The PEM System for Chemical Engineering Problem Solving – Five Examples

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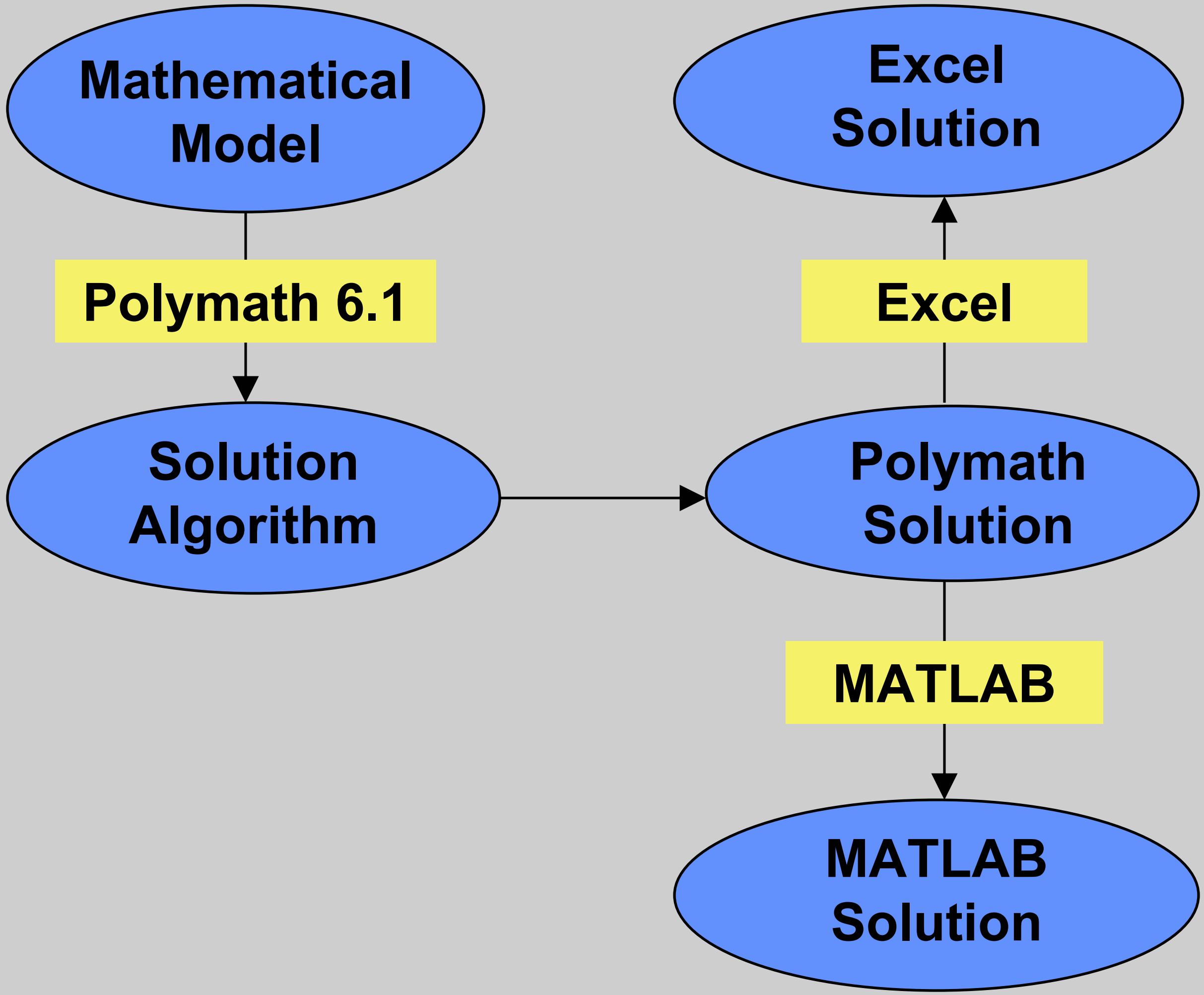
PEM - Increases Problem Solving Efficiency and Capabilities with a Novel Combination of Software Tools

- **Polymath© (easy problem formulation)**
- **Excel™ (familiar spreadsheet environment)**
- **MATLAB™ (advanced problem solving)**

Students and professionals at their personal computers or in computer labs can now effectively solve problems using all the above packages.

PEM Desktop Problem Solving Involving Polymath, Excel, and MATLAB



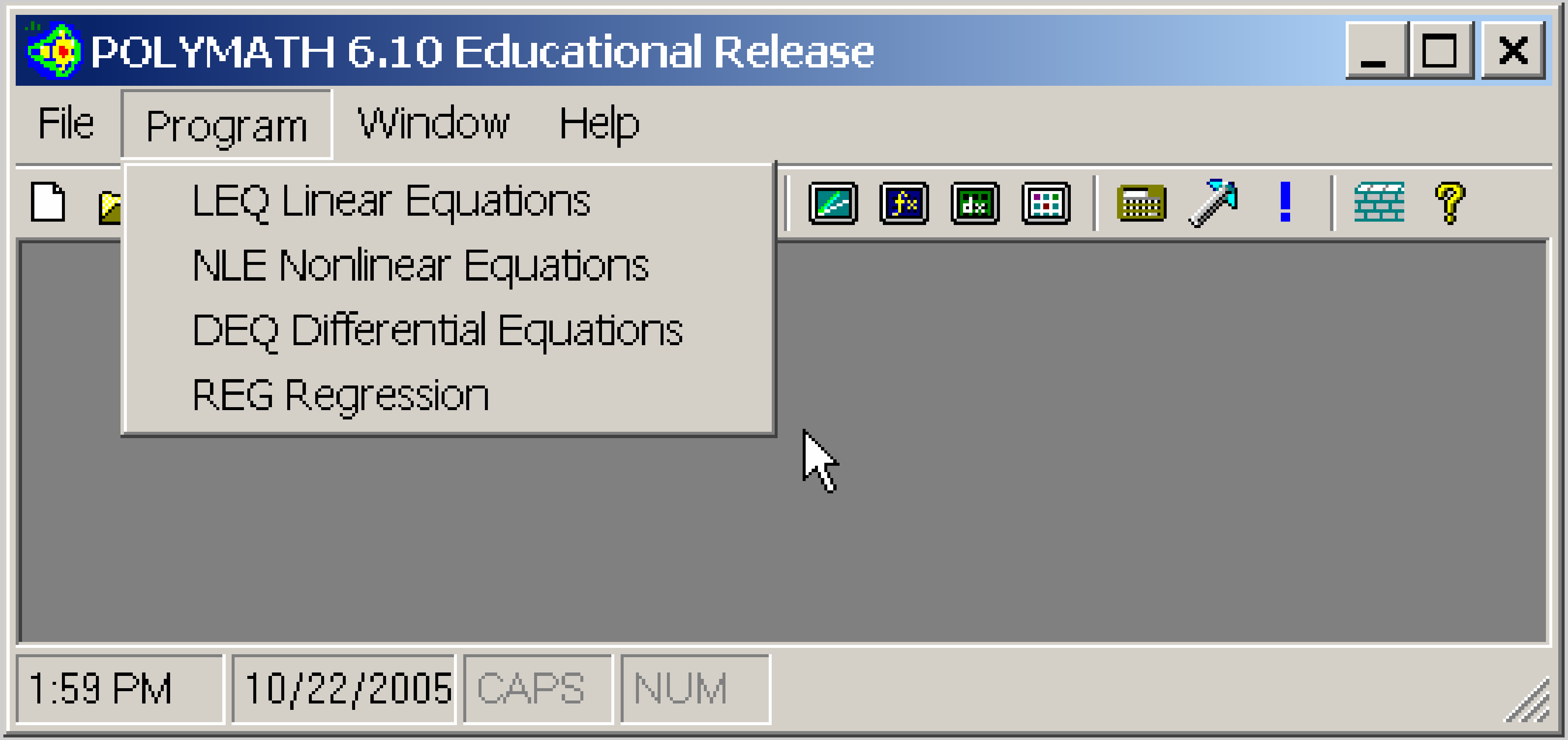
POLYMATH Educational (EDU) or POLYMATH Professional (PRO)

- **Extremely Easy-to-Use**
- **Excellent Problem Solving Capabilities**
  - Linear Equations – 100 (264 **PRO**)
  - Nonlinear Equations – 30 (300 **PRO**)
  - Differential Equations – 30 (300 **PRO**
  - Regressions (Linear, Polynomial, Multiple Linear, Nonlinear) - 301 data points (1001 **PRO**)
- **Automated Export of Problems to Working Excel Spreadsheets Enabling Stand-Alone Excel Calculations (Provides Add-In for Excel that Solves ODEs). (EDU and PRO)**
- **Enables the Use MATLAB by Automatically Translating Problems to Code for Use in M-files. (EDU and PRO)**

POLYMATH 6.1 features include:

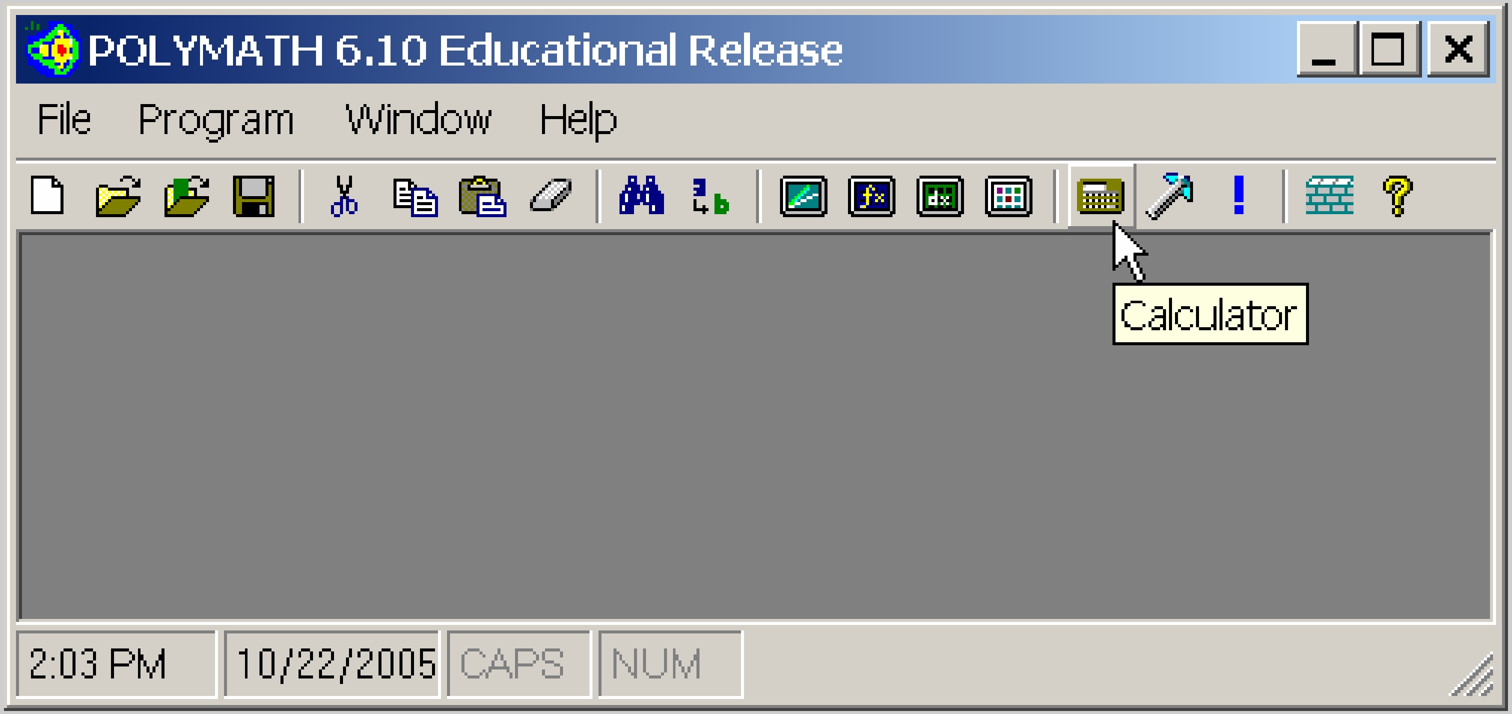
- EASE OF USE WITHOUT ANY PROGRAMMING LANGUAGES OR CONTROL LANGUAGES TO REMEMBER
- STANDARD WINDOWS EDITING
- EXTENSIVE USER ALGORITHM SELECTION AND CONTROL
- EXECUTION WITH ALL 32-BIT WINDOWS OPERATING SYSTEMS INCLUDING VISTA
- COMPATIBILITY WITH PREVIOUS VERSIONS
- THREE ON-BOARD UTILITIES: POWERFUL CALCULATOR, UNIT CONVERTER, AND EXTENSIVE ENGINEERING CONVERSION FACTORS
- EXTENSIVE ON-LINE DOCUMENTATION
- AUTOMATIC PROBLEM EXPORT TO EXCEL – EXCEL ADD-IN FOR DIFFERENTIAL EQUATIONS
- MATLAB OUTPUT GIVING ORDERED AND FORMATTED EQUATIONS

Polymath Software has Four Main Programs

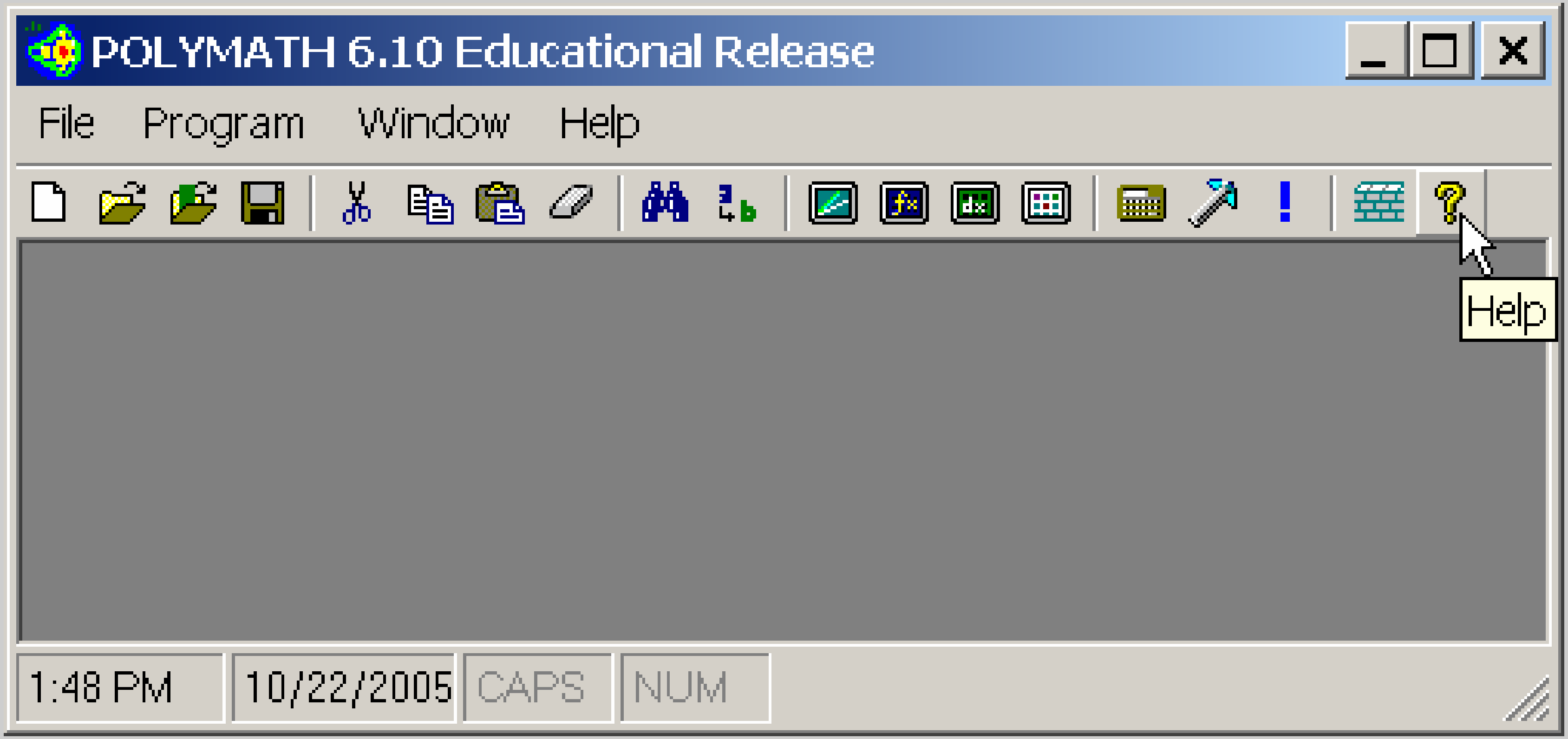


Polymath Software also has Three Utilities:

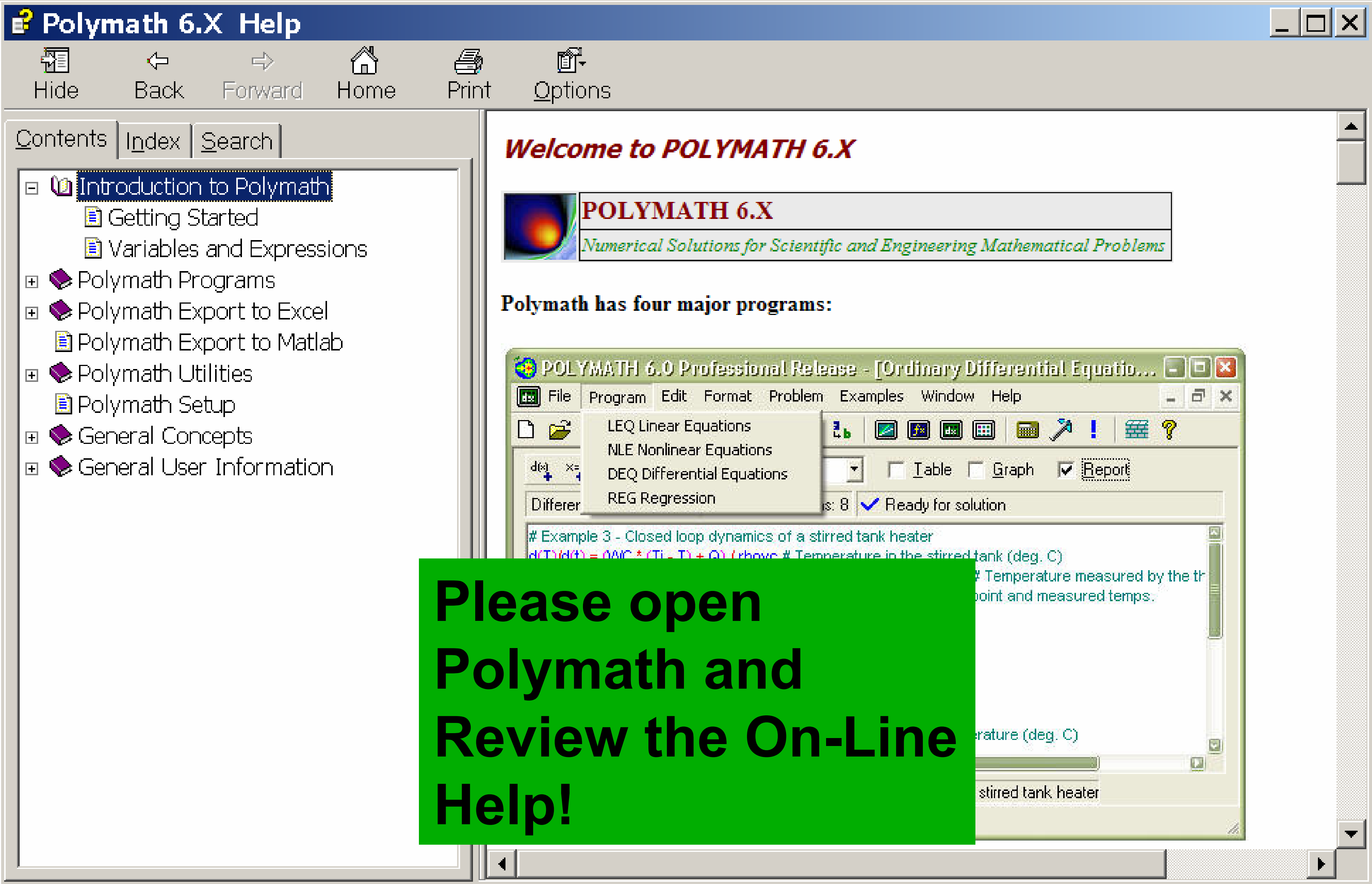
- Calculator
- Units Converter
- Scientific Constants



Initial Polymath Software Display with Help that Gives Detailed Information on the Software



Extensive On-Line HELP



Please open Polymath and Review the On-Line Help!

Five Sample Problems

1. Linear Equations – Material Balances for Distillation Columns – Polymath
2. Explicit Calculations – Equation of State – Polymath and Excel
3. Nonlinear Equations – Pressure Drop for Pipe Flow – Polymath and Excel
4. Differential Equations – Series Reactions in a Batch Reactor - Polymath, Excel, and MATLAB
5. Regressions – Vapor Pressure Data (Linear and Nonlinear) - Polymath, Excel

Working the Sample Problems

You will be able to work with the five sample problems if you have access to POLYMATH, Excel and MATLAB on your personal computer.

POLYMATH Educational (for students and faculty) or POLYMATH Professional can be downloaded for 15-days of free use from

POLYMATH Educational 15-dayTrial

POLYMATH Professional 15-day Trial

It is recommended that you download and install POLYMATH Software and the ODE_Solver Add-In in preparation for solving the example problems. Also you should install Excel and MATLAB if possible.

Clicking on the green boxes with the file names below in the following pages will automatically load the files directly into the appropriate program. You should try to keep this presentation in one window and work on the problem in another window while keeping both visible. This will be very convenient for working the sample problems.

Please close the programs and related windows when each sample problem is completed.

Workshop Problem 1

Numerical Solution: Linear Equations

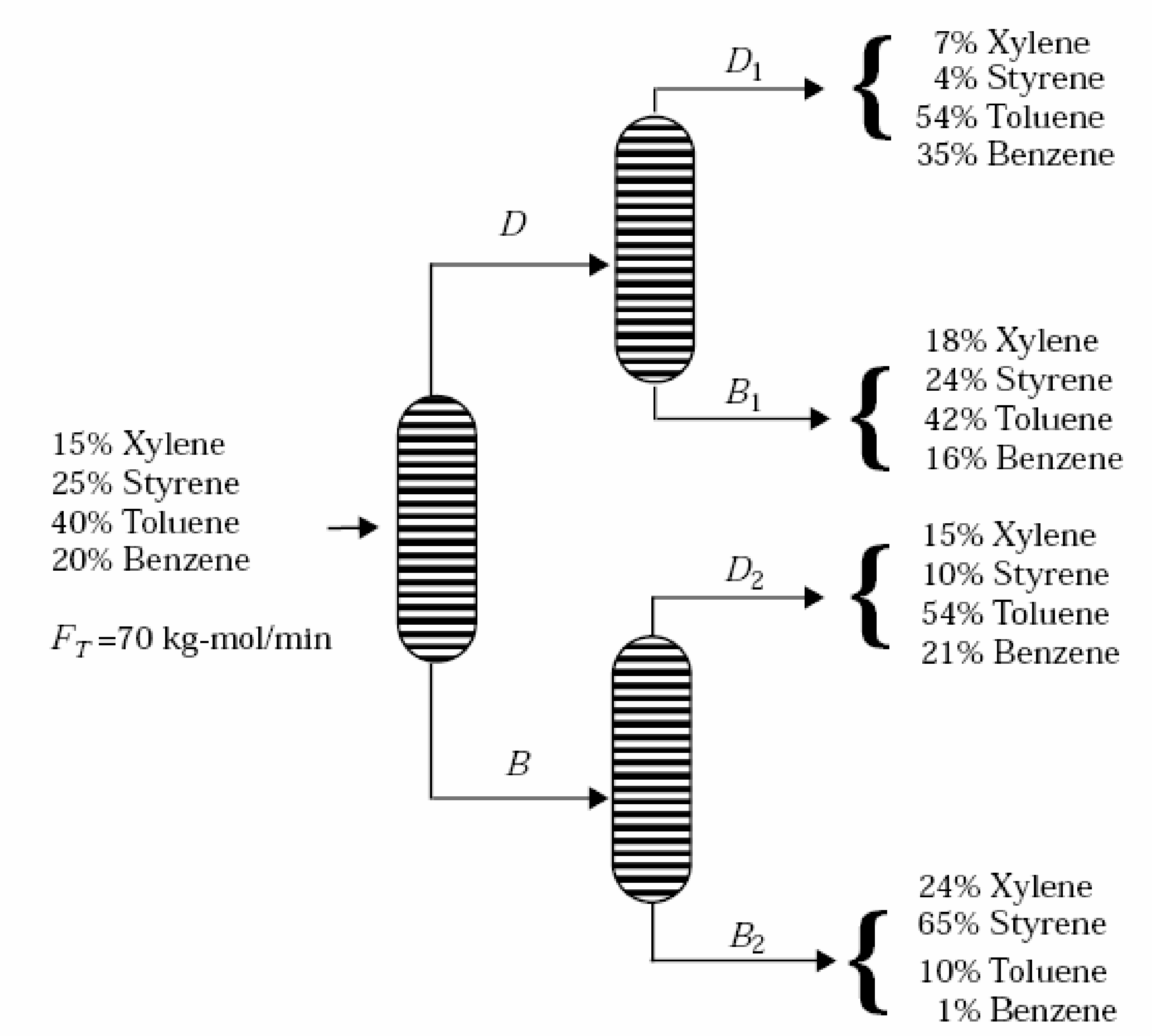
Title: Material Balances for a Train of Distillation Columns

Software Used:

Polymath

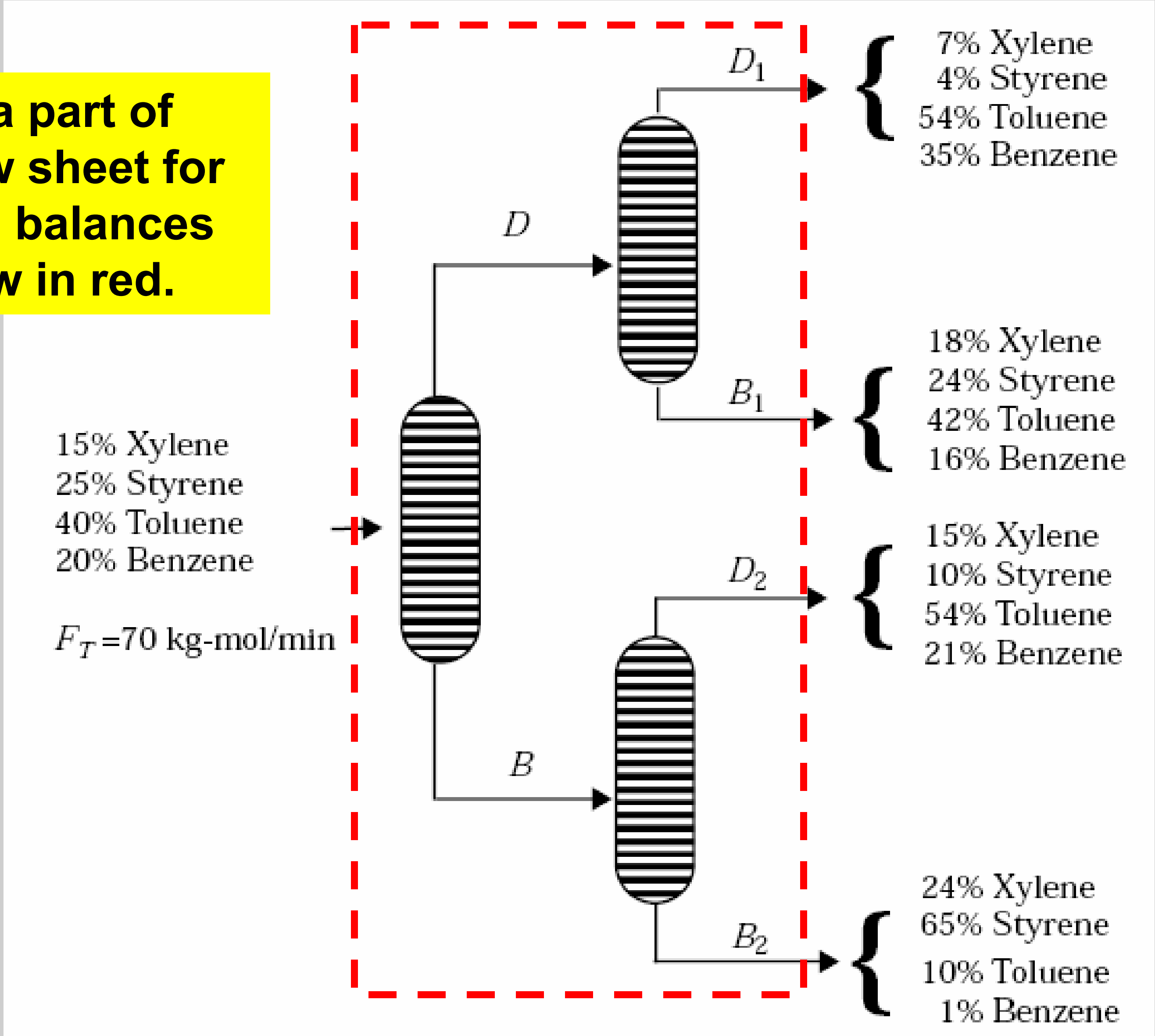
Problem 1 – Linear Equations for Material Balances for a Train of Distillation Columns

Determine Molar Flow Rates B_1, D_1, B_2, and D_2



Problem 1 – Linear Equations for Material Balances for a Train of Distillation Columns

Select a part of the flow sheet for making balances as show in red.



Problem 1 – Linear Equations for Material Balances for a Train of Distillation Columns

Make Balances on Each Species:

- **Xylene**
- **Styrene**
- **Toluene**
- **Benzene**

Determine Flow Rates B1, D1, B2, and D2

$$\text{Xylene: } 0.07\,D_1 + 0.18\,B_1 + 0.15\,D_2 + 0.24\,B_2 = 0.15 \times 70$$

$$\text{Styrene: } 0.04\,D_1 + 0.24\,B_1 + 0.10\,D_2 + 0.65\,B_2 = 0.25 \times 70$$

$$\text{Toluene: } 0.54\,D_1 + 0.42\,B_1 + 0.54\,D_2 + 0.10\,B_2 = 0.40 \times 70$$

$$\text{Benzene: } 0.35\,D_1 + 0.16\,B_1 + 0.21\,D_2 + 0.01\,B_2 = 0.20 \times 70$$

Problem 1 – Linear Equations for Material Balances for a Train of Distillation Columns

Xylene: $0.07D_1 + 0.18B_1 + 0.15D_2 + 0.24B_2 = 10.5$

Styrene: $0.04D_1 + 0.24B_1 + 0.10D_2 + 0.65B_2 = 17.5$

Toluene: $0.54D_1 + 0.42B_1 + 0.54D_2 + 0.10B_2 = 28$

Benzene: $0.35D_1 + 0.16B_1 + 0.21D_2 + 0.01B_2 = 14$

Polymath Program Exercise

Use Polymath to Enter and Solve Equations

Select Program LEQ – Linear Equations, Change Number of Equations to 4 and Press Enter. Then Enter Problem Data.

OR

Click Here to Use Polymath Solution File to Solve Equations

LinearEquations01.pol

Workshop Problem 2

Numerical Solution: Explicit Equations

Title: Explicit Calculations for an Equation of State

Software Used:

Polymath and Excel

Problem 2 - Explicit Calculations for an Equation of State

Calculate P when the other variables and parameters of the van der Waals equation of state are known.

