

University of Baghdad
College of Engineering
Department of Chemical Engineering

MATLAB for Chemical engineer

Basic and Applications

Lecture No. 8

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Example 1: Write a script file to calculate the volume of a cylinder given its radius and height. Test your function with $r=0.5$ m and $h=3$ m.

MATLAB session:

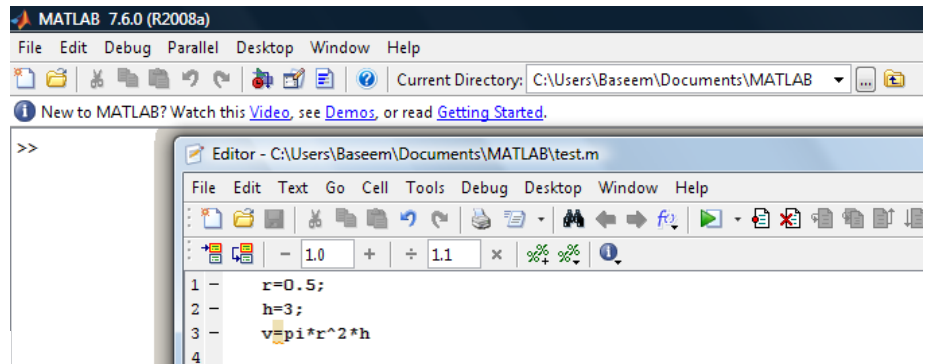
```
>> test

v =

2.3562
```



You must store your m-files in the MATLAB current directory.



Example 2: Write a function to calculate the volume of a cylinder given its radius and height. Test your function with $r=0.5$ m and $h=3$ m.

MATLAB session:

```
>> cyl_vol(0.5,3)

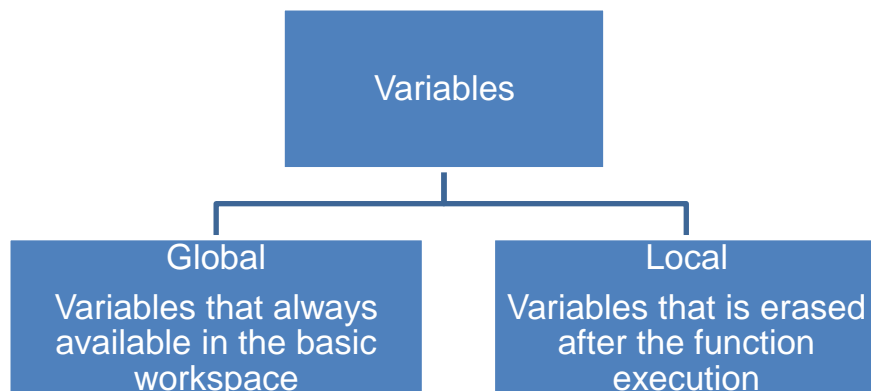
ans =

2.3562
```

```
function v=cyl_vol(r,h)
% r the cylinder radius
```

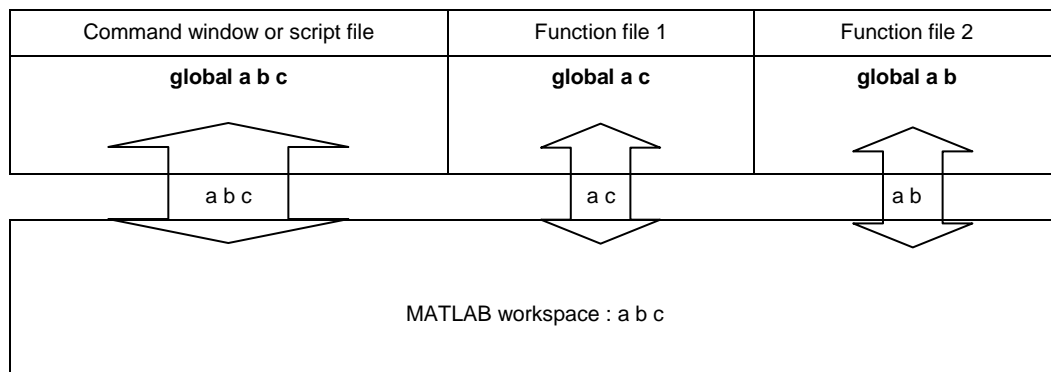
Could you modify the function so that it can accept vectors of r and h to return the result as a vector?

2. Global and local variables





Use the **global** command to share variables between the command window or script files and function files. The global command should be inserted at the beginning of each one to determine which variables are shared.



