Tutorial: 10 SCILAB Programming – Chemical Engineering Applications

Date :19/09/2016

Aim

To solve the algebraic explicit relations (or equations) used in chemical engineering problems using SCILAB

Problem statements

Exercise 1:

Use of `input` and `disp` commands in Dimensionless number calculations. Create a script file incorporating the above-mentioned commands to calculate the Reynolds, Prandtl, Nusselt, Grashof, Schmidt and Archimedes number in U.S. customary units as well as in SI units.

a) Calculation of Reynolds Number

$$N_{Re} = \frac{DV\rho}{\mu}$$

U.S. customary units

$D = 3$ in. $= 3/12$ ft

$V = 6$ ft/s

$\rho = 0.08$ lbm/ft^3

$\mu = 0.015$ cp $= (0.015)(0.000672)$ lbm/ft·s

$$N_{Re} = \frac{(3/12)(6)(0.08)}{(0.015)(0.000672)} = 11{,}904$$

SI units

$D = (3)(0.0254)$ m

$V = (6)(0.3048)$ m/s

$\rho = (0.08)(16.018)$ kg/m^3

$\mu = (0.015)(0.001)$ kg/m·s

$$N_{Re} = \frac{(3 \times 0.0254)\,(6 \times 0.3048)\,(0.08 \times 16.018)}{(0.015)\,(0.001)} = 11{,}904$$

Similary, try the following dimensionless numbers using the `input` and `disp` commands

Open SciNotes and type the following

```
D = input('Diameter, (ft) = ');
V = input('Velocity, (ft/s) = ');
Rho = input('Density, (lbm/cubic feet) = ');
Mu = input('Viscosity, (lbm/ft.s) = ');
disp(' ')
disp('Reynolds no. = ')
disp(D*V*Rho/Mu)
```

Press, Save and execute the function (Play button) in SCINOTES window and then goto console window. Provide the input values to execute the above function as given below:

```
-->exec('/Users/admin/Desktop/reynolds.sce', -1)
```

```
Diameter, (ft) = 3/12
Velocity, (ft/s) = 6
Density, (lbm/cubic feet) = 0.08
Viscosity, (lbm/ft.s) = 0.015*0.000672

 Reynolds no. =
        11904.762
```

Open SciNotes and type the following

```
D = input('Diameter, (m) = ');
V = input('Velocity, (m/s) = ');
Rho = input('Density, (kg/cubic meter) = ');
Mu = input('Viscosity, (kg/m.s) = ');
disp(' ')
disp('Reynolds no. = ')
disp(D*V*Rho/Mu)
```

Press, Save and execute the function (Play button) in SciNotes window and then goto console window. Provide the input values to execute the above function as given below:

```
-->exec('/Users/admin/Desktop/reynoldssi.sce', -1)
Diameter, (m) = 3*0.0254
Velocity, (m/s) = 6*0.3048
Density, (kg/cubic meter) = 0.08*16.018
Viscosity, (kg/m.s) = 0.015*0.001

 Reynolds no. =
    11904.967
```

Exercise 2:

Calculation of a Prandtl Number

$$N_{Pr} = \frac{C_p \mu}{k}$$

U.S. customary units

$\gamma_p = 0.47$ Btu/lbm °F

$\mu = 15$ centipoise $= (15)\ (0.000672)\ (3600)$ lbm/ft·hr

$k = 0.065$ Btu/hr·ft² (°F/ft)

$$N_{Pr} = \frac{(0.47)\ (15 \times 0.000672 \times 3600)}{0.065} = 262.4$$

SI units

$\gamma = (0.47)(4184)$ J/kg °C

$\mu = (15)(0.001)$ kg/m·s

$k = (0.065)(1.728)$ J/s·m² (°C/m)

$$N_{Pr} = \frac{(0.47)\ (4184)\ (15)\ (0.001)}{(0.065)\ (1.728)} = 262.6$$

Open SciNotes and type the following

```
Cp=input('Heat Capacity,(Btu/lbm deg. F) = ');
Mu=input('Viscosity, (lbm/ft h)=');
k=input('Thermal conductivity, (Btu/hr sq. ft)=');
disp(' ');
disp('Prandtl No. =');
disp((Cp*Mu)/(k))
```