Hint: Use POLYMATH Nonlinear Equations Solver (even when there are no nonlinear equations).

$$R = 0.08206$$

$$T_c = 304.2$$

$$P_c = 72.9$$

$$T = 350$$

$$V = 0.6$$

$$a = (24/64)((R^2 T_c^2)/P_c)$$

$$b = (R T_c)/(8 P_c)$$

$$P = (R T)/(V - b) - a/V^2$$

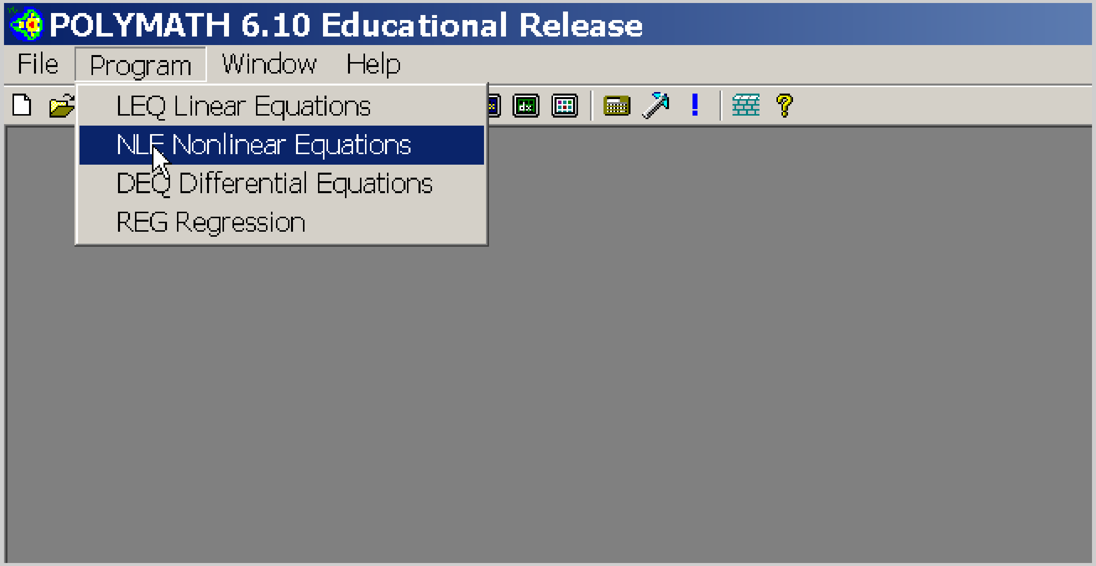
Problem 2 - Explicit Calculations for an Equation of State

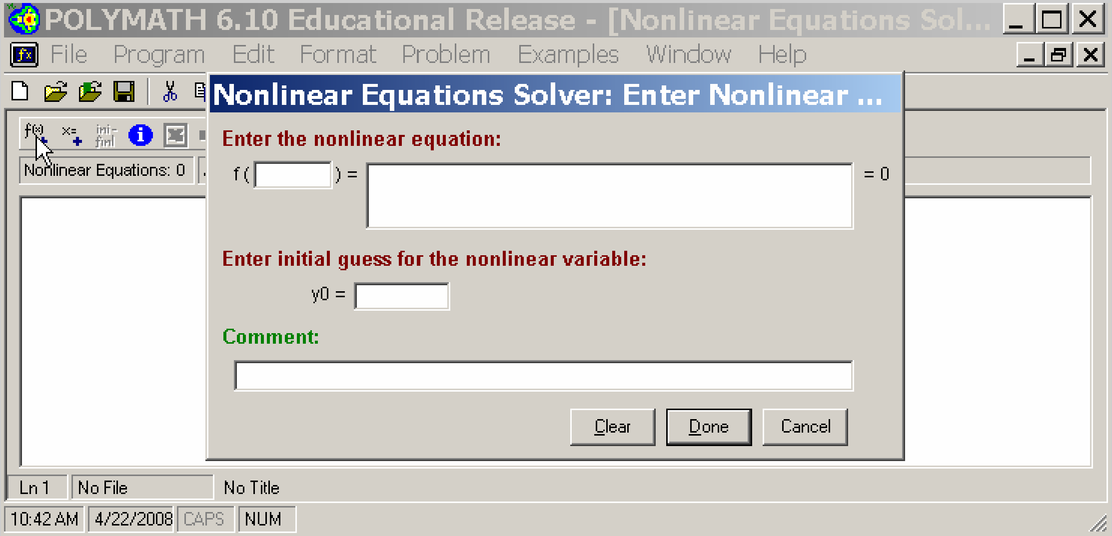
Polymath Solution Demonstration

Enter the equations into Polymath.

Note that the equations can be entered in any order. Polymath orders equations before solution.

Use templates or full screen editor.





Problem 2 - Explicit Calculations for an Equation of State

Polymath Solution Exercise

POLYMATH 6.10 Educational Release - [Nonlinear Equations Solver]

File Program Edit Format Problem Examples Window Help

safenewt

Nonlinear Equations: 0 | Auxiliary Equations: 8 | Ready for solution

```
R = 0.08206
Tc=304.2
Pc=72.9
T=350
V=0.6
a=(24/64)*((R^2*Tc^2)/Pc)
b=(R*Tc)/(8*Pc)
P=(R*T)/(V-b)-a/V^2
```

POLYMATH Report

Explicit Equations

Calculated values of explicit variables

	Variable	Value
1	a	3.205422
2	b	0.0428029
3	P	42.64155
4	Pc	72.9
5	R	0.08206
6	T	350.
7	Tc	304.2
8	V	0.6

Explicit equations

1 R = 0.08206

2 Tc = 304.2

3 Pc = 72.9

4 T = 350

5 V = 0.6

6 a = (24/64)*((R^2*Tc^2)/Pc)

7 b = (R*Tc)/(8*Pc)

8 P = (R*T)/(V-b)-a/V^2

Click here to use Polymath to enter and solve equations

PolymathNonlinear.pol

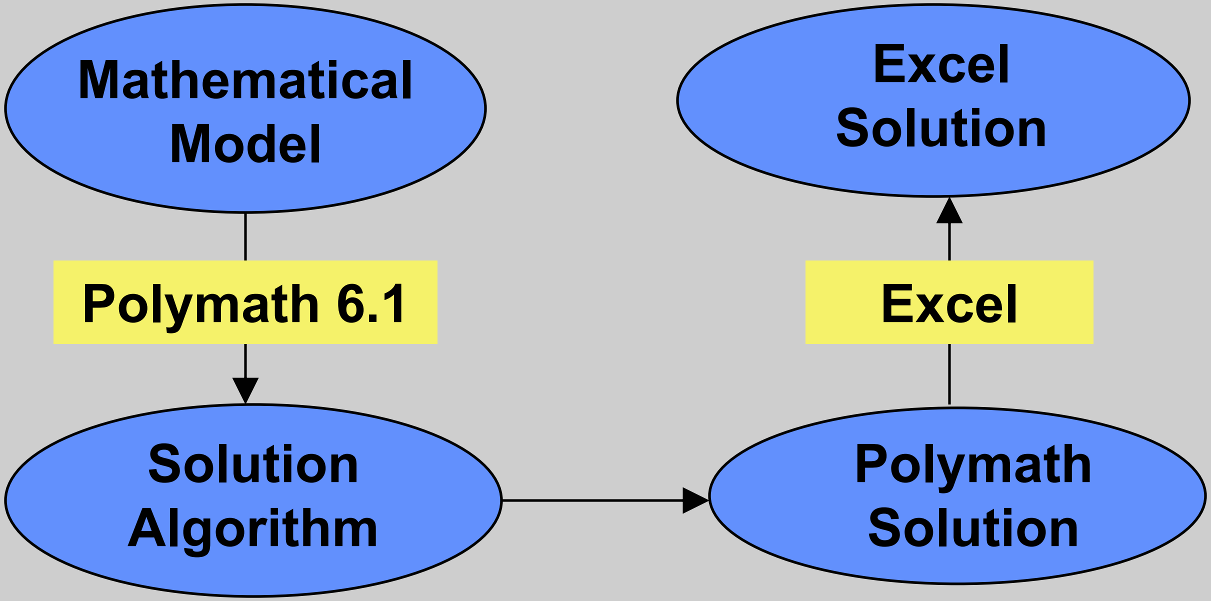
OR

Click here to import this problem solution into POLYMATH and solve problem to verify given solution.

NonlinearEquations01.pol

Problem 2 - Explicit Calculations for an Equation of State

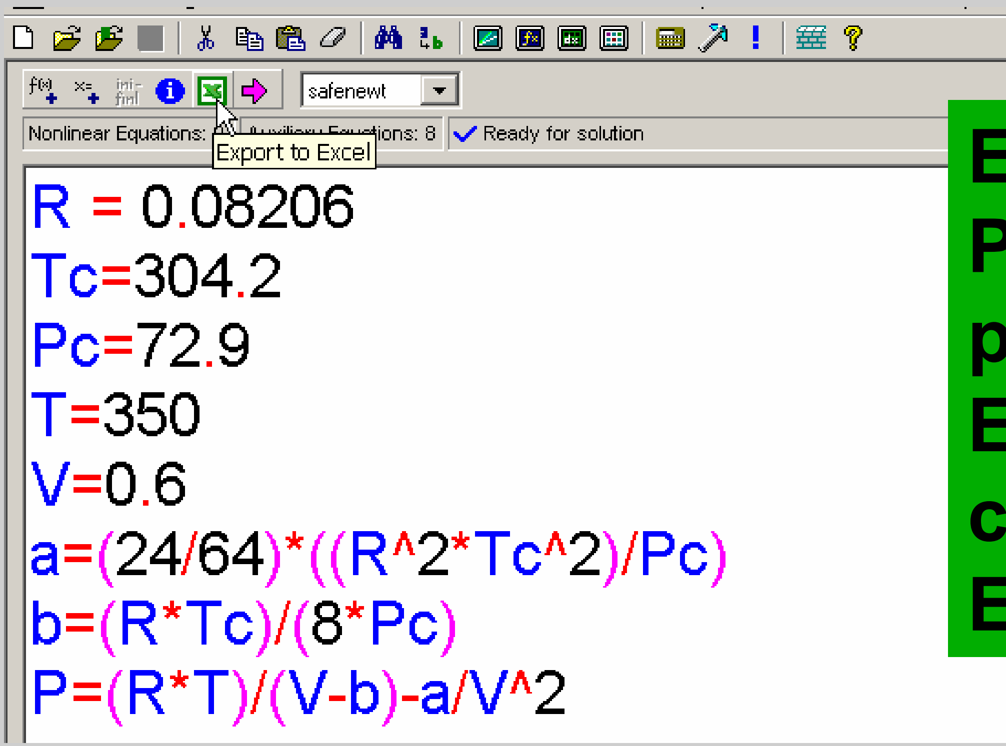
Polymath Solution then Export to Excel for Solution



Problem 2 - Explicit Calculations for an Equation of State

Polymath Solution then Export to Excel for Solution

Exercise



Export the POLYMATH problem to EXCEL by clicking the EXCEL icon.

Hint – Be sure to have an open EXCEL Spreadsheet running on your computer before exporting problem.

Problem 2 - Explicit Calculations for an Equation of State

Polymath Solution then Export to Excel for Solution

Exercise

Microsoft Excel - Book1

	A	B	C	D	E
1	POLYMATH NLE Migration Document				
2		Variable	Value		Polymath Equation
3	Explicit Eqs	R	0.08206		R=0.08206
4		Tc	304.2		Tc=304.2
5		Pc	72.9		Pc=72.9
6		T	350		T=350
7		V	0.6		V=0.6
8		a	3.20542178		a=(24/64)*((R^2*Tc^2)/Pc)
9		b	0.0428029		b=(R*Tc)/(8*Pc)
10		P	42.6415451		P=(R*T)/(V-b)-a/V^2
11					

Compare your EXCEL results to the POLYMATH results.

POLYMATH Report
Explicit Equations

Calculated values of explicit variables

	Variable	Value
1	a	3.205422
2	b	0.0428029
3	P	42.64155
4	Pc	72.9
5	R	0.08206
6	T	350.
7	Tc	304.2
8	V	0.6

Explicit equations

1 R = 0.08206
2 Tc = 304.2
3 Pc = 72.9
4 T = 350
5 V = 0.6
6 a = (24/64)*((R^2*Tc^2)/Pc)
7 b = (R*Tc)/(8*Pc)
8 P = (R*T)/(V-b)-a/V^2

Workshop Problem 3

Numerical Solution: Nonlinear Equations

Title: Pressure Drop Calculations for Pipe Flow

Software Used:

Polymath and Excel

Problem 3 – Nonlinear Equations - Pressure Drop Calculations for Pipe Flow

Polymath Solution for Two Nonlinear Equations – Simultaneous Solution with If… Then… Else… Statement

Pressure Drop Equation

dp = 2 * fF * rho * v * v * L / D

becomes in Polymath

f(D) = dp - 2 * fF * rho * v * v * L / D

The nonlinear equation is always rearranged to equal zero.

Problem 3 – Nonlinear Equations - Pressure Drop Calculations for Pipe Flow

Polymath Solution for Two Nonlinear Equations – Simultaneous Solution with If… Then… Else… Statement

The second nonlinear equation uses the If… Then... Else Statement

Friction Factor Equation

fF = 16 / Re if Re < 2100

= 1 / (4 * *log*(Re * *sqrt*(fF)) - 0.4) ^ 2 if Re >= 2100

becomes in Polymath

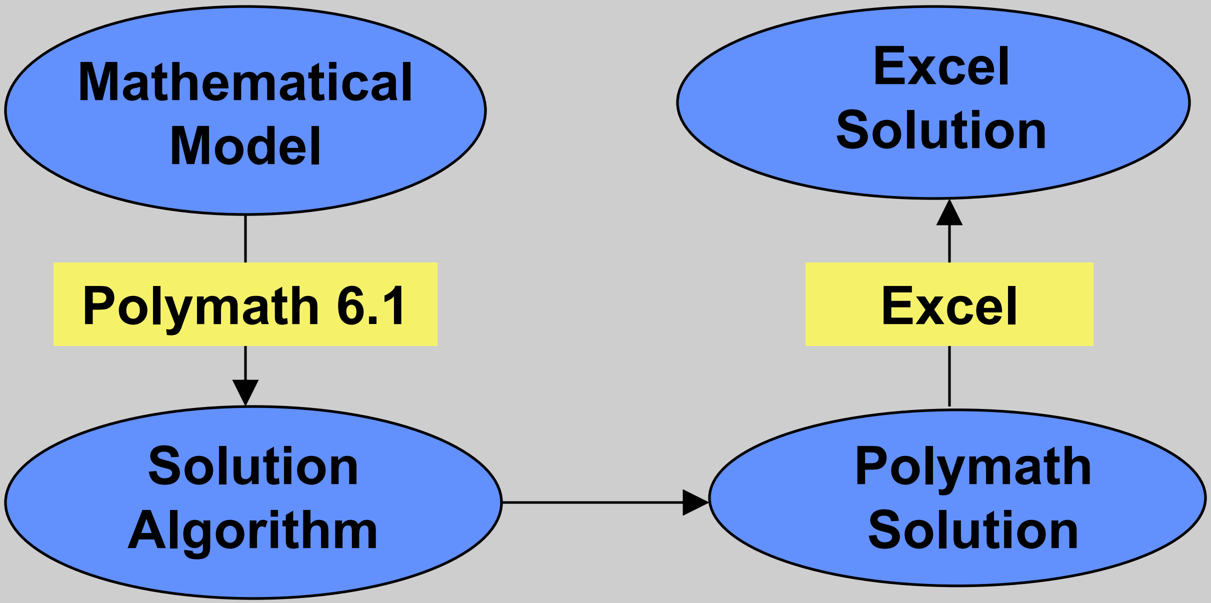
f(fF) = **If** (Re < 2100) **Then** (fF - 16 / Re)

Else (fF - 1 / (4 * *log*(Re * *sqrt*(fF)) - 0.4) ^ 2)

Problem 3 – Nonlinear Equations - Pressure Drop Calculations for Pipe Flow

Polymath Solution for Two Nonlinear Equations – Simultaneous Solution with If… Then… Else… Statement

Solution will be made in Polymath and Excel



Problem 3 – Nonlinear Equations - Pressure Drop Calculations for Pipe Flow

POLYMATH Demonstration - Two Nonlinear Equations – Simultaneous Solution with If… Then… Else… Statement

safenewt

Nonlinear Equations: 2 | Auxiliary Equations: 9 | Ready for solution

```
# Calculation of pipe diameter to have Pressure Drop of 103000 Pa over Length of 100 meters.
f(D) = dp - 2 * fF * rho * v * v * L / D # Calculation of pipe diameter for specified flowrate (D in m)
f(fF) =  If (Re < 2100) Then (fF - 16 / Re) Else (fF - 1 / (4 * log(Re * sqrt(fF)) - 0.4) ^ 2) # Fanning's friction factor

# The explicit equations
rho = 46.048 + T * (9.418 + T * (-0.0329 + T * (4.882e-5 - T * 2.895e-8))) # Liquid density (kg/cu-m)
vis = exp(-10.547 + 541.69 / (T - 144.53)) # Liquid viscosity (Pa-s)
Re = D * v * rho / vis # Reynold's number
v = q / (pi * D ^ 2 / 4) # Flow velocity (m/s)
dp = 103000 # Pressure drop (Pa)
L = 100 # Pipe length (m)
T = 25 + 273.15 # Temperature (K)
pi = 3.1416
q = 0.0025 # Flow rate (cu-m/s)

# Initial Guess for nonlinear equations variables
D(0) = 0.04
fF(0) = 0.004
```

This is an example of two nonlinear equations plus nine explicit equations.

