

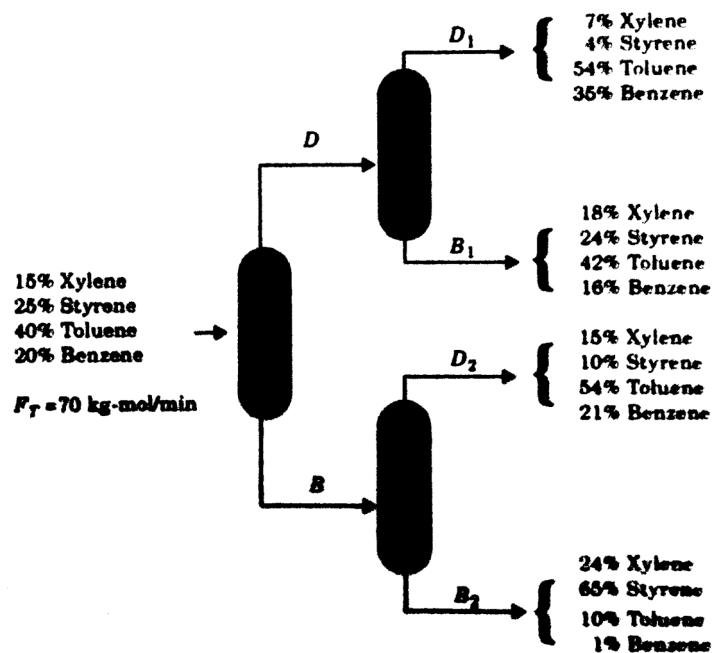
Date : 26/09/2016

Aim

To solve the chemical engineering problems (steady state and unsteady state) using SCILAB

Problem statements

1. Paraxylene, styrene, toluene, and benzene are to be separated with the array of distillation column as shown in figure given below:



Calculate the molar flow rates of D_1 , D_2 , B_1 and B_2 using SCILAB.

Solution

Applying general mass (component) balance equation to the above separation train we have,

$$\text{Balance on Xylene: } 0.70 \times 0.15 = 0.07 x_1 + 0.18 x_2 + 0.15 x_3 + 0.24 x_4$$

$$\text{Balance on Styrene: } 0.70 \times 0.25 = 0.04 x_1 + 0.24 x_2 + 0.10 x_3 + 0.65 x_4$$

Balance on Toluene: $0.70 \times 0.40 = 0.54 x_1 + 0.42 x_2 + 0.54 x_3 + 0.10 x_4$

Balance on Benzene: $0.70 \times 0.80 = 0.35 x_1 + 0.16 x_2 + 0.21 x_3 + 0.01 x_4$

Where $x_1, x_2, x_3,$ and x_4 are D_1, B_1, D_2 and B_2 respectively

Now, open console window of SCILAB and type the following to obtain the solution

```
-->A=[0.07 0.18 0.15 0.24; 0.04 0.24 0.10 0.65; 0.54 0.42 0.54  
0.10; 0.35 0.16 0.21 0.01];
```

```
-->B=[70*0.15; 70*0.25; 70*0.40; 70*0.20];
```

```
-->x=[A\B]
```

```
x =
```

```
26.25
```

```
17.5
```

```
8.75
```

```
17.5
```

2. Weight Reduction Model

Assume that a person who is having 100 kg now is interested to reduce his weight by 10% per month for two years. Write a model (First order initial value) describing the loss in weight. Determine $x(t)$ as a function of t . Where x is weight of the person and t is the time. Also plot the data for two years, i.e. for 24 months, show the grid lines and label the axis Using SCILAB.

Solution

Weight of person = x kg

Tries to reduce weight

Weight loss per month = 10% of weight

Starting weight = 100 kg

Now,

$$\frac{dx}{dt} = -0.1x$$

Initial conditions:

$x = 100$ at $t = 0$

Determine $x(t)$ as a function of t .