Example 3: Write a function that uses the ideal gas law to calculate the pressure of a gas at two temperatures if $n=1$, $V=20$ liter, at $T=300$ and 330 K.

MATLAB session:

```
>> global R

>> R=0.08206;

>> ideal(1,[300 330],20)

ans =

    1.2309    1.3540
```

```
function P=ideal(n,T,V)

global R
```

3. Finding the zero of a function of one unknown

MATLAB uses the function `fzero` to solve the problem of $f(x)=0$ for x starting from an initial guess. The function syntax is:

fzero ('function_name', guess)

The name of the function file which contains the equation to be solved

An initial guess for the solution

The solution steps are as follows:

1. Make the function equal to zero.
2. Define your function in a function file using the m-file editor (e.g. test.m).
3. Suggest an initial guess for the solution (e.g. 0).
4. Issue the following command in the command window or your script file: `>>fzero('test',0)`
Then MATLAB will return a value of x that makes the function equal to zero.

Example 4: Find the roots of the equation: $x + 2e^{-x} = 3$ near $x = -0.5$ and $x = 3$.

```
function f=ex4(x)
```

MATLAB session:

```
>> x=fzero('ex4',-0.5)
```

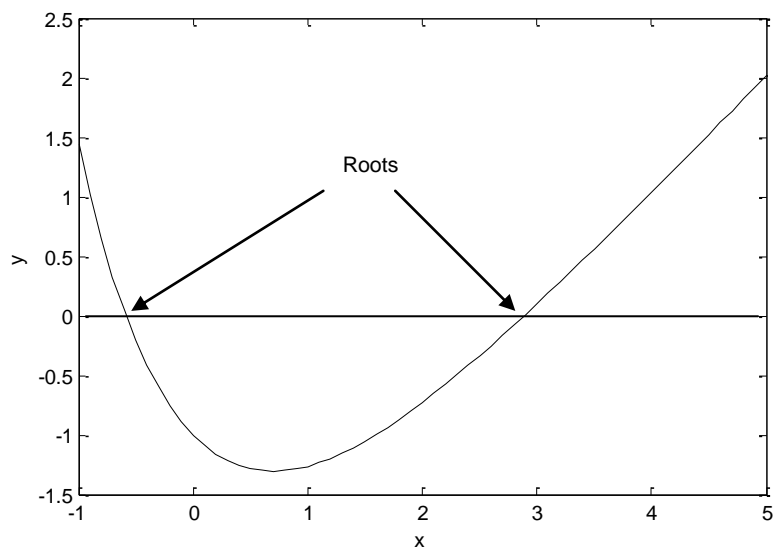
```
x =
```

```
-0.5831
```

```
>> x=fzero('ex4',3)
```

```
x =
```

```
2.8887
```



If the function have more than one solution, fzero will return the nearest solution to the guess

Example 5: Lee and Duffy (1976) relate the friction factor c_f for flow of suspension of fibrous particles to the Reynolds number Re by this empirical equation:

$$\sqrt{\frac{1}{c_f}} = \left(\frac{1}{k}\right) \ln(Re \sqrt{c_f}) + \left(14 - \frac{5.6}{k}\right)$$

Comput c_f for $Re=3750$ and $k=0.28$.

MATLAB session:

```
>> global Re k
>> Re=3750;k=0.28;
>> guess=0.0396*Re^-0.25;
>> cf=fzero('ex5',guess)

cf =

    0.0051
```

```
function f=ex5(cf)

global Re k
```



A good starting guess for the iterative solution of the equation may be found from the Blasius equation: $c_f = 0.0396 Re^{-0.25}$

4. Finding solution for a system of nonlinear equations

MATLAB uses the function `fsolve` to solve a system of nonlinear equations of several variables which takes the form $f(x)=0$ where f or x may be vectors or matrices. The function syntax is:

`fsolve('function_name',guess)`

The name of the function file which contains the equations to be solved

An initial guess for each variable in the system.

Example 7: Solve the equations: (take 0.8 and 0.2 as initial guesses for x_1 and x_2)

$$x_1^2 + 4x_2^2 = 5$$

$$2x_1^2 - 2x_1 - 3x_2 = 2.5$$

MATLAB session:

```
>> x=fsolve('ex7',[0.8 0.2])

Equation solved.
```

```
function f = ex7(x)
```

```
f(1)=x(1)^2+4*x(2)^2-5;
```

fsolve completed because the vector of function values is near zero
as measured by the default value of the function tolerance, and
the problem appears regular as measured by the gradient.

