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MATLAB Applications in Chemical Engineering

Table of Contents

Section I: How MATLAB Works

» Basic MATLAB: The Language
» Mfiles (Function files)
» Dealing with Functions
- The ‘plot’ function
- The ‘fzero’ function
- Solving linear equations in MATLAB
- The ‘fsolve’ function

Section II: Numerical and Symbolic Integration

» Numerical Integration; Quadrature
- The Simpson’s Rule and Lobotto Quadrature

» Symbolic Integration and Differentiation

Section III: Numerically Solving Differential Equations and Systems of Differential Equations

» First order ode’s

» Higher order ode’s

Appendix

» Glossary of Commands, Parts I, II and II

» Line Markers

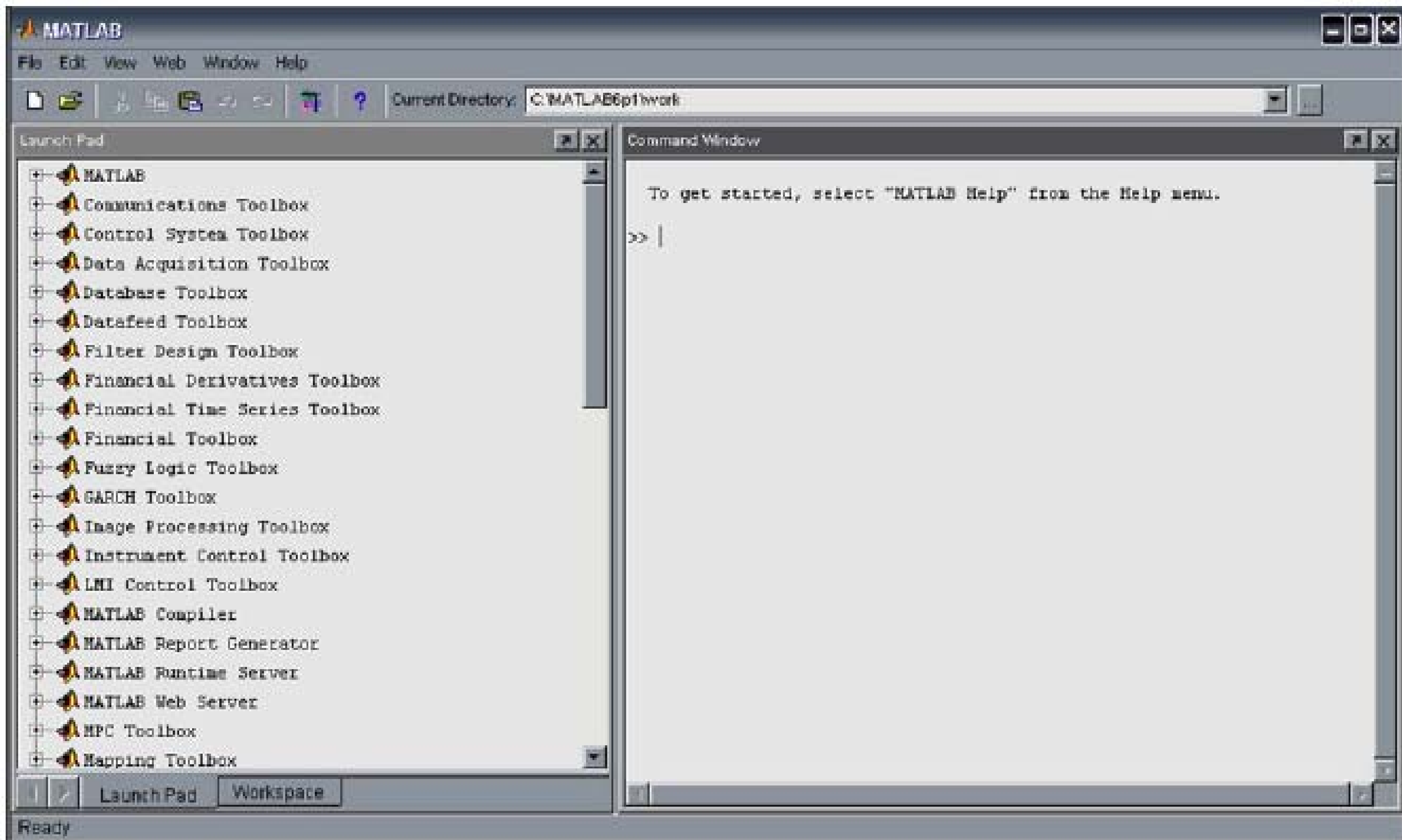
Section I: How MATLAB works

Most MATLAB commands can be run from the command window (shown below, on the right hand side of the interface).

MATLAB commands can also be entered into a text file labeled with the '.m' extension. These files are known as 'm-files'.

These commands can be broken down into scripts and programming. Scripts can be thought of as commands that instruct MATLAB to execute a particular function or pre-made program, and programming can be thought of as the raw code required to construct functions and programs within MATLAB.

Generally, all programming must be contained within a file used by MATLAB (called an m-file), but script can be entered either in an m-file or directly into the command window. An image of the MATLAB interface is shown below.



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MATLAB contains many ready-made programs or functions that are conveniently arranged into different toolboxes. When using MATLAB, these toolboxes and their functions can be called upon and executed in any MATLAB script. In the above image, the toolbox selection or launch pad is shown (at the left hand side of the interface).

Basic MATLAB: The language

MATLAB uses a language that is somewhat similar to that of Maple1. The scripts or calling functions have a particular name and argument that must be entered into the function execution call. For example, to plot the sine function in MATLAB between 0 and 6 using the ***fplot*** *command, the following code can be entered directly into the* command window, or into an m-file:

```
fplot('sin(x)',[0,6])
```

(One can define the function sin(x) in an m-file and replace the *fplot command to be fplot('filename',[0,6]))*

Before going much further, an understanding of the structure of a MATLAB simulation or execution must be developed.

