BITS Pilani

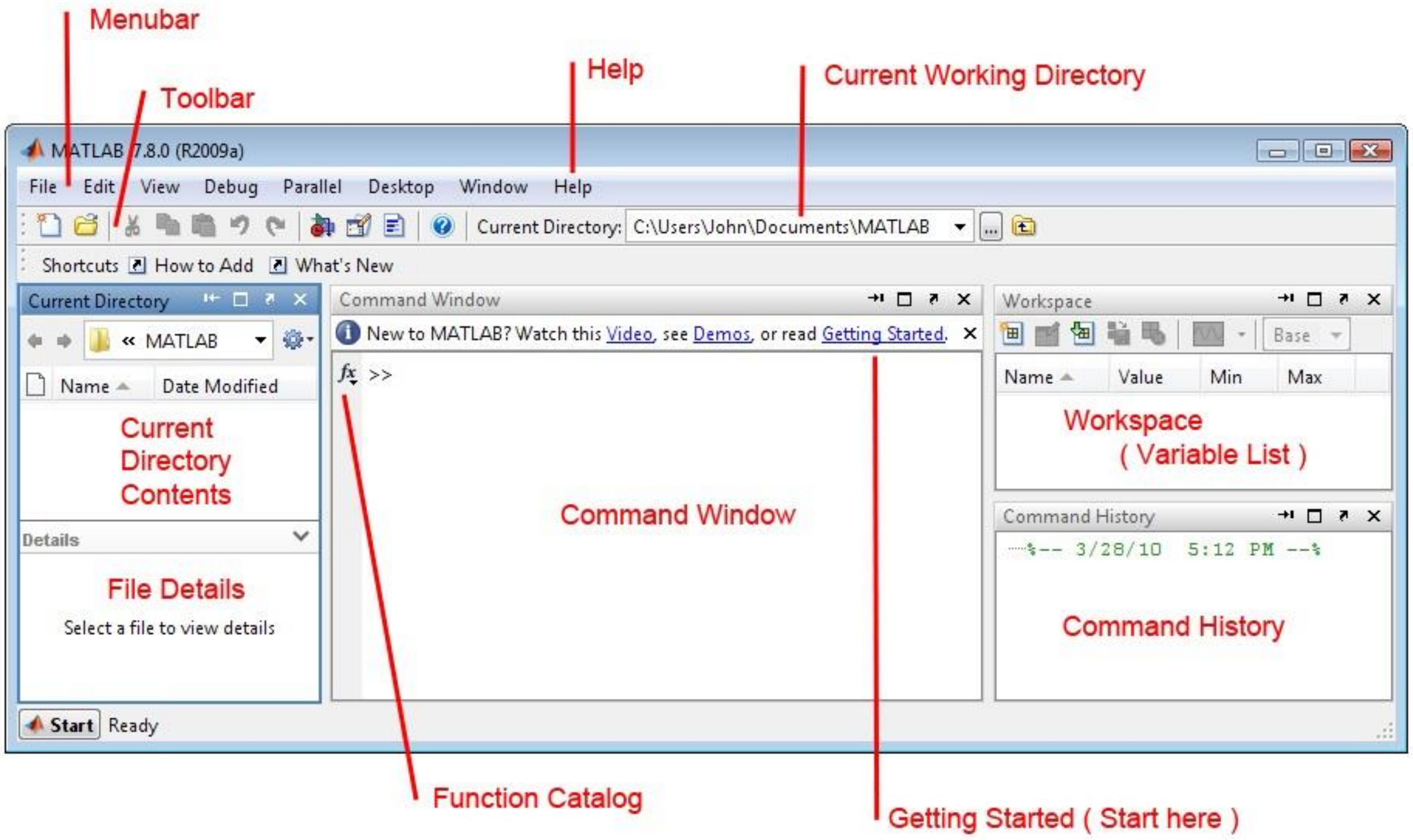
Pilani Campus

Modeling & Simulation in Chemical Engineering

(CHE-F418)

“Introduction to MATLAB-Computing”