<stopping criteria details>

x =

2.0000 0.5000

Example 8: For turbulent flow of fluids in an interconnected network, the flow rate v from one node to another is about proportional to the square root of the difference in pressures at the nodes. For the conduits shown, find the pressure at each node. The values of b represent conductance factors in the relation $v_{ij} = b_{ij}\sqrt{(p_i - p_j)}$.

Solution: setting up the equations for the pressures at each node gives:

Node 1:

$$0.3\sqrt{500 - p_1} = 0.2\sqrt{p_1 - p_2} + 0.1\sqrt{p_1 - p_3}$$

Node 2:

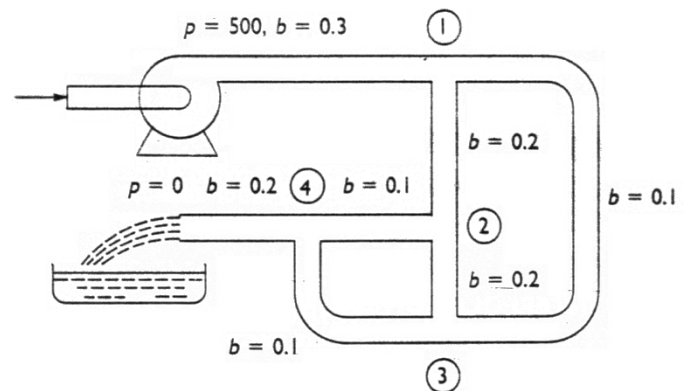
$$0.2\sqrt{p_1 - p_2} = 0.1\sqrt{p_2 - p_4} + 0.2\sqrt{p_2 - p_3}$$

Node 3:

$$0.1\sqrt{p_1 - p_3} + 0.2\sqrt{p_2 - p_3} = 0.1\sqrt{p_3 - p_4}$$

Node 4:

$$0.1\sqrt{p_2 - p_4} + 0.1\sqrt{p_3 - p_4} = 0.2\sqrt{p_4 - 0}$$



MATLAB session:

```
>> p=abs(fsolve('ex8',[400 200 200 0]))
```

Equation solved.

fsolve completed because the vector of function values is near zero

as measured by the default value of the function tolerance, and

the problem appears regular as measured by the gradient.

<stopping criteria details>

p =

423.1898 347.7937 343.5118 172.8230

```
function f = ex8(p)
f(1)=0.3*sqrt(500-p(1))-0.2*sqrt(p(1)-p(2))-0.1*sqrt(p(1)-p(3));
f(2)=0.2*sqrt(p(1)-p(2))-0.1*sqrt(p(2)-p(4))-0.2*sqrt(p(2)-p(3)).
```

PROBLEMS

1. Find a root of $f(x) = \sin x - x/2$, near $x = 2.0$. (ans 1.8955)
2. DeSantis (1976) has derived a relationship for the compressibility factor of real gases of the form:

$$z = \frac{1 + y + y^2 - y^3}{(1 - y)^3}$$

where $y = b/(4v)$, b being the van der Waals correction and v is the molar volume. If $z = 0.892$, what is the value of y ? What answer is the reliable one if you take 0 and 1.5 as initial guesses.

3. In studies of solar-energy collection by focusing a field of plane mirrors on a central collector, Vant-Hull (1976) derives an equation for the geometrical concentration factor C :

$$C = \frac{\pi(h/\cos A)^2 F}{0.5\pi D^2(1 + \sin A - 0.5 \cos A)}$$

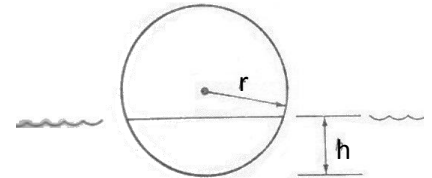
where A is the rim angle of the field, F is the fractional coverage of the field with mirrors, D is the diameter of the collector, and h is the height of the collector. Find A if $h=300$, $C=1200$, $F=0.8$, and $D=14$.

4. Based on the work of Frank-Kamenetski in 1955, temperatures in the interior of a material with embedded heat sources can be determined if we solve this equation:

$$e^{-(1/2)t} \cosh^{-1}(e^{(1/2)t}) = \sqrt{\frac{1}{2} L_{er}}$$

Given that $L_{er} = 0.088$, find t .