M-files

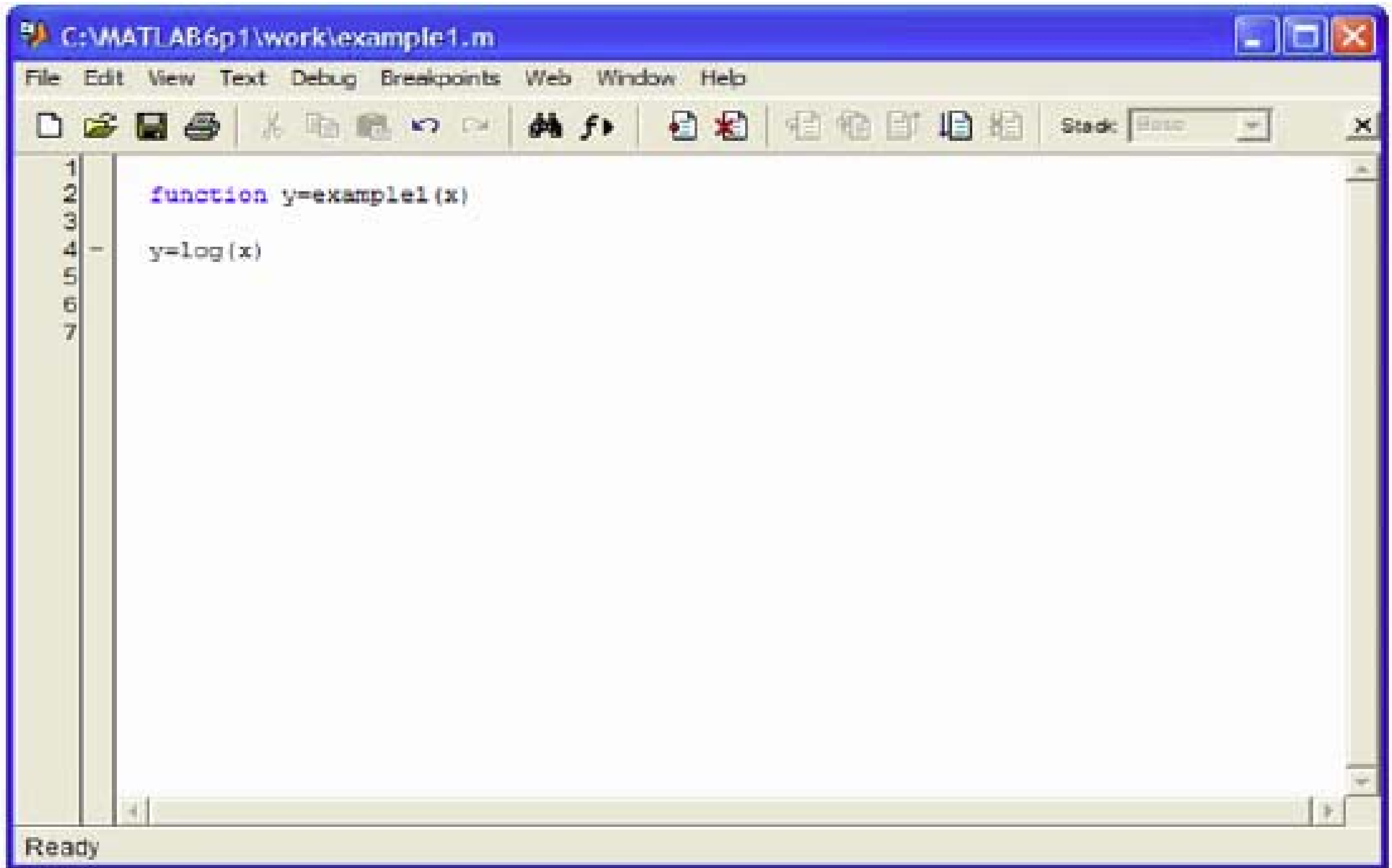
M-files contain programming, scripts, equations or data that are called upon during an execution.

If the m-file is a function definition, then the most important part of this type of m-file is the first line.

The first line **must contain the function definition** so that MATLAB can find those m-files that are called upon. These types of m-files are called **function m-files or function files**. The code used to define the function file is as follows:

```
function z=file_name(x,y)
```

'file_name' is simply the name of the m-file (the filename *must be the same in the* definition and the file-name), z is the dependant variable, and x and y are the independent variables. (Of course, one can have less or more independent variables depending upon the complexity of the problem and the equations involved.) The next few lines of script in the m-file can define the function or functions and label any required variables. The following is an example of an m-file used to plot the *natural logarithm function.*



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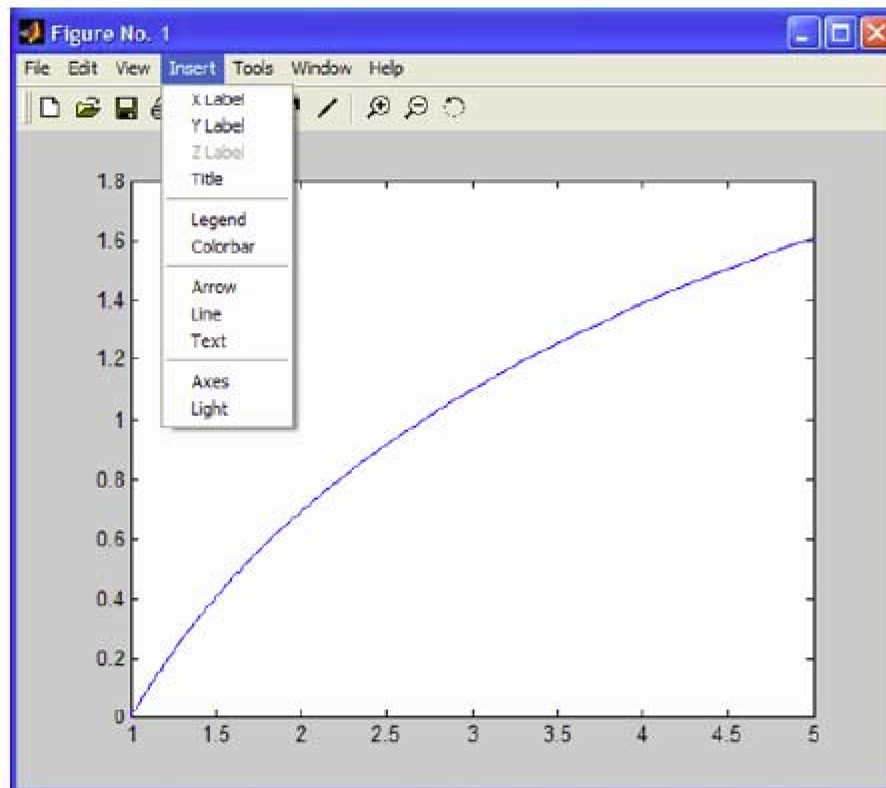
To produce a plot of this function, the following code is entered into the command window:

```
fplot('example1',[1,5])
```

This yields a plot of ln(x) between x= 1 and x= 5.



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Using the ‘insert’ menu one can add a title, x and y axis titles, and if necessary a legend.