Ln 18 | NonLinearEquation02.pol | Calculation of Pipe Diameter

Problem 3 – Nonlinear Equations - Pressure Drop Calculations for Pipe Flow

POLYMATH Demonstration - Two Nonlinear Equations – Simultaneous Solution with If… Then… Else… Statement

safenewt

Nonlinear Equations: 2 | Auxiliary Equations: 9 | Ready for solution

```
# Calculation of pipe diameter to have Pressure Drop of 103000 Pa over Length of 100 meters.
f(D) = dp - 2 * fF * rho * v * v * L / D # Calculation of pipe diameter for specified flowrate (D in m)
f(fF) = If (Re < 2100) Then (fF - 16 / Re) Else (fF - 1 / (4 * log(Re * sqrt(fF)) - 0.4) ^ 2) # Fanning's friction factor

# The explicit equations
rho = 46.048 + T * (9.418 + T * (-0.0329 + T * (4.882e-5 - T * 2.895e-8)))
vis = exp(-10.547 + 541.69 / (T - 144.53)) # Liquid viscosity (Pa-s)
Re = D * v * rho / vis # Reynold's number
v = q / (pi * D ^ 2 / 4) # Flow velocity (m/s)
dp = 103000 # Pressure drop (Pa)
L = 100 # Pipe length (m)
T = 25 + 273.15 # Temperature (K)
pi = 3.1416
q = 0.0025 # Flow rate (cu-m/s)

# Initial Guess for nonlinear equations variables
D(0) = 0.04
fF(0) = 0.004
```

The nonlinear equations for pressure drop and for Fanning friction factor will be solved to be zero.

Ln 18 | NonLinearEquation02.pol | Calculation of Pipe Diameter

Problem 3 – Nonlinear Equations - Pressure Drop Calculations for Pipe Flow

POLYMATH Demonstration - Two Nonlinear Equations – Simultaneous Solution with If… Then… Else… Statement

Here is the Polymath solution

Calculated values of NLE variables

	Variable	Value	f(x)	Initial Guess
1	D	0.0389653	4.133E-09	0.04
2	fF	0.0045905	-8.674E-19	0.004

	Variable	Value
1	dp	1.03E+05
2	L	100.
3	pi	3.1416
4	q	0.0025
5	Re	9.097E+04
6	rho	994.5715
7	T	298.15
8	v	2.096491
9	vis	0.0008931

Nonlinear equations

1 f(D) = dp - 2 * fF * rho * v * v * L / D = 0

Calculation of pipe diameter for specified flowrate (D in m)

2 f(fF) = If (Re < 2100) Then (fF - 16 / Re) Else (fF - 1 / (4 * log(Re * sqrt(fF)) - 0.4) ^ 2) = 0

Fanning's friction factor

Explicit equations

1 T = 25 + 273.15

Temperature (K)

2 rho = 46.048 + T * (9.418 + T * (-0.0329 + T * (4.882e-5 - T * 2.895e-8)))

Liquid density (kg/cu-m)

3 pi = 3.1416

4 q = 0.0025

Flow rate (cu-m/s)

5 dp = 103000

Pressure drop (Pa)

6 L = 100

Pipe length (m)

7 vis = exp(-10.547 + 541.69 / (T - 144.53))

Liquid viscosity (Pa-s)

8 v = q / (pi * D ^ 2 / 4)

Flow velocity (m/s)

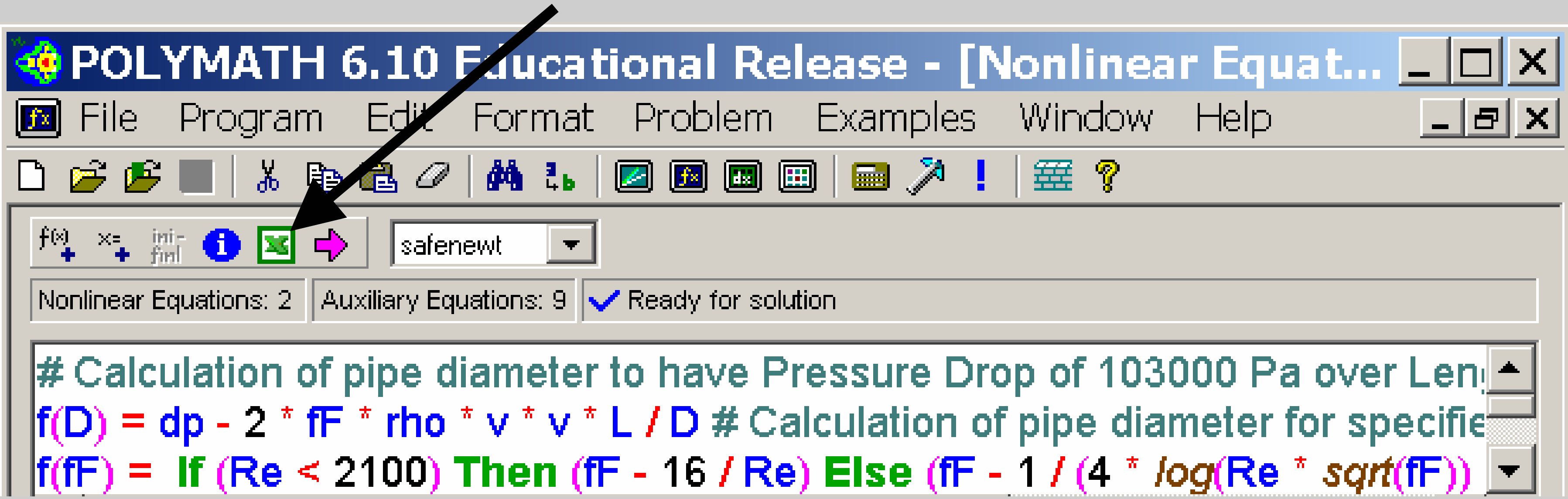
9 Re = D * v * rho / vis

Reynold's number

Problem 3 – Nonlinear Equations - Pressure Drop Calculations for Pipe Flow

POLYMATH/Excel Demonstration - Two Nonlinear Equations – Simultaneous Solution with If… Then… Else… Statement

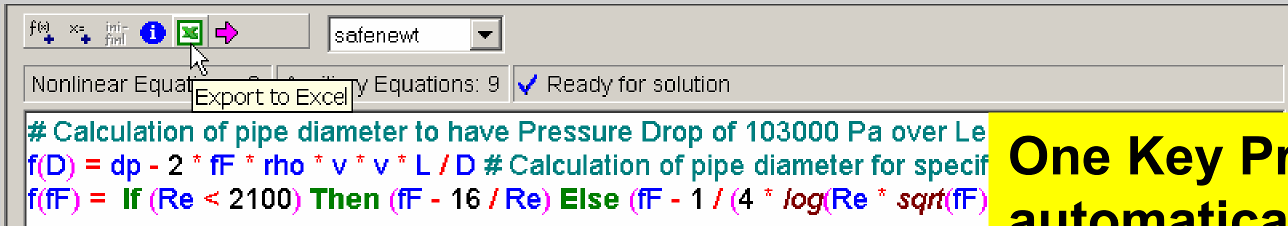
Polymath Software has the option of automatically sending a problem to Excel where the problem is ready to be solved. For Nonlinear Equations, you will use the Solver Add-In to obtain Excel solution.



Problem 3 – Nonlinear Equations - Pressure Drop Calculations for Pipe Flow

POLYMATH/Excel Demonstration - Two Nonlinear Equations – Simultaneous Solution with If… Then… Else… Statement

From Polymath



One Key Press automatically creates problem in Excel.

To Excel

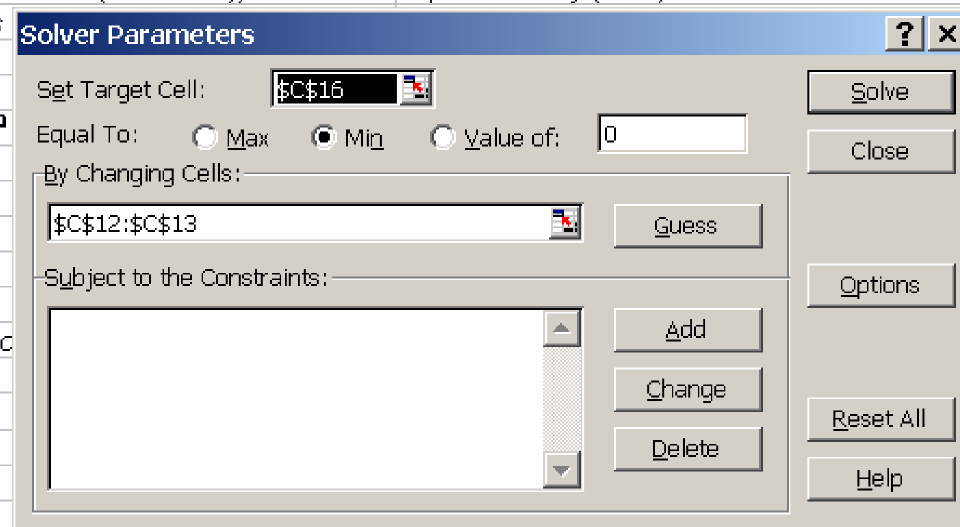
C16 =((C14 ^ 2) + (C15 ^ 2))

	A	B	C	D	E
1	POLYMATH NLE Migration Document				
2		Variable	Value		Polymath Equation
3	Explicit Eqs	rho	994.5715		rho=46.048 + T * (9.418 + T * (-0.0329 + T * (4.8
4		vis	0.0008931		vis=exp(-10.547 + 541.69 / (T - 144.53))
5		Re	88620.363		Re=D * v * rho / vis
6		v	1.9894321		v=q / (pi * D ^ 2 / 4)
7		dp	103000		dp=103000
8		L	100		L=100
9		T	298.15		T=25 + 273.15
10		pi	3.1416		pi=3.1416
11		q	0.0025		q=0.0025
12	Implicit Vars	D	0.04		D(0)=0.04
13		fF	0.004		fF(0)=0.004
14	Implicit Eqs	f(D)	24272.898		f(D)=dp - 2 * fF * rho * v * v * L / D
15		f(fF)	-0.000695		f(fF)=If (Re < 2100) Then (fF - 16 / Re) Else (fF -
16	Sum of Squares:		589173571		F = f(D)^2+f(fF)^2

Problem 3 – Nonlinear Equations - Pressure Drop Calculations for Pipe Flow Excel Demonstration

Use Excel Add-In Solver For Solution

	A	B	C	D	E	
1	POLYMATH NLE Migration Document					
2		Variable	Value		Polymath Equation	Comments
3	Explicit Eqs	rho	994.571504		rho=46.048 + T * (9.418 + T * (-0.0329 + T * (4.882e	Liquid density (kg
4		vis	0.00089308		vis=exp(-10.547 + 541.69 / (T - 144.53))	Liquid viscosity (
5		Re	88620.3631		Re=D * v * rho / vis	
6		v	1.98943214		v=q / (pi * D ^ 2 / 4)	
7		dp	103000		dp=103000	
8		L	100		L=100	
9		T	298.15		T=25 + 273.15	
10		pi	3.1416		pi=3.1416	
11		q	0.0025		q=0.0025	
12	Implicit Vars	D	0.04		D(0)=0.04	
13		fF	0.004		fF(0)=0.004	
14	Implicit Eqs	f(D)	24272.8979		f(D)=dp - 2 * fF * rhc	
15		f(fF)	-0.000695		f(fF)=If (Re < 2100)	
16	Sum of Squares:		589173571		F = f(D)^2+f(fF)^2	
17						
18						
19						



Excel Solution

12	Implicit Vars	D	0.03952106	D(0)=0.04
13		fF	0.00492738	fF(0)=0.004
14	Implicit Eqs	f(D)	0.00374439	f(D)=dp - 2 * fF * rho * v * v * L / D
15		f(fF)	0.00035971	f(fF)=If (Re < 2100) Then (fF - 16 / Re) Else (fF - 1 /
16	Sum of Squares:		1.415E-05	F = f(D)^2+f(fF)^2

Problem 3 – Nonlinear Equations - Pressure Drop Calculations for Pipe Flow - Excel EXCERCISE

1) Obtain the Polymath Solution

Click here for Polymath Problem Solution File

NonlinearEquations02.pol

2) Export the Problem to Excel by Clicking on Excel Icon

First Open Excel (click here) before Export and Have Solver Add-In Available for Use in Solution

Excel.xls

3) Solve the Same Problem in Excel

Or Click here for Excel Solution File

NonlinearEquations02.xls

Workshop Problem 4

Numerical Solution: Simultaneous
Ordinary Differential Equations

Title: Batch Reactor

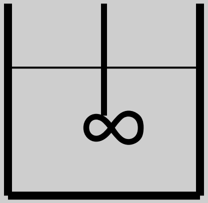
Software Used:

Polymath, Excel and MATLAB

Problem 4 - Differential Equations - Batch Reactor

Differential Equations – Simultaneous ODEs

Consider a Batch Reactor that initially has only reactant A at a value of 1. The reactions are first order and irreversible. Reaction time t is from 0 to 3.



