Introduction to Problem Solving with POLYMATH, Excel and MATLAB

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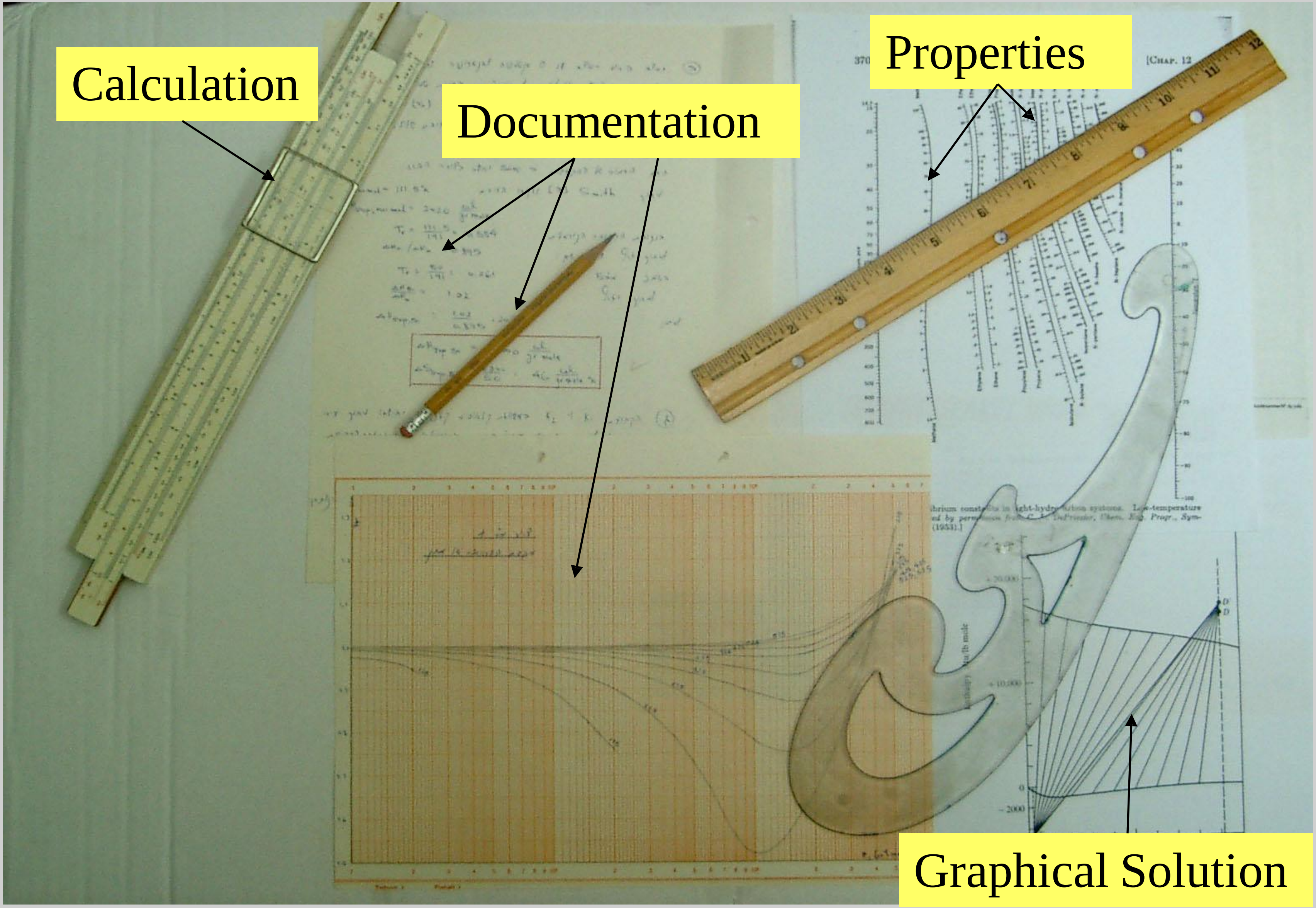
Engineer's Tools - THEN in early 1960's