One can also use commands nested within the *fplot command to title the chart, add axis* titles, or decide upon curve characteristics such as line color or marker.

Dealing with functions

Standard functions such as the sine, cosine, logarithmic, exponential, and userdefined functions within MATLAB will now be covered. *fplot has already been* introduced; now *plot, fzero and fsolve will be introduced The ‘plot’ function*

The plot function produces a 2-D plot of a y-vector versus either its real index or a specified x-vector. The plot function can be used for data, standard functions, or userdefined functions. Let’s look at a simple example of using *plot to model data.*

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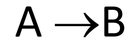
Example

The following reaction data has been obtained from a simple decay reaction:



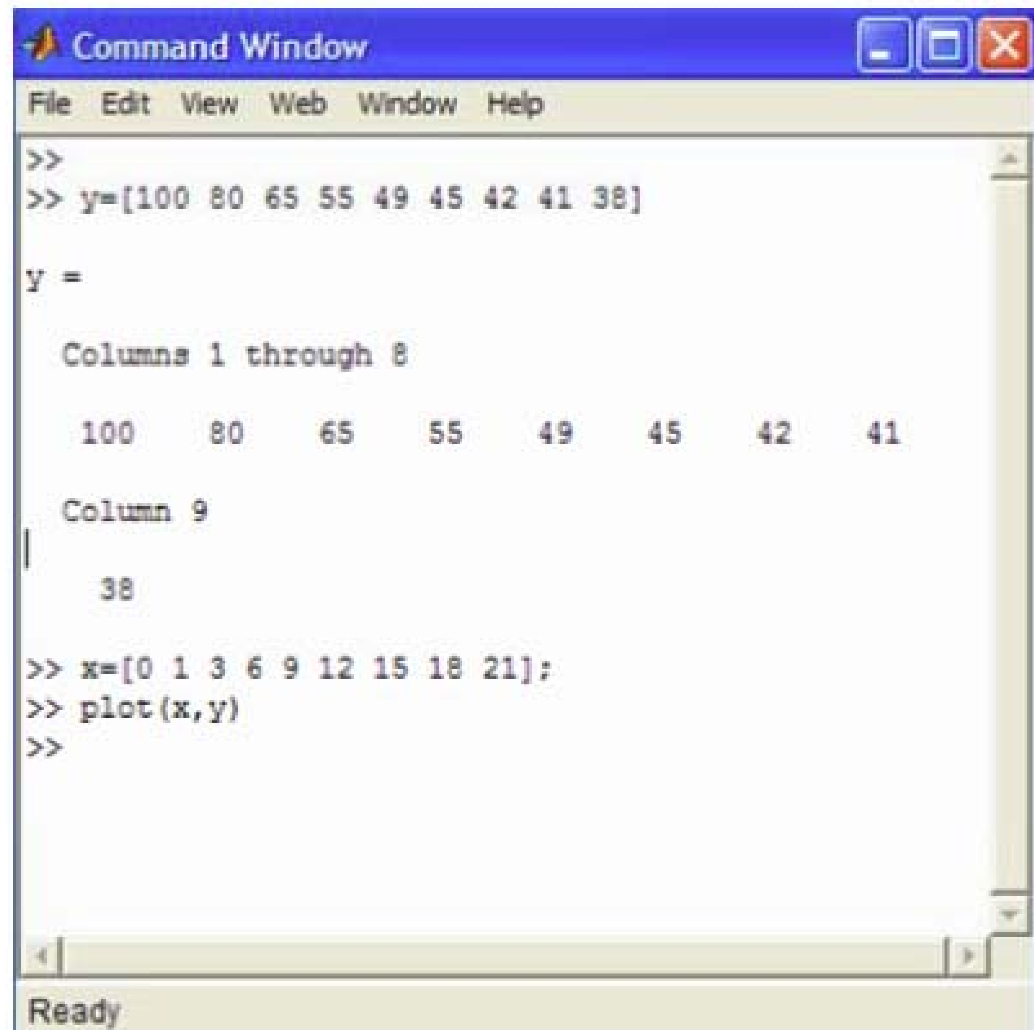
$$A \rightarrow B$$

Use MATLAB to plot the concentration of component A in mol/L against the reaction time, t, in minutes. Title the plot, label the axes, and obtain elementary statistics for the data.

Time (Minutes)	Concentration (Moles/Liter)
0	100
1	80
3	65
6	55
9	49
12	45
15	42
18	41
21	38

Solution

First, the data must be entered into MATLAB as two vectors. The vectors x and y are defined in the command window, followed by the command to plot the data. The following graph is displayed:



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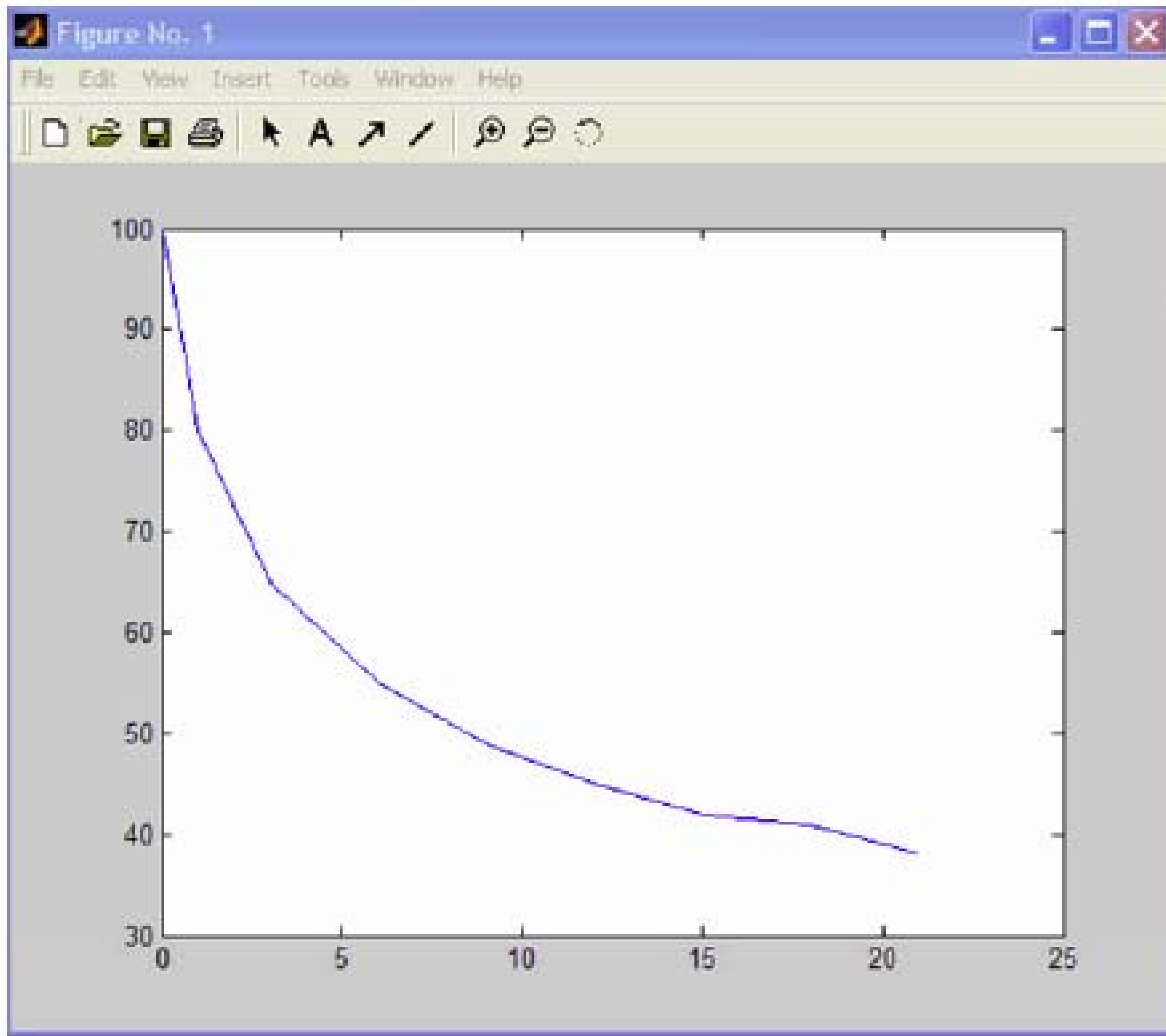


Figure No. 1
File Edit View Insert Tools Window Help
100
90
80
70
60
50
40
30
0
5
10
15
20
25

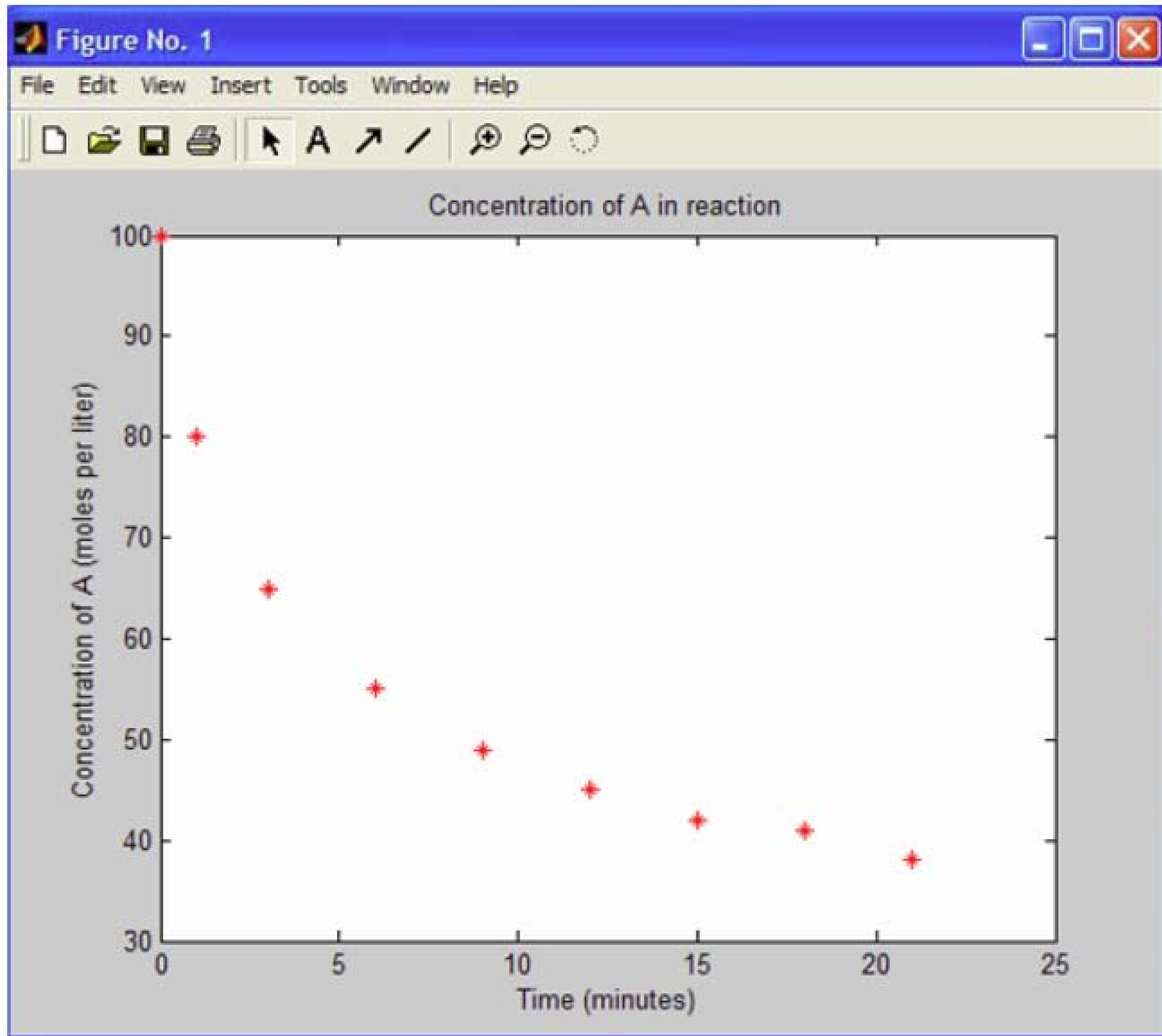
The ‘x’ row matrix (or vector*) has its display output suppressed using the ‘;’ at the end of the line.

Syntax can be used to specify the title and labels, but an easier GUI (Graphical User Interface) based approach is to simply edit the figure.

- Select the ‘Edit Plot’ command found in the ‘Tools’ menu, or click the north-west facing arrow icon on the figure.

- Double click on the white-space in the graph. This enables the property editor. Now the title and axes can be inserted under the ‘labels’ command.