Press, Save and execute the function (Play button) in SciNotes window and then goto console window. Provide the input values to execute the above function as given below:

```
-->exec('C:\Users\asus\Desktop\prandtl.sce', -1)
      Heat Capacity,(Btu/lbm deg. F) = 0.47
      Viscosity, (lbm/ft h)=15*0.000672*3600
      Thermal conductivity, (Btu/hr sq. ft)=0.065
       Prandtl No. =
           262.39015
```

Open SciNotes and type the following

```
Cp=input('Heat Capacity,(J/kg deg. C) = ');
Mu=input('Viscosity, (kg/m s)=');
k=input('Thermal conductivity, (J/s sq. m)=');
disp(' ');
disp('Prandtl No. =');
disp((Cp*Mu)/(k))
```

Press, Save and execute the function (Play button) in SciNotes window and then goto console window. Provide the input values to execute the above function as given below:

```
-->exec('C:\Users\asus\Desktop\prandtl1.sce', -1)
      Heat Capacity,(J/kg deg. C) = 0.47*4184
      Viscosity, (kg/m s)=15*0.001
      Thermal conductivity, (J/s sq. m)=0.065*1.728
```

```
Prandtl No. =
   262.61752
```

Exercise 3:

"Diffusion of water through stagnant, non-diffusing air"

Water in the bottom of a narrow metal tube is held at constant temperature of 293 K. The total pressure of air (assumed dry) is 1.01325×10^5 Pa (1.0 atm) and the temperature is 293 K (20 ^oC). Water evaporates and diffuses through the air in tube, and the diffusion path Z_2-Z_1 is 0.1524 m (0.5 ft) long. Calculate the rate of evaporation at steady state in kg mol/s · m^2. The diffusivity of water vapor at 293 K and 1 atm pressure is 0.250 × 10^{-4} m^2/s. Assume the system is isothermal.

Data: $P_{BM} = 1.001 \times 10^5$, $P_{A1} - P_{A2} = 2.341 \times 10^3$ Pa

Solution

$$N_A = \frac{D_{AB}P}{RT(z_2 - z_1)P_{BM}}(P_{A1} - P_{A2})$$

$$N_A = \frac{(0.250 \times 10^{-4})(1.01325 \times 10^5)(2.314 \times 10^3)}{8314(293)(0.1524)(1.001 \times 10^5)} = 1.595 \times 10^{-7}\,\text{kgmol/s} \cdot \text{m}^2$$

Open SciNotes and type the following

```
DAB=input('Diffusivity,(sq. m/s ) = ');
P=input('Total Pressure, (Pa)=');
PA=input('Vapor pressure of water at 20 deg.C. - Vapor
Pressure of Air at 20 deg.C, (PA1-PA2), (Pa)=');
R=input('Universal gas constant,(R)(cubic meter Pa/kg
mole K)=');
T=input('Temperature, (K)=');
Z=input('Diffusion path (Z1-Z2), (m)=');
Pbm=input('Log mean Pressure, (Pa)=');
disp(' ');
disp('Rate of evaporation at steady state. =');
disp((DAB*P*PA)/(R*T*Z*Pbm))
```

Press, Save and execute the function (Play button) in SciNotes window and then goto console window. Provide the input values to execute the above function as given below:

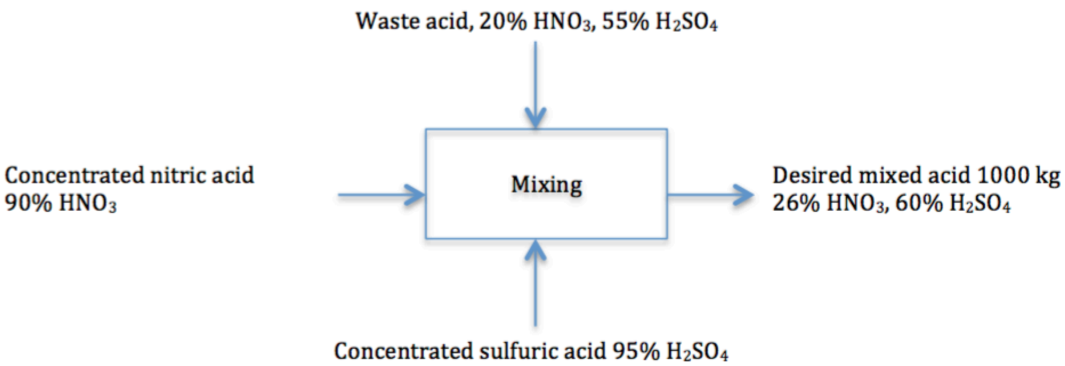
```
-->exec('C:\Users\asus\Desktop\prandtl1.sce', -1)
     Diffusivity,(sq. m/s ) = 0.250*10^-4
```

```
Total Pressure, (Pa)=1.01325*10^5
Vapor pressure of water at 20 deg.C. - Vapor Pressure of
Air at 20 deg.C=2.341*10^3
Universal gas constant, (cubic meter Pa/kg mole K)=8314
Temperature, (K)=293
Diffusion path (Z1-Z2), (m)=0.1524
Log mean Pressure, (Pa)=1.001*10^5
Rate of evaporation at steady state. =
0.0000002
```

The above result can also be written as 2E-07 kg mol/s.m^2

Exercise 4:

The waste acid from a nitrating process containing 20% HNO_3, 55% H_2SO_4 and 25% H_2O by weight is to be concentrated by the addition of concentrated H_2SO_4 containing 95% H_2SO_4 and concentrated HNO_3 containing 90% HNO_3 to get desired mixed acid containing 26% HNO_3 and 60% H_2SO_4. Calculate the quantities of waste and concentrated acids required for 1000 kg of desired mixed acid.



By overall Balance;

$$x + y + z + = 1000$$

By H_2SO_4 balance;

$$0.55x + 0.95y = 600$$

By HNO_3 balance;

$$0.2x + 0.9z = 260$$

Write the above equation in the matrix form as given below

$$\begin{bmatrix} 1 & 1 & 1 \\ 0.57 & 0.95 & 0 \\ 0.2 & 0 & 0.9 \end{bmatrix} \begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \begin{bmatrix} 1000 \\ 600 \\ 260 \end{bmatrix}$$

Obtain the solution using SCILAB.

Open Console window in SCILAB and try the following

```
-->A=[1 1 1; 0.55 0.95 0.0; 0.2 0 0.9];

-->B=[1000 600 260]';

-->X=A\B
 X  =

    400.
    400.
    200.
```

Exercise 5:

It is general practice in engineering and science that equations be plotted as lines and discrete data as symbols. Here is some data for concentration (*c*) versus time (*t*) for the photodegradation of aqueous bromine

***t*, min**	**10**	**20**	**30**	**40**	**50**	**60**
***c*, ppm**	3.4	2.6	1.6	1.3	1.0	0.5

The above data can be described by the following function

$$c = 4.84e^{-0.034t}$$

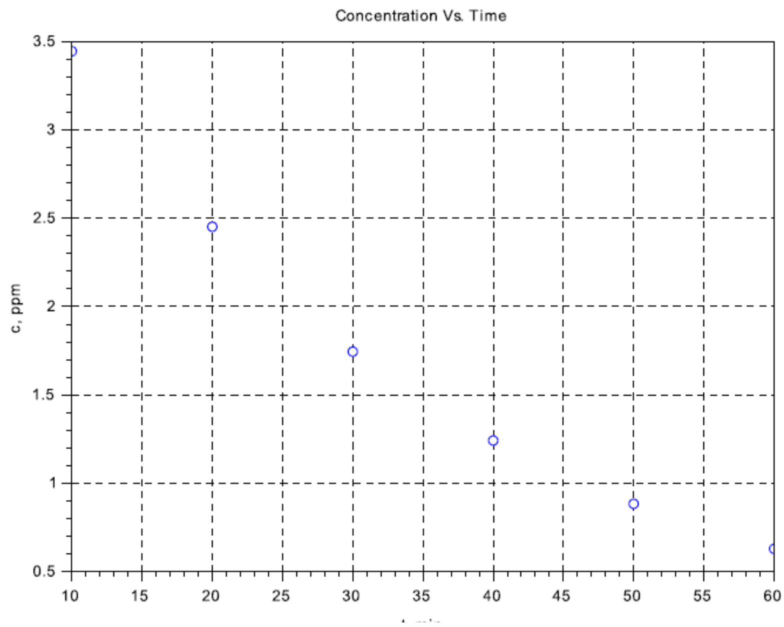
Use SCILAB to create a plot displaying both the data (using circle 'o' symbol).