Interface of MATLAB



➢ **File name: *.m**
*name of file

Fundamentals of Programming

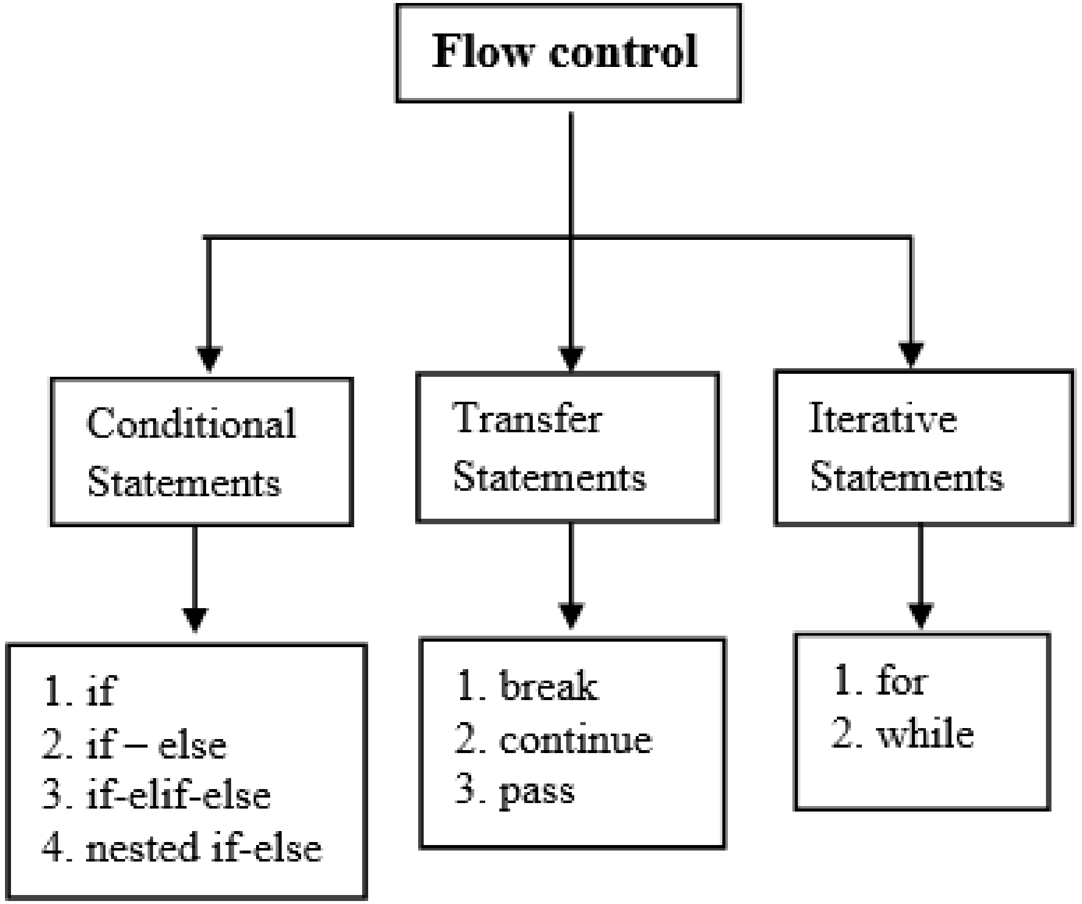
1. Variables (numerical/catagorical)
2. Data types (scaler, vector, array, matrix)
3. Operators (arithmetic & conditional)
4. Flow controls (loops)
5. Functions (solvers, optimizers, plots….)

Operators & Function

Symbol	Operation	Symbol	Operation
+	Addition	.^	Array exponentiation
–	Subtraction	\	Backslash, left division
*	Multiplication	/	Slash, right division
.*	Array Multiplication	.\	Array left division
^	Exponentiation	./	Array right division

Functions	Solution Method
ode23	Runge–Kutta lower order (2nd and 3rd order)
ode45	Runge–Kutta higher order (4th and 5th order)
ode113	Adams–Bashforth–Moulton

Flow controls



- MATLAB uses *mostly* standard relational operators

➢ equal	==
➢ **not** equal	~=
➢ greater than	>
➢ less than	<
➢ greater or equal	>=
➢ less or equal	<=

- Logical operators

Logical operators	elementwise	short-circuit (scalars)
➢ And	&	&&
➢ Or	|	||
➢ **Not**	~	
➢ Xor	xor	
➢ All true	all	
➢ Any true	any	

Problem Statements: 1

Please print output of following commands in “MATLAB”,

- Any indexed/assigned variable (numeric/non-numeric)
- A variable with a scaler element
- A variable with vector elements
- Create an array of 10 random numbers

Please print the matrix in “MATLAB” ,

- Create a matrix of size 1x4
- Create a matrix of size 2x1
- Create a matrix of size 2x3