Analytical solution of weight reduction model

Recall the model:

$$\frac{dx}{dt} = -0.1x$$

$$x(t = 0) = 100$$

Cross multiplying,

$$\frac{dx}{x} = -0.1dt$$

Integrating both sides from 0 to t ,

$$\int \frac{dx}{x} = -0.1 \int dt$$

$$C + \ln [x(t)] = -0.1t$$

Using initial conditions

$$C = -\ln 100$$

Thus the final solution is

$$\ln \frac{x(t)}{100} = -0.1t$$

or

$$x(t) = 100e^{-0.1t}$$

Summary of Weight Reduction Problem

Weight of person = x kg

Tries to reduce weight

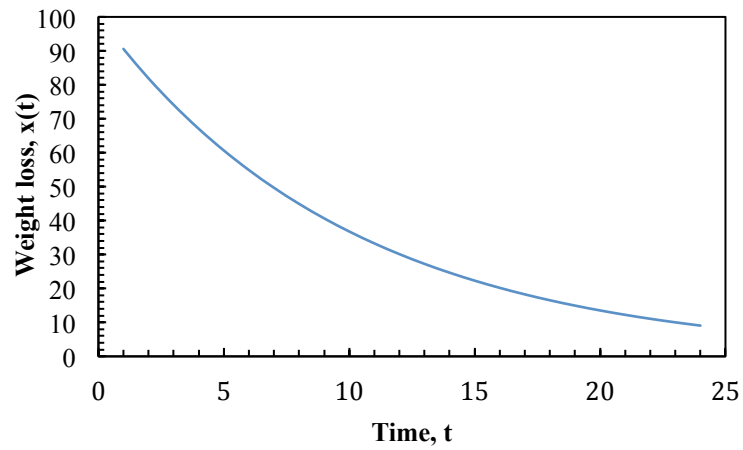
Weight loss per month = 10% of weight

Starting weight = 100 kg, Model describing the weight loss is:

$$x(t) = 100e^{-0.1t}$$

Compute and plot for two years, i.e. for 24 months

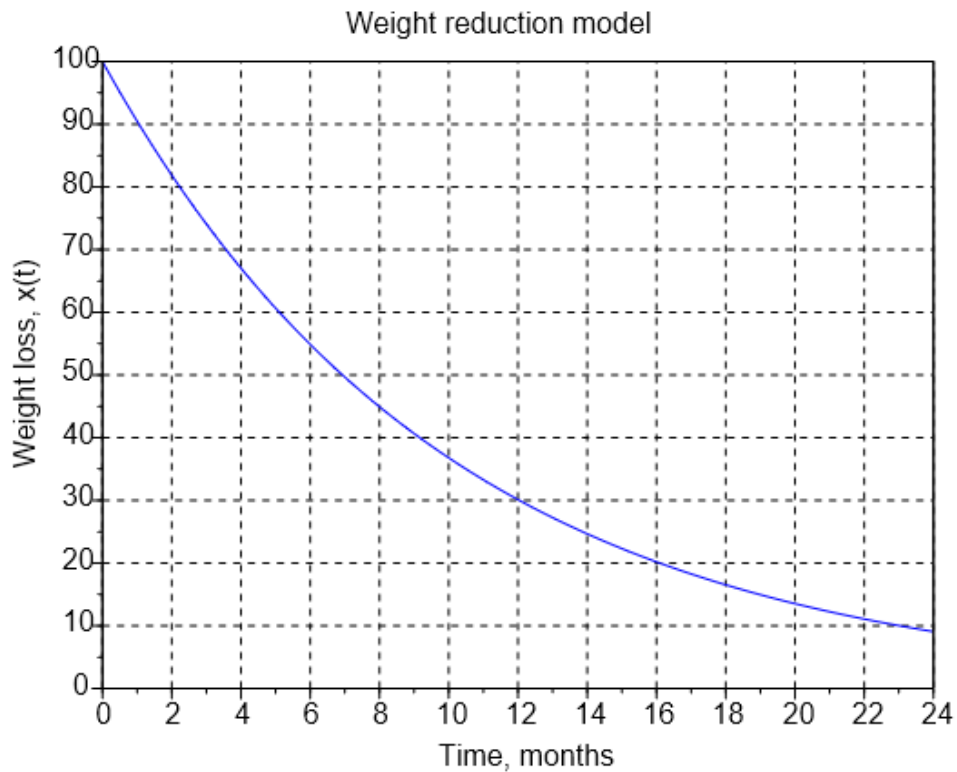
Time (t), Months	$x(t)$
0	100.00
1	90.483
2	81.873
3	74.081
4	67.032
5	60.653
6	54.881
7	49.658
8	44.932
9	40.656
10	36.787
11	33.287
12	30.119
13	27.253
14	24.659
15	22.313
16	20.189
17	18.268
18	16.529
19	14.956
20	13.533
21	12.245
22	11.080
23	10.025
24	9.071



```
T=0:0.1:24;
B=100*exp(-0.1*T)
plot(T,B);
```