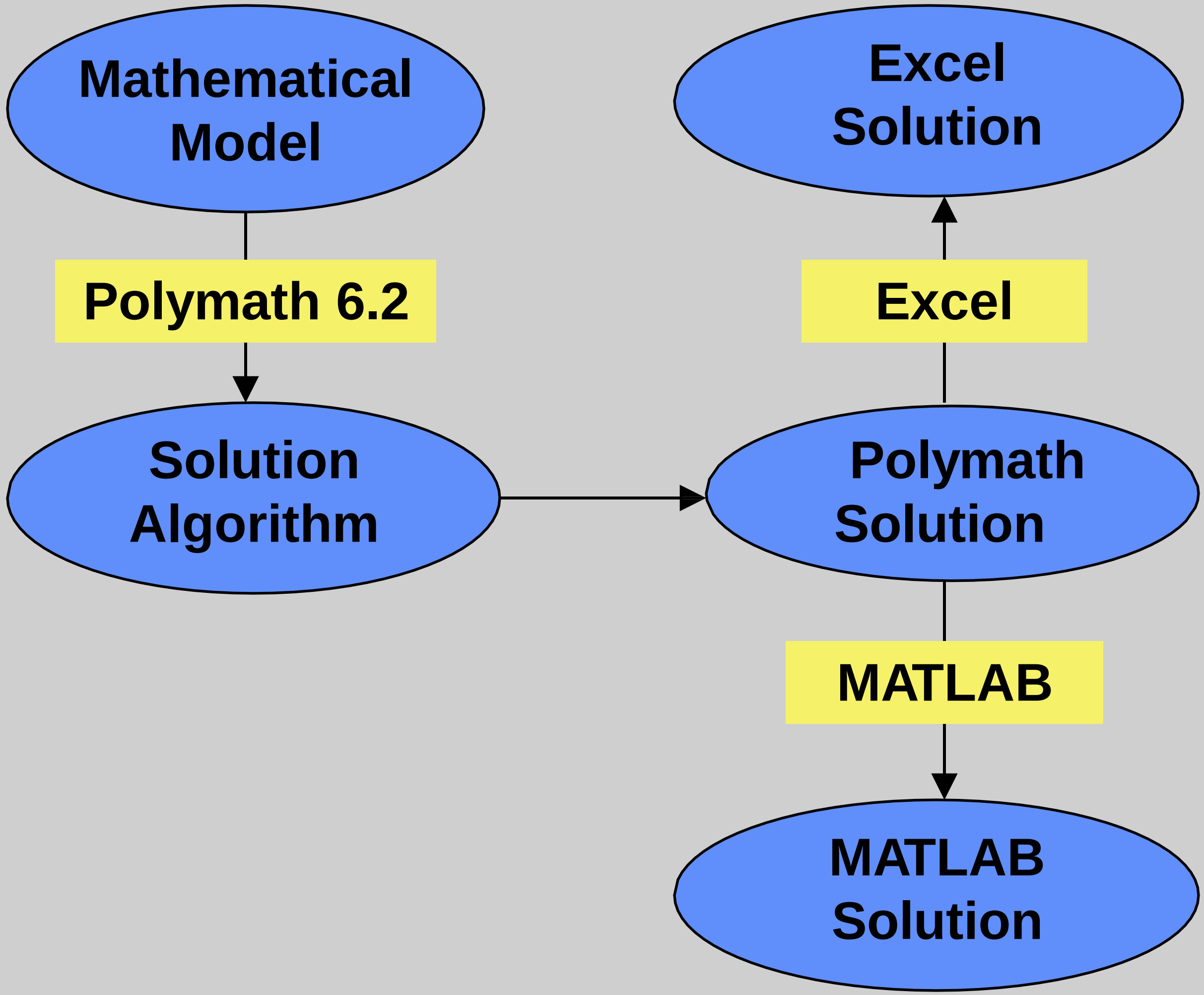


NOW! Increasing Problem Solving Efficiency and Capabilities with a Novel Combination of Software Tools

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

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

Desktop Problem Solving Involving Polymath, Excel, and MATLAB



POLYMATH Educational 6.2

Numerical Computation Package

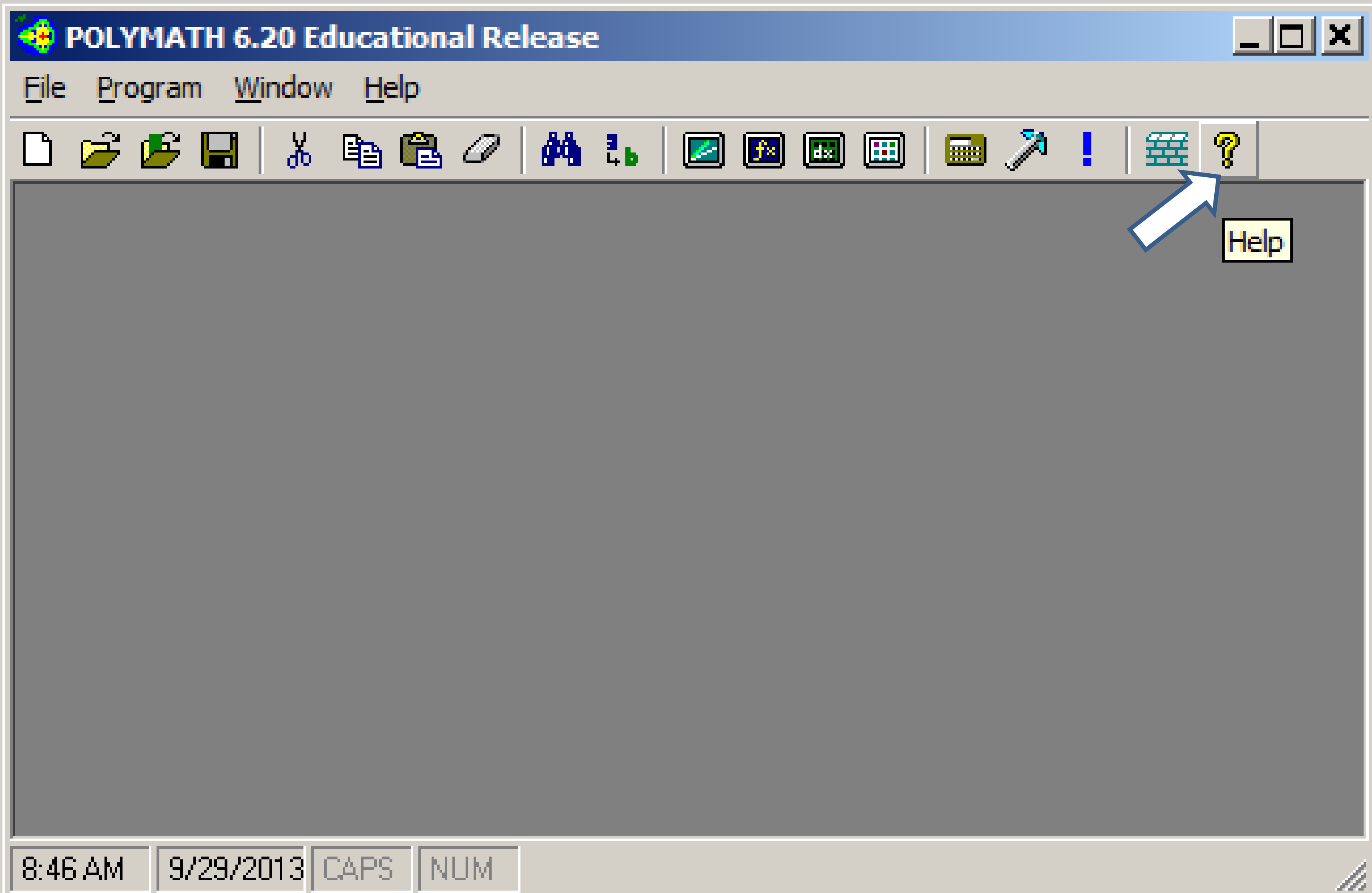
- Extremely Easy-to-Use
- Excellent Problem Solving Capabilities
  - Linear Equations – 100 (264) Professional Version
  - Nonlinear Equations – 30 (300)
  - Differential Equations – 30 (300)
  - Regressions (Linear, Polynomial, Multiple Linear, Nonlinear) - 301 data points (1001)

