

Department of Chemical Engineering  
ChE-101: Approaches to Chemical Engineering Problem Solving  
**MATLAB Tutorial VI**

**Solving a System of Linear Algebraic Equations** (last updated 5/19/05 by GGB)

Objectives:

These tutorials are designed to show the introductory elements for any of the topics discussed. In almost all cases there are other ways to accomplish the same objective, or higher level features that can be added to the commands below. Read Chapter 3 of the textbook to learn more about matrix operations

Any text below appearing after the double prompt (>>) can be entered in the Command Window directly or in an m-file.

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The following topics are covered in this tutorial;

**Introduction**

**Solving Using Matrix Algebra Commands**

**Solved Problems (guided tour)**

**Proposed Problems**

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**Introduction:**

There are a number of common situations in chemical engineering where systems of linear equations appear. Any system of 'n' linear equations in 'n' unknowns can be expressed in the general form:

$$\begin{array}{rcl}
 a_{11} x_1 + a_{12} x_2 + \dots + a_{1n} x_n & = & b_1 \\
 a_{21} x_1 + a_{22} x_2 + \dots + a_{2n} x_n & = & b_2 \\
 & & \vdots \\
 & & \vdots \\
 a_{n1} x_1 + a_{n2} x_2 + \dots + a_{nn} x_n & = & b_n
 \end{array}$$

where  $x_j$  is the  $j^{\text{th}}$  variable,  
 $a_{ij}$  is the constant coefficient on the  $j^{\text{th}}$  variable in the  $i^{\text{th}}$  equation, and  
 $b_j$  is the constant term.

There are at least three ways in Matlab of solving these systems;

- (1) using matrix algebra commands, (the preferred method)
- (2) using the symbolic algebra **solve** command,
- (3) using the numerical equation solver, ie. the **fsolve** command.

Only the matrix algebra method will be demonstrated in this tutorial.

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## Method Using Matrix Algebra Commands

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

$$\begin{bmatrix} a_{11} & a_{12} & \dots & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & \dots & a_{2n} \\ & & : & & \\ & & : & & \\ a_{n1} & a_{n2} & \dots & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ : \\ : \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ : \\ : \\ b_n \end{bmatrix}$$

In short\_hand notation this is listed as  $[A]\{x\} = \{b\}$ .

Remember that the rules of matrix multiplication dictate that the '[A]' matrix be consistent with the '{x}' and '{b}' vectors. The first column of 'A' contains the coefficients for  $x_1$ . The first row of 'A' and element of 'b' contain the coefficients for the first equation.

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

- Create the coefficient matrix '[A]'. Also remember to include zeroes where an equation doesn't contain a variable.
- Calculate the determinant of the coefficient matrix to make sure that you have an independent set of equations. If the determinant is zero you have a singular matrix. The meaning of this is that your equations are not independent therefore; you will have to verify each of your equations. You will start learning how to formulate equations to understand different processes when you take ChE-200.

The command used in Matlab to calculate the determinant of a matrix is *det*. See the example given below:

Calculate the determinant of the matrix  $A = \begin{bmatrix} 3 & 1 & 1 \\ 2 & 0 & 1 \\ 2 & 3 & 4 \end{bmatrix}$

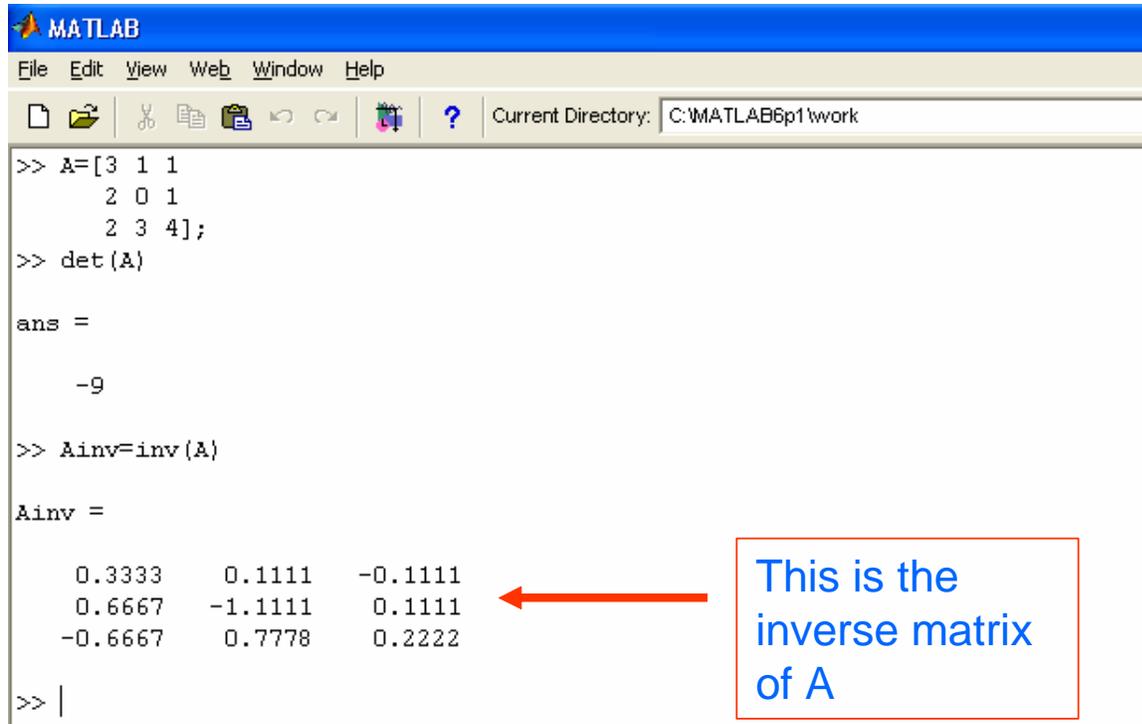
```
MATLAB
File Edit View Web Window Help
Current Directory: C:\MATLAB6p1\work
>> A=[3 1 1
      2 0 1
      2 3 4];
>> det(A)
ans =
     -9
>> |
Ready
```

