Exercise 9. Assume that a fluid with constant density enters into a tank at the rate of 10 L/min. A control valve at the outlet of the tank controls the flow at a constant rate of 6 L/min. Derive an equation describing this process and solve the same over a 100 min interval. Write a program for the process in MATLAB

Solution

We know that, Material balance equation under unsteady state condition is written as

$$Accumulation = input - output$$

$$\frac{d(\rho V)}{dt} = (10\rho - 6\rho)$$

$$\frac{d(\rho V)}{dt} = (10 - 6)\rho$$

$$\frac{d(V)}{dt} = (10 - 6) \because \rho = constant$$

$$\frac{d(V)}{dt} = 4$$

MATLAB Code

Open the editor window and create a function file as shown below and save the file in the name of unsteady.

```
function vdot = unsteady (t,v);
%vdot = dv/dt
vdot=4;
```

After saving the above function file, return to command window and run the program as given below

```
>> tspan=[0 100];
>> v0=0;
>> [t,v]=ode23('unsteady',tspan,v0);
>> plot(t,v);
>> grid
>> xlabel('Time, min')
>> ylabel('volume, L/min')
```

Exercise 10: The following set of differential equations describes the change in concentration of three species in a reactor. The reactions $A \rightarrow B \rightarrow C$ occur within the reactor. The rate constants k_1 and k_2 describe the reaction rate for $A \rightarrow B$ and $B \rightarrow C$ respectively. The following ODE are obtained

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

Where k_1 = hr^{-1} and k_2 =2hr^{-1} and at time t = 0, Ca = 5 mol and Cb = Cc = 0mol. Solve the system of equations and the plot the change in concentration of each species over time.

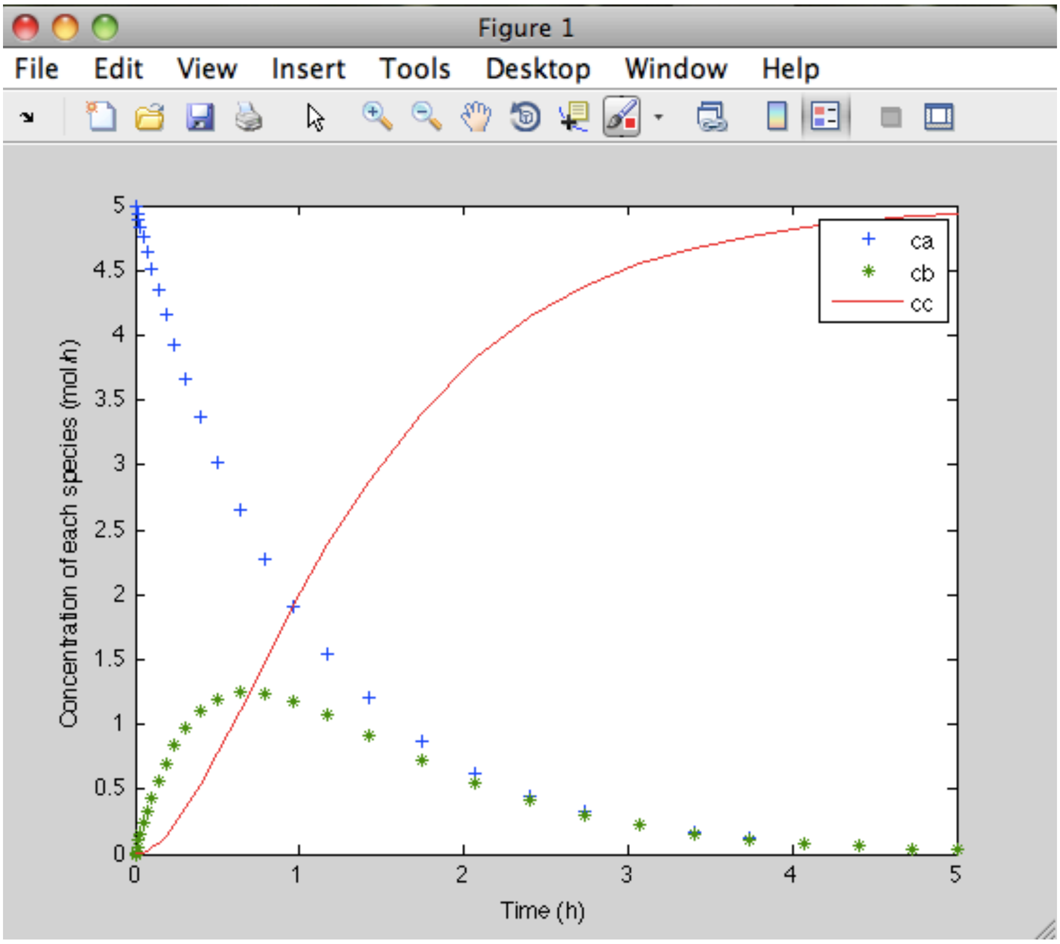
MATLAB Code

Create the following function file in editor window to as given below

```
function dcdt=kinetics(t,c)
global k1 k2
dcdt=[-k1*c(1);k1*c(1)-k2*c(2);k2*c(2)];
```

