Matrix Algebra

1. Introduction

There are a number of common situations in chemical engineering where systems of linear equations appear. There are at least three ways in MATLAB for solving this system of equations;

(1) Using matrix **algebra commands** (Also called matrix inverse or Gaussian Elimination method)

(2) Using the **solve** command (have been discussed).

(3) Using the **numerical** equation solver.

The first method is the preferred; therefore we will explain and demonstrate it. Remember, you always should work in an m-file.

2. Solving Linear Equations Using Matrix Algebra

One of the most common applications of matrix algebra occurs in the solution of linear simultaneous equations. Consider a set of n equations in which the unknowns are x_1, x_2, ... x_n.

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots\ldots\ldots\ldots\ldots a_{1n}x_n = b_1$$
$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \ldots\ldots\ldots\ldots\ldots a_{2n}x_n = b_2$$
$$a_{31}x_1 + a_{32}x_2 + a_{33}x_3 + \ldots\ldots\ldots\ldots\ldots a_{3n}x_n = b_3$$
$$\cdot \qquad \cdot \qquad \cdot \qquad\qquad\qquad \cdot \qquad \cdot$$
$$a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \ldots\ldots\ldots\ldots\ldots a_{nn}x_n = b_n$$

where

x_j is the j^{th} variable.

a_{ij} is the constant coefficient of the j^{th} variable in the i^{th} equation.

b_j is constant "right-hand-side" coefficient for equation i.

The system of equations given above can be expressed in the matrix form as.

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & : & a_{1n} \\ a_{21} & a_{22} & a_{23} & : & : \\ : & : & : & : & : \\ : & : & : & : & : \\ a_{n1} & a_{n2} & a_{n3} & : & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ : \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ : \\ b_n \end{bmatrix}$$

Or

$AX = b$

Where

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & : & a_{1n} \\ a_{21} & a_{22} & a_{23} & : & a_{2n} \\ : & : & : & : & : \\ : & : & : & : & : \\ a_{n1} & a_{n2} & a_{n3} & : & a_{nn} \end{bmatrix} \qquad b = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ : \\ b_n \end{bmatrix} \qquad X = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ : \\ x_n \end{bmatrix}$$

To determine the variables contained in the column vector 'x', complete the following steps.

(a) Create the coefficient matrix 'A'. Remember to include zeroes where an equation doesn't contain a variable.

(b) Create the right-hand-side column vector 'b' containing the constant terms from the equation. This must be a ***column*** vector, ***not*** a ***row***.

(c) Calculate the values in the 'x' vector by left dividing 'b' by 'A', by typing x = A\b.

Note: this is different from x = b/A.

As an example of solving a system of equations using the matrix inverse method, consider the following system of three equations.

$x_1 - 4x_2 + 3x_3 = -7$

$3x_1 + x_2 - 2x_3 = 14$

$2x_1 + x_2 + x_3 = 5$

These equations can be written in matrix format as;

$$\begin{bmatrix} 1 & -4 & 3 \\ 3 & 1 & -2 \\ 2 & 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -7 \\ 14 \\ 5 \end{bmatrix}$$

To find the solution of the following system of equations type the code.

```
A =[1,-4, 3; 3, 1, -2; 2, 1, 1]
B = [ -7;14; 5]
x = A\B
```

the results will be results in

```
x = [ 3
      1
     -2 ]
```

In which $x_1=3$, $x_2=1$, $x_3= -2$

To extract the value of each of x_1, x_2, x_3 type the command:

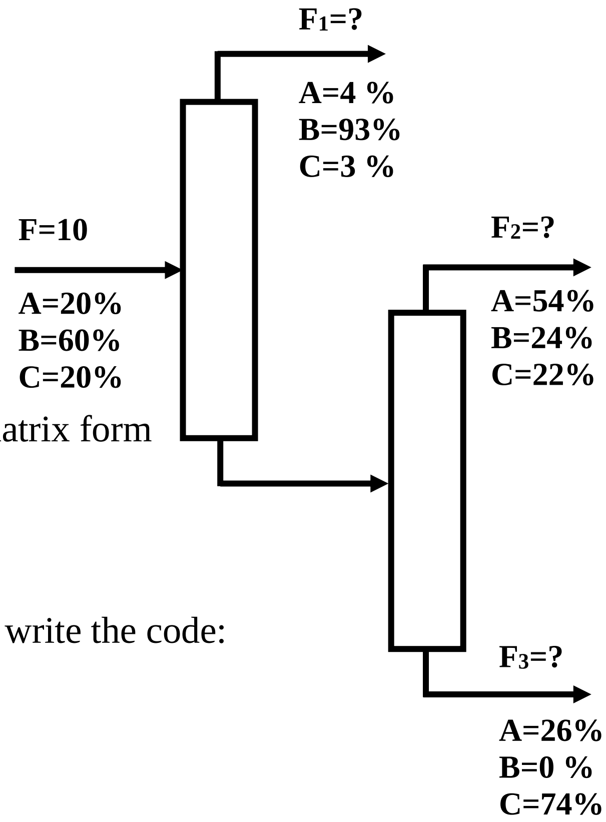
```
x1=x(1)
x2=x(2)
x3=x(3)
```

The results will be:

```
x1 =
     3
x2 =
     1
x3 =
    -2
```

Exercise 1:

For the following separation system, we know the inlet mass flow rate (in Kg/hr) and the mass fractions of each species in the inlet flow (F) and each outlet flow (F_1, F_2 and F_3). We want to calculate the unknown mass flow rates of each outlet stream.



Solution:

Set up the mass balances for

1. the total mass flow rate

$F_1 \quad +F_2 \quad +F_3 \quad =10$

2. the mass balance on species A

$0.04F_1+0.54F_2+0.26F_3=0.2*10$

3. the mass balance on species B

$0.93F_1+0.24F_2 \qquad =0.6*10$

These three equations can be written in matrix form

$$\begin{bmatrix} 1 & 1 & 1 \\ 0.04 & 0.54 & 0.26 \\ 0.93 & 0.24 & 0 \end{bmatrix} \begin{bmatrix} F1 \\ F2 \\ F3 \end{bmatrix} = \begin{bmatrix} 10 \\ 2 \\ 6 \end{bmatrix}$$

To find the values of unknown flow rates write the code:

```
A=[1, 1, 1; .04, .54, .26; .93, .24 ,0];
B=[10; .2*10; .6*10];
X=A\B;
F1=X(1),F2=X(2),F3=X(3)
```

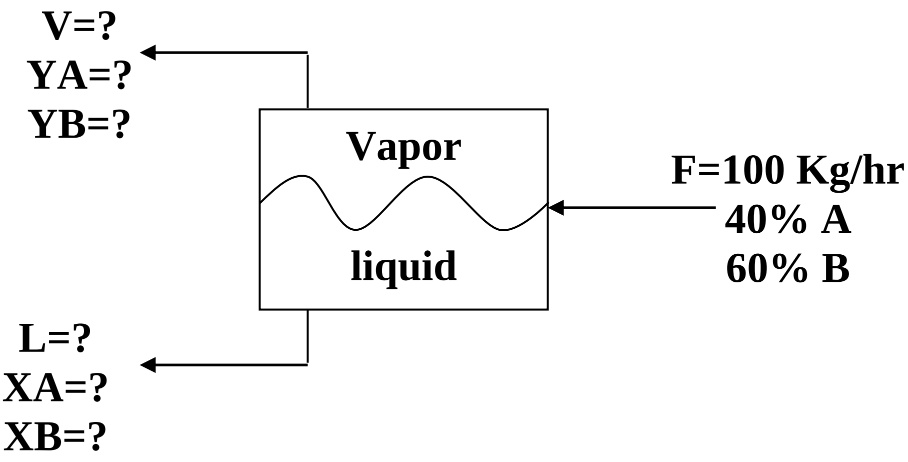
The results will be:

```
F1 =
   5.8238
F2 =
   2.4330
F3 =
   1.7433
```

Exercise 2:

Write a program to calculate the values of XA, XB,YA, YB, L and V for the vapor liquid separator shown in fig.