Now, put the x - y labels, grid lines and title for the plot. Put the title for the plot as “Weight reduction model”.

```
-->plot(T,B);
-->xlabel('Time, months','fontsize',3);
-->ylabel('Weight loss, x(t)','fontsize',3);
-->title('Weight reduction model','fontsize',4);
-->xgrid(1)
```



A SCILAB function for the model can be written as stated below:

Open the SCINOTES and create a function file by typing the following:

```
function xdot=f(t,x)
    xdot=-0.1*x
endfunction
```

Save the above function, goto console and provide the initial conditions

```
-->exec('/Users/admin/Desktop/f.sci', -1)
-->x0=100;
-->t0=0;
-->t=0:0.1:24;
-->x=ode(x0,t0,t,f);
-->plot(t,x);
-->xlabel('Time, months','fontsize',3);
-->ylabel('Weight loss, x(t)','fontsize',3);
-->title('Weight reduction model','fontsize',4);
-->xgrid(1)
```

3. Write a SCILAB program for the weight gain model. The approach is similar to the problem 2 as stated above. The model is considered as:

$$\frac{dx}{dt} = 0.1x$$
$$x(t = 0) = 9.071 \text{ kg}$$

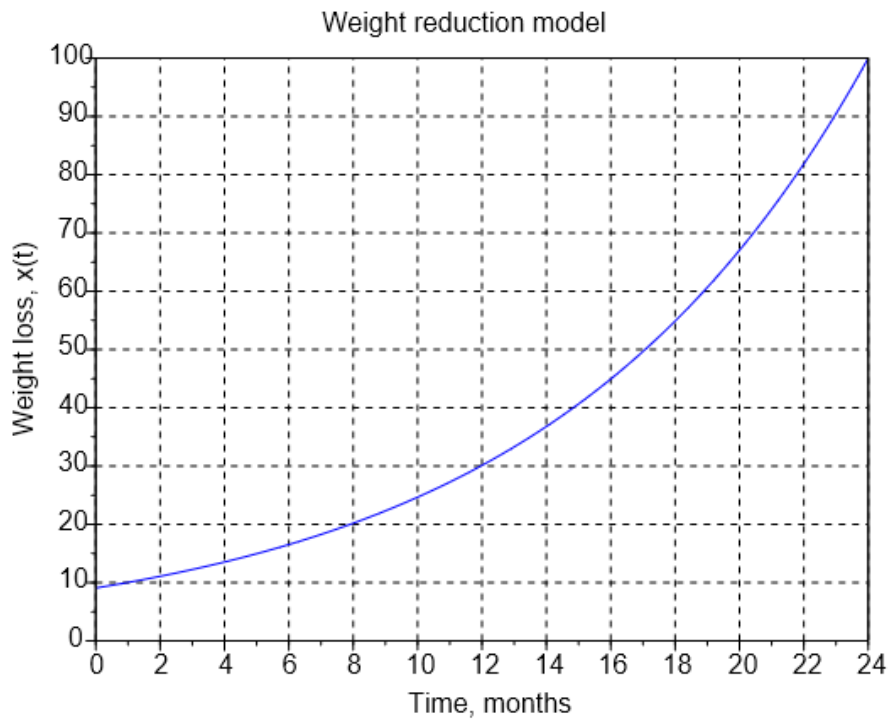
Where x is the weight gain, initial weight at time $t = 0$ and $x = 9.071\text{kg}$. Determine and plot the graph for 24 months time period. Put the x - y labels, grid lines and title for the plot. Title for the plot is weight gain model.

Open the SCINOTES and create a function file by typing the following:

```
function xdot=f(t, x)  
    xdot=0.1*x  
endfunction
```

Open console window and try the following:

```
-->exec('C:\Users\User-Pc\Desktop\f.sci', -1)  
-->x0=9.071;  
-->t0=0;  
-->T=0:0.1:24;  
-->x=ode(x0,t0,T,f);  
-->plot(t,x);  
-->plot(t,x);  
-->xlabel('Time, months','fontsize',3);  
-->ylabel('Weight loss, x(t)','fontsize',3);  
-->title('Weight reduction model','fontsize',4);  
-->xgrid(1)
```