Solution

Open Console window in SCILAB and try the following:

```
-->x=[10:10:60]'
 x  =

    10.
    20.
    30.
    40.
```

```
     50.
     60.

-->y=[2.4,2.6,1.6,1.3,1.0,0.5]';

-->y=4.84*exp(-0.034*x);

-->plot(x,y,'o');

-->xgrid(1)

-->xlabel('t, min');

-->ylabel('c, ppm');

-->xtitle('Concentration Vs. Time')
```



Exercise 6:

The temperature dependence of chemical reactions can be computed with the

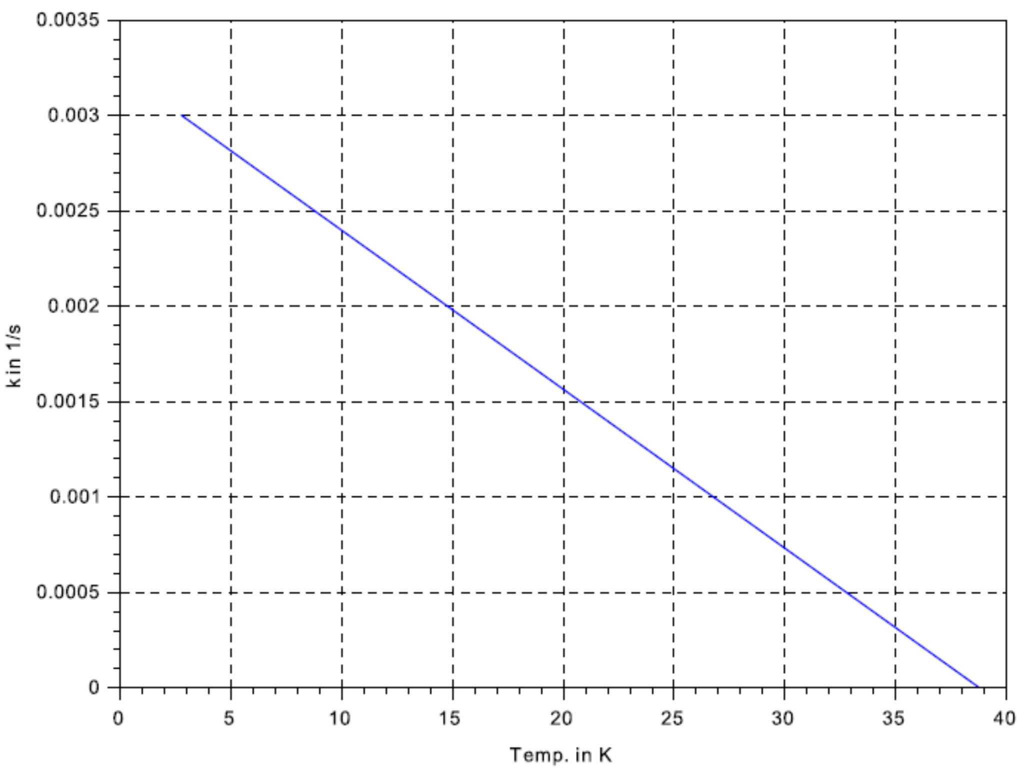
Arrhenius equation:

$$k = Ae^{-E/(RT_a)}$$

where k = reaction rate (s-1), A = preexponential factor (or frequency factor), E = Activation energy (J/mol), R = gas constant [8.314 J/mol . K], and T_a = absolute temperature (K). A compound has 1×10^5 J/mol and $A = 7 \times 10^{16}$ J/mol. Use SCILAB command window to generate values of reaction rates ranging for temperature ranging from 273 to 333 K. Use plot to generate a graph of $\log_{10}k$ versus $1/T_a$.