If you know:
XA+XB=1
YA+YB=1
YA=KA*XA=1.9XA
YB=KB*XB=0.6XB



Solution:

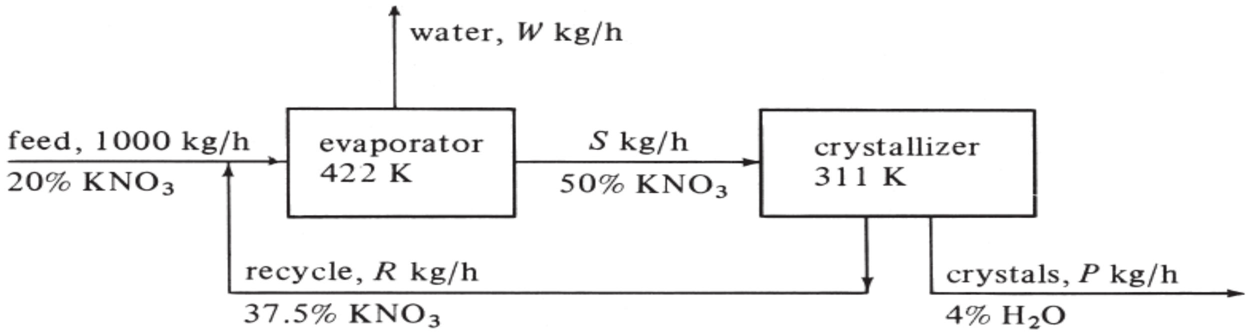
```
A=[1,1,0,0;0,0,1,1;-1.9,0,1,0;0,-0.6,0,1];
B=[1;1;0;0];
X=A\B;
xa=X(1)
xb=X(2)
ya=X(3)
yb=X(4)
a=[xa,ya;xb,yb];
b=[.4*100;.6*100];
x=a\b;
L=x(1),
V=x(2)
```

Gives the results

```
xa =
   0.3077
xb =
   0.6923
ya =
   0.5846
yb =
   0.4154
L =
  66.6667
V =
  33.3333
```

Exercise 3:

In a process producing KNO_3 salt, 1000 kg/h of a feed solution containing 20 wt % KNO_3 is fed to an evaporator, which evaporates some water at 422 K to produce a 50 wt % KNO_3 solution. This is then fed to a crystallizer at 311 K, where crystals containing 96 wt % KNO_3 is removed. The saturated solution containing 37.5 wt % KNO_3 is recycled to the evaporator. Write a code to calculate the amount of recycle stream R in kg/h and the product stream of crystals P in kg/h.



Solution:

Set up the total mass balances for KNO_3 and water:

0.2*1000 = 0.96*P

0.8*1000 = 0.04*P +W

Mass balances on crystallizer for KNO_3 and water:

0.5*S=0.375*R+0.96*P

0.5*S=0.625*R+0.04*P

To find the values of unknown W, S, R and P write the code:

```
A=[0.96, 0, 0, 0;-0.04,1,0,0;-0.96, 0, 0.5,-0.375;-0.04, 0,0.5,-0.625];
B=[200; 800;0;0];
X=A\B;
P=X(1),W=X(2),S=X(3), R=X(4),
```

The results will be:

```
P =
   208.33
W =
   808.3333
S =
   975
R =
   766.6667
```

Exercise 4:

Balance the following chemical equation:

$x1\ CH_4 + x2\ O_2 \rightarrow x3\ CO_2 + x4\ H_2O$

Solution:

There are three elements involved in this reaction: carbon (C), hydrogen (H), and oxygen (O). A balance equation can be written for each of these elements:

Carbon (C): $1 \cdot x1 + 0 \cdot x2 = 1 \cdot x3 + 0 \cdot x4$

Hydrogen (H): $4 \cdot x1 + 0 \cdot x2 = 0 \cdot x3 + 2 \cdot x4$

Oxygen (O): $0 \cdot x1 + 2 \cdot x2 = 2 \cdot x3 + 1 \cdot x4$

Re-write these as homogeneous equations, each having zero on its right hand side:

$x1 - x3 = 0$

$4x1 - 2x4 = 0$

$2x2 - 2x3 - x4 = 0$

At this point, there are three equations in four unknowns.