    - **Automated Export of Problems to Working Excel Spreadsheets Enabling Stand-Alone Excel Calculations (Provides Add-In for Excel that Solves ODEs.**
    - **Enables the Use MATLAB by Automatically Translating Problems to Code for Use in M-files.**

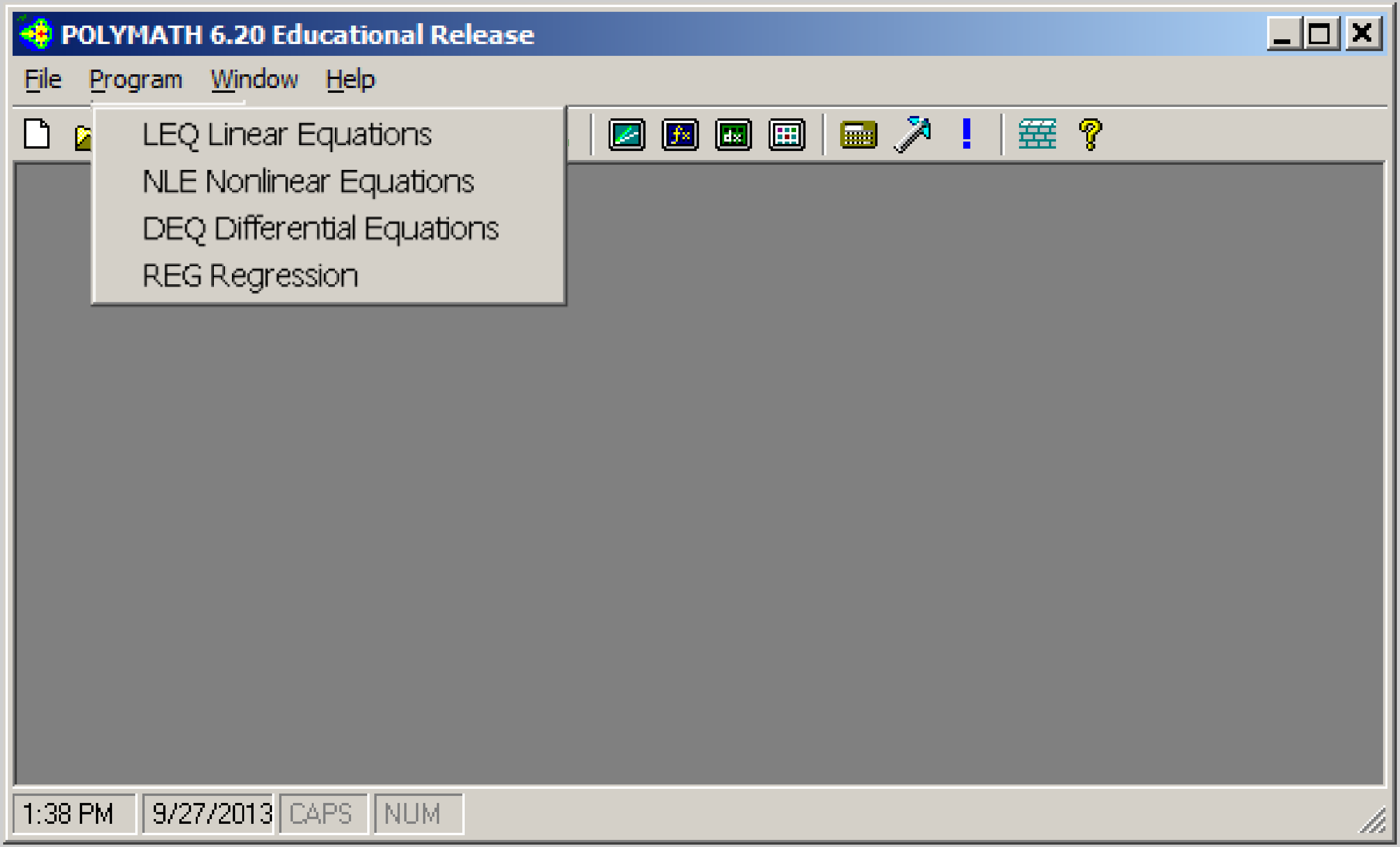
POLYMATH 6.2 features include:

- 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 AND 64-BIY WINDOWS OPERATING SYSTEMS INCLUDING WIN 8
- 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

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

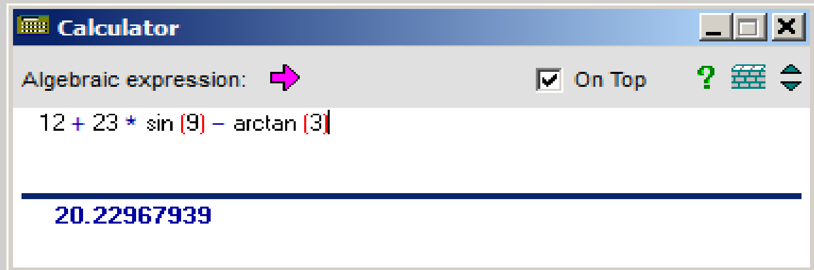


Polymath Software has Four Main Programs

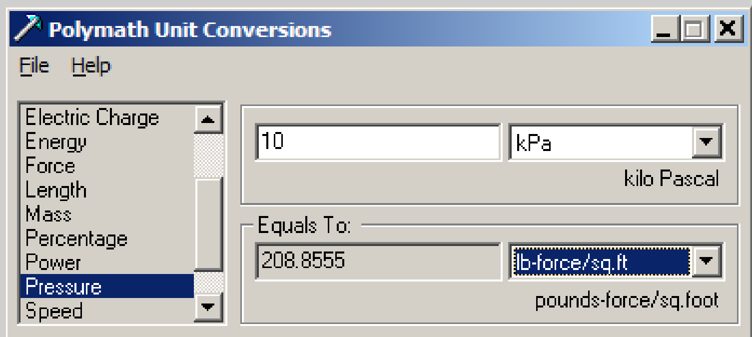


Polymath Software also has Three Utilities:

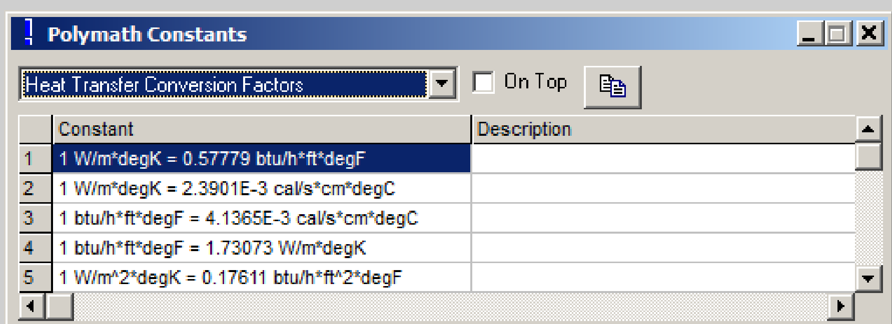
- Calculator



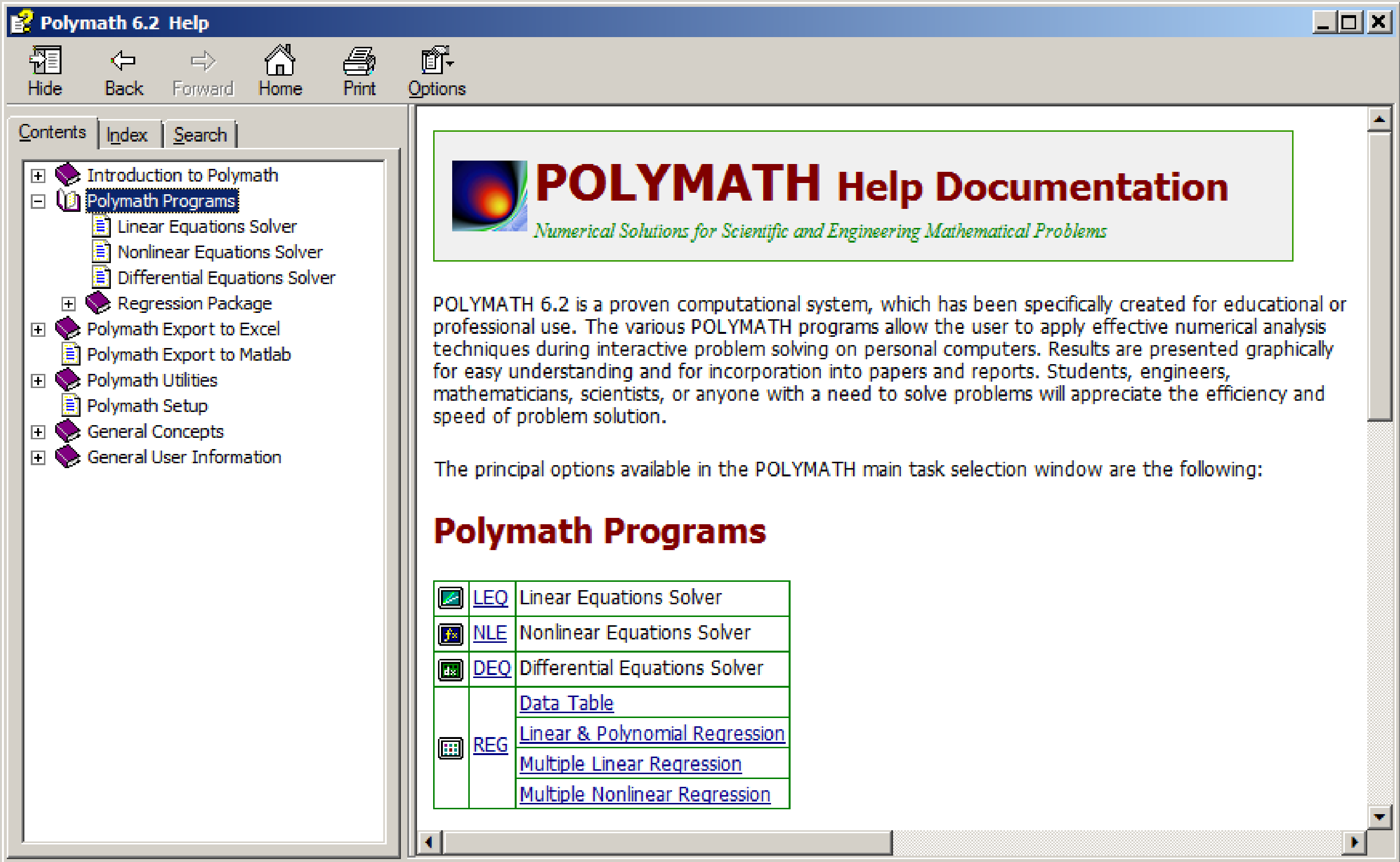
- Units Converter



- Scientific Constants



Polymath Software has Extensive HELP



Open Polymath on your computer and look at the HELP to learn more about the program.