Because the determinant is different to zero the inverse matrix of A exists.

- (c) Create the right\_hand\_side column vector '{b}' containing the constant terms from the equation. This must be a column vector, not a row.
- (d) Calculate the values in the '{x}' vector of unknowns by performing the following matrix operation:  $\{x\} = [A]^{-1} \{b\}$

Where  $[A]^{-1}$  is the inverse matrix of the coefficient matrix A.

The command used in Matlab to calculate the inverse of a matrix is *inv*. See the example given below:



```

MATLAB
File Edit View Web Window Help
Current Directory: C:\MATLAB6p1\work
>> A=[3 1 1
      2 0 1
      2 3 4];
>> det(A)

ans =

    -9

>> Ainv=inv(A)

Ainv =

    0.3333    0.1111   -0.1111
    0.6667   -1.1111    0.1111
   -0.6667    0.7778    0.2222

>> |
  
```

This is the inverse matrix of A

Therefore, if the {b} vector is given by:  $\{b\} = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$ . The solution of the system of LAEs can be calculated in Matlab as shown below:

```

MATLAB
File Edit View Web Window Help
Current Directory: C:\MATLAB6p1\wo

>> A=[3 1 1
      2 0 1
      2 3 4];
>> det(A)

ans =

    -9

>> Ainv=inv(A)

Ainv =

    0.3333    0.1111   -0.1111
    0.6667   -1.1111    0.1111
   -0.6667    0.7778    0.2222

>> b=[1
      0
      -1];
>> x=Ainv*b

x =

    0.4444
    0.5556
   -0.8889

```

This must be a column vector

This is the operational symbol for the product of matrices (see Tutorial 3)

Solution for the system of LAEs

The *inv* command will give you an error message if the matrix that you are trying to calculate the inverse to is singular. See the example given below:

```

MATLAB
File Edit View Web Window Help
Current Directory: C:\MATLAB6p1\work

>> A=[1 0 0
      0 1 0
      -1 0 0];
>> Ainv=inv(A)
Warning: Matrix is singular to working precision.

Ainv =

    Inf    Inf    Inf
    Inf    Inf    Inf
    Inf    Inf    Inf

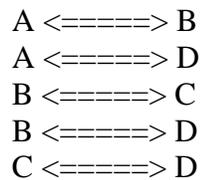
>> |

```

Remember: This means that you don't have a set of independent equations

**SOLVED PROBLEMS**

1. The following series of reversible reactions occurs;



Assume that the reactions are carried out in a batch reactor at constant temperature and pressure, and that the reactor initially contains only component A at a concentration of 1 mole/liter. Given the first order rate constants for each reaction, determine the equilibrium concentration of each component.

Given an example set of rate constants, and applying a mass balance on three of the components and the constraint that the concentration of all four species must sum to one, results in the following system of linear equations.

$$\begin{aligned} C_A + C_B + C_C + C_D &= 1 \\ -0.3C_A + 0.02C_B + 0.05C_D &= 0 \\ 0.1C_A - 0.82C_B + 0.1C_C + 0.1C_D &= 0 \\ 0.5C_B - 0.11C_C + 0.1C_D &= 0 \end{aligned}$$

Write a program in Matlab to calculate the concentration of each of the components in the reactor. .

