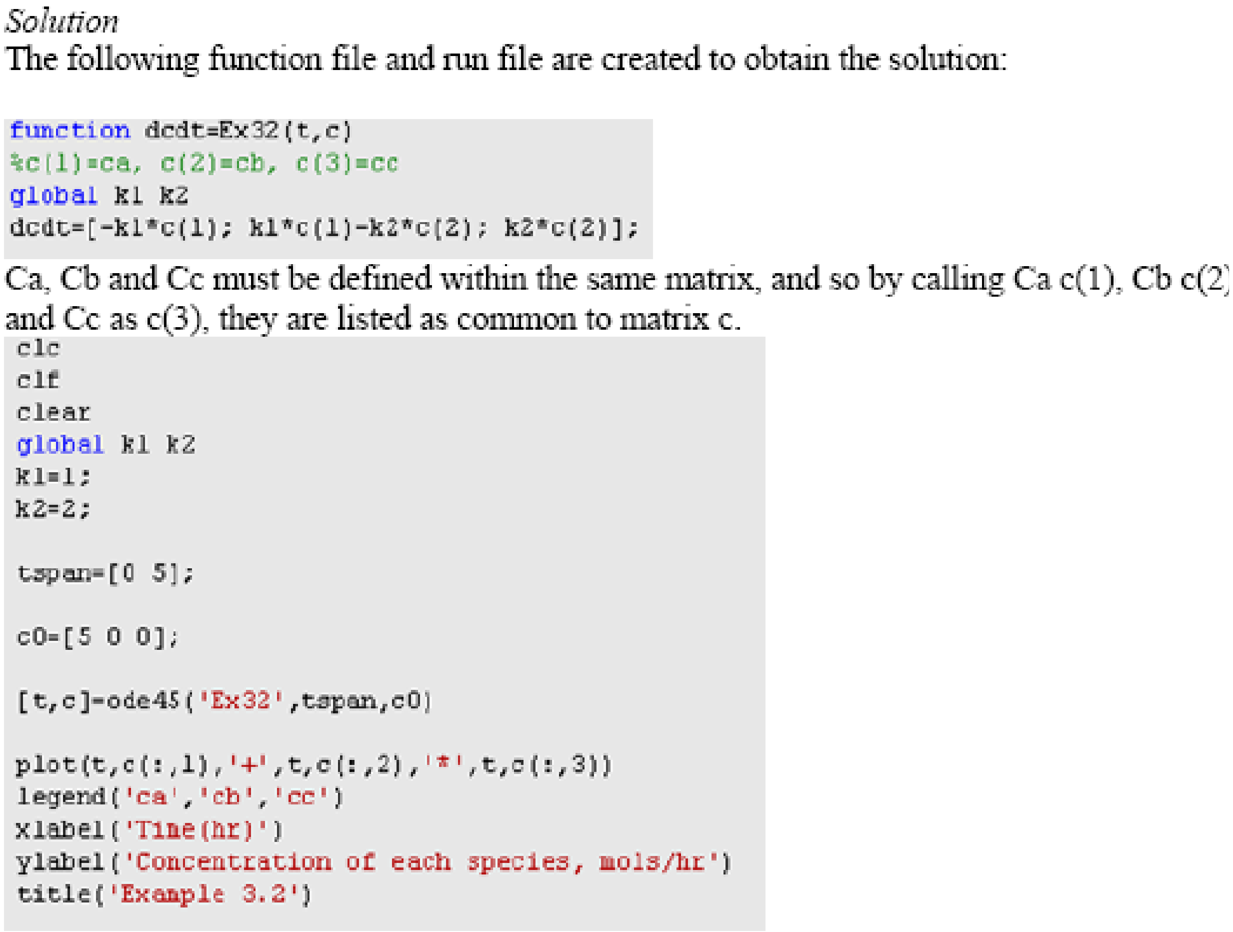
The following set of differential equations describes the change in concentration three species in a tank. The reactions A→B→C occur within the tank. The constants k1, and k2 describe the reaction rate for A→B and B→C respectively. The following ode's are obtained:

$$\frac{dCa}{dt} = -k1Ca$$

$$\frac{dCb}{dt} = k1Ca - k2Cb$$

$$\frac{dCc}{dt} = k2Cb$$

Where k1=1 hr^{-1} and k2=2 hr^{-1} and at time t=0, Ca=5mol and Cb=Cc=0mol. Solve the system of equations and plot the change in concentration of each species over time. Select an appropriate time interval for the integration.



Solution

The following function file and run file are created to obtain the solution:

```
function dcdt=Ex32(t,c)
%c(1)=ca, c(2)=cb, c(3)=cc
global k1 k2
dcdt=[-k1*c(1); k1*c(1)-k2*c(2); k2*c(2)];
```

Ca, Cb and Cc must be defined within the same matrix, and so by calling Ca c(1), Cb c(2 and Cc as c(3), they are listed as common to matrix c.

