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 these 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 explained and demonstrated 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.

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

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)
```

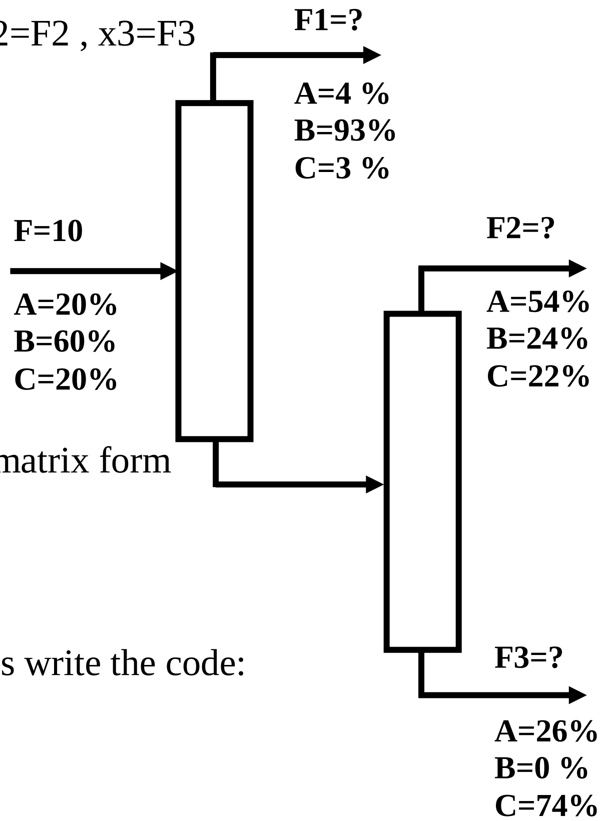
The results will be:

```
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 (F1, F2 and F3). We want to calculate the unknown mass flow rates of each outlet stream.

<u>Solution:</u>



If we define the unknowns as x1=F1, x2=F2 , x3=F3 and set up the mass balances for

1. the total mass flow rate

x1 +x2 +x3 =10

2. the mass balance on species 1

0.04x1+0.54x2+0.26x3=0.2*10

3. the mass balance on species 2

0.93x1+0.24X2 =0.6*10

These three equations can be written in matrix form

$$\begin{bmatrix} 1 & 1 & 1 \\ 0.04 & 0.54 & 0.26 \\ 0.93 & 0.24 & 0 \end{bmatrix} \begin{bmatrix} x1 \\ x2 \\ x3 \end{bmatrix} = \begin{bmatrix} 10 \\ 2 \\ 6 \end{bmatrix}$$

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:

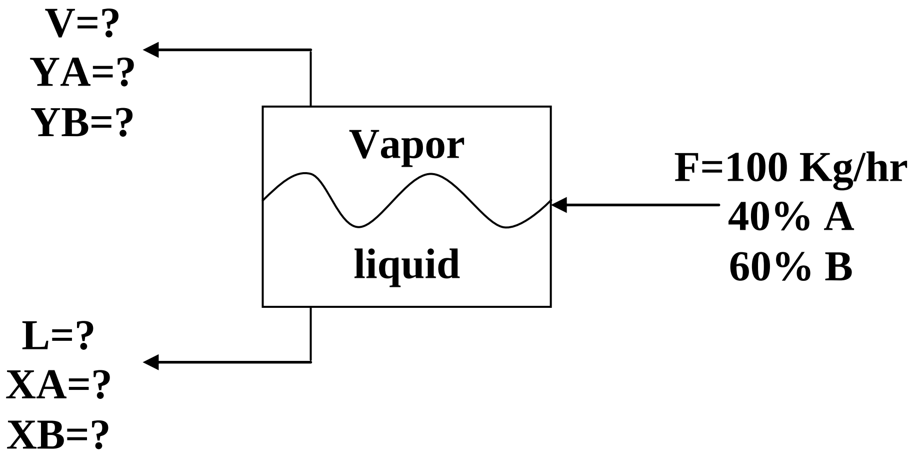
```
F1 =
   5.8238
F2 =
   2.4330
F3 =
   1.7433
```