Save the file in the name of kinetics and return to the command window to run the program

```
>> global k1 k2
>> k1=1;
>> k2=2;
>> tspan=[0 5];
>> c0=[5 0 0];
>> [t,c]=ode23('kinetics',tspan,c0);
>> plot(t,c(:,1),'+',t,c(:,2),'*',t,c(:,3));
>> legend('ca','cb','cc');
>> xlabel('Time (h)');
>> ylabel('Concentration of each species (mol/h)')
```



Exercise 11: The dynamic model for an isothermal, constant volume, chemical reactor with a single second order reaction is:

$$\frac{dC_A}{dt} = \frac{F}{V}C_{Af} - \frac{F}{V}C_A - kC_A^2$$

$$\frac{F}{V} = 1\min^{-1}, C_{Af} = 1gmol/liter, k = 1liter/gmol.\min$$

Find the steady-state $f(x) = -x2$ and substituting the parameter and input values we find

$$1 - C_{As} - C_{As}^2 = 0$$

where the subscript *s* is used to denote the steady-state solution. For notational convenience, let $x = C_{As}$ and write the algebraic equation as

$$f(x) = -x^2 - x + 1 = 0$$

We can directly solve this equation using the quadratic formula to find *x*.

MATLAB Code

Go to the command window and solve for x as shown below

```
>> solve('-x^2-x+1')


ans =


 - 5^(1/2)/2 - 1/2
   5^(1/2)/2 - ½
```

Therefore, x = - 0.6I8 and x = +0.618 to be the solutions. Obviously a concentration cannot be negative, so the only physically meaningful solution is $x = 0.618$

Exercise 11. The heat capacity of gas is tabulated as series of temperature

T (°C)	20	50	80	110	140	170	200	230
Cp[J/(mol.°C)	28.95	29.13	29.30	29.48	29.65	29.82	29.99	30.16

Calculate the change in enthalpy for 3.00 g – moles of this gas from 20 °C to 230 °C

$$\Delta H(J) = n \int_{20\ ^oC}^{230\ ^oC} C_P\, dT$$

Solution

MATLAB Code

Goto command window and do the following

```
>> x=linspace(20,230,8)'


x =


    20
    50
    80
   110
   140
   170
   200
   230

>> y=[28.95,29.13,29.30,29.48,29.65,29.82,29.99,30.16]'
```

```
y =

   28.9500
   29.1300
   29.3000
   29.4800
   29.6500
   29.8200
   29.9900
   30.1600

>> area=trapz(x,y)

area =

   6.2078e+03

>> format short g
>> area=trapz(x,y)

area =

       6207.8

>> format short
>> area*3

ans =

   1.8623e+04

>> format short g
>> area*3

ans =

        18623
```

Therefore,

$$\Delta H = 1.8623\times10^{-4} J$$
$$or$$
$$\Delta H(J) = 18623J$$

Exercise 12. 100 moles of benzene (A) and toluene (B) mixture containing 50% mole 0f benzene is subjected to a differential distillation at atmospheric pressure till the composition of the benzene residue is 33%. Calculate the total moles of the mixture distilled. Average relative volatility is 2.16

Solution

The equilibrium relation (x vs y) is computed with the help of α ,

i.e.