Problem Statements: 2

Create a matrix “A” of size 3x3 and another matrix “B” of size 3x1 and carry out following calculations,

- Addition of matrix A & B
- Multiplication of matrix A & B
- Division of matrix A & B
- Inverse of matrix A & B

Problem Statement: 3 (linear algebra)

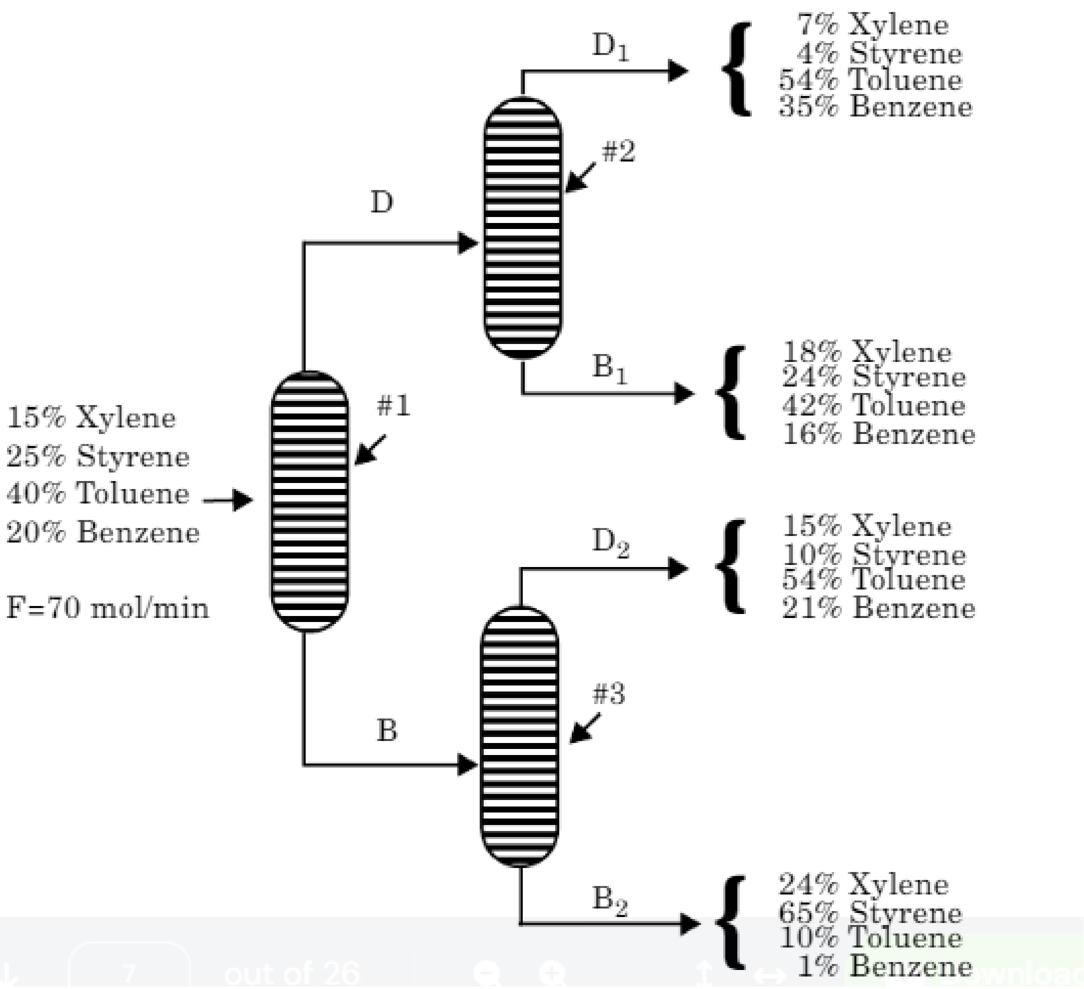
$$-x_1 - 3x_3 = -2$$

$$5x_1 + 2x_2 - 6x_3 = 1$$

$$-4x_1 + x_2 + 8x_3 = 3$$

Numerical methods: Gauss Elimination & Gauss Siedel method (Matlab function: **"inv" in matrix**)
Physical significations: Mass and energy balance equations in chemical engineering

Problem Statement: 4 (Mass Balance across Separators)



Problem Statements: 5 (Nonlinear Algebra)

A non-linear function “y” is given below,

$$y = x^3 – 4*t + t/8$$

Create a function in matlab and compute the given function for predicting y at x= 5 & t=10.