<u>Exercise 2:</u>

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



<u>Solution:</u>

```
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:

Xylene, styrene, toluene and benzene are to be separated with the array of distillation columns that is shown below. Write a program to calculate the amount of the streams D, B, D1, B1, D2 and B2 also to calculate the composition of streams D and B.

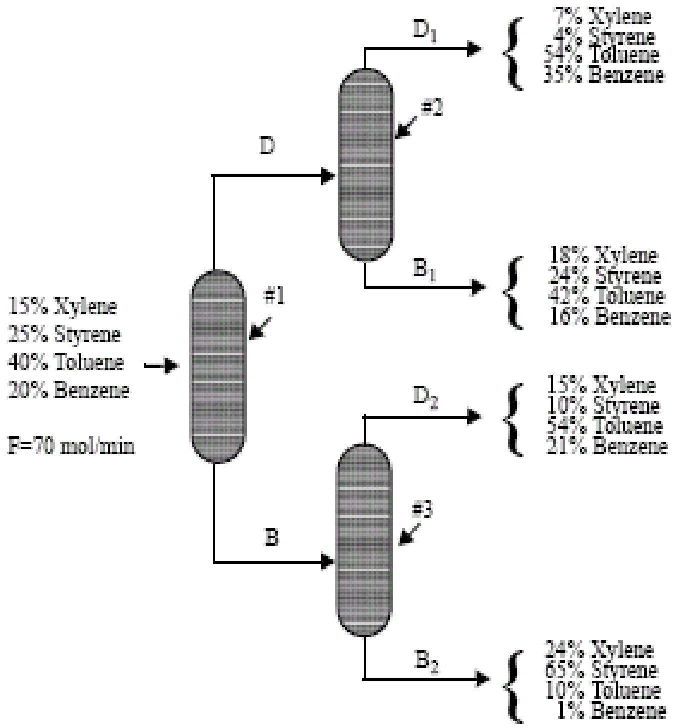


Figure A1 Separation Train

Solution:

By making material balance on individual components on the overall separation train yield the equation set

Xylene: 0.07D1+ 0.18B1+ 0.15D2+ 0.24B2= 0.15× 70

Styrene: 0.04D1+ 0.24B1+ 0.10D2+ 0.65B2= 0.25× 70

Toluene: 0.54D1+ 0.42B1+ 0.54D2+ 0.10B2= 0.40× 70

Benzene: 0.35D1+ 0.16B1+ 0.21D2+ 0.01B2= 0.20× 70

Overall material balances and individual component balances on column 2 can be used to determine the molar flow rate and mole fractions from the equation of stream D.

Molar Flow Rates: D = D1 + B1

Xylene: XDxD = 0.07D1 + 0.18B1

Styrene: XDsD = 0.04D1 + 0.24B1

Toluene: XDtD = 0.54D1 + 0.42B1

Benzene: XDbD = 0.35D1 + 0.16B1

where

XDx = mole fraction of Xylene.

XDs = mole fraction of Styrene.

XDt = mole fraction of Toluene.

XDb =mole fraction of Benzene.

Similarly, overall balances and individual component balances on column 3 can be used to determine the molar flow rate and mole fractions of stream B from the equation set.

Molar Flow Rates: B = D2 + B2

Xylene: XBxB = 0.15D2 + 0.24B2

Styrene: XBsB = 0.10D2 + 0.65B2

Toluene: XBtB = 0.54D2 + 0.10B2

Benzene: XBbB = 0.21D2 + 0.01B2

where F, D, B, D1, B1, D2 and B2 are the molar flow rates in mol/min.

Now type the following code in command window

```
A=[0.07, 0.18, 0.15, 0.24; 0.04, 0.24, 0.10, 0.65; 0.54, 0.42, 0.54, 0.1;0 .35,
0.16, 0.21, 0.01];
B=[0.15*70; 0.25*70; 0.4*70; 0.2*70];
X=A\B;
D1=X(1),B1=X(2),D2=X(3),B2=X(4),
D=D1+B1
B=D2+B2
XDx=(.07*D1+.18*B1)/D
XDs=(.04*D1+.24*B1)/D
XDt=(.54*D1+.42*B1)/D
XDb=(.35*D1+.16*B1)/D
XBx=(.15*D2+.24*B2)/B
XBs=(.1*D2+.65*B2)/B
XBt=(.54*D2+.1*B2)/B
XBb=(.21*D2+.01*B2)/B
```

The results will be