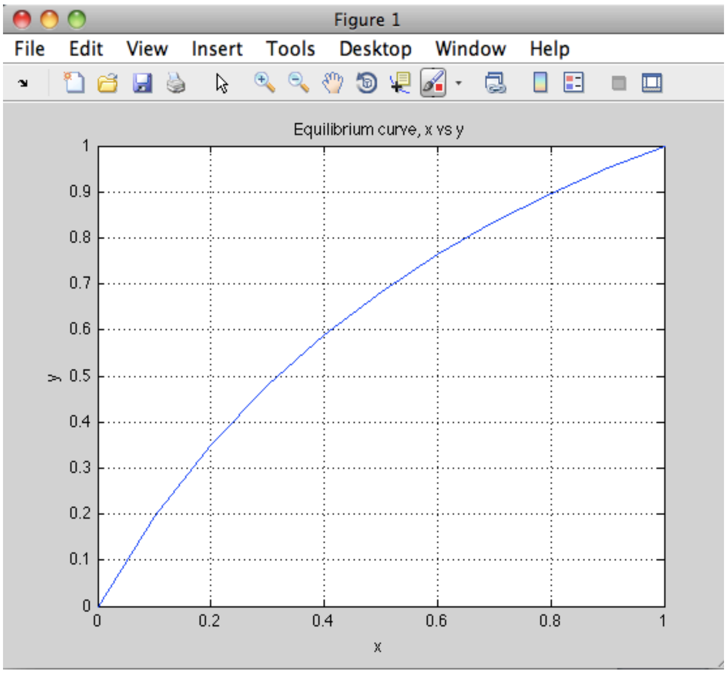
$$y = \frac{\alpha x}{1+(\alpha-1)x}$$

$$y = \frac{2.16x}{1+1.16x} \because \alpha = 2.16$$

The equilibrium curve is plotted in MATLAB as follows, Go to command window and try the following

```
>> x=linspace(0,1.0,11)'
x =

         0
    0.1000
    0.2000
    0.3000
    0.4000
    0.5000
    0.6000
    0.7000
    0.8000
    0.9000
    1.0000
```

```
>> y = (2.16.*x)./(1+1.16*x)

y =

     0
0.1935
0.3506
0.4807
0.5902
0.6835
0.7642
0.8344
0.8963
0.9511
1.0000
>> plot(x,y)
>> xlabel('x')
>> ylabel('y')
>> title('Equilibrium curve, x vs y')
>> grid
```



From the given problem statement we know that

$x_f = 0.50$

$x_w = 0.33$

The Rayleigh Equation is

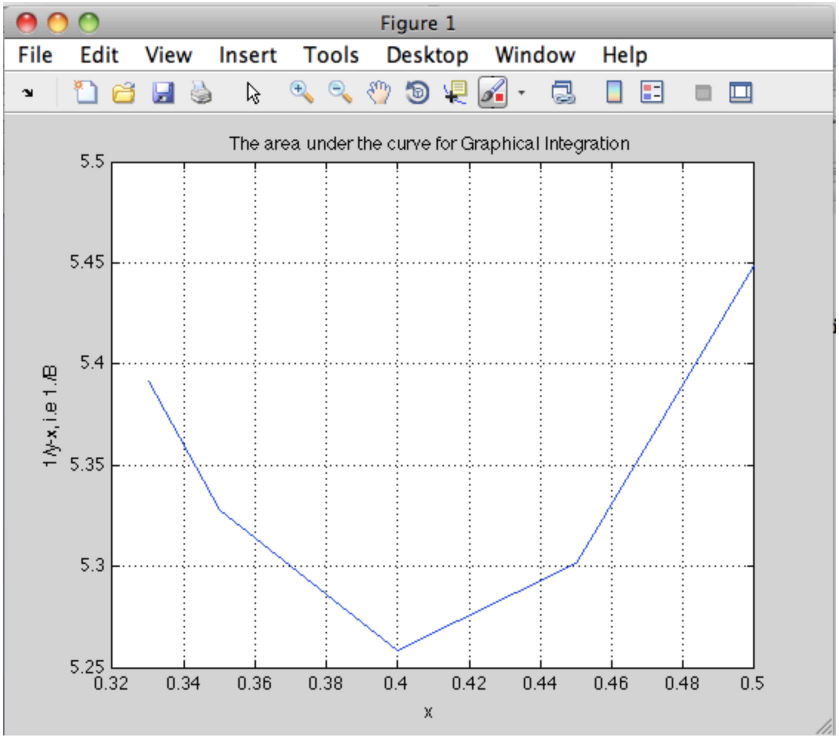
$$\ln\frac{F}{w}=\int_{0.50}^{0.33}\frac{dx}{y-x}$$

The R.H.S of the equation is evaluated by graphical integration (Trapezoidal rule)

i.e. Area under the curve = $\int_{0.50}^{0.33}\frac{dx}{y-x}$

To find the area under the curve go to command window in MATLAB and do the following

```
>> clc

>> x=[0.33,0.35,0.40,0.45,0.50]

x =

    0.3300    0.3500    0.4000    0.4500    0.5000

>> y = (2.16*x)./(1+1.16*x)

y =

    0.5155    0.5377    0.5902    0.6386    0.6835

>> B=y-x

B =

    0.1855    0.1877    0.1902    0.1886    0.1835

>> 1./B

ans =

    5.3915    5.3278    5.2586    5.3013    5.4483

>> plot(x,1./B)
>> xlabel('x');
>> ylabel('1/y-x, i.e 1./B')
>> Title('The area under the curve for Graphical Integration')
>> grid
```




```
>> area=trapz(x,1./B)

area =

    0.9046
```

Therefore, Area under the curve = 0.9046

$$\ln\left(\frac{F}{w}\right) = 0.904$$

$$\left(\frac{F}{w}\right) = 2.4709$$

$$W = \frac{100}{2.4709} = 40.4711$$

Moles distilled = 100 – W

= 100 – 40.7111 = 60 moles/h