To complete the system, we define an auxiliary equation by arbitrarily choosing a value for one of the coefficients:

$x4 = 1$

To solve these four equations write the code:

```
A =[1,0,-1,0;4,0,0,-2;0,2,-2,-1;0,0,0,1];
B=[0;0;0;1];
X=A\B
```

The result will be

```
X =
   0.5000
   1.0000
   0.5000
   1.0000
```

Finally, the stoichiometric coefficients are usually chosen to be integers.

Divide the vector X by its smallest value:

```
X =X/min(X)
X =
    1
    2
    1
    2
```

Thus, the balanced equation is

$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

Exercise 5:

Balance the following chemical equation:

$x1\ P_2I_4 + x2\ P_4 + x3\ H_2O \rightarrow x4\ PH_4I + x5\ H_3PO_4$

Solution:

We can easily balance this reaction using MATLAB:

```
A = [2 4 0 -1 -1
4 0 0 -1 0
0 0 2 -4 -3
0 0 1 0 -4
0 0 0 0 1];
B= [0;0;0;0;1];
X = A\B;
X =
   0.3125
   0.4063
   4.0000
   1.2500
   1.0000
```

We divide by the minimum value (first element) of **x** to obtain integral coefficients:

```
X=X/min(X)
X =
   1.0000
   1.3000
  12.8000
   4.0000
   3.2000
```

This does not yield integral coefficients, but multiplying by 10 will do the trick:

```
x = x * 10
X =
   10
   13
  128
   40
   32
```

The balanced equation is

$10\ P_2I_4 + 13\ P_4 + 128\ H_2O \rightarrow 40\ PH_4I + 32\ H_3PO_4$

Practice Problems

1) Solve each of these systems of equations by using the matrix inverse method.

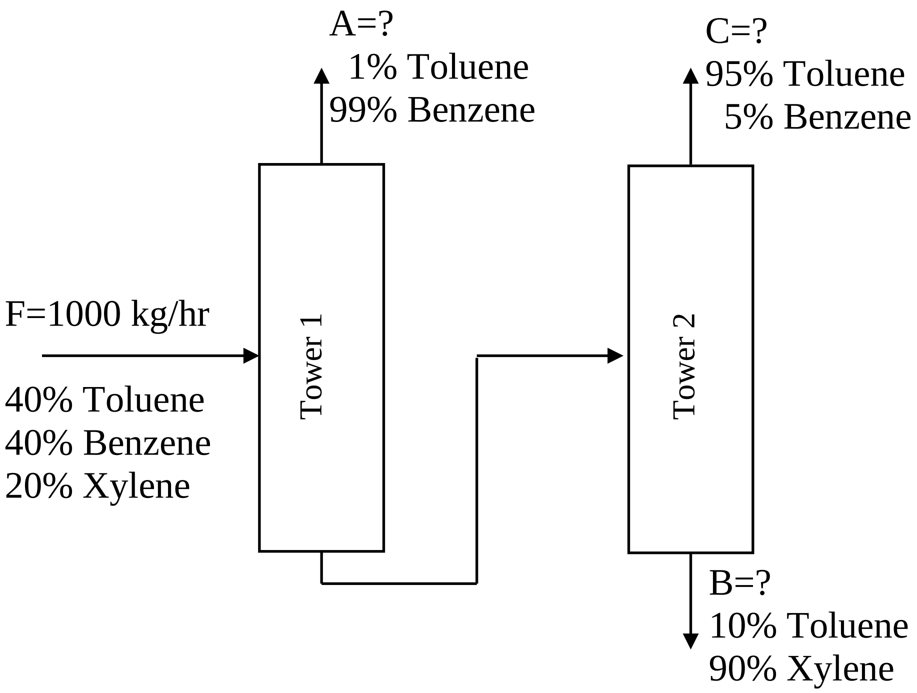
A)
$$\begin{aligned} r + s + t + w &= 4 \\ 2r - s + w &= 2 \\ 3r + s - t - w &= 2 \\ r - 2s - 3t + w &= -3 \end{aligned}$$