$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

I. C. for t = 0, $t_{final} = 3$

$$\frac{dC_A}{dt} = -k_1 C_A \qquad \text{I. C. } C_A\big|_{t=0} = 1$$

$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B \qquad \text{I. C. } C_B\big|_{t=0} = 0$$

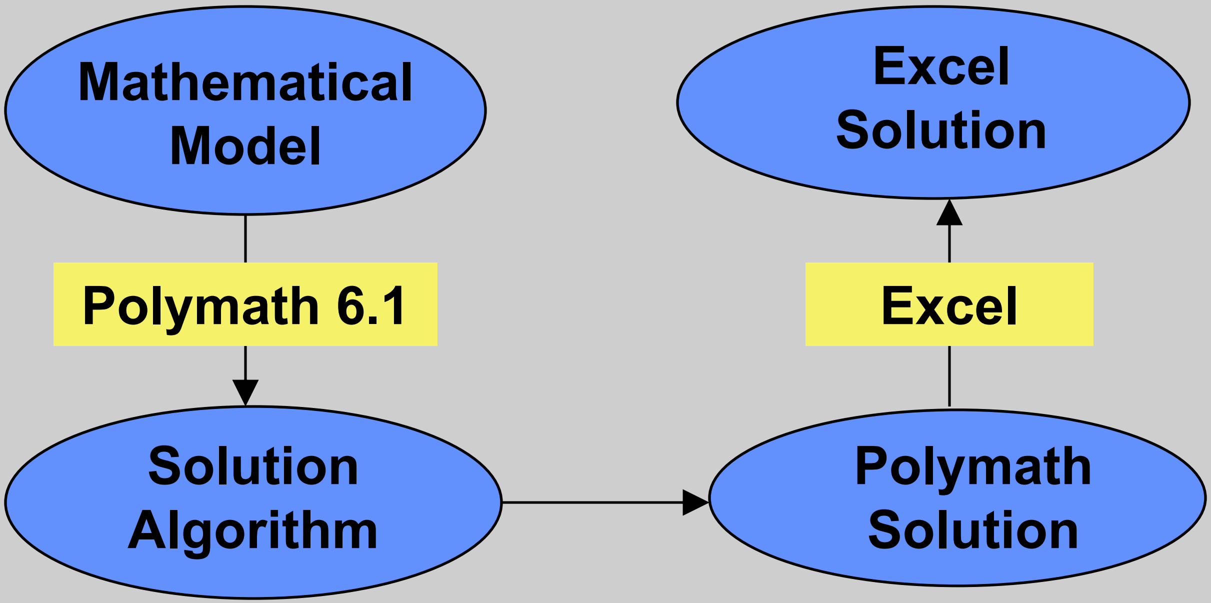
$$\frac{dC_C}{dt} = k_2 C_B \qquad \text{I. C. } C_C\big|_{t=0} = 0$$

$$k_1 = 2 \qquad k_2 = 3$$

Problem 4 - Differential Equations - Batch Reactor

Differential Equations – Simultaneous ODEs

POLYMATH/Excel Solution EXERCISE



Click Here to Enter and Solve this Problem in POLYMATH

PolymathDifferential.pol

Or Open Polymath

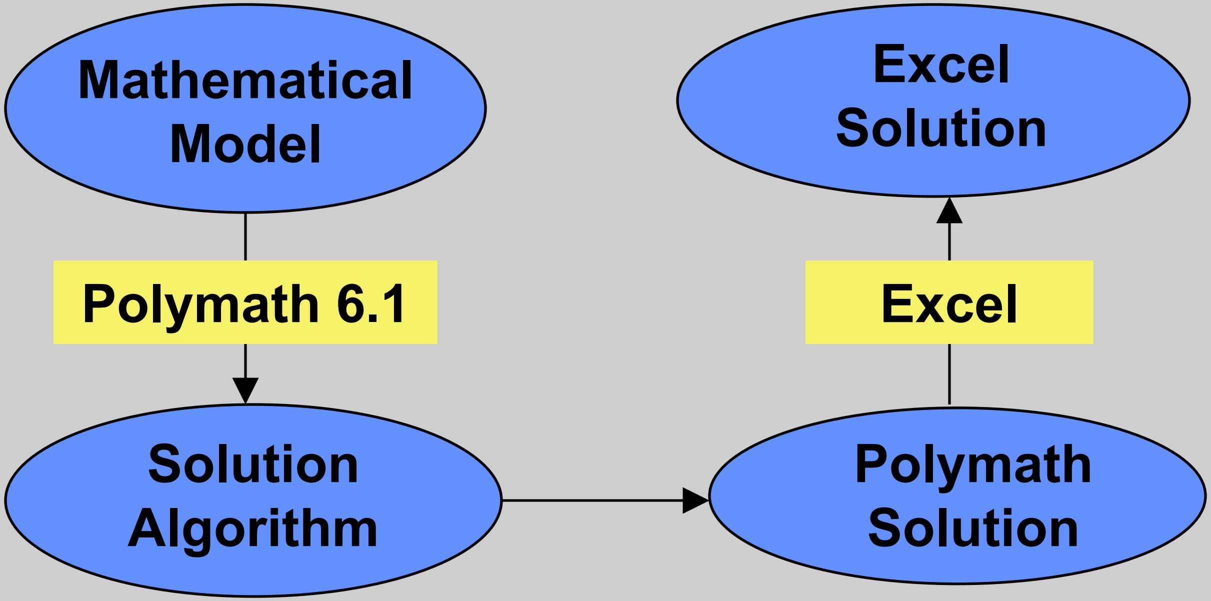
OR

Click Here to Use Problem Solution in POLYMATH

DifferentialEquations01.pol

Problem 4 - Differential Equations - Batch Reactor

POLYMATH/Excel Solution EXERCISE



1) Open Excel, 2) Export Polymath Problem to Excel, and 3) Solve with Polymath ODE_Solver Add-In.

Click here to Open Excel

Excel.xls or Open Excel

Click here to Open Problem, Export and Solve in Excel

DifferentialEquations01.pol

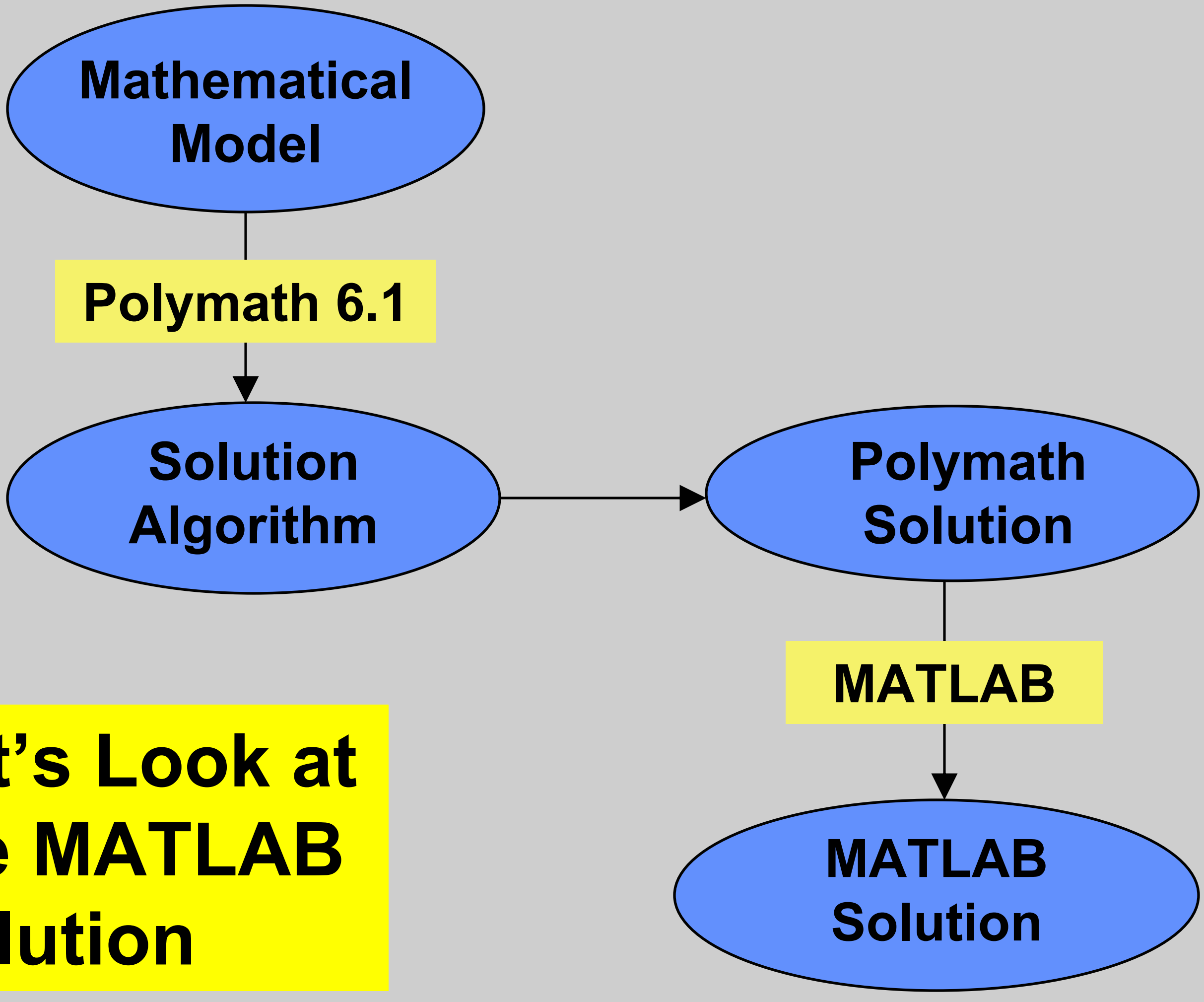
OR

Click here for Excel Solution File

DifferentialEquation01.xls

Problem 4 - Differential Equations - Batch Reactor

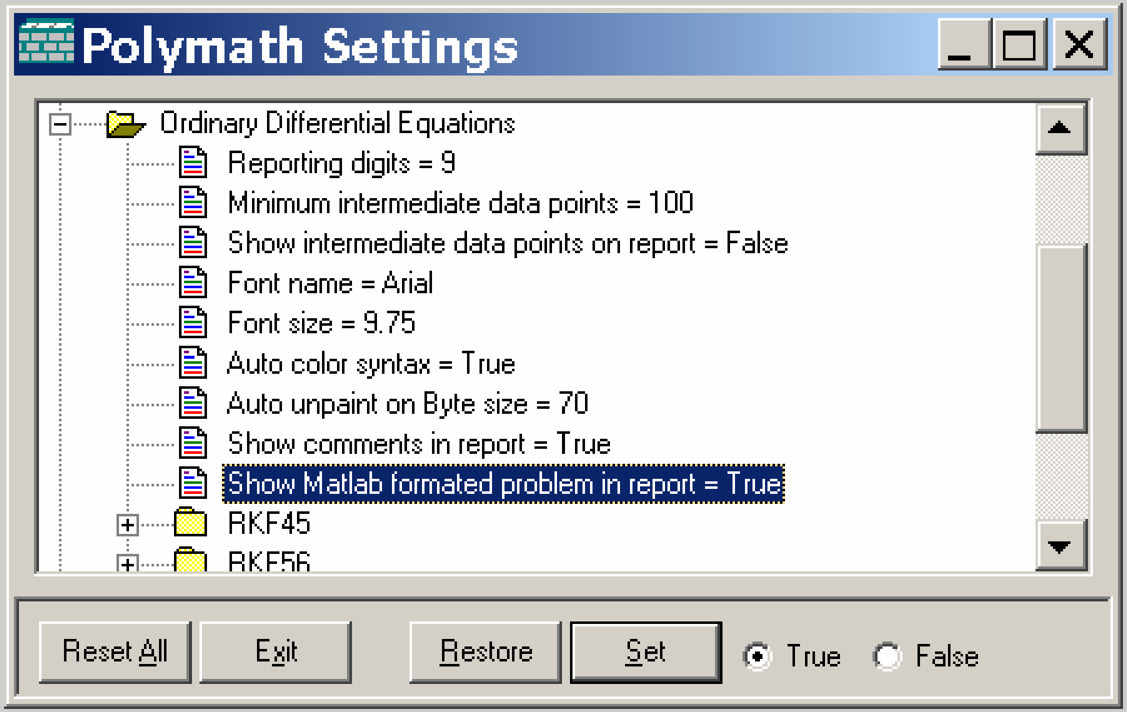
POLYMATH/MATLAB Solution Demonstration



Let's Look at the MATLAB Solution

Problem 4 - Differential Equations - Batch Reactor
POLYMATH/MATLAB Solution Demonstration

MATLAB problem solution is obtained by first requesting MATLAB output in the Polymath Setting window found with the Settings Icon.



Problem 4 - Differential Equations - Batch Reactor
POLYMATH/MATLAB Solution Demonstration

This option for MATLAB formatted output results in the MATLAB code to be generated automatically at the end of the POLYMATH report.

Matlab Formatted Problem Code

```
tspan = [0 4.]; % Range for the independent variable
y0 = [1.; 0; 0]; % Initial values for the dependent
variables
function dYfuncvecdt = ODEfun(t,Yfuncvec);
CA = Yfuncvec(1);
CB = Yfuncvec(2);
CC = Yfuncvec(3);
k1 = 2;
k2 = 3;
dCAdt = 0 - (k1 * CA);
dCBdt = k1 * CA - (k2 * CB);
dCCdt = k2 * CB;
dYfuncvecdt = [dCAdt; dCBdt; dCCdt];
```

Problem 4 - Differential Equations - Batch Reactor

POLYMATH/MATLAB Solution Demonstration

The MATLAB formatted output is copied and pasted into the MATLAB template that is provided within the Polymath HELP materials.

3. Differential Equations

The MATLAB program template for a Polymath program involving differential equations is given in the box below. This can be copied into the MATLAB editor and saved as **MultipleDEQtemplate.m** for future use.

```
function % Insert here your file name after function (Use Alphanumberic names only)
clear, clc, format short g, format compact
tspan= % Replace this line with tspan line from Polymath report
y0= % Replace this line with y0 line from Polymath report
disp(' Variable values at the initial point ');
disp([' t = ' num2str(tspan(1))]);
disp(' y dy/dt ');
disp([y0 ODEfun(tspan(1),y0)]);
[t,y]=ode45(@ODEfun,tspan,y0);
for i=1:size(y,2)
disp([' Solution for dependent variable y' int2str(i)]);
disp([' t y' int2str(i)]);
disp([t y(:,i)]);
plot(t,y(:,i));
title([' Plot of dependent variable y' int2str(i)]);
xlabel(' Independent variable (t)');
ylabel([' Dependent variable y' int2str(i)]);
pause
end
%- - - - - - - - - - - - - - - - - - - - - - -
% Replace this and the following line with the function copied from the Polymath report
% Do not include the tspan and y0 lines
```