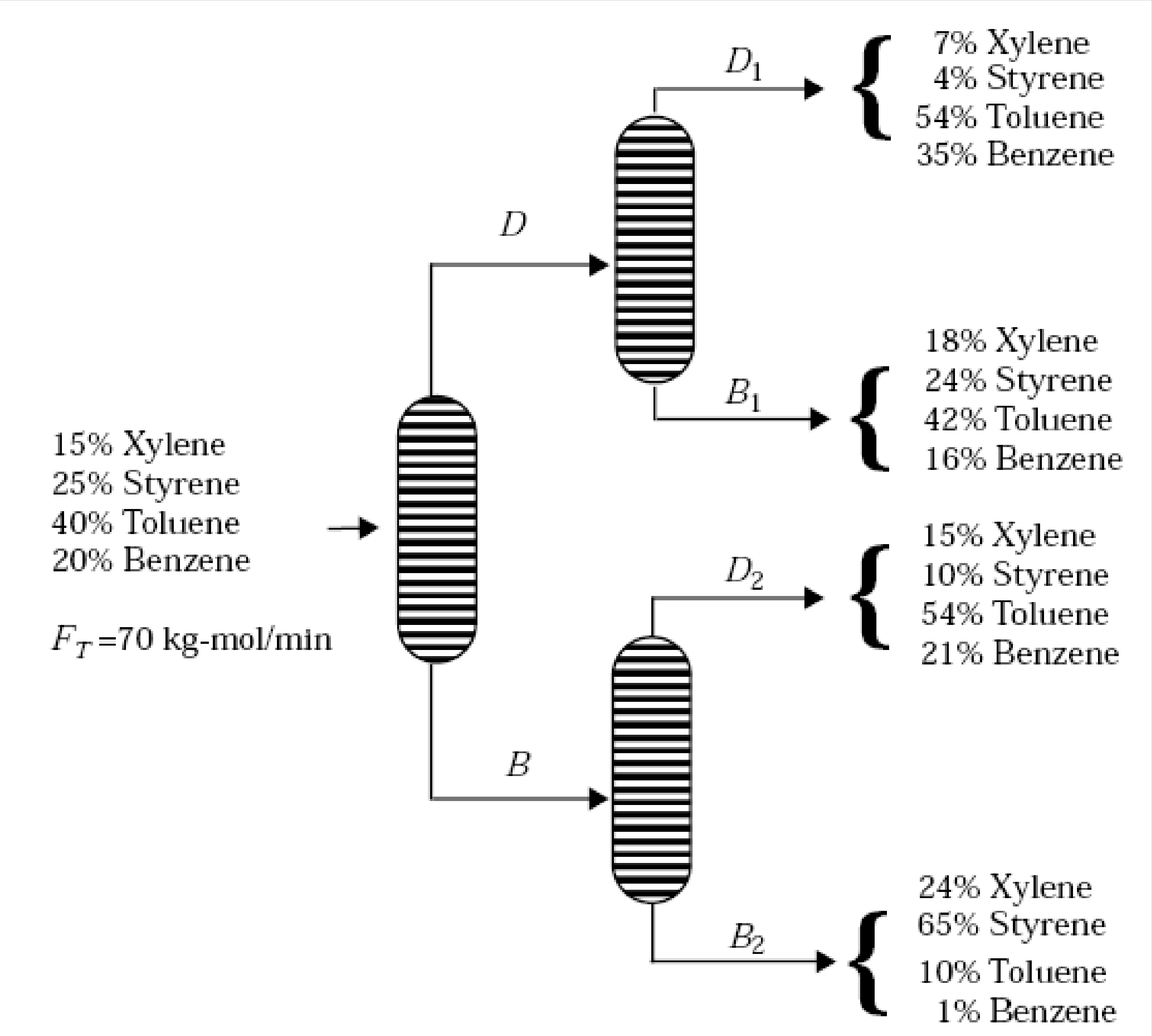
You can open Polymath from the Programs Menu (Start/Polymath Software directory) and click on the question mark icon on the main Polymath display to access HELP. Alternately you can open Polymath from the Attachements list on this Acrobat file by clicking on the paper clip and then double clicking on Polymath.pol.

Introductory 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. Regression – Hardening of Concrete (Multiple Linear Regression) - Polymath, Excel
6. Regressions – Vapor Pressure Data (Linear and Nonlinear) - Polymath, Excel