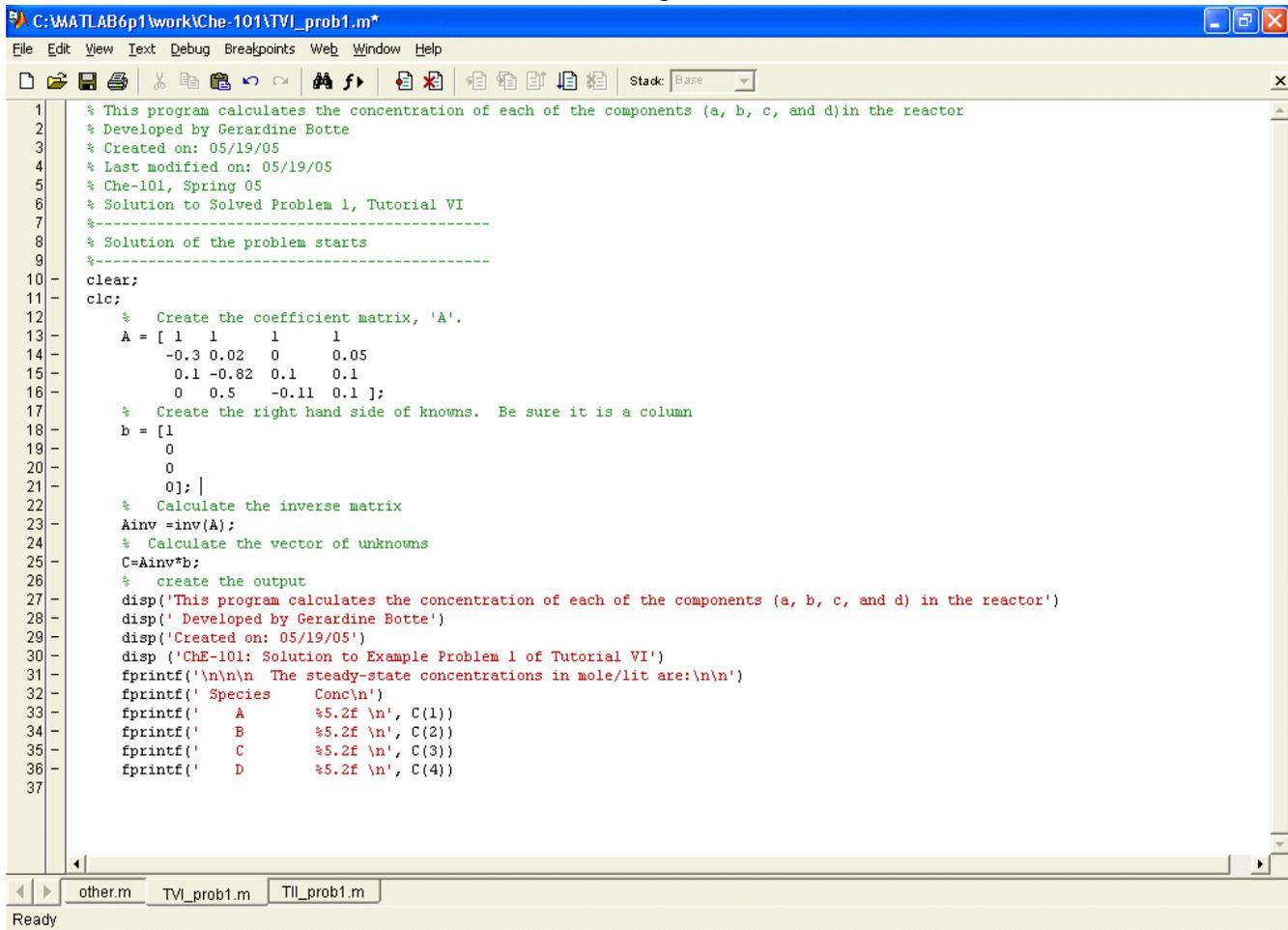
Solution:

1. The first step is to express the system of linear algebraic equations in matrix form:

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ -0.3 & 0.02 & 0 & 0.05 \\ 0.1 & -0.82 & 0.1 & 0.1 \\ 0 & 0.5 & -0.11 & 0.1 \end{bmatrix} \begin{bmatrix} C(1) \\ C(2) \\ C(3) \\ C(4) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

