

ChE 400: Applied Chemical Engineering Calculations Tutorial 1: Basic Operations with Matlab and Excel

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Learning objectives:

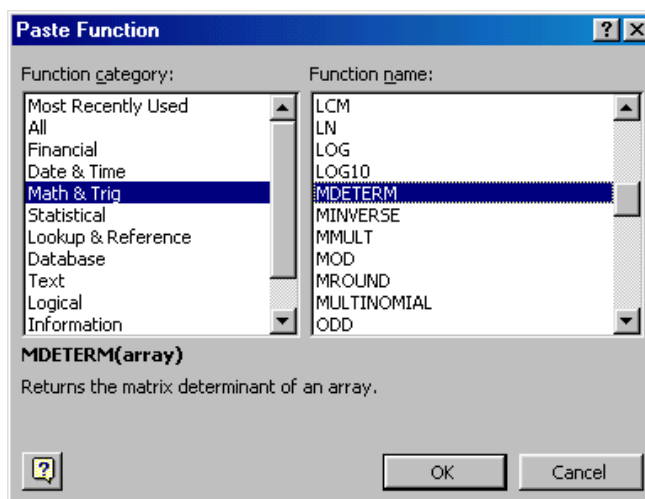
After completing the exercises given in this tutorial you should be able to:

1. Perform different matrix operations using excel
2. Build plots in Matlab
3. Build functions in Matlab

It is important that you review Tutorials IV of ChE-101 (Function Files, see your ChE-101 binder, web: <http://webche.ent.ohiou.edu/WEB-che101/T4-Function%20Files.pdf>) and Vb (Making Plots with Matlab, see your ChE-101 binder, web: <http://webche.ent.ohiou.edu/WEB-che101/T5b-Making%20PLOTS.pdf>)

It is also important that you review the rules from producing quality plots and tables (see your handout H-4 ChE-101 binder, web: <http://webche.ent.ohiou.edu/WEB-che101/H-4.pdf>)

1. Matrix Operations. Excel can be used to perform different matrix operations such as: inverse matrix (minverse()), matrix determinant (mdeterm()), and product of two matrices (mmult()). All these functions are in the “insert” menu, “function”, “math&trig”, as shown below:



For instance, given the following matrices:

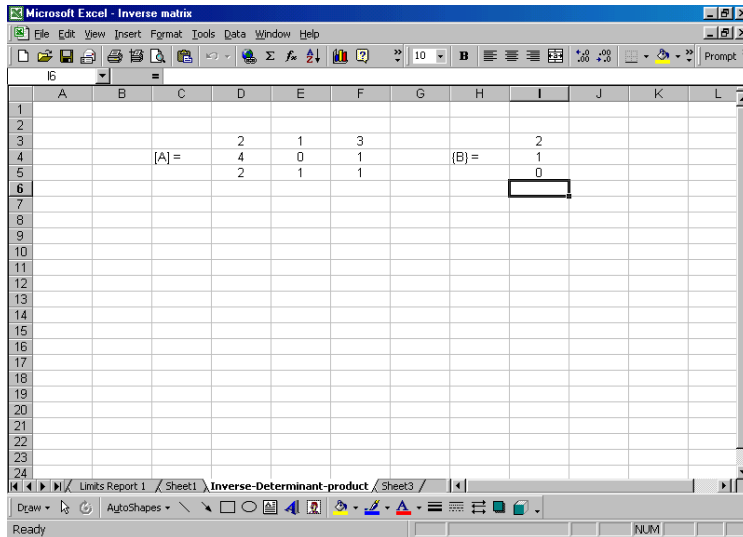
$$[A] = \begin{bmatrix} 2 & 1 & 3 \\ 4 & 0 & 1 \\ 2 & 1 & 1 \end{bmatrix} \quad \{B\} = \begin{Bmatrix} 2 \\ 1 \\ 0 \end{Bmatrix}$$

use Excel to:

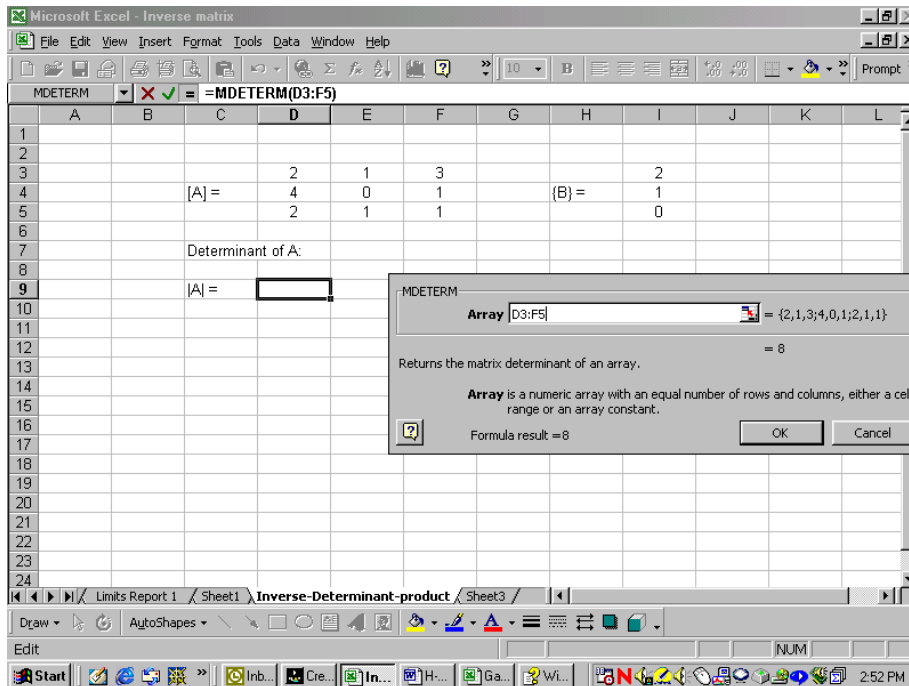
- 1.1 Calculate the determinant and the inverse matrix of [A].
- 1.2 Evaluate [C] and [E] defined as: [C] = [A] {B} and [E] = [A]⁻¹ {B}.

Solution:

Each cell in “excel” represents an element of the matrix [A] and the vector {B}. Input your elements as shown below:

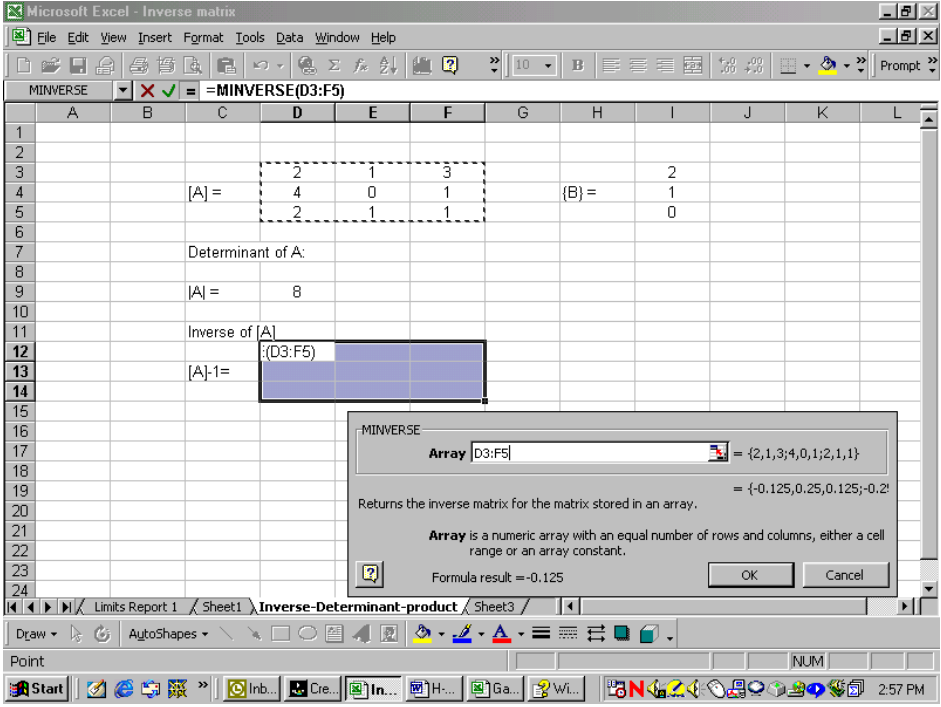


To calculate the determinant of [A] use the function mdeterm() from the function palette as shown below:



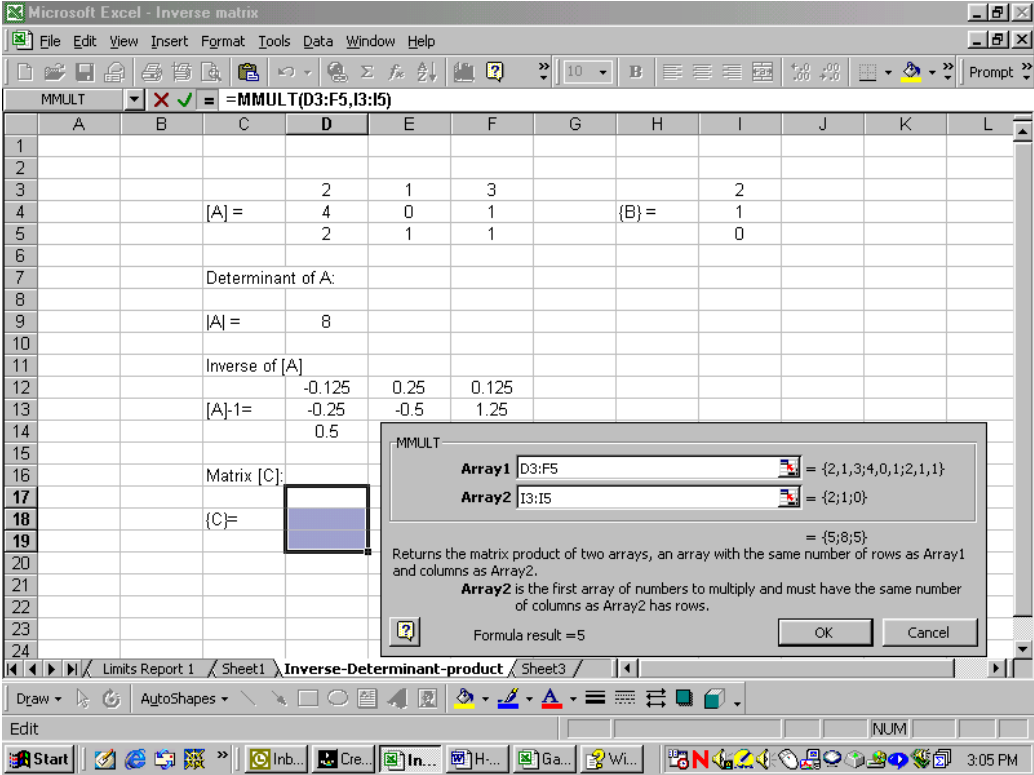
The determinant of [A] = 8. Click “OK” to accept your results.

To calculate the inverse of [A] select the range of the cells that will contain the inverse matrix and use the function minverse() from the function palette as shown below:

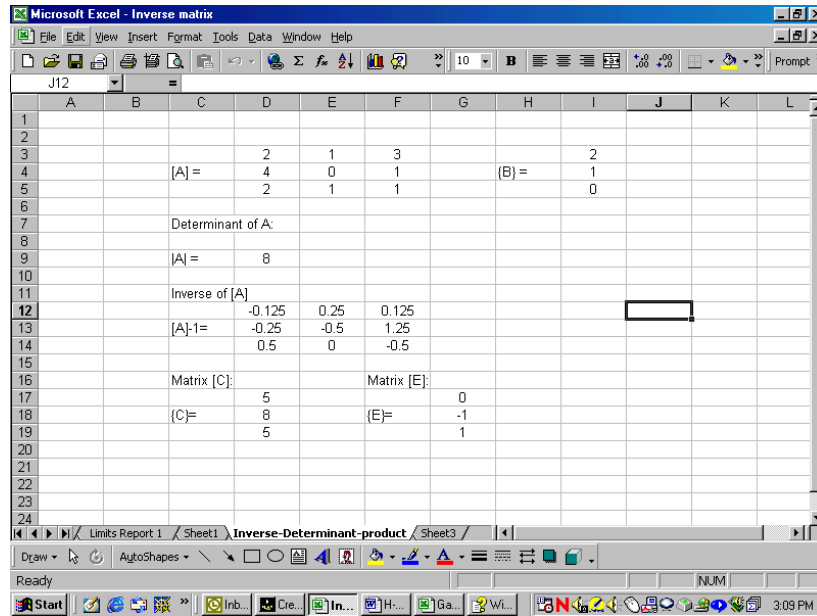


The results of the inverse are shown in the screen. To accept the results click “**Ctrl+Shift+OK**”.