Problem 4 - Differential Equations - Batch Reactor

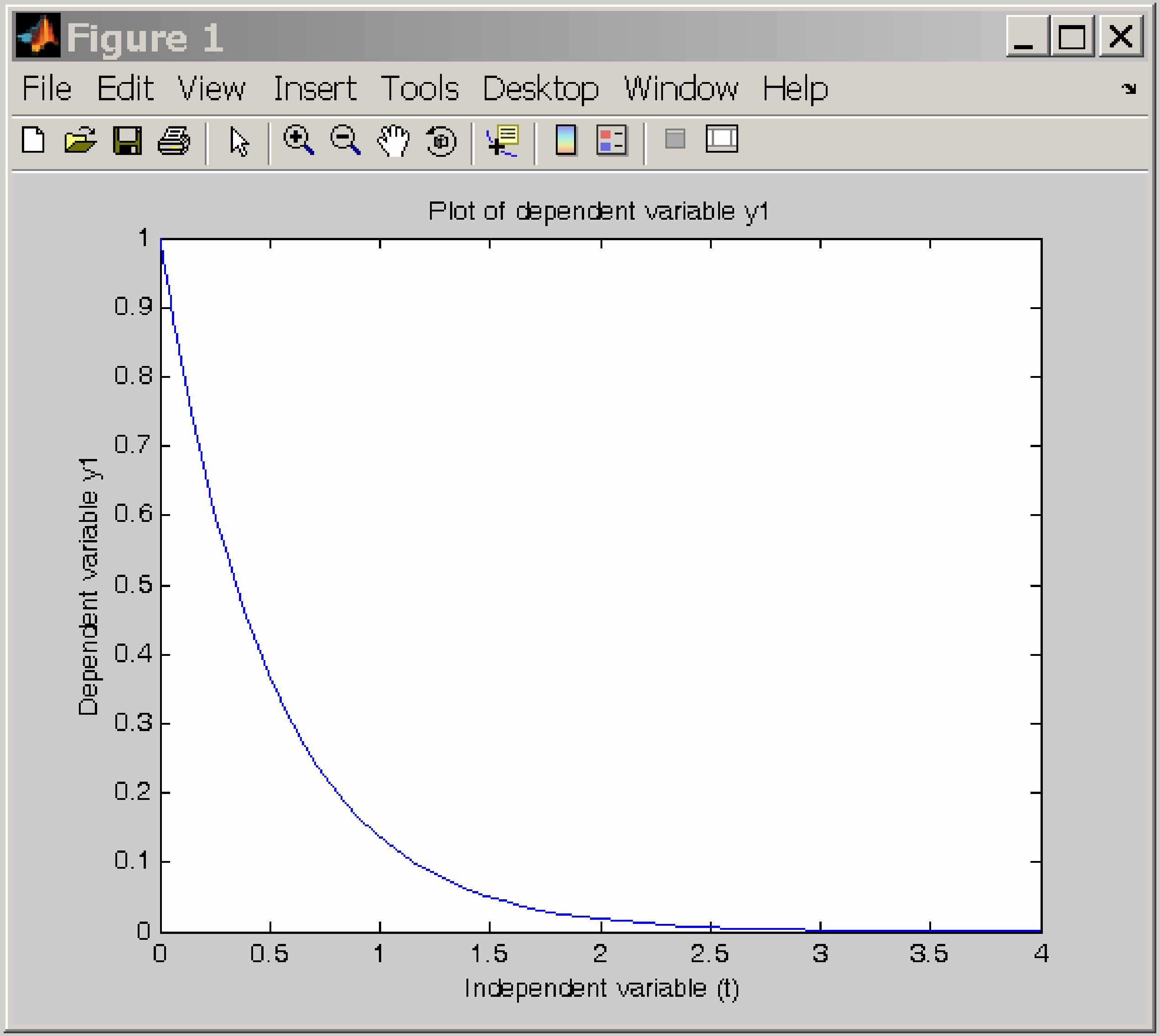
MATLAB Solution Demonstration

```
function MATLAB01
clear, clc, format short g, format compact
tspan = [0 4.]; % Range for the independent variable
y0 = [1.; 0; 0]; % Initial values for the dependent variables
disp(' Variable values at the initial point ');
disp([' t     = ' num2str(tspan(1))]);
disp('           y                   dy/dt         ');
disp([y0 ODEfun(tspan(1),y0)]);
[t,y]=ode45(@ODEfun,tspan,y0);
for i=1:size(y,2)
    disp([' Solution for dependent variable y' int2str(i)]);
    disp(['            t                   y' int2str(i)]);
    disp([t y(:,i)]);
    plot(t,y(:,i));
    title([' Plot of dependent variable y' int2str(i)]);
    xlabel(' Independent variable (t)');
    ylabel([' Dependent variable y' int2str(i)]);
    pause
end
%- - - - - - - - - - - - - - - - - - - - - -
function dYfuncvecdt = ODEfun(t,Yfuncvec);
CA = Yfuncvec(1);
CB = Yfuncvec(2);
CC = Yfuncvec(3);
k1 = 2;
k2 = 3;
dCAdt = 0 - (k1 * CA);
dCBdt = k1 * CA - (k2 * CB);
dCCdt = k2 * CB;
dYfuncvecdt = [dCAdt; dCBdt; dCCdt];
```

MATLAB Code from Polymath is Entered into Template. Yellow bars indicate copied code.

Problem 4 - Differential Equations - Batch Reactor

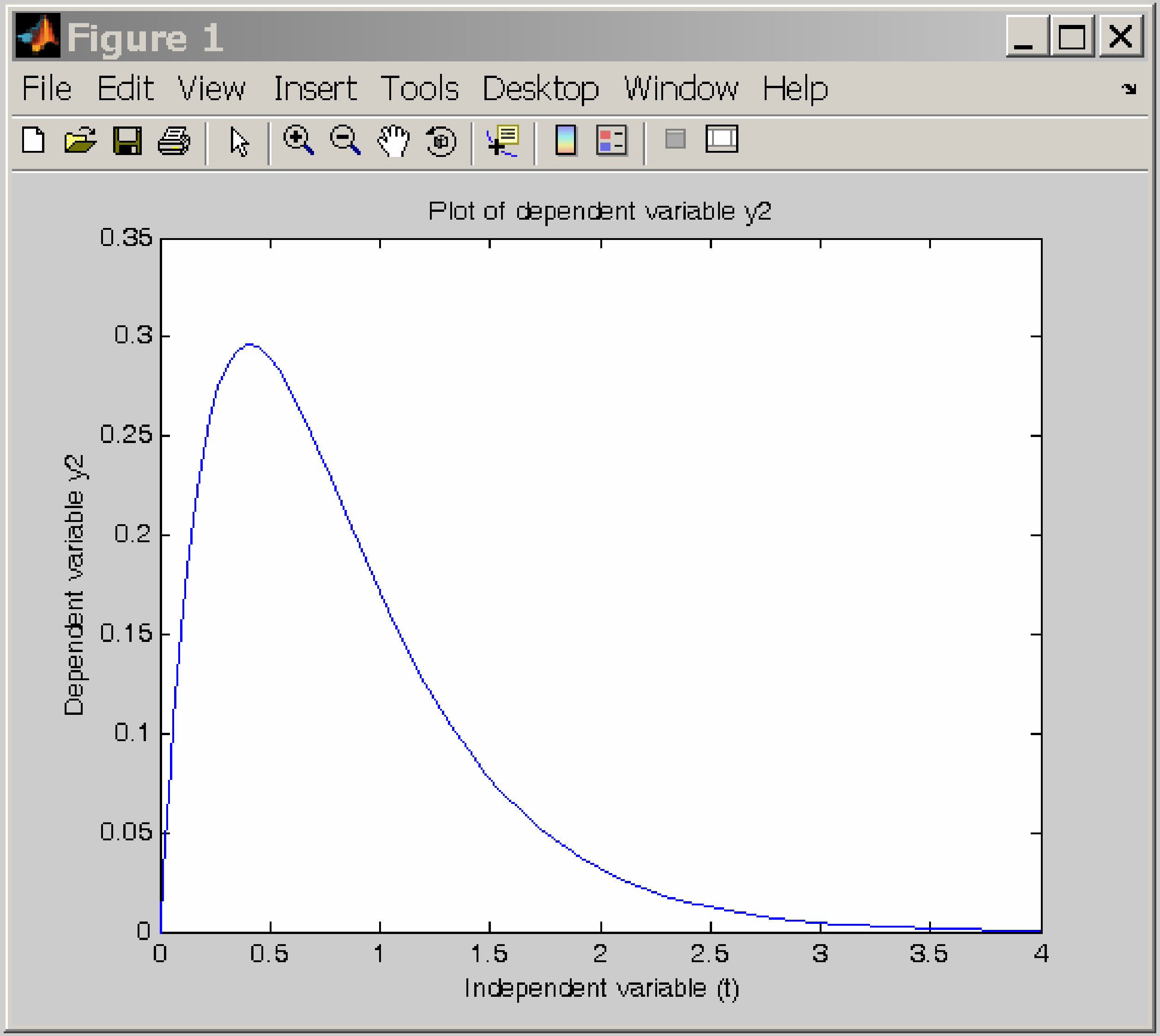
The MATLAB m-file thus created provides graphical output for all differential variables.



MATLAB Solution Demonstration

Problem 4 - Differential Equations - Batch Reactor

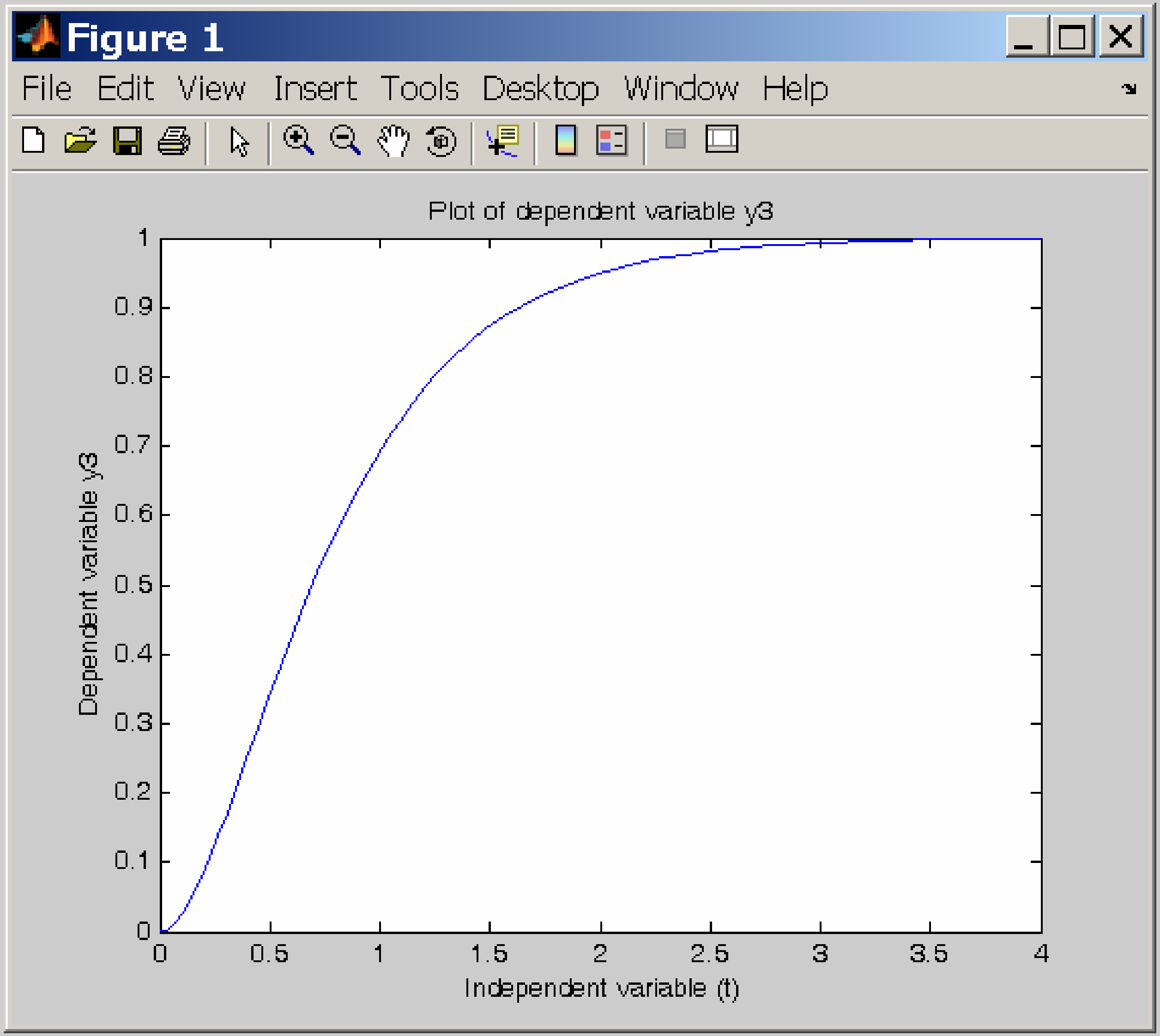
The MATLAB m-file thus created provides graphical output for all differential variables.



MATLAB Solution Demonstration

Problem 4 - Differential Equations - Batch Reactor

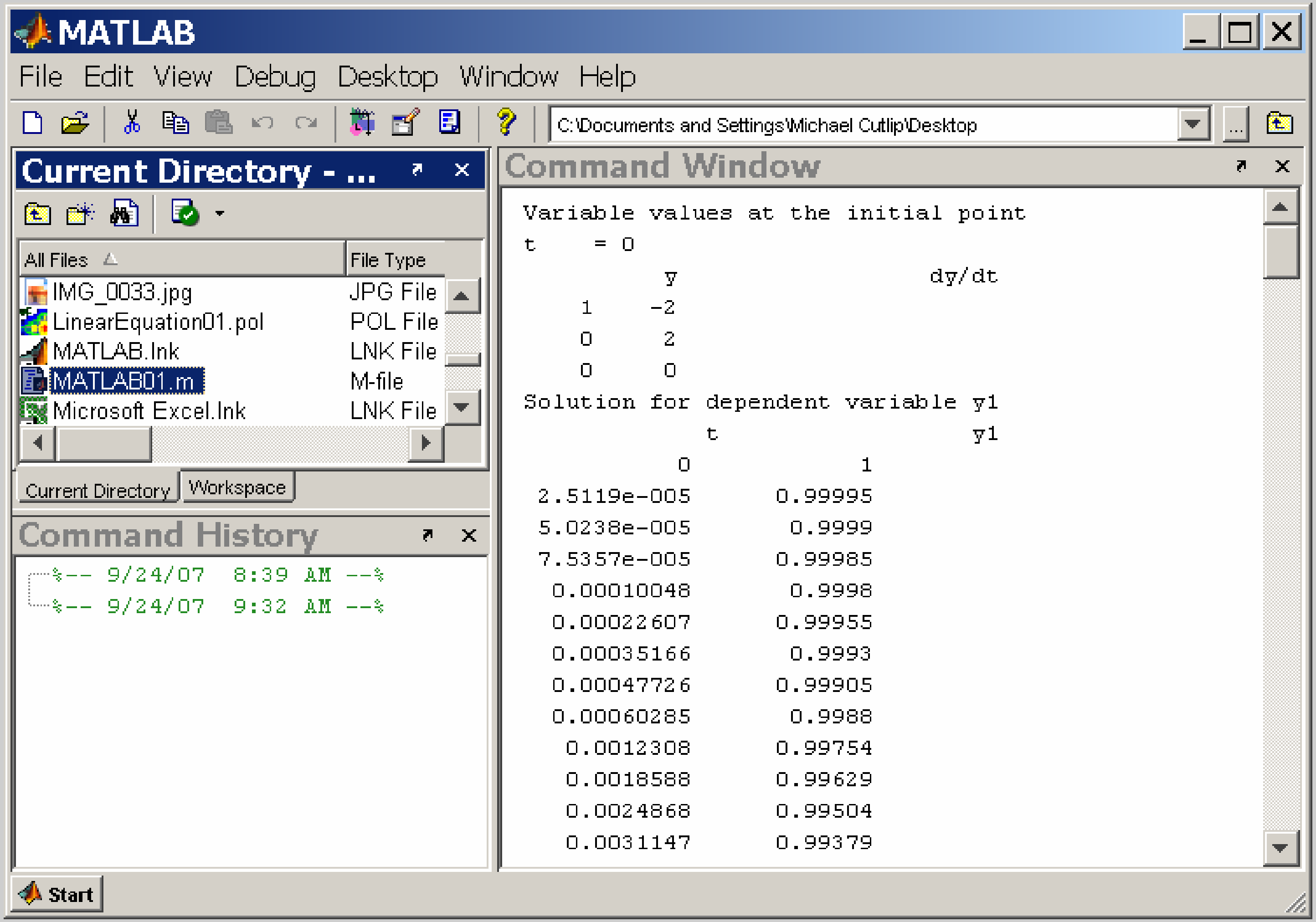
The MATLAB m-file thus created provides graphical output for all differential variables.



MATLAB Solution Demonstration

Problem 4 - Differential Equations - Batch Reactor
MATLAB Solution Demonstration

The MATLAB m-file thus created also provides tabular output within the MATLAB editor.



Problem 4 - Differential Equations - Batch Reactor
POLYMATH/MATLAB Solution EXERCISE

1) Obtain the Polymath Solution with options to generate MATLAB Code

Click here for Polymath Solution File

DifferentialEquations01.pol

2) Start MATLAB, Open MATLAB Template for Multiple Differential Equations, Enter MATLAB Code from Polymath, and Solve Problem.

Click here for MATLAB files that need to be placed in your working MABLAB directory. For MATLAB, a right mouse click should be used to 'Save Target As..' to indicate the location of your desired working directory for MATLAB.