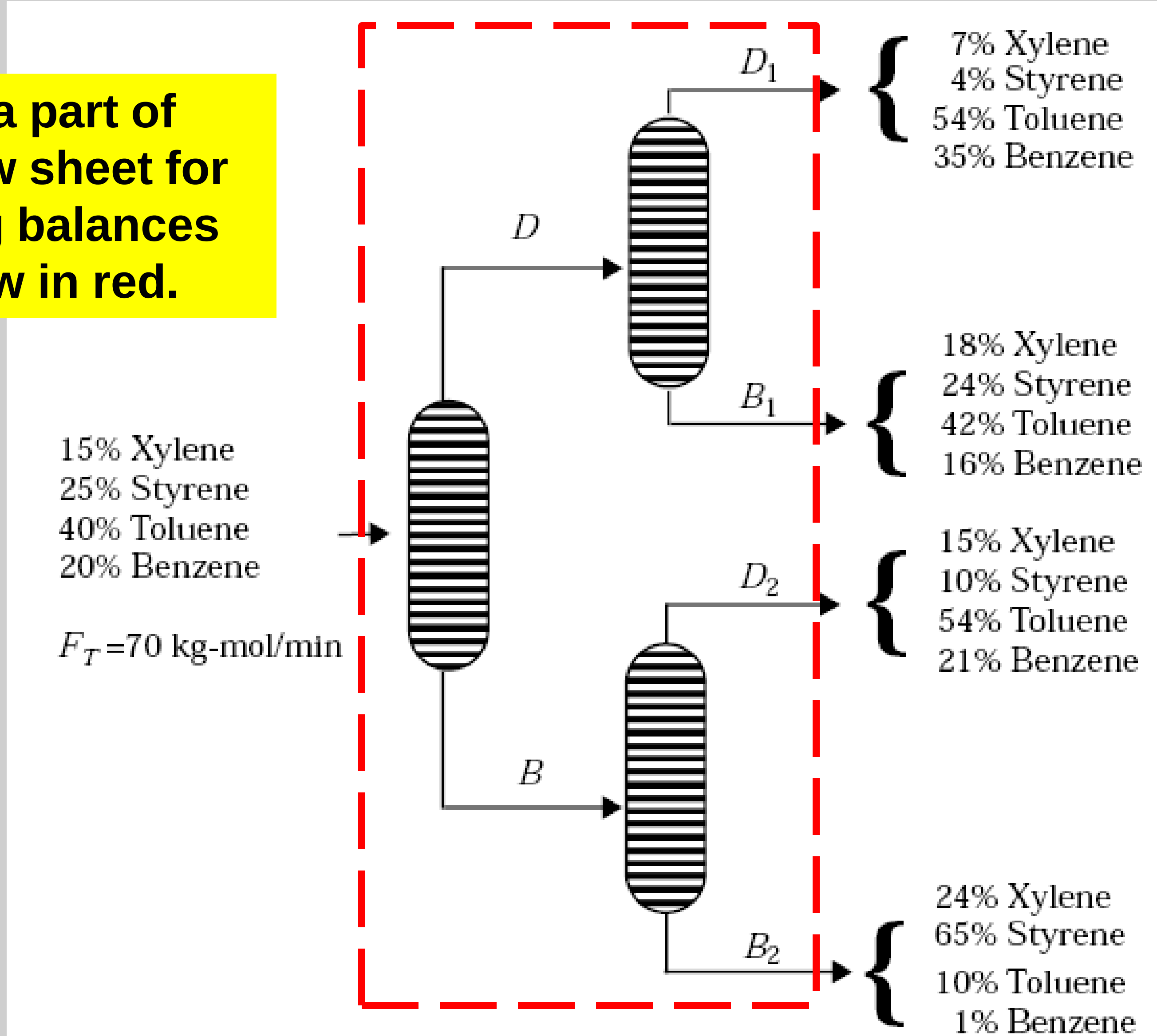
Problem 1 – Material Balances for Distillation Columns

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



Linear Equations – Material Balance Problem
Determine the Flow Rates B_1, D_1, B_2, and D_2

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



Linear Equations – Material Balance Problem to Determine the Flow Rates B_1, D_1, B_2, and D_2

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

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

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

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

Make Balances on Each Species:
Xylene
Styrene
Toluene
Benzene

Linear Equations – Material Balance Problem to Determine the Flow Rates B_1, D_1, B_2, and D_2

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

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

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

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

Demonstrate the Actual Polymath Program

Let's Go to POLYMATH with the program ready for solution. Double click on file name from attachments list.

POLYMATH – This file name is LinearEquation01.pol

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).

$$R = 0.08206$$

$$T_c = 304.2$$

$$P_c = 72.9$$

$$T = 350$$

$$V = 0.6$$

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

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

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

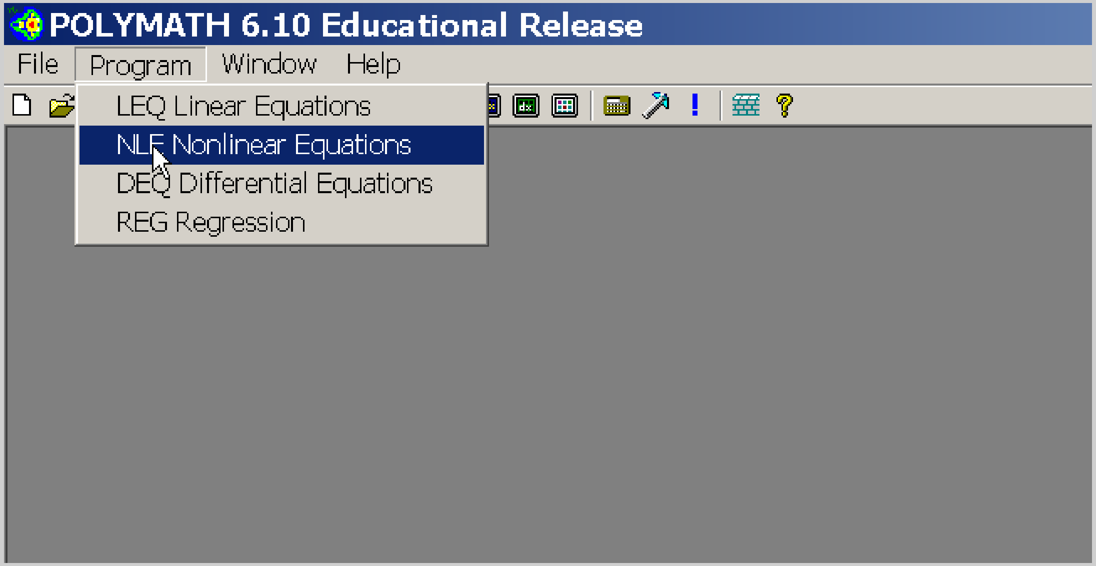
Problem 2 - Explicit Calculations for an Equation of State