Problem Statements: 6 (Nonlinear Algebra)

A non-linear function "y" as given below,

$$y_1 = x^3 + 3x+5$$
$$y_2 = 5x+1$$

Compute the given function y_1 and y_2 for the x values ranging from 1 to 10 and plot the graph x vs y_1 & y_2.

Problem Statements: 7 (Nonlinear Algebra)

Find the roots of the following equation:

$$f(x) = x^5 - 3x^4 + 3x^3 - 2x^2 - 4x + 1 = 0$$

Numerical methods: Newton Raphson's method (Matlab function: **"fzero" or "roots")**
Physical significations: Cubic EOS in thermodynamics

Problem Statements: 8 (Implicit functions)

The van der Waals equation of state is given by

$$\left(p+\frac{a}{v^2}\right)(v-b)=RT$$

In this equation, $v = (V/n)$ (n: number of moles), $R = 0.082054$ liter·atm/(mol·K), and $a = 3.592$ and $b = 0.04267$ for CO_2. Find the specific volume (liter/mol) of CO_2 when $P = 12$ atm and $T = 315.6$ K.

$$Pv^3-\left(bP+RT\right)v^2+av-ab=0$$

Numerical methods: Newton Raphson's method (Matlab function: **"fzero" & "roots")**
Physical significations: Friction factor calculations in fluid-flow

Problem Statements: 9 (Polynomial Equations)

Estimate the vapor pressure (MPa) of acetone at 273.15 K. For acetone, T_c = 508.1 K, P_c = 4.6924 MPa, and values of parameters of the Wagner equation are $A = -7.670734$, $B = 1.965917$, $C = -2.445437$, and $D = -2.899873$.

$$\ln \frac{P_v}{P_c} = \frac{1}{T_r}\left[A(1-T_r) + B(1-T_r)^{1.5} + C(1-T_r)^{2.5} + D(1-T_r)^{5}\right]$$

Numerical methods: Newton Raphson's method (Matlab function: **"fzero" & "roots")**
Physical significations: Friction factor calculations in fluid-flow

Problem Statements: 10 (Polynomial Equations)

The Colebrook equation is given by

$$\frac{1}{\sqrt{f}} = -0.86 \ln\left(\frac{\epsilon/D}{3.7} + \frac{2.51}{N_{Re}\sqrt{f}}\right)$$

Find the friction factor f for $N_{Re} = 6.5 \times 10^4$ and $\epsilon/D = 0.00013$. As the first guess for f, use $f_0 = 0.1$.

Numerical methods: Newton Raphson's method (Matlab function: **"fzero")**
Physical significations: Friction factor calculations in fluid-flow

Problem Statements: 11 (Mass & Energy Balance Equ_ODEs)

$$\frac{dV}{dt} = F_f - F_o$$

$$A\frac{dL}{dt} = F_f - F_o$$

$$F_o = \alpha\sqrt{L}$$

Data given,

A = 30^{o}C
F_f= 100^{o}C
ά = 0.025
h(t=0) = 0

$$\frac{dT_1}{dt} = \frac{\dot{m}}{m}(T_o - T_1) + \frac{UA}{mC_p}(T_s - T_1)$$

Data given,

$\dot{m}$= 2 kg/s
m= 1000 kg
T_o = 20^{o}C
T_s = 0.025
T_1(t=0)= 20^{o}C

Numerical methods: Euler's & RK methods (Matlab function: **"ode45 or ode23")**
Physical significations: Solving material & energy balance derived sets of ODEs (reaction engineering, heat/mass/momentum transport)

Problem Statements: 12 (Heat Equation_PDE)

$$\alpha \frac{\partial^2 T}{\partial x^2} = \frac{\partial T}{\partial t}$$

Dirichlet conditions

$$T = T_0 \quad (t = 0, 0 \le x \le 1)$$

$$T = T_1 \quad (x = 1, t > 0)$$

Neumann conditions

$$\frac{\partial T}{\partial x} = 0 \quad (x = 1, t \ge 0)$$

<u>Data given,</u>

T_o = 30°C
T_1 = 100°C
ά = 0.025

Numerical methods: Finite difference methods (Matlab function: **“pdepe”)**
Physical significations: Solving material & energy balance derived sets of PDEs (reaction engineering, heat/mass/momentum transport)