MultipleDEQtemplate.m **MATLAB01.m**

Workshop Problem 5

Numerical Solution: Linear and Nonlinear Regression

Title: Vapor Pressure Data

Software Used:

Polymath and Excel

Problem 5 – Regressions - Vapor Pressure Data

The Clapeyron equation is commonly used to correlate vapor pressure (P_v) with absolute temperature (T) in °C where ΔH_v is the latent heat of vaporization and R is the gas constant. This equation can be written with two parameters, D and E, when ΔH_v is constant with temperature. P_v is typically in mm Hg and T is usually in °C.

$$\log P_v = -\frac{\Delta H_v}{RT} + B = \frac{D}{T} + E$$

Another common vapor pressure correlation is the Antoine equation, which utilizes three parameters given by A, B, and C.

$$\log P_v = A + \frac{B}{T + C}$$

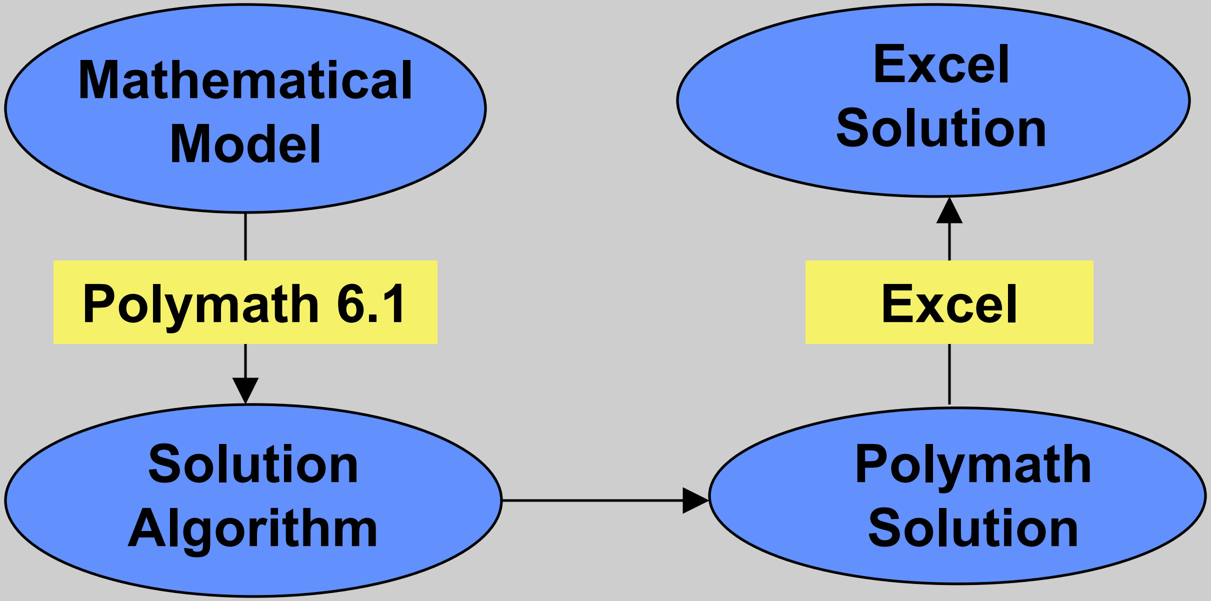
Determine the values of D and E for the Clapeyron equation and the values of A, B, and C for the Antoine equation using the data given below. Compare these correlations.

Vapor Pressure Data

T (°C)	41.77	56.69	69.66	84.78	95.65	100.18	114.79	123.40
P (mm Hg)	100	200	300	500	700	900	1200	1500

Problem 5 – Regressions - Vapor Pressure Data

Regressions – Linear and Nonlinear



Problem 5 – Regressions - Vapor Pressure Data

POLYMATH Clapeyron Equation Linear Regression **EXERCISE**

Utilize the Polymath Regression Program to input the data to the Data Table.

Create a new column for a variable logP that is the log of the pressure.

$$logP = \log(P)$$

Then create another column for a variable invT that is the inverse of the temperature in ^{o}C.

$$InvT = 1/T$$

POLYMATH 6.10 Educational Release - [Data Table]

File Program Edit Row Column Format Analysis Examples

R001 : C001 P 100

	P	T	C03	C04	C05	C06	C07
01	100	41.77					
02	200	56.69					
03	300	69.66					
04	500	84.78					
05	700	95.65					
06	900	100.18					
07	1200	114.79					
08	1500	123.40					

R001 : C003 logP = log(P)

	P	T	logP	invT	C05	C06	C07
01	100	41.77	2.	0.0239406			
02	200	56.69	2.30103	0.0176398			
03	300	69.66	2.477121	0.0143554			
04	500	84.78	2.69897	0.0117952			
05	700	95.65	2.845098	0.0104548			
06	900	100.18	2.954243	0.009982			
07	1200	114.79	3.079181	0.0087116			
08	1500	123.40	3.176091	0.0081037			

Problem 5 – Regressions - Vapor Pressure Data

POLYMATH/Excel Solution EXERCISE

Utilize the Polymath Regression Program to make a Linear Regression of logP versus invTK to yield the parameters D and E of the Clapeyron equation.

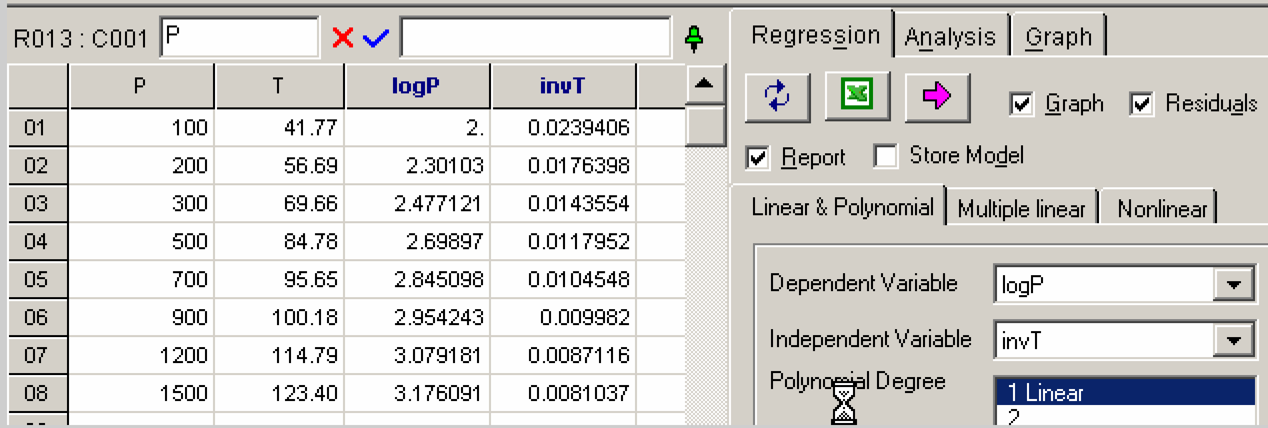
E = a0 = 3.658

D = a1 = -73.61

Click here for Polymath Problem Data File

OR

Click here for Polymath Solution File



	P	T	logP	invT
01	100	41.77	2.	0.0239406
02	200	56.69	2.30103	0.0176398
03	300	69.66	2.477121	0.0143554
04	500	84.78	2.69897	0.0117952
05	700	95.65	2.845098	0.0104548
06	900	100.18	2.954243	0.009982
07	1200	114.79	3.079181	0.0087116
08	1500	123.40	3.176091	0.0081037

Results

Model: logP = a0 + a1*invT

Variable	Value	95% confidence
a0	3.657529	0.2373364
a1	-73.61662	16.88797

General

Regression including a free parameter

Number of observations = 8

Statistics

R^2	0.949908
R^2adj	0.9415594
Rmsd	0.0300589
Variance	0.0096377

Source data points and calculated data points

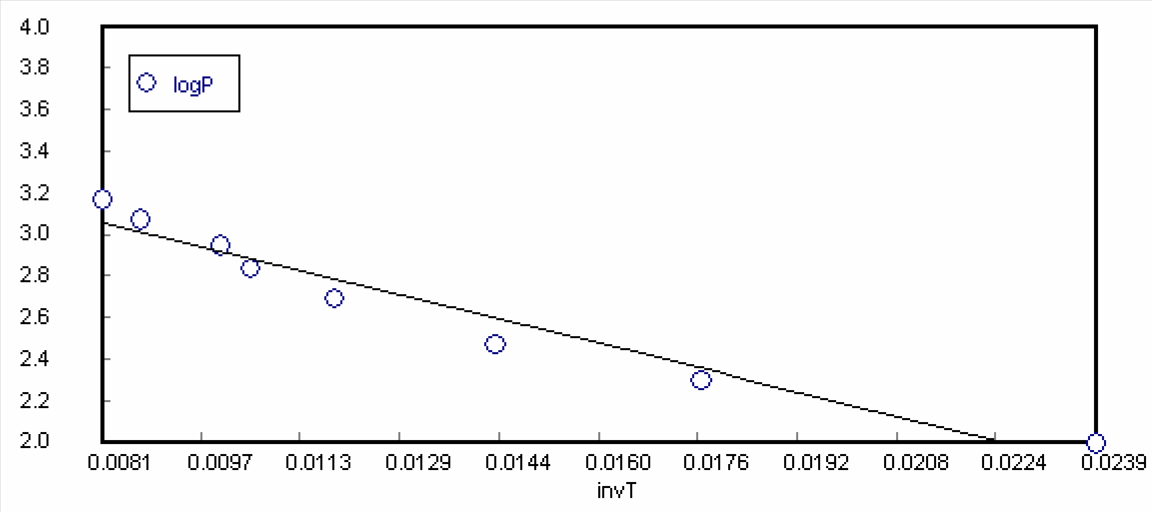
	invT	logP	logP calc	Delta logP
1	0.0239406	2	1.895103	0.1048967
2	0.0176398	2.30103	2.358947	-0.0579169
3	0.0143554	2.477121	2.600733	-0.1236123
4	0.0117952	2.69897	2.789207	-0.0902366
5	0.0104548	2.845098	2.887882	-0.0427843
6	0.009982	2.954243	2.922688	0.0315547
7	0.0087116	3.079181	3.016211	0.0629702
8	0.0081037	3.176091	3.060962	0.1151286

Polymath Data File is RegressionData01.pol   **Polymath Solution File is Regression01.pol**

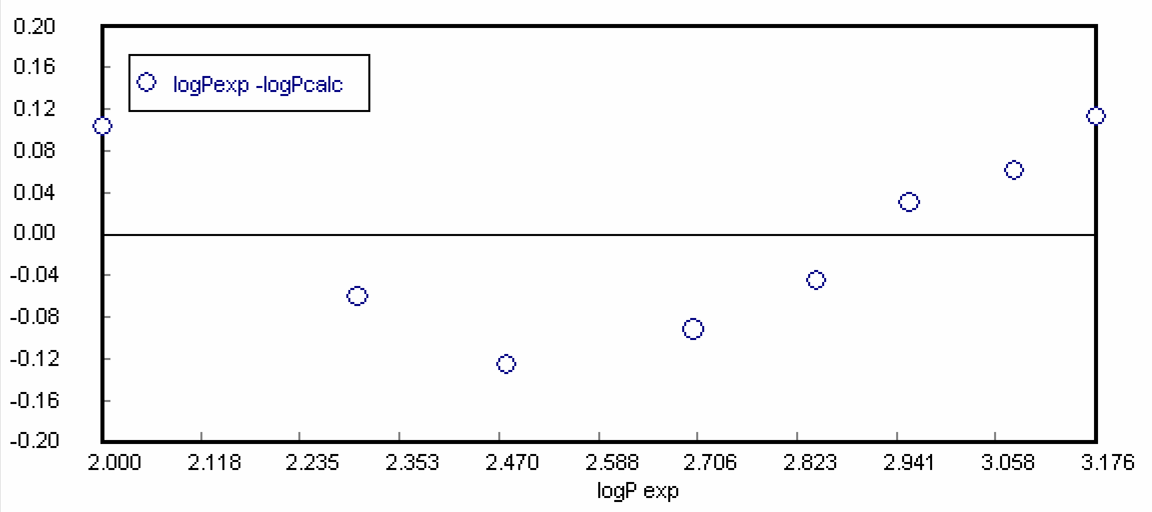
Problem 5 – Regressions - Vapor Pressure Data

POLYMATH/Excel Solution EXERCISE

The Graph Option from the Polymath Regression Program indicates a reasonable representation of the data.



However, the Residuals Plot Option shows a trend in the errors.



Problem 5 – Regressions - Vapor Pressure Data

POLYMATH/Excel Solution EXERCISE

Utilize the Export to EXCEL Option from the Polymath Regression Program to make a Linear Regression of logP versus invTK. The results, shown below, are essentially the same as those obtained with Polymath.

	A	B	C	D	E	F	G	H	I
1	POLYMATH Polynomial Regression Migration Document								
2							Linear Regression. Including a free parameter.		
3	invT	logP	logP calc	logP residual	logP residual ^2			a1	a0
4	0.0239406	2	1.895103293	-0.104896707	0.011003319		Coefficients	-73.6166	3.657529
5	0.0176398	2.30103	2.358946908	0.057916908	0.003354368		Std.dev.s	6.9015	0.096991
6	0.0143554	2.477121	2.600733343	0.123612343	0.015280011		R2, SE (y)	0.949908	0.098172
7	0.0117952	2.69897	2.789206619	0.090236619	0.008142647		95% conf. int.	16.88797	0.237336
8	0.0104548	2.845098	2.88788234	0.04278434	0.0018305		Variance	0.009638	
9	0.009982	2.954243	2.922688279	-0.031554721	0.0009957		Sum of Squares	0.057826	
10	0.0087116	3.079181	3.016210836	-0.062970164	0.003965242		Model	logP = a1 * invT + a0	
11	0.0081037	3.176091	3.060962381	-0.115128619	0.013254599				
12									

Click here for EXCEL Problem Solution File

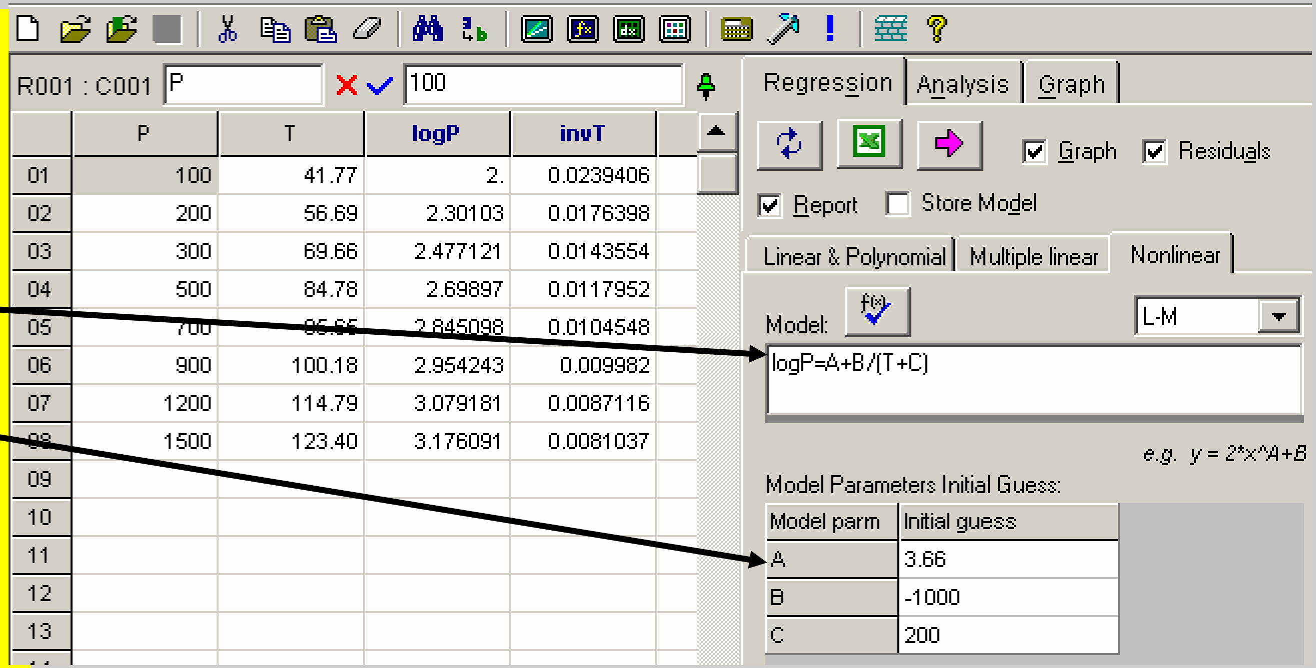
(for those who need it)

File is Regression01.xls

Problem 5 – Regressions - Vapor Pressure Data

POLYMATH/Excel Solution EXERCISE

Utilize the Polymath Regression Program to make a Nonlinear Regression of the Antoine Equation. Use the initial guesses as shown. Plot the Graph and the Residual for this regression.