Open Console window in SCILAB and try the following

```
--> T=[273:10:333]'
 T  =

    273.
    283.
    293.
    303.
    313.
    323.
    333.

-->A=(7)*(10^16);

-->E=1*10^5;

-->R=8.314;

-->x=[(-10^5)/(8.314.*T)]'

-->k=[A*exp(x)]'

-->log1p(k);

-->1/T;

-->plot(log1p(k),1/T)

-->xgrid(1)

-->xlabel('Temp. in K')

-->ylabel('k in 1/s')
```



Exercise 7:

Find the specific volume of n-butane at 500 K and 18 atm using the Redlich-Kwong equation of state.

$$p = \frac{RT}{\hat{v} - b} - \frac{a}{\hat{v}(\hat{v} + b)}$$

$$\hat{v}^3(p) - \hat{v}^2(RT) + \hat{v}(a - pb^2 - RTb) - ab = 0$$

where

$$a = 0.42748\left(\frac{R^2T_c^2}{p_c}\right), \quad b = 0.08664\left(\frac{RT_c}{p_c}\right),$$

take $T_c = 425.2$, and p_c=37.5.

Solution

Open SciNotes and create the function file

```
function [y]=specvol(v)
Tc=425.2
pc=37.5
T=500
p=18
R=0.08206
aRK=0.42748*(R*Tc)^2/pc
bRK=0.08664*(R*Tc/pc)
y=p*v^3-R*T*v^2+(aRK-p*bRK^2-R*T*bRK)*v-aRK*bRK;
```

Console

```
-->v=0.2;
-->y=fsolve(v,specvol)
 y  =
     0.1404458
```

Note: The command `fsolve` is used to solve a nonlinear equation or model using an initial guess. Here the initial guess is v=0.2.

Example for `fsolve` command

Solve F(x) = x^3 - 3x - 2. Clearly the solution is 2 try the solution with SCILAB.

```
function [f]=F(x)
```

```
    f=x^3-3*x-2
endfunction
```

Goto console

```
x = 100; //initial guess
-->x=100;

-->y=fsolve(x,F)

 y  =

    2.
```

Exercise 8: Use function command in SCINOTES and obtain the solutions for the problems listed in exercise1a, 2a, 3a and

Exercise 1a: Reyno lds number (SI Units)

Exercise 2a: Prandtl number (SI Units)

Exercise 3a: Diffusion of water through, non-diffusing air (SI Units)

Exercise 1a: Reynolds number

Open SciNotes and try the following:

```
function Nre=reynolds(D, V, Rho, mu)
    Nre=D*V*Rho/(mu)
endfunction
```

Press, Save and execute the function (Play button) in SCINOTES window and then goto console window. Provide the input values to execute the above function as given below:

Console window:

```
-->reynolds(3*0.0254,6*0.3048,0.08*16.018,0.015*0.001)
 ans  =
     11904.967
```

Exercise 2a: Prandtl number (SI Units)

Open SciNotes and try the following:

```
function Pr=Prandtl(Cp, Mu, k)
    Pr=Cp*Mu/(k)
endfunction
```

Press, Save and execute the function (Play button) in SCINOTES window and then goto console window. Provide the input values to execute the above function as given below:

```
-->Prandtl(0.47*4184,15*0.001,0.065*1.728)
 ans  =
     262.61752
```

Exercise 3a: Diffusion of water through stagnant. Non-diffusing air (SI Units)
Open SciNotes and try the following:

```
function Na=diffusion(DAB, P, PA, R, T, Z, Pbm)
    Na=(DAB*P*PA)/(R*T*Z*Pbm)
endfunction
```

Press, Save and execute the function (Play button) in SCINOTES window and then goto console window. Provide the input values to execute the above function as given below:

```
-->
diffusion(0.250*10^4,1.01325*10^5,2.341*10^3,8314,293,0.1524,1
.001*10^5)
 ans  =

    0.0000002
```

Result

Thus we learned the use of SCILAB in solving algebraic equations in chemical engineering problems.