- Now click directly on the line, and the line property editor will come up. Now the lines color, pattern, or the markers can be edited. The final curve is presented below:



Solution curve to example 1.1

NOTE: These figures can be exported in .bmp or .jpg format so they can be made part of a document. Find these under the 'File→Export' menu.

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To display simple statistics of the data, follow the path, ‘Tools → Data Statistics’ and the minimum, maximum, mean, median, standard deviation, and range of x and y will be displayed. Within this box, each statistic can be added to the curve as a data point/line.

To plot functions using *plot, an m-file can be created defining the function, or the* definition can be specified in the command window. This is done in a similar fashion as seen in '*fplot'. The following code entered into the command window yields a plot of the* exponential function between 0 and 10, at intervals of 1.

```
>> x = [0:10]

x =

  Columns 1 through 8

     0     1     2     3     4     5     6     7

  Columns 9 through 11

     8     9    10

>> y = exp(x);
>> plot(x,y)
>>
```

There are many other 2-D plotting functions in Matlab, but ***fplot, plot and ezplot*** *are the* most useful. ‘ezplot’ is another way to quickly plot functions between specified or nonspecified ($-2\pi<x<2\pi$) intervals. The syntax key for *ezplot is shown below.*

```
ezplot(f)
ezplot(f,[min,max])
ezplot(f,[xmin,xmax,ymin,ymax])
ezplot(x,y)
ezplot(x,y,[tmin,tmax])
```

This can be used to plot f(x) or f(x(t),y(t)).

The **fzero** function is a convenient function used to find **local zeros** of a one variable function. The general syntax that can be used for fzero (entered into the command window) is

x=fzero(‘function’,initial guess)

Matlab will then return the solution or a NaN result. An **NaN** result is ‘not a number’ and represents a **‘no solution’** for the function. Below are a few examples relating to fzero.

Example

Find the zero of the function $y(x) = x^2-1$ using an m-file and fzero.

Solution

Create the m-file, ‘myfunction.m’

```
function y = myfunction(x)
y = x^2-1
```

In the command window, use fzero to find the zero of the function ‘myfunction’

```
x = fzero(‘myfunction’,3)
```

Matlab returns a few iterations and then produces the result ‘x = 1’

Example

Find the zero of the function y(x) = sin(x) closest to x=3 using the fzero command directly in the command window. Do not use an m-file for this example.

Solution

Enter into the command window ***x = fzero('sin(x)',3)*** Matlab returns a value of 3.1416. This is the zero of sin(x) closest to our initial guess of 3.

Solving linear equations in Matlab

Matlab has the ability to easily solve linear equations directly on the command window. The following example will demonstrate how to do this in Matlab.

Example

Solve the system of linear equations given below using Matlab.

$$
\begin{aligned}
3.5u + 2v \qquad\qquad &= 5 \\
-1.5u + 2.8v + 1.9w &= -1 \\
-2.5v + 3w &= 2
\end{aligned}
$$

Solution

Enter the following code directly into the clear Matlab command window. (If the window is not clear, enter the command ‘clear’ to clear the memory of any variables).

The matrix ‘a’ contains the coefficients of u, v and w respectively. Each row in the matrix (there are three) corresponds to the coefficients of u, v and w in that order. Matrix ‘b’ contains the solution to each row or equation, 5, -1 and 2. The matrix ‘x’ that is divided out can be thought of as containing the values for u, v and w.

```
>> a = [3.5 2 0; -1.5 2.8 1.9; 0 -2.5 3];
>>
>> b = [5 -1 2]

b =

     5    -1     2

>> a\b'

ans =

    1.4421
   -0.0236
    0.6470
```

The command **a\b′** performs reverse matrix division. The **′** command transposes matrix b, this is required to perform matrix division. It is a property of matrices.

Essentially, the matrix is in the form **Ax=B,** the command a\b′ can be thought of as 'dividing out' the values of x. (Alternatively, the command 'b/a″ will also yield the correct solution set.)

The 'fsolve' function

The 'fsolve' function will probably be the most useful function for simple chemical engineering problems. It is essentially a numeric solver, capable of solving systems of non-linear *continuous equations.*

For the system of n continuous equations (f1--fn) with n unknown variables (x_1--x_n) given by

$$f(1) \equiv f_1(x_1, x_2, x_3, \ldots, x_n) = 0$$

$$f(2) \equiv f_2(x_1, x_2, x_3, \ldots, x_n) = 0$$

$$f(3) \equiv f_3(x_1, x_2, x_3, \ldots, x_n) = 0$$

$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$

$$f(n) \equiv f_n(x_1, x_2, x_3, \ldots, x_n) = 0$$

Matlab’s solver can be used to determine the unknown variables, x_1 through x_n.

The following example will illustrate the use of the ***fsolve** function.*

Example

Solve the system of equations below using ***fsolve.***

$$2a - b - e^{-a} = 0$$

$$2b - a - e^{-b} = 0$$

Solution

The most efficient way to solve these types of systems is to create a function **mfile** that contains the equations.

```
function f=example15(x)

f = [2*x(1)-x(2)-exp(-x(1)); -x(1)+2*x(2)-exp(-x(2))];
```

The equations are separated within the matrix **'f'** using the *semi-colon* operator. Now the **'fsolve'** command must be used to solve the system.

```
>>
>> x0 = [-5 -5]; %Initial guess, arbitrary
>>
>> fsolve('example15',x0,optimset('fsolve'))  %Command calls m-file to solve
Optimization terminated successfully:
 Relative function value changing by less than OPTIONS.TolFun

ans =

    0.5671    0.5671
```

The solutions to the system are ***a*** = *0.5671 and* ***b*** = *0.5671. Using the* ***'fsolve'*** *command,* much more complicated systems can be easily solved in Matlab.

NOTE: 'optimset' is used to change the default solver in Matlab to the optimization toolbox solver.

Section II: Numerical and Symbolic integration

Numerical Integration-Quadrature

MATLAB can perform in-depth numerical integrations or quadrature effortlessly and accurately. The first part of this section will look at some of the simple methods of numerical integration within MATLAB.

The Simpson's Rule and Lobotto Quadrature

In MATLAB, the functions **'quad'** or in more recent versions, **'quadl'** perform numerical integration based on the Simpson's rule and the adaptive Lobatto quadrature respectively. The syntax for the Simpson's based approximation and the Lobotto quadrature are the same. The difference is in each function's name. The syntax below is for the Lobotto quadrature (quadl), and it is the same for the Simpson's quadrature (quad).

```
q = quadl(fun,a,b)
q = quadl(fun,a,b,tol)
q = quadl(fun,a,b,tol,trace)
q = quadl(fun,a,b,tol,trace,p1,p2,...)
[q,fcnt] = quadl(fun,a,b,...)
```

The functions can be defined in function m-files or as inline functions (those functions entered directly into the command).