Click here for Polymath Problem Data File

File is RegressionData01.pol

OR

Click here for Polymath Solution File

File is Regression02.pol

Model: logP = A+B/(T+C)

Variable	Initial guess	Value	95% confidence
A	3.66	6.376557	2.317467
B	-1000.	-971.542	1202.155
C	200.	180.4905	159.0569

Nonlinear regression settings

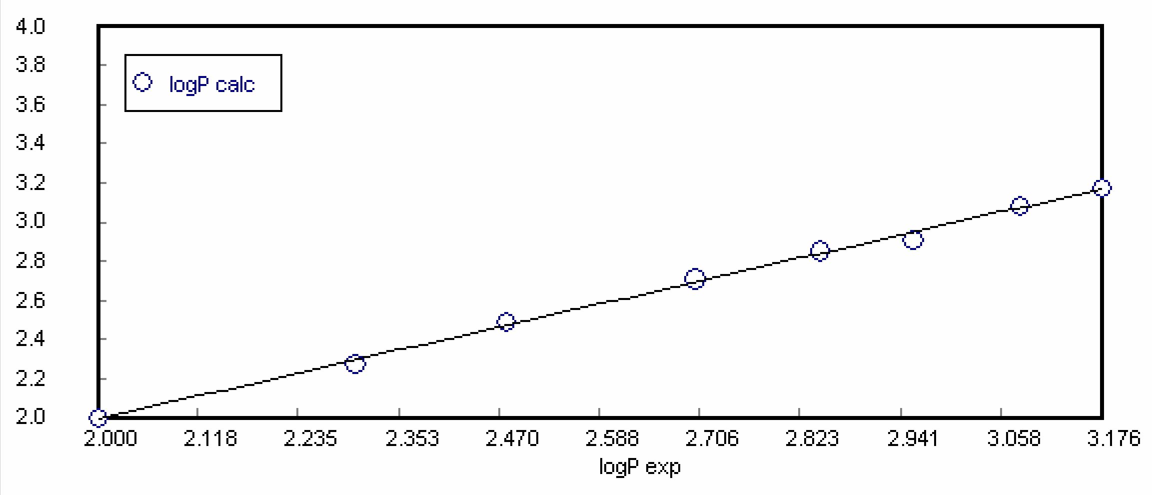
Max # iterations = 64

Precision

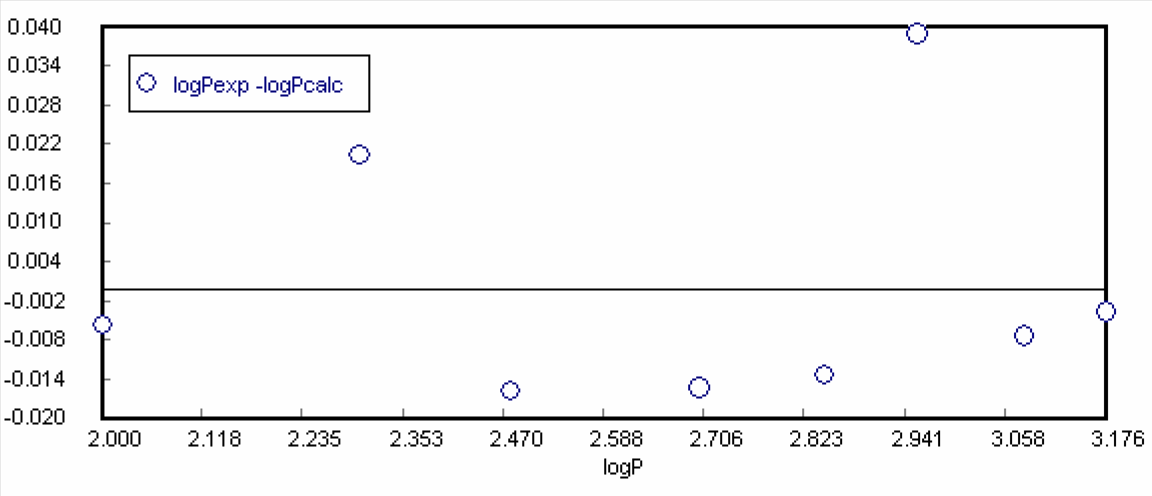
R^2	0.9976599
R^2adj	0.9967238
Rmsd	0.0064969
Variance	0.0005403

Problem 5 – Regressions - Vapor Pressure Data
POLYMATH/Excel Solution EXERCISE

The Graph Option from the Polymath Nonlinear Regression Program indicates a reasonable representation of the data.



The Residuals Plot Option shows a more random distribution of the errors.

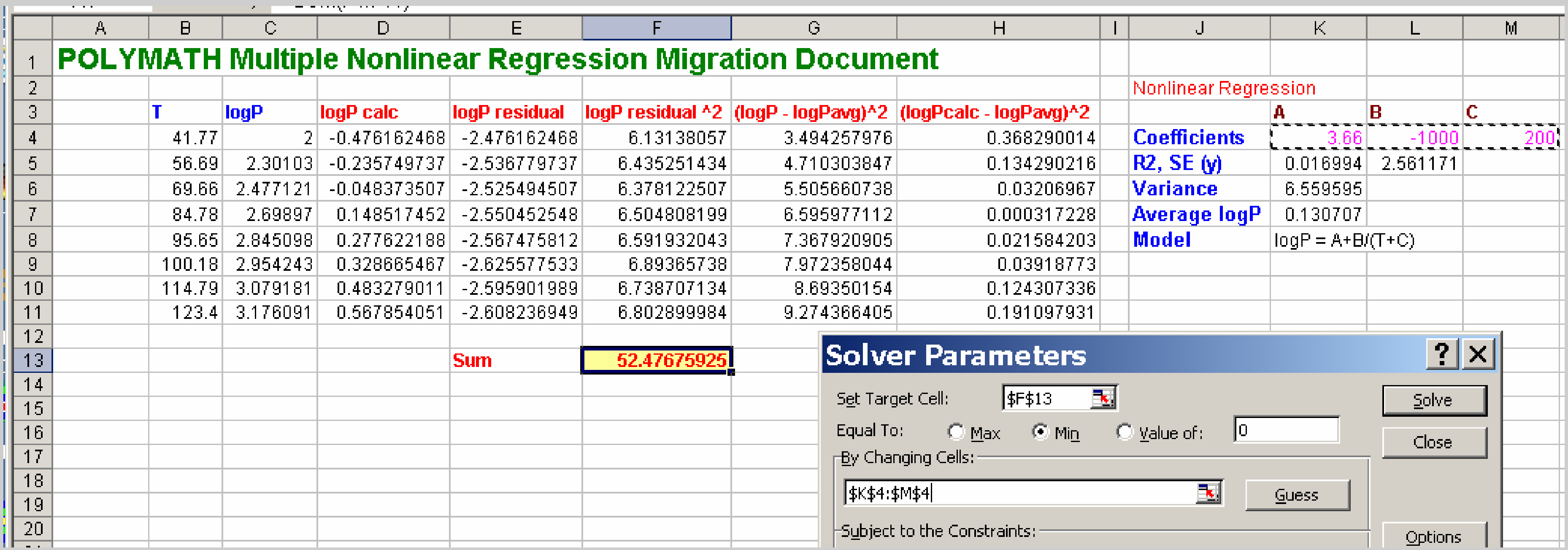


These graphs plus the lower variance for the Antoine equation indicate that the data are well represented.

Problem 5 – Regressions - Vapor Pressure Data

POLYMATH/Excel Solution EXERCISE

Utilize the Export to EXCEL Option from the Polymath Regression Program to make a Nonlinear Regression of logP versus invTK. The results, shown below, are essentially the same as those obtained with Polymath. Note that the EXCEL Add-In Solver must be used to complete the Nonlinear Regression.



POLYMATH Multiple Nonlinear Regression Migration Document

	T	logP	logP calc	logP residual	logP residual ^2	(logP - logPavg)^2	(logPcalc - logPavg)^2		J	K	L	M
2									Nonlinear Regression			
3										A	B	C
4	41.77	2	-0.476162468	-2.476162468	6.13138057	3.494257976	0.368290014		Coefficients	3.66	-1000	200
5	56.69	2.30103	-0.235749737	-2.536779737	6.435251434	4.710303847	0.134290216		R2, SE (y)	0.016994	2.561171	
6	69.66	2.477121	-0.048373507	-2.525494507	6.378122507	5.505660738	0.03206967		Variance	6.559595		
7	84.78	2.69897	0.148517452	-2.550452548	6.504808199	6.595977112	0.000317228		Average logP	0.130707		
8	95.65	2.845098	0.277622188	-2.567475812	6.591932043	7.367920905	0.021584203		Model	logP = A+B/(T+C)		
9	100.18	2.954243	0.328665467	-2.625577533	6.89365738	7.972358044	0.03918773					
10	114.79	3.079181	0.483279011	-2.595901989	6.738707134	8.69350154	0.124307336					
11	123.4	3.176091	0.567854051	-2.608236949	6.802899984	9.274366405	0.191097931					
13				Sum	52.47675925							

Problem 5 – Regressions - Vapor Pressure Data

POLYMATH/Excel Solution EXERCISE

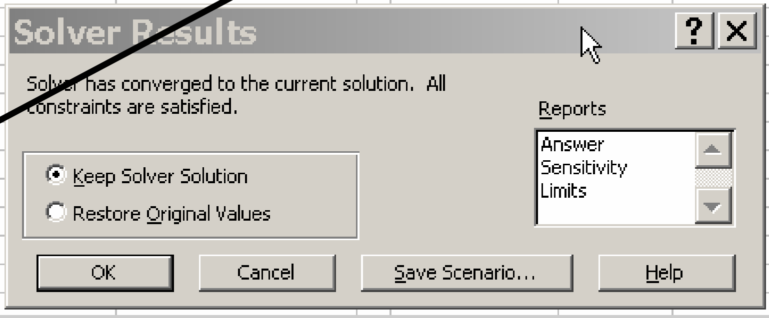
The EXCEL Nonlinear Regression results obtained with Solver, shown below in spreadsheet and magnified view, are essentially the same as those obtained with Polymath.

POLYMATH Multiple Nonlinear Regression Migration Document

T	logP	logP calc	logP residual	logP residual ^2	(logP - logPavg)^2	(logPcalc - logPavg)^2
41.77	2	2.006165146	0.006165146	3.8009E-05	0.478129438	0.469641432
56.69	2.30103	2.280127127	-0.020902873	0.00043693	0.152442647	0.169202172
69.66	2.477121	2.492149822	0.015028822	0.000225865	0.045945084	0.039728152
84.78	2.69897	2.713535931	0.014565931	0.000212166	5.62644E-05	0.000486948
95.65	2.845098	2.857928733	0.012830733	0.000164628	0.023601856	0.027708828
100.18	2.954243	2.914848329	-0.039394671	0.00155194	0.069050152	0.049898305
114.79	3.079181	3.086683783	0.007502783	5.62918E-05	0.150320561	0.156194691
123.4	3.176091	3.180313475	0.004222475	1.78293E-05	0.234858441	0.238908878
			Sum	0.00270366		

Nonlinear Regression

	A	B	C
Coefficients	6.435009	-1002.14	184.5053
R2, SE (y)	0.997769	0.018384	
Variance	0.000338		
Average logP	2.691469		
Model	logP = A+B/(T+C)		



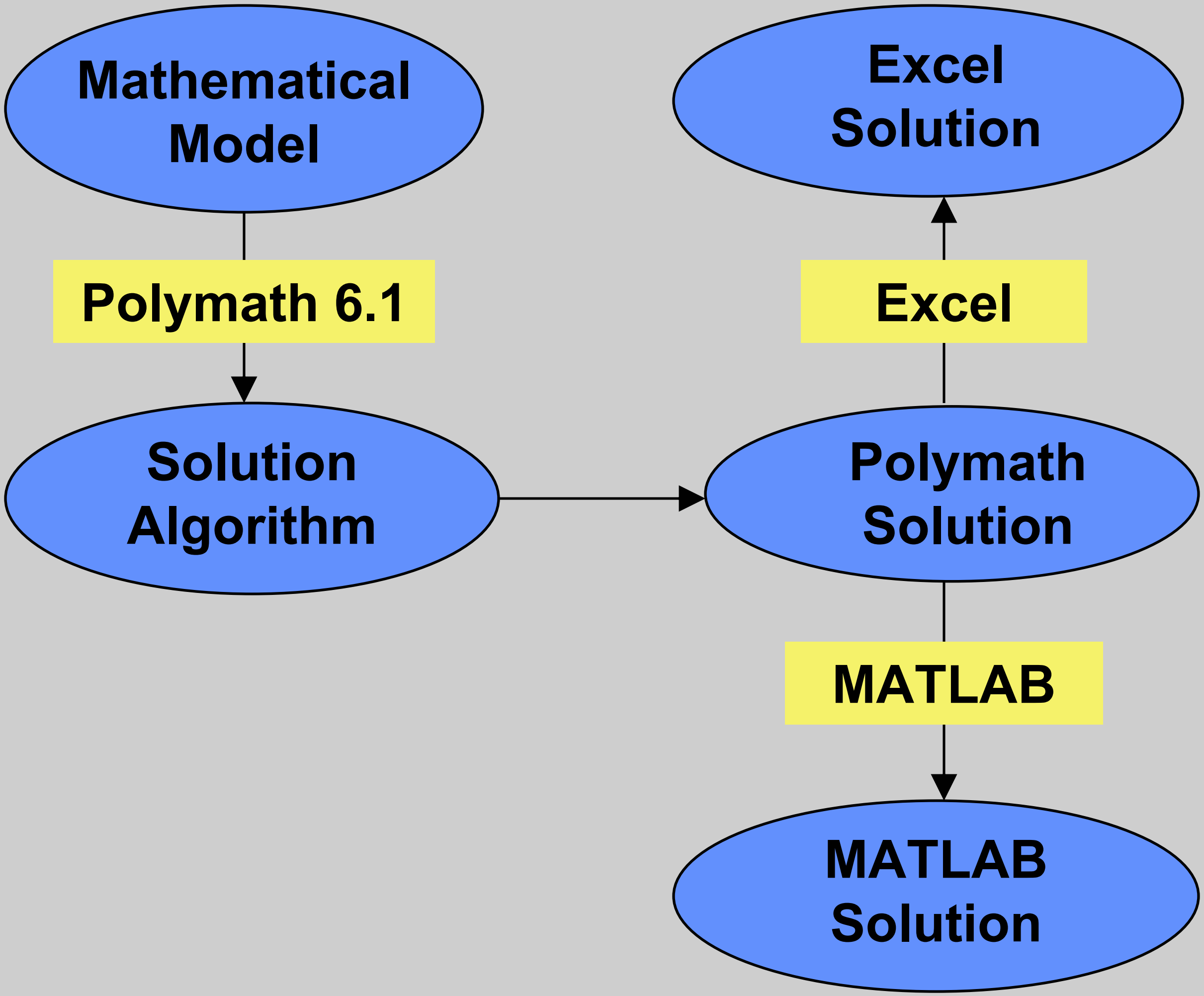
Nonlinear Regression

	A	B	C
Coefficients	6.435009	-1002.138	184.5053
R2, SE (y)	0.997769	0.018384	
Variance	0.000338		
Average logP	2.691469		
Model	logP = A+B/(T+C)		

Click here for EXCEL Solution File

File is Regression02.xls

SUMMARY - Desktop Problem Solving Involving Polymath, Excel and MATLAB



Happy Future Problem Solving!