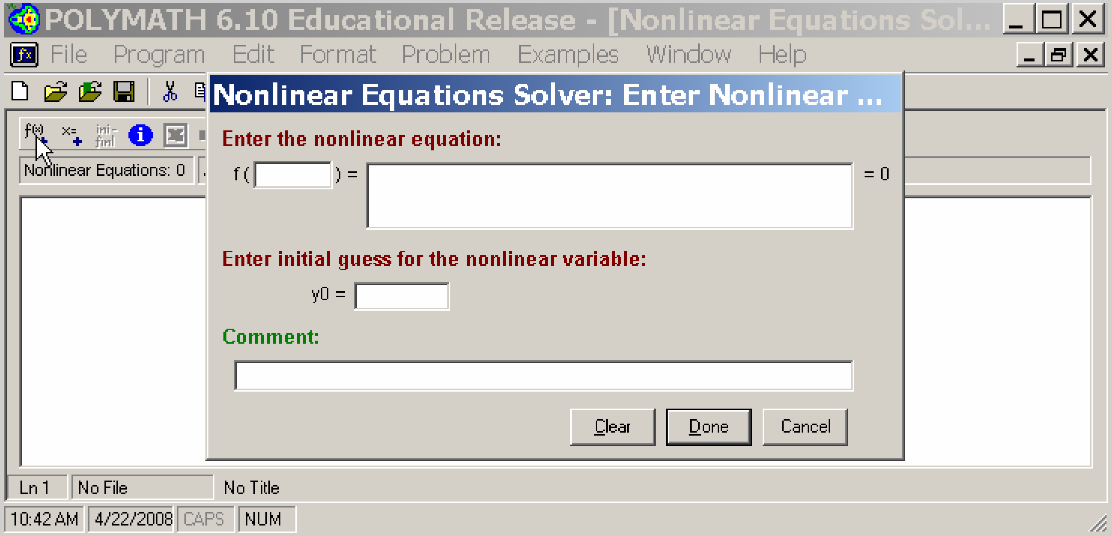
Polymath Solution Demonstration

Enter the equations into Polymath.

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

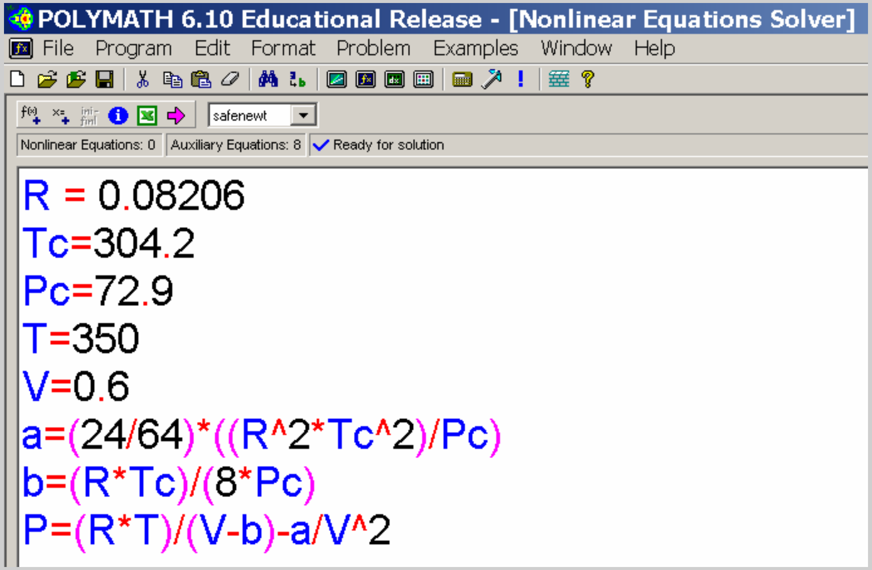
Use templates or full screen editor.





Problem 2 – Explicit Calculations for an Equation of State

Polymath Solution Exercise



POLYMATH 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

Use Polymath to enter and solve equations

OR

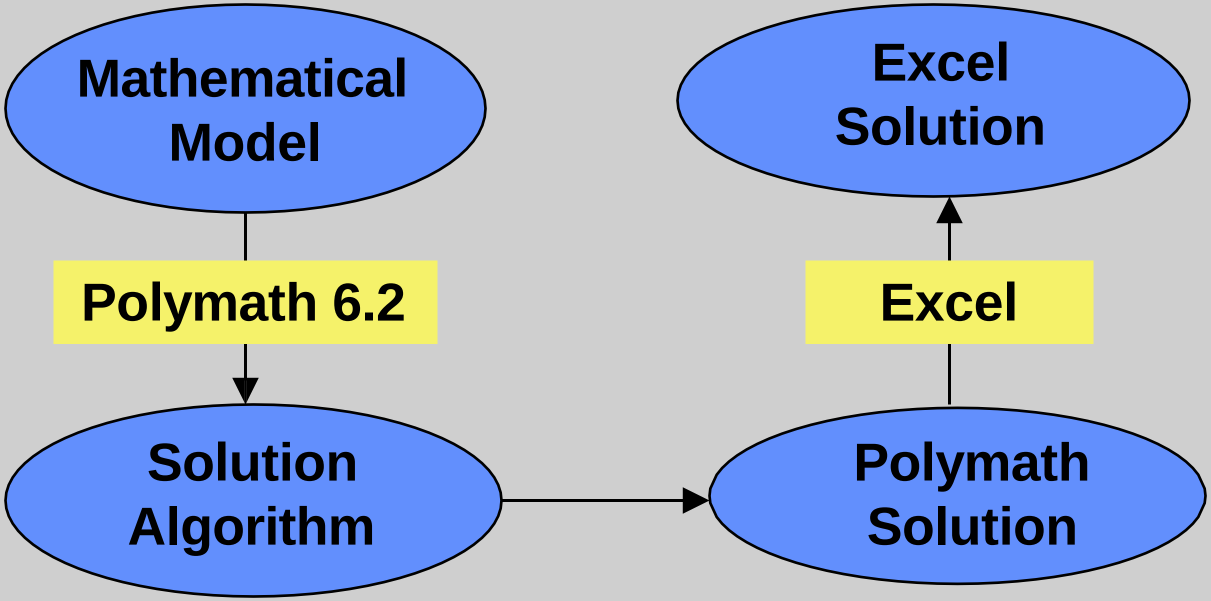
Execute this problem solution with Polymath and verify the given Polymath Report solution.