MATLAB also has a function called **‘trapz’** which enables numerical integration using the trapezoid rule. More information about ‘trapz’ can be found in the MATLAB help files.

Symbolic Integration and differentiation

Matlab has the ability to perform symbolic integration and differentiation thanks to the Maple® engine located in the symbolic toolbox.

Matlab can solve differential equations symbolically, providing general or unique solutions.

First, let’s look at symbolic integration and differentiation.

Using the **‘diff’** command, symbolic differentiation of a function can be achieved, and analogously, using the **‘int’** command symbolic integration of a function can be achieved.

Example

Integrate ax^2+bx, with respect to x, (where a and b are constant) and then differentiate the solution obtained with respect to x to regain the initial function.

Solution

To begin with, the symbolic variables within the expression must be defined within MATLAB as symbolic variables. This is done using the **syms** command. In the expression, a, b, and x are the symbolic variables that must be defined. The following code is used directly at the command prompt to obtain the solution:

```
>> syms a b x
>> diff(a*x^2+b*x)

ans =

2*a*x+b

>> int(2*a*x+b)

ans =

a*x^2+b*x
```

The **syms** command is used to define a, b and x as variables for symbolic purposes. The expression is differentiated to obtain the solution 2ax+b, which upon integration with respect to x yields ax^2+bx as expected.

MATLAB can solve **ordinary differential equations symbolically** with or without boundary conditions or initial value parameters. The **'dsolve'** command is used for thispurp ose. Within **dsolve**, the letter **'D*ij*'** *is used to indicate a derivative, where i is the* order of differentiation, and j is the dependent variable. 'D' implicitly specifies first order derivative, 'D2' signifies a second order derivative and so on. The letter **t** is the default independent variable for dsolve. So D2y is analogous to

$$\frac{d^2 y}{dt^2}$$

The following example illustrates the use of **dsolve**.

Example 2.2

Solve the ode $\frac{d^2y}{dx} = 6y - \frac{dy}{dx}$, where y(x) using dsolve

Solution

```
>> dsolve('D2y=6*y-Dy','x')

ans =

C1*exp(-3*x)+C2*exp(2*x)
```

Where C1 and C2 are constants of integration.

The next example shows how to solve an initial value problem for a second order ode.

Example 2.3

Solve the ode $\frac{d^2m}{dx^2} + m = 0$, m(0)=2 and $\frac{dm}{dx}(0) = 3$, where m(x).

Solution

```
>> dsolve('D2m+m=0','m(0)=2','Dm(0)=3','x')

ans =

3*sin(x)+2*cos(x)
```

Within dsolve, m(0)=2 and Dm(0)=3 define the initial conditions of the ode.

In the assignment of the initial conditions, labeled variables could have been inserted rather than numeric values. For example, if the initial conditions for example 2.3 were m(0)=a and $\frac{dm}{dx}(0) = b$, then the command chain `dsolve('D2m+m=0','m(0)=a','Dm(0)=b','x')` could have been used to yield the solution `b*sin(x)+a*cos(x)`.

Section III: Numerically Solving Differential Equations and Systems of Differential Equations

First order ode's

One of the best engineering uses of MATLAB is its application to the numeric solution of ordinary differential equations (ode's). MATLAB has multiple different ode solvers that allow ode's to be solved accurately and efficiently depending on the stiffness of the ode. Stiffness is the relative change in the solution of a differential equation. A stiff differential equation is one that the solution changes greatly when close to the point of integration, but need not change significantly over the duration of the integration. For this type of solution, a numerical method that takes small integration intervals rather than large intervals would be required.

Stiffness and solver selection are mainly a matter of efficiency. In solving ode's, selecting a solver that takes the largest step, yet still maintains an accurate solution is the key to increased efficiency.

There are different ways to set up and execute the ode solvers, but for this guide, a system that uses multiple m-files per each ode solution will be employed. The main two m-files that are needed are a run file and a function file. For the solution of ode's in MATLAB *all ode's must be defined in a function m-file.*

When entered into the function file, the ode's must have the first order form

$$\frac{dy}{dx} = f(y,x)$$

The function file must contain

i) The function definition e.g. , `function dmdt=file_name(t,m)` where **t** is the independent variable and m is the dependent variable of first order

ii) If global variables are used, the global command must be inserted after the function definition

iii) The ode or ode's in the form described above e.g. `dmdt=f(m,t)`

The filename, variables (m and t) and dmdt are arbitrary. ‘dmdt’ is also arbitrary and can equivalently be called ‘A’ or any other non-reserved name. One stipulation that exists is that the definition within the ***‘function dmdt=file_name(t,m)’*** MUST be the same as that defined when the ode’s are listed.

For example, the following function m-file is incorrect

```
function dmdt=myfile(t,m)
A=4*m
```

But, the following function file is correct:

```
function dmdt=myfile(t,m)
dmdt=4*m
```

(It may appear that from this MATLAB is unable to solve any more than a first order ode, but all ode's of second order or higher can be written in the form of multiple ode's, each of first order. This will be covered once an introduction using first order ode's has been accomplished).

Once a suitable function file has been created, a run-file or executable file is created that is used to solve the ode or ode's that are within the function file. The run file must contain the following items:

i) If global variables are used, the global command must be inserted at this point.

ii) Depending on how the tspan, the integration interval. is defined. the lower and upper limits can be defined here. E.g. , `tspan=[t0 tf];` where t0 and tf are predefined vectors for the integration limits. Forward or reverse integration can be used; t0 does not have to be less than tf in the case of reverse integration

iii) The initial conditions must be defined as vectors or single direction matrices
.
iv) The ode solver must then be called. The following is the syntax for the solver, and ode45 is the solver that will be used. It is a good place to start as a general solver:

```
[independent, dependent]=ode45('file_name',tspan,initial_condition_vector)
```

v) The solution can now be plotted using the ‘plot’ command and then formatted either using the GUI interface or by the commands ‘legend’,
‘xlabel’, ‘ylabel’, ‘title’ and ‘axis’. E.g.

```
plot(independent, dependent(:,n),independent,dependent(:,n+1))
```

where n denotes the 1st dependent variable, then second and so on.

The following example demonstrates the setup and execution for the solution of a set of differential equations.

Example

A fluid of constant density starts to flow into an empty and infinitely large tank at 8 L/s. A valve regulates the outlet flow to a constant 4L/s. Derive and solve the differential equation describing this process over a 100 second interval.

Solution

The accumulation is described as input – output, so the ode describing the process becomes $\frac{d(\rho V)}{dt} = (8-4)\rho$

Since density is constant, then $\frac{dv}{dt}$ *= 8 − 4 = 4 in liters per* second.

The initial condition is that at time t=0, the volume inside the tank =0.

The following function file 'ex31' is used to set up the ode solver.

```
function dvdt=ex31(t,v)

dvdt=4
```

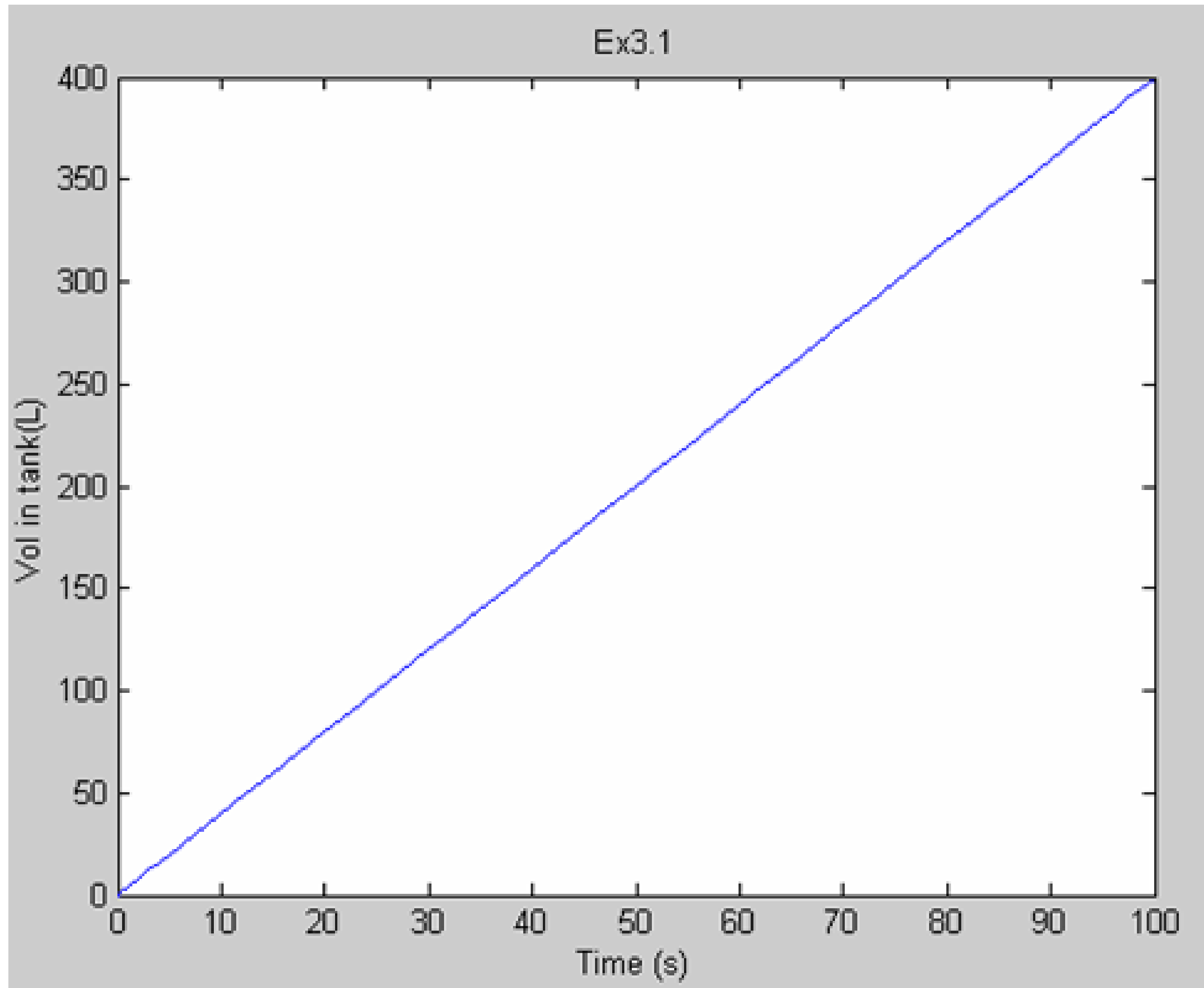
The file ex31run is used to execute the solver. The code for this file is overleaf.

```
t0=0;
tf=100;
tspan=[t0 tf]; %Integration interval
v0=0 %Initial condition

[t,v]=ode45('ex31',tspan,v0)

plot(t,v(:,1))
xlabel('Time (s)')
ylabel('Vol in tank(L)')
title('Ex3.1')
```

The plot produced is


Ex3.1
Vol in tank(L)
Time (s)
0
50
100
150
200
250
300
350
400
0
10
20
30
40
50
60
70
80
90
100

Systems of ode's can also be easily solved in MATLAB using the same setup as described for a single ode.

The next example demonstrated how to solve a system of simultaneous ode's. In this example the 'global' command is used to define certain variables as 'shared' or 'in common' between the run file and the function file.

Global variables are not necessary, but they are convenient. Using the 'global' command variables can be defined once in the run file and the global command will link them to the function file. If used, the global command *must not contain the independent or dependent* variables.

Example

The following set of differential equations describes the change in concentration three species in a tank. The reactions A →B → C occur within the tank. The constants k1, and k2 describe the reaction rate for A → B and B → C respectively.

The following ode's are obtained:

$$\frac{dCa}{dt} = -k1Ca$$

$$\frac{dCb}{dt} = k1Ca - k2Cb$$

$$\frac{dCc}{dt} = k2Cb$$

Where k1=1 hr^{-1} and k2=2 hr^{-1} and at time t=0, Ca=5mol and Cb=Cc=0mol.

Solve the system of equations and plot the change in concentration of each species over time.
Select an appropriate time interval for the integration.

Solution

The following function file and run file are created to obtain the solution:

```
function dcdt=Ex32(t,c)
%c(1)=ca, c(2)=cb, c(3)=cc
global k1 k2
dcdt=[-k1*c(1); k1*c(1)-k2*c(2); k2*c(2)];
```

Ca, Cb and Cc must be defined within the same matrix, and so by calling Ca c(1), Cb c(2) and Cc as c(3), they are listed as common to matrix c.

```
clc
clf
clear
global k1 k2
k1=1;
k2=2;

tspan=[0 5];

c0=[5 0 0];

[t,c]=ode45('Ex32',tspan,c0)

plot(t,c(:,1),'+',t,c(:,2),'*',t,c(:,3))
legend('ca','cb','cc')
xlabel('Time(hr)')
ylabel('Concentration of each species, mols/hr')
title('Example 3.2')
```

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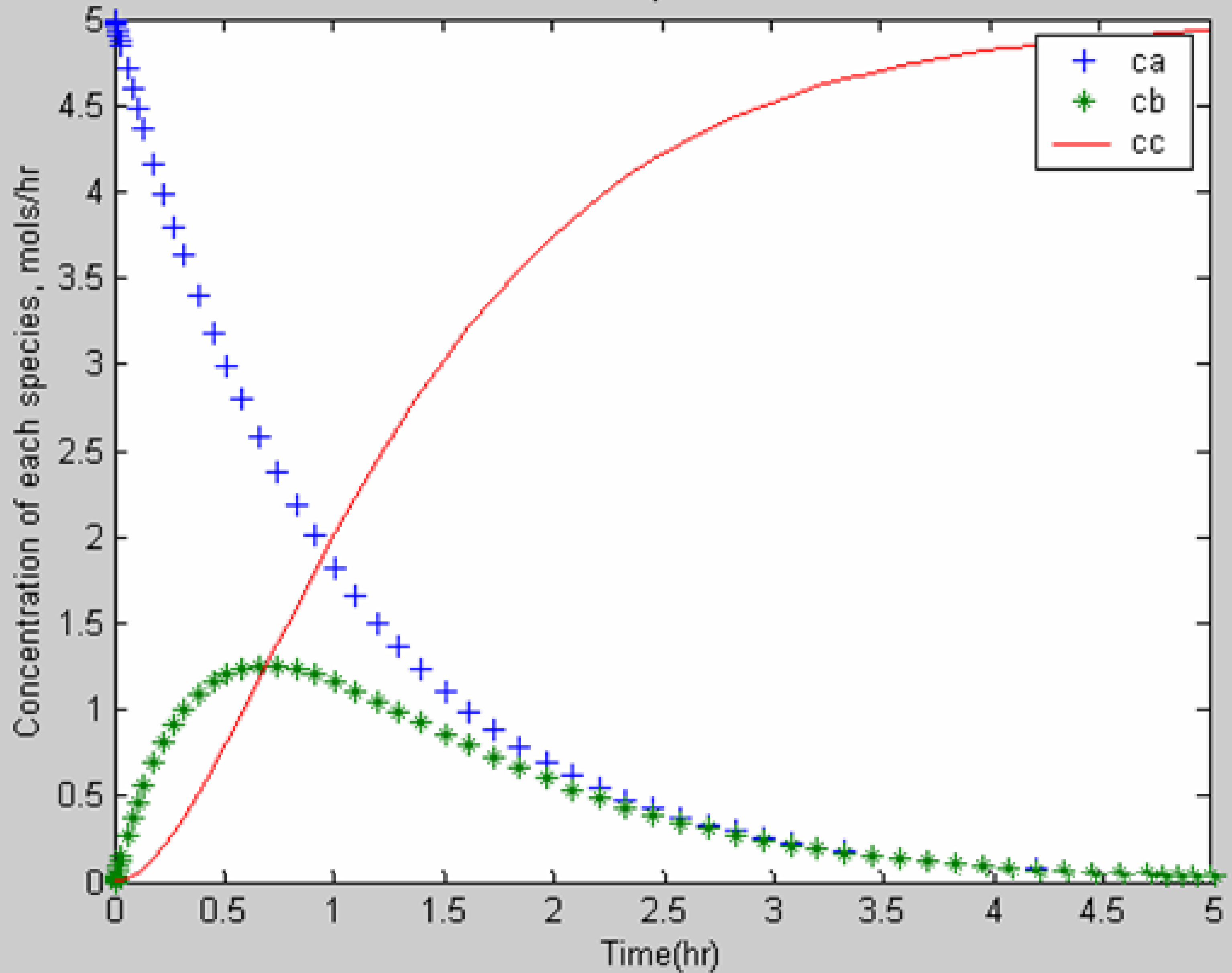
Notice that the constants k1 and k2 are defined (only once) in the run file, and using the 'global' command they are linked to the function file. The following curve is produced upon execution. In the 'plot' command, the + and * change the line markers so that they can be easily distinguished using a non-color printer. The appendix contains a list of available markers for plotting.



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Higher order ode's

To be able to solve higher order ode's in MATLAB, they must be written in terms of a system of first order ordinary differential equations. An ordinary differential equation can be written in the form

$$\frac{d^n y}{dx^n} = f(x, y, y', y'', y''', \ldots, y^{n-1})$$

and can also be written as a system of first order differential equations such that

$$y_1 = y, y_2 = y', y_3 = y'', \ldots. y_n = y^{n-1}.$$

From here, the system can then be represented as an arrangement such that

$$y_1' = y_2, y_2' = y_3, \ldots y_{n-1}' = y_n, \text{ where } y'_n = f(x, y_1, y_2, \ldots y_n).$$

Example

Solve the following differential equation by converting it to a system of first order differential equations, then using a numeric solver to solve the system. Plot the results.

$$Y'' + Y' + Y = 0 \text{ , Y(0)=1 and Y'(0)=0}$$

To convert this 2nd order ode to a system of 1st order ode's, the following assignment is made:

$$Y = y_1 = y(1) \text{ and } Y' = y_2 = y(2),$$

then the ode can be written as the first-order system:

$$Y = y(1)$$

$$\frac{dY}{dt} = Y' = y(2)$$

$$\frac{d^2Y}{dt^2} = Y'' = -(y(2) + y(1))$$

The function file containing this system can now be created and solved. The function file and run file are shown below:

```
function dmdt=Ex33(t,y)
%Solving Y" + Y' + Y = 0
%Assign Y=y(1), Y'=y(2), Y"=y(3)
dYdt=y(2);
dY2dt=-(y(2)+y(1));
dmdt=[dYdt; dY2dt];
```

The variable dmdt is a ‘dummy’ variable that is used to describe the system as a whole,

```
clc
clf
clear
tspan=[0 10];
y0=[1 0];
[t,Y]=ode45('Ex33',tspan,y0)
plot(t,Y(:,1),'+',t,Y(:,2))
legend('Y','dYdt')
xlabel('t')
ylabel('Y and dY/dt')
```