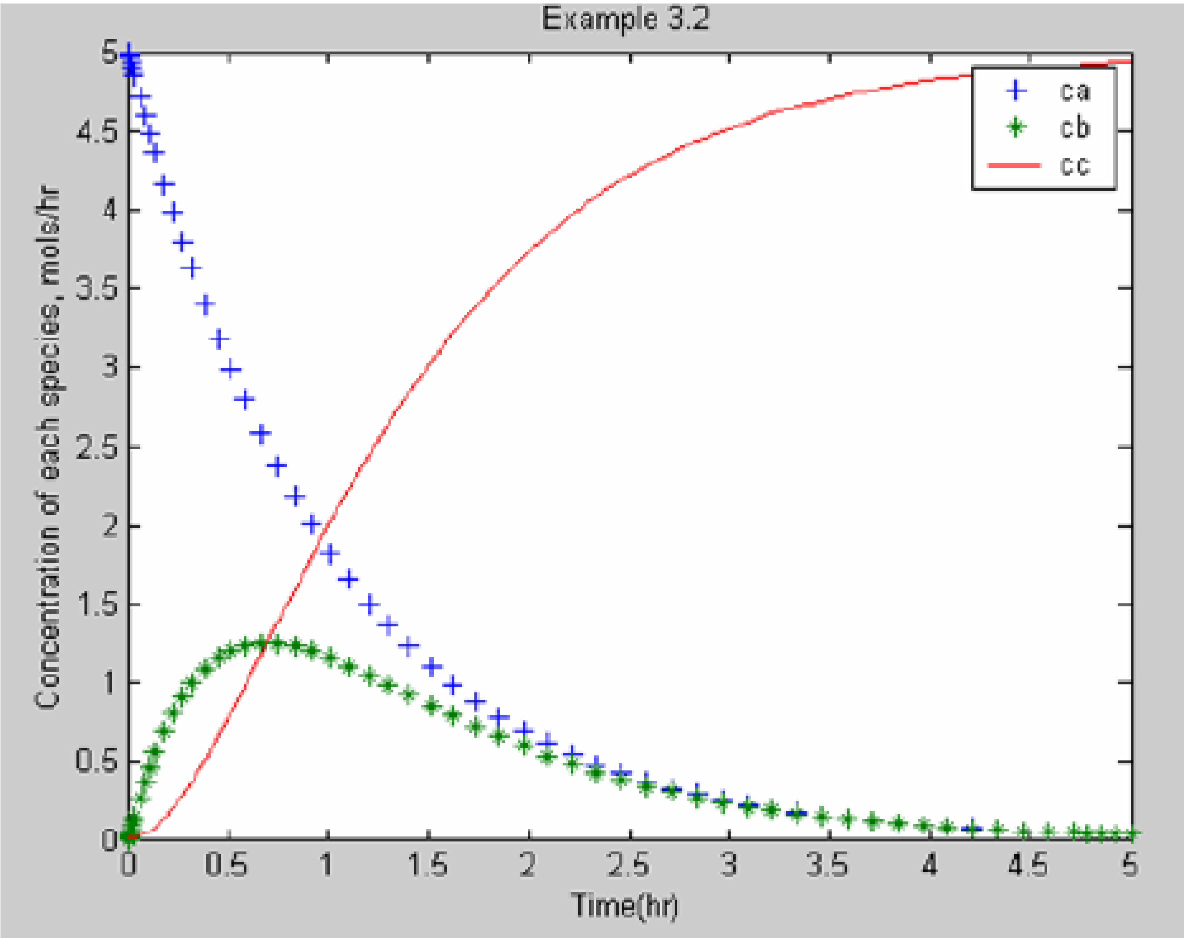
```
clc
clf
clear
global k1 k2
k1=1;
k2=2;

tspan=[0 5];

c0=[5 0 0];

[t,c]=ode45('Ex32',tspan,c0)

plot(t,c(:,1),'+',t,c(:,2),'*',t,c(:,3))
legend('ca','cb','cc')
xlabel('Time(hr)')
ylabel('Concentration of each species, mols/hr')
title('Example 3.2')
```


Example 3.2
Concentration of each species, mols/hr
Time(hr)
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
ca
cb
cc

Nonlinear ODE: Initial value Problems

$$\frac{dy}{dx} = f(x,y), \qquad y(x_o) = y_o$$

$$\int_{y_i}^{y_{i+1}} dy = \int_{x_i}^{x_{i+1}} f(x,y)dx \rightarrow y_{i+1} - y_i = \int_{x_i}^{x_{i+1}} f(x,y)dx$$

Approximated using Finite differences

Euler Method

$$y_{i+1} = y_i + hf(x_i, y_i)$$

Implicit Euler Method

$$y_{i+1} = y_i + hf(x_{i+1}, y_{i+1})$$

Modified Euler method

$$y_{i+1,pr} = y_i + hf(x_i, y_i)$$

$$y_{i+1,cor} = y_i + hf(x_{i+1}, y_{i+1})$$