PolymathNonlinear.pol

NonlinearEquations01.pol

Problem 2 - Explicit Calculations for an Equation of State

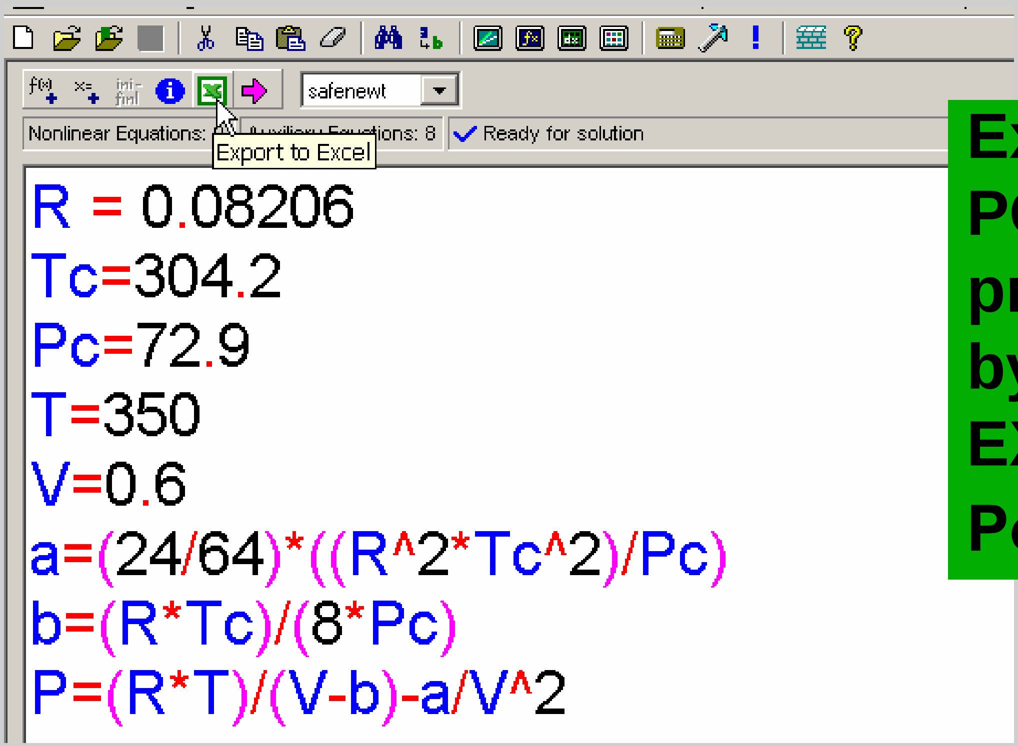
Polymath Solution then Export to Excel for Solution



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 in the Polymath Program.

Hint – Be sure to have an open Excel Spreadsheet running on your computer before exporting problem. Open Excel or click on attachment Excel.xls.

Problem 2 – Explicit Calculations for an Equation of State

Polymath Solution then Export to Excel for Solution

Exercise

Microsoft Excel - Book1

File Edit View Insert Format Tools Data Window Help Adobe PDF

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B21

	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

Problem 3 – Pressure Drop Calculation 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 – Pressure Drop Calculation 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

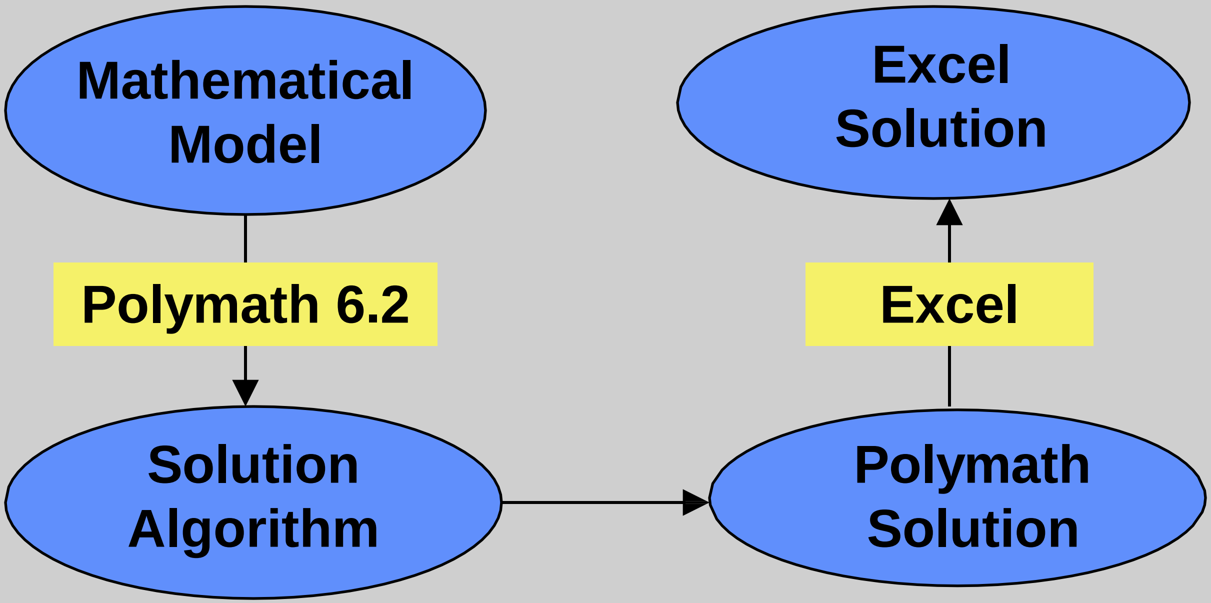
The nonlinear equation is rearranged to equal zero.

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

Problem 3 – Pressure Drop Calculation 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 – Pressure Drop Calculation for Pipe Flow 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 – Pressure Drop Calculation for Pipe Flow Two Nonlinear Equations – Simultaneous Solution with If… Then… Else… Statement

safenewt