To evaluate the product of [A] and {B} select the range where the new matrix will be locate, and use the function mmult() from the function palette as shown below:



The results of the product are shown in the screen. To accept the results click “**Ctrl+Shift+OK**”. The results of the calculations are shown below:



2. Proposed Exercises with Excel. Calculate the value of {x} according to:

$$\{x\} = [A]^{-1} \{b\}$$

$$A = \begin{bmatrix} 3 & -0.1 & -0.2 \\ 0.1 & 7 & -0.3 \\ 0.3 & -0.2 & 10 \end{bmatrix} \quad \{b\} = \begin{bmatrix} 7.85 \\ -19.3 \\ 71.4 \end{bmatrix}$$

Solution

$$[A] = \begin{matrix} & 3 & -0.1 & -0.2 \\ & 0.1 & 7 & -0.3 \\ & 0.3 & -0.2 & 10 \end{matrix} \quad \{B\} = \begin{matrix} 7.85 \\ -19.3 \\ 71.4 \end{matrix}$$

$$[A]^{-1} = \begin{matrix} 0.332489 & 0.004944 & 0.006798 \\ -0.00518 & 0.142903 & 0.004183 \\ -0.01008 & 0.00271 & 0.09988 \end{matrix} \quad \{X\} = \begin{matrix} 3 \\ -2.5 \\ 7 \end{matrix}$$

$$[A] = \begin{matrix} & 3 & -0.1 & -0.2 \\ & 0.1 & 7 & -0.3 \\ & 0.3 & -0.2 & 10 \end{matrix} \quad \{B\} = \begin{matrix} 7.85 \\ -19.3 \\ 71.4 \end{matrix}$$