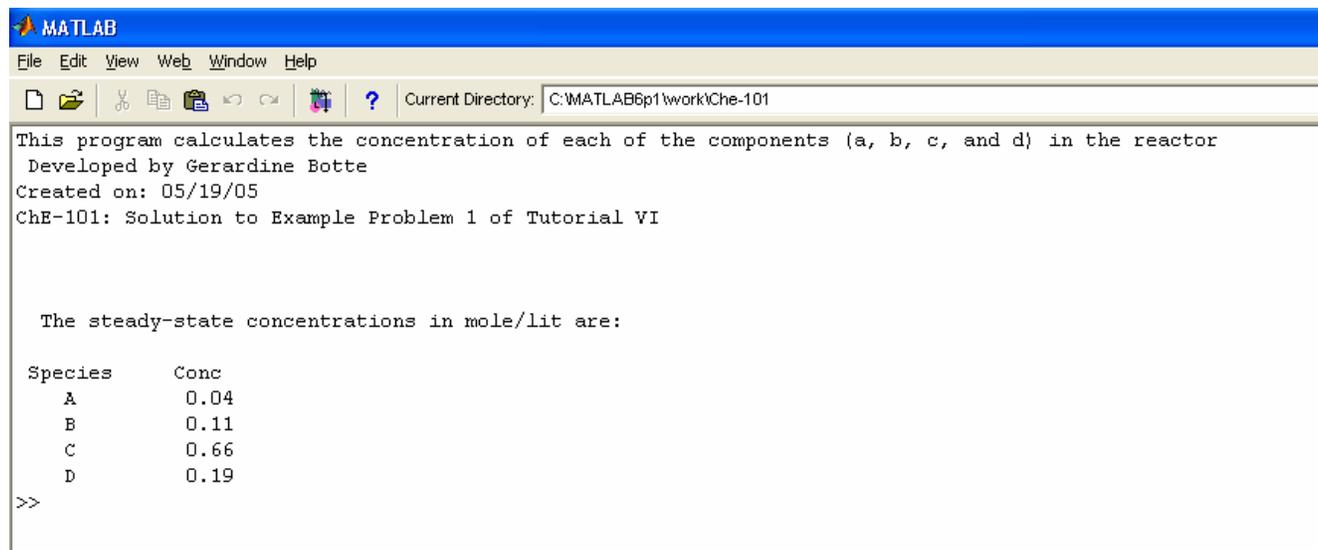
2. Follow the “tips for solving problems”
3. Write a flowchart diagram (see H-2). In the space given below draw your flowchart diagram

#### 4. Write the code in Matlab. See the solution given below.



```
C:\MATLAB6p1\work\Che-101\TVI_prob1.m
File Edit View Text Debug Breakpoints Web Window Help
[Icons] Stack: Base
1 % This program calculates the concentration of each of the components (a, b, c, and d) in the reactor
2 % Developed by Gerardine Botte
3 % Created on: 05/19/05
4 % Last modified on: 05/19/05
5 % Che-101, Spring 05
6 % Solution to Solved Problem 1, Tutorial VI
7 %-----
8 % Solution of the problem starts
9 %-----
10 clear;
11 clc;
12 % Create the coefficient matrix, 'A'.
13 A = [ 1 1 1 1
14      -0.3 0.02 0 0.05
15      0.1 -0.82 0.1 0.1
16      0 0.5 -0.11 0.1 ];
17 % Create the right hand side of knows. Be sure it is a column
18 b = [1
19      0
20      0
21      0];
22 % Calculate the inverse matrix
23 Ainvs = inv(A);
24 % Calculate the vector of unknowns
25 C=Ainvs*b;
26 % create the output
27 disp('This program calculates the concentration of each of the components (a, b, c, and d) in the reactor')
28 disp(' Developed by Gerardine Botte')
29 disp('Created on: 05/19/05')
30 disp('ChE-101: Solution to Example Problem 1 of Tutorial VI')
31 fprintf('\n\n The steady-state concentrations in mole/lit are:\n\n')
32 fprintf(' Species      Conc\n')
33 fprintf('  A      %5.2f \n', C(1))
34 fprintf('  B      %5.2f \n', C(2))
35 fprintf('  C      %5.2f \n', C(3))
36 fprintf('  D      %5.2f \n', C(4))
37
other.m TVI_prob1.m TII_prob1.m
Ready
```

#### 5. This is the solution of the problem



```
MATLAB
File Edit View Web Window Help
[Icons] ? Current Directory: C:\MATLAB6p1\work\Che-101
This program calculates the concentration of each of the components (a, b, c, and d) in the reactor
Developed by Gerardine Botte
Created on: 05/19/05
ChE-101: Solution to Example Problem 1 of Tutorial VI

The steady-state concentrations in mole/lit are:

Species      Conc
  A      0.04
  B      0.11
  C      0.66
  D      0.19
>>
```

**PROPOSED PROBLEMS**

The analysis of a reactor used to chlorinate ethane results in the following set of equations:

$$0.87N_1 = N_3$$

$$13.3N_4 = 100$$

$$2N_1 = 2N_3 = 200 + 2N_4$$

$$6N_1 = 6N_3 + 500 + 4N_4 + N_5$$

where  $N_1$  through  $N_5$  represents the flowrates in moles/hr of ethane fed, chlorine fed, ethane remaining, dichloroethane produced, and hydrogen chloride produced respectively. Is the system of equations linear or nonlinear? Justify your answer. If linear express the system of equations in matrix form and develop a program in Matlab to obtain the solution for the flowrates.