5. Using the formula for the volume of a segment of a sphere, it can be shown that the depth h to which a floating sphere of radius r sinks in water is a root of the equation: $h^3 - 3rh^2 + 4r^3d = 0$. Where d is the specific gravity of the sphere. Suppose a wooden sphere of radius 0.5 m has specific gravity of 0.75. Calculate the depth (h) to which the sphere will sink.



6. Consider Q gpm of water flowing from point 1 to point 2 in an inclined pipe of length L ft and diameter D in. The equation below can be hold approximately for turbulent flow in pipes of average roughness:

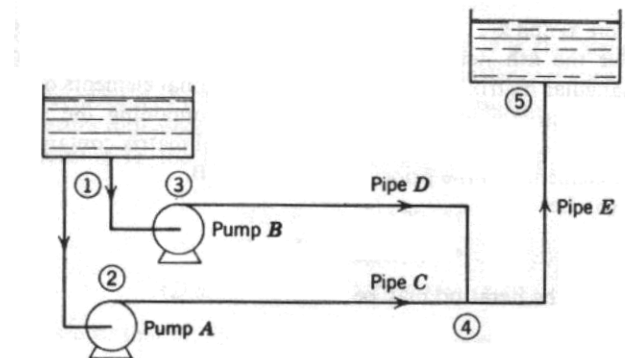
$$(z_2 - z_1) + 2.3(p_2 - p_1) + 8.69 \times 10^{-4} Q^2 L / D^5 = 0$$

Here, p is the pressure in psig and z is the elevation in feet. Also, a typical head-discharge curve for a centrifugal pump can be represented by:

$$\Delta p = \alpha - \beta Q^2$$

In which Δp is the pressure increase in psig across the pump, Q is the flow rate in gpm, and α and β are constants depending on the particular pump.

For the piping system shown, the pressures p_1 and p_5 are both essentially atmospheric (0 psig); there is an increase in elevation between points 4 and 5, but pipes C and D are horizontal. Write a program that will accept values of $\alpha_A, \beta_A, \alpha_B, \beta_B, (z_5 - z_4), D_C, L_C, D_D, L_D, D_E,$ and L_E , and that will solve the resulting equations for the unknowns $Q_C, Q_D, Q_E, p_2, p_3,$ and p_4 . One suggested set of test data is $(z_5 - z_4) = 70$ ft, with the given data.



Pump	α , psi	β , psi/(gpm) ²
A	156.6	0.00752
B	117.1	0.00427

Pipe	D , in.	L , ft
C	1.278	125
D	2.067	125
E	2.469	145

Assume that the above pipe lengths have already included the equivalent lengths of all fittings and valves.

7. When a pure sample gas is bombarded by low energy electrons in a mass spectrometer, the galvanometer shows peak heights that correspond to individual mass-to-charge ratios for the resulting mixture of ions. For the i th peak produced by a pure sample j , one can then assign a sensitivity s_{ij} (peak height per micron of Hg sample pressure). These coefficients are unique for each type of gas. A distribution of peak heights may also be obtained for n -components gas mixture that is to be analyzed for the partial pressures $p_1, p_2, p_3, \dots, p_n$ on each of its constituents. The height of h_i of certain peak is a linear combination of the products of the individual sensitivities and partial pressures:

$$\sum_{j=1}^n s_{ij} p_j = h_i$$

Write a program that will accept values for the number of components, the sensitivities, and peak heights. The program then should calculate the values for individual partial pressures from the following data. Take $h_1=17.1$, $h_2=65.1$, $h_3=186$, $h_4=82.7$, $h_5=84.2$, $h_6=63.7$, $h_7=119.7$. Check your answer with a total mixture pressure of 39.9 microns of Hg.

Peak Index i	Component Index, j						
	1 Hydrogen	2 Methane	3 Ethylene	4 Ethane	5 Propylene	6 Propane	7 n -Pentane
1	16.87	0.1650	0.2019	0.3170	0.2340	0.1820	0.1100
2	0.0	27.70	0.8620	0.0620	0.0730	0.1310	0.1200
3	0.0	0.0	22.35	13.05	4.420	6.001	3.043
4	0.0	0.0	0.0	11.28	0.0	1.110	0.3710
5	0.0	0.0	0.0	0.0	9.850	1.684	2.108
6	0.0	0.0	0.0	0.0	0.2990	15.98	2.107
7	0.0	0.0	0.0	0.0	0.0	0.0	4.670