4. In the following example, we solve the Ordinary Differential Equation

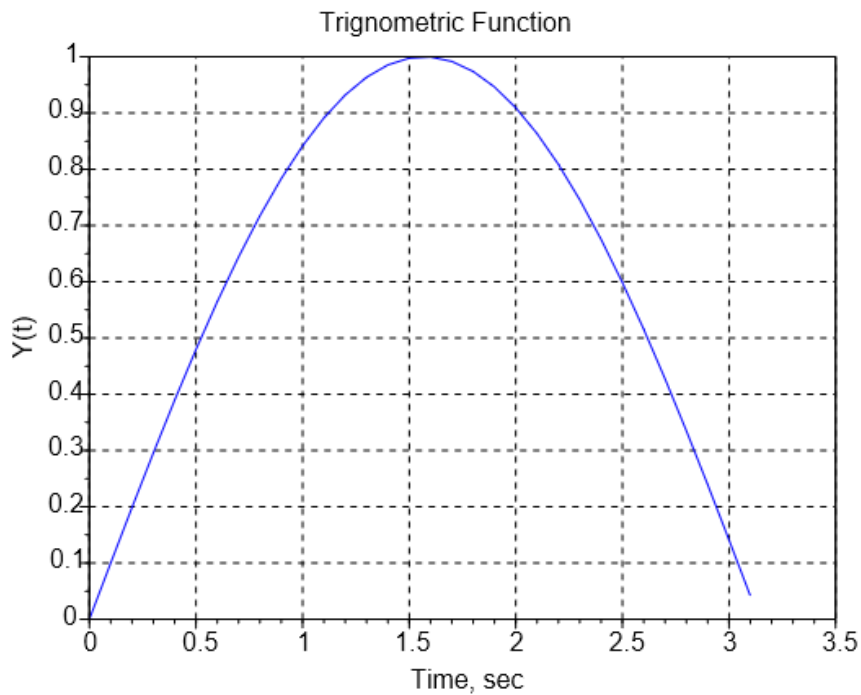
$$\frac{dy}{dt} = y^2 - y\sin(t) + \cos(t) \text{ with the initial condition } y(0) = 0.$$

Open SCINOTES and create a function file by type the following

```
function ydot=f(t,y)
    ydot=y^2-y*sin(t)+cos(t)
endfunction
```

Now go to console window and give the following conditions

```
-->y0=0;
-->t0=0;
-->t=0:0.1:%pi;
-->y = ode(y0,t0,t,f);
-->plot(t,y);
-->xlabel('Time, sec','fontsize',3);
-->ylabel('Y(t)','fontsize',3);
-->title('Trignometric Function','fontsize',4);
-->xgrid(1)
```



5. 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 SCILAB.

Solution

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

$$\text{Accumulation} = \text{input} - \text{output}$$

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

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

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

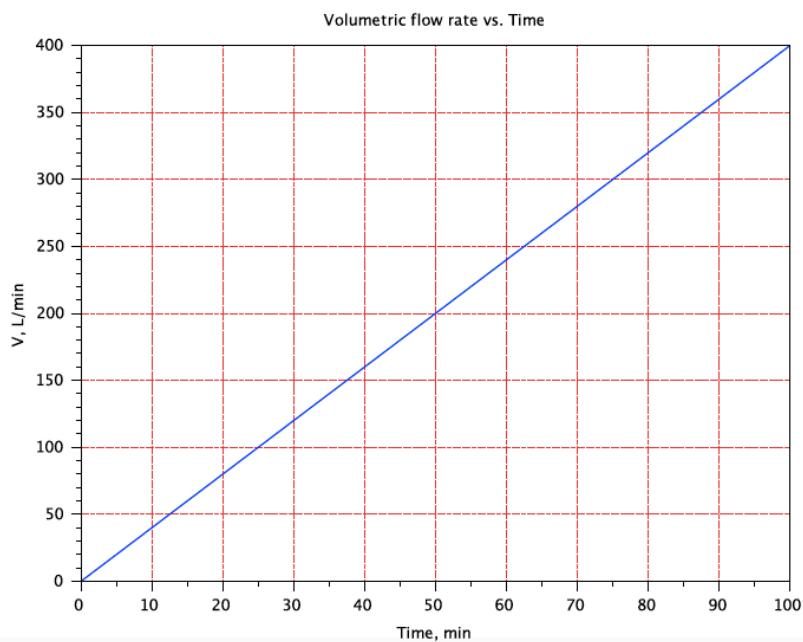
$$\frac{d(V)}{dt} = 4$$

Open SCINOTES and type the following:

```
function vdot=unsteady(t, v)
    vdot=4
endfunction
```