3. Making a plot with Excel

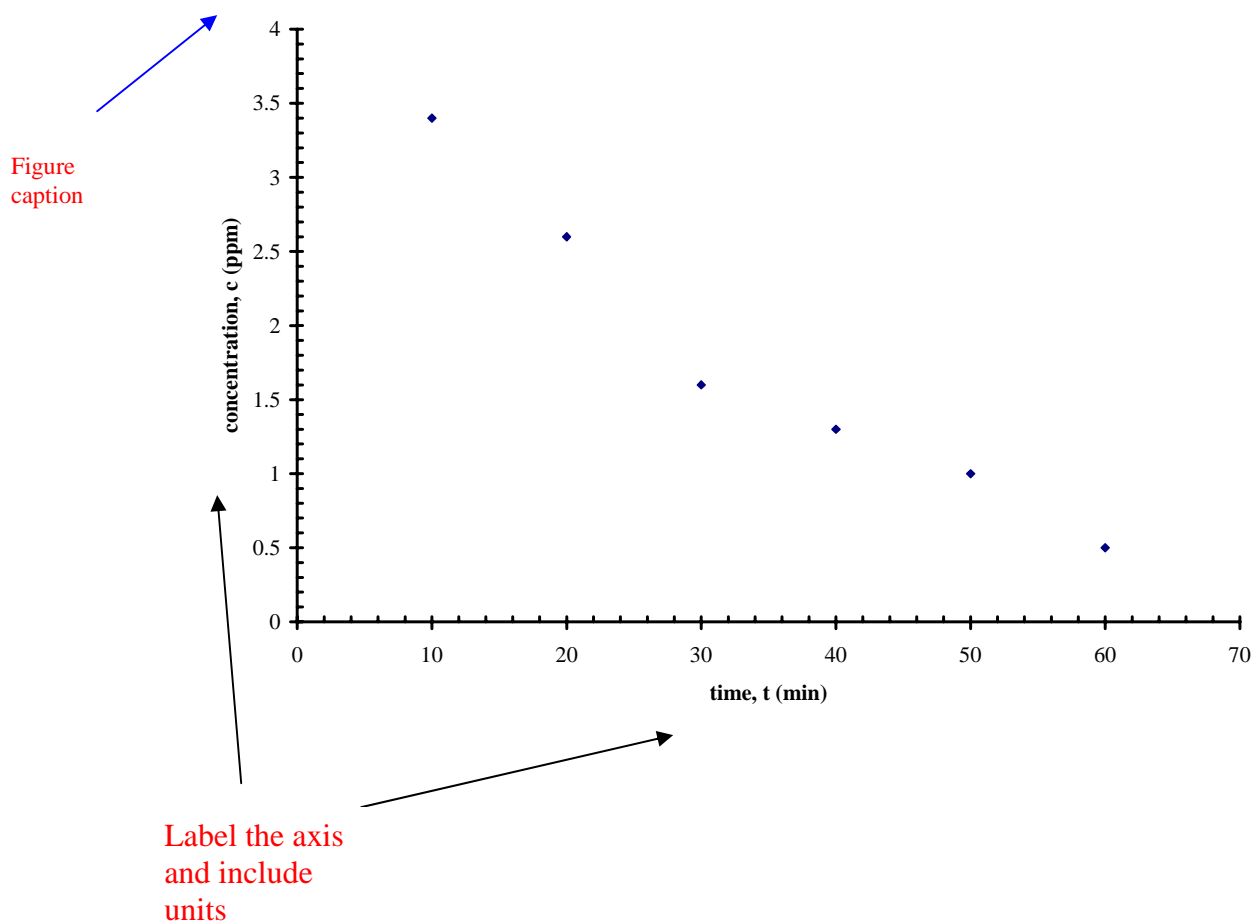
When making plots it is very important to:

1. Label the axis, including the units
2. Provide a caption of the graph. A caption of the graph gives the reader a short interpretation of the important information from the graph.
3. Use different line types or symbols to distinguish multiple sets of data on the same graph. Use a legend.

Exercise: Here is some data for concentration c , versus time for the photo-degradation of aqueous bromine. Build a graph with the information

t, min	10	20	30	40	50	60
C (ppm)	3.4	2.6	1.6	1.3	1.0	0.5

Figure 1. Variation of the concentration of aqueous bromine as a function of time. The data indicates that there is a strong decrease in the concentration of bromine at short times (less than 30 minutes)

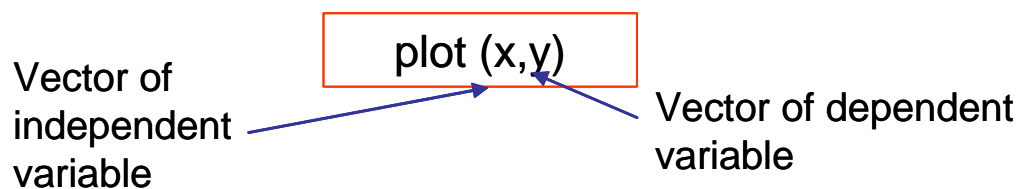


Notice that the graph is assigned a figure number. This is a recommended practice to refer the reader to the graph during the narrative of a document (e.g., report). It is a common practice in science and engineering to plot discrete data as symbols (that is the reason why the points are not joined in the figure). On the other hand equations are plotted as lines.

It is also important that you review the rules from producing quality plots and tables (see your handout H-4 ChE-101 binder, web: <http://webche.ent.ohiou.edu/WEB-che101/H-4.pdf>)

4. Making plots with Matlab.

The *plot* command is used to create two dimensional plots. The simplest form of the command is



See Tutorial Vb (Making Plots with Matlab, see your ChE-101 binder, web: <http://webche.ent.ohiou.edu/WEB-che101/T5b-Making%20PLOTS.pdf>)

Reproduce the exercise 3 of this tutorial using Matlab.

5. Function m files

Reproduce the exercises given in Tutorial IV of ChE-101 (Function Files, web: <http://webche.ent.ohiou.edu/WEB-che101/T4-Function%20Files.pdf>)