B)
$$\begin{aligned} x_1+2x_2-x_3&=3 \\ 3x_1-x_2+2x_3&=1 \\ 2x_1-2x_2+3x_3&=2 \\ x_1-x_2+x_4&=-1 \end{aligned}$$

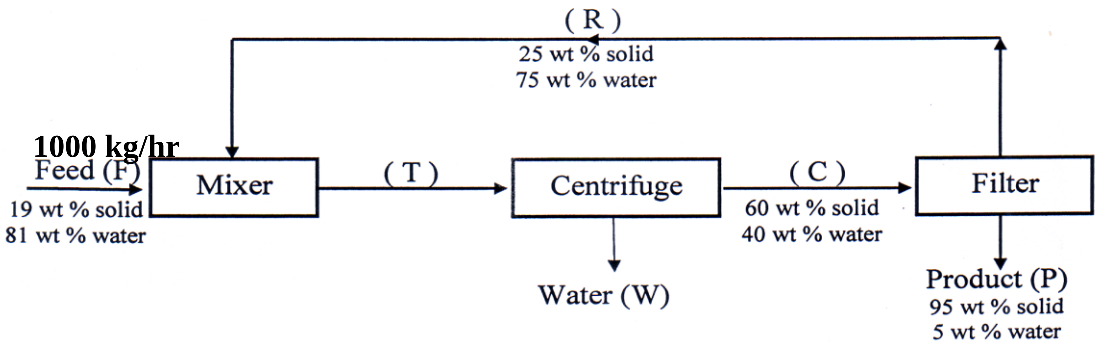
C)
$$\begin{aligned} 5x_1+3x_2+7x_3-4&=0 \\ 3x_1+26x_2-2x_3-9&=0 \\ 7x_1+2x_2+10x_3-5&=0 \end{aligned}$$

D)
$$\begin{aligned} 2x_1 + x_2 - 4x_3 + 6x_4 + 3x_5 - 2x_6 &= 16 \\ -x_1 + 2x_2 + 3x_3 + 5x_4 - 2x_5 &= -7 \\ x_1 - 2x_2 - 5x_3 + 3x_4 + 2x_5 + x_6 &= 1 \\ 4x_1 + 3x_2 - 2x_3 + 2x_4 + x_6 &= -1 \\ 3x_1 + x_2 - x_3 + 4x_4 + 3x_5 + 6x_6 &= -11 \\ 5x_1 + 2x_2 - 2x_3 + 3x_4 + x_5 + x_6 &= 5 \end{aligned}$$

2) For the following figure calculate the values of the unknown flow rates A, B, C by using matrix inverse method.



3) Write a program to calculate the flow rates of streams W, P, C, R and T in the following flow diagram using **matrix inverse method**.



4) Balance the following chemical equations using the matrix inverse method:

a) $Pb(NO_3)_2 \rightarrow PbO + NO_2 + O_2$

b) $MnO_2 + HCl \rightarrow MnCl_2 + H_2O + Cl_2$

c) $As + NaOH \rightarrow Na_3AsO_3 + H_2$

d) $C_4H_{10} + O_2 \rightarrow CO_2 + H_2O$

e) $BaCl_2 + Al_2(SO_4)_3 \rightarrow BaSO_4 + AlCl_3$