Goto console window and call the above written function by clicking the play button in the SciNotes (or editor) window. Provide all the initial conditions and execute the result from console window as shown below:

```
-->exec('/Users/admin/Desktop/unsteady.emf', -1)
-->v0=0;
-->t0=0;
-->t=0:10:100;
-->v=ode(v0,t0,t,unsteady);
-->xgrid(5,1,7);
-->plot(t,v)
-->xlabel('Time, min');
-->ylabel('V, L/min')
-->title('Volumetric flow rate vs. Time')
```



6. 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

$$\begin{aligned}\frac{dC_a}{dt} &= -k_1 C_a \\ \frac{dC_b}{dt} &= k_1 C_a - k_2 C_b \\ \frac{dC_c}{dt} &= k_2 C_b\end{aligned}$$

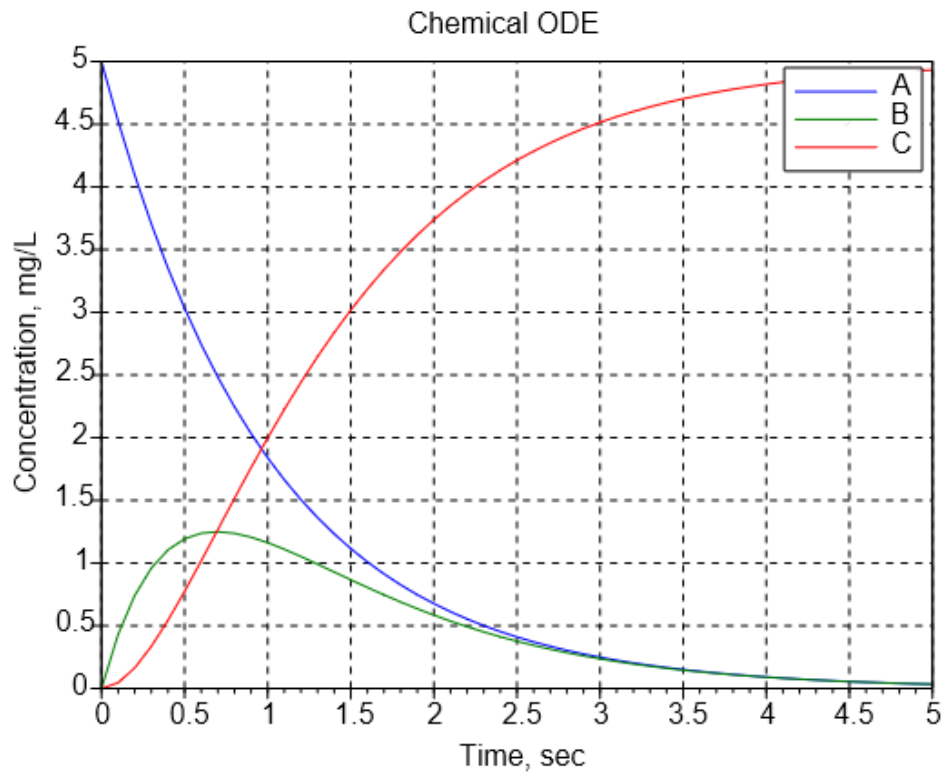
Where $k_1 = \text{hr}^{-1}$ and $k_2 = 2\text{hr}^{-1}$ and at time $t = 0$, $C_a = 5 \text{ mol}$ and $C_b = C_c = 0 \text{ mol}$. Solve the system of equations and plot the change in concentration of each species over time.

Open the SCINOTES and create the function file

```
Function dx=chemical(t,x)
f1=k1*x(1)
f2=k2*x(2)
dx(1)=-f1
dx(2)=f1-f2
dx(3)=f2
endfunction
```

Now go to console window and provide the initial conditions

```
-->exec('C:\Users\User-Pc\Desktop\chemical.sci', -1)
-->k1=1;
-->k2=2;
-->t=0:0.1:5;
-->x0=[5;0;0];
-->x=ode(x0,0,t,chemical);
-->plot(t,x);
\or you can also use-->plot(t,[x(1,:) 'x(2,:) 'x(3,:)'])
-->legends(['A','B','C','D'],[1 2 3 4],"ur");
-->xgrid(1);
-->xlabel('time, min',"fotsize",4);
-->ylabel('Concentration, mg/L',"fotsize",4);
-->xtitle('Chmical ODE',"fotsize",4);
```



Result

Thus we learned the use of SCILAB in solving steady and unsteady (or transient) examples from chemical engineering problems.