```
D1 =
  26.2500
B1 =
  17.5000
D2 =
   8.7500
B2 =
  17.5000
D =
  43.7500
```

```
B =
  26.2500
XDx =
   0.1140
XDs =
   0.1200
XDt =
   0.4920
XDb =
   0.2740
XBx =
   0.2100
XBs =
   0.4667
XBt =
   0.2467
XBb =
   0.0767
```

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
$CH4 + 2O_2 \rightarrow CO_2 + 2H_2O$

<u>Exercise 5:</u>

Balance the following chemical equation:
$x1\ P_2I_4 + x2\ P_4 + x3\ H_2O \rightarrow x4\ PH_4I + x5\ H_3PO_4$

<u>Solution:</u>

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:

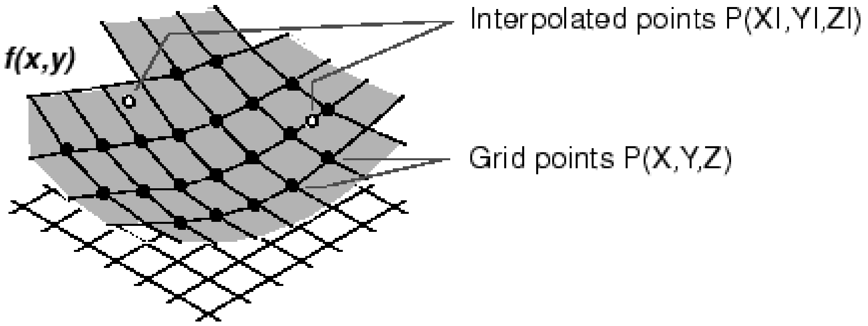
```
x = x * 10
X =
   10
   13
  128
   40
   32
```

The balanced equation is

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

3.Two-Dimensional Interpolation

The **interp2** command performs two-dimensional interpolation between data points. It finds values of a two-dimensional function underlying the data at intermediate points>



Its most general form is:

Zi = interp2(X, Y, Z, Xi, Yi)

Zvector = interp2(X, Y, Z, Xvector, Yvector)

Note: the number of elements of the X vector and Z matrix rows must be the same, while the number of elements of the Y vector and Z matrix columns must be the same.

Exercise 6:

Calculate the values of z corresponding to (x,y)=(1.3, 1.5) and (1.5,2.3) from data as following:

x=1, 2

y= 1, 2, 3

z = 10 20

  40 50

  70 80

Solution

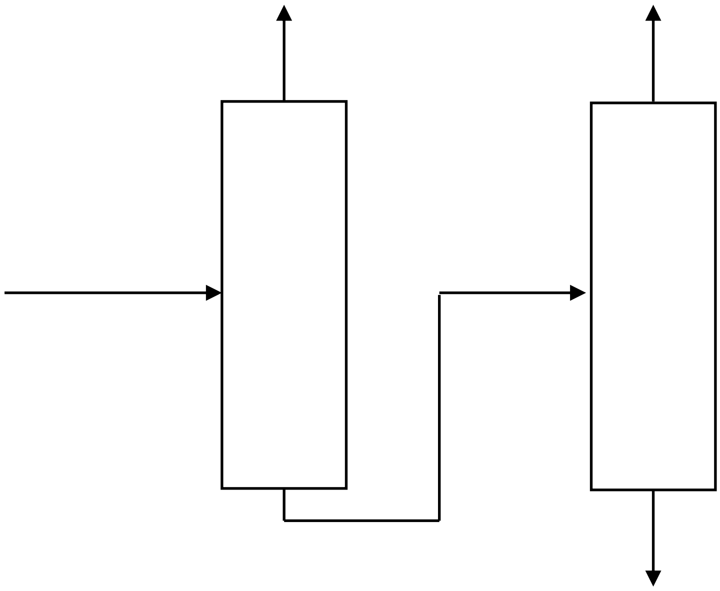
```
x = [1 2];
y = [1 2 3];
z = [10 20
     40 50
     70 80];
z1 = interp2(x,y,z,1.3,1.5)
```

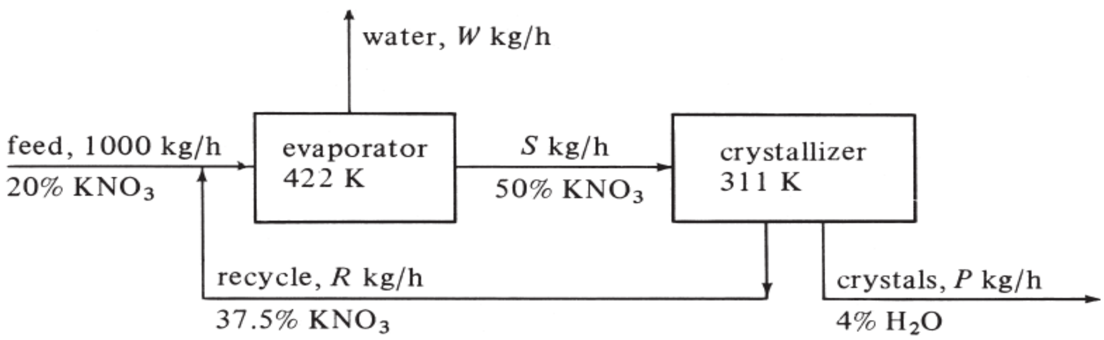
The results will be

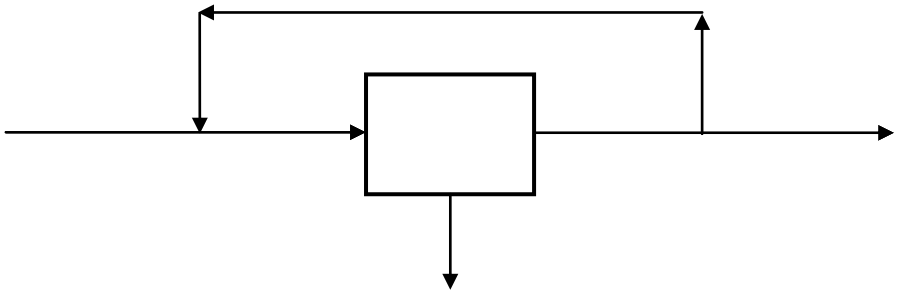
```
z1 =
   28000
```

To interpolate a vector of x, y point repeat the same code with small change:

```
z12 = interp2(x,y,z,[1.3,1.5],[1.5,2.3])
z12 =
   28.0000    54.0000
```




water, W kg/h
feed, 1000 kg/h
20% KNO3
evaporator
422 K
S kg/h
50% KNO3
crystallizer
311 K
recycle, R kg/h
37.5% KNO3
crystals, P kg/h
4% H2O



P(bar) ($T_{sat.}$°C)		Sat'd Water	Sat'd Steam	Temperature (°C)→ 50	75	100	150	200	250	300	350
0.0	$\hat{H}$	—	—	2595	2642	2689	2784	2880	2978	3077	3177
(—)	$\hat{U}$	—	—	2446	2481	2517	2589	2662	2736	2812	2890
	$\hat{V}$	—	—	—	—	—	—	—	—	—	—
0.1	$\hat{H}$	191.8	2584.8	2593	2640	2688	2783	2880	2977	3077	3177
(45.8)	$\hat{U}$	191.8	2438.0	2444	2480	2516	2588	2661	2736	2812	2890
	$\hat{V}$	0.00101	14.7	14.8	16.0	17.2	19.5	21.8	24.2	26.5	28.7
0.5	$\hat{H}$	340.6	2646.0	209.3	313.9	2683	2780	2878	2979	3076	3177
(81.3)	$\hat{U}$	340.6	2484.0	209.2	313.9	2512	2586	2660	2735	2811	2889
	$\hat{V}$	0.00103	3.24	0.00101	0.00103	3.41	3.89	4.35	4.83	5.29	5.75
1.0	$\hat{H}$	417.5	2675.4	209.3	314.0	2676	2776	2875	2975	3074	3176
(99.6)	$\hat{U}$	417.5	2506.1	209.2	313.9	2507	2583	2658	2734	2811	2889
	$\hat{V}$	0.00104	1.69	0.00101	0.00103	1.69	1.94	2.17	2.40	2.64	2.87
5.0	$\hat{H}$	640.1	2747.5	209.7	314.3	419.4	632.2	2855	2961	3065	3168
(151.8)	$\hat{U}$	639.6	2560.2	209.2	313.8	418.8	631.6	2643	2724	2803	2883
	$\hat{V}$	0.00109	0.375	0.00101	0.00103	0.00104	0.00109	0.425	0.474	0.522	0.571
10	$\hat{H}$	762.6	2776.2	210.1	314.7	419.7	632.5	2827	2943	3052	3159
(179.9)	$\hat{U}$	761.5	2582	209.1	313.7	418.7	631.4	2621	2710	2794	2876
	$\hat{V}$	0.00113	0.194	0.00101	0.00103	0.00104	0.00109	0.206	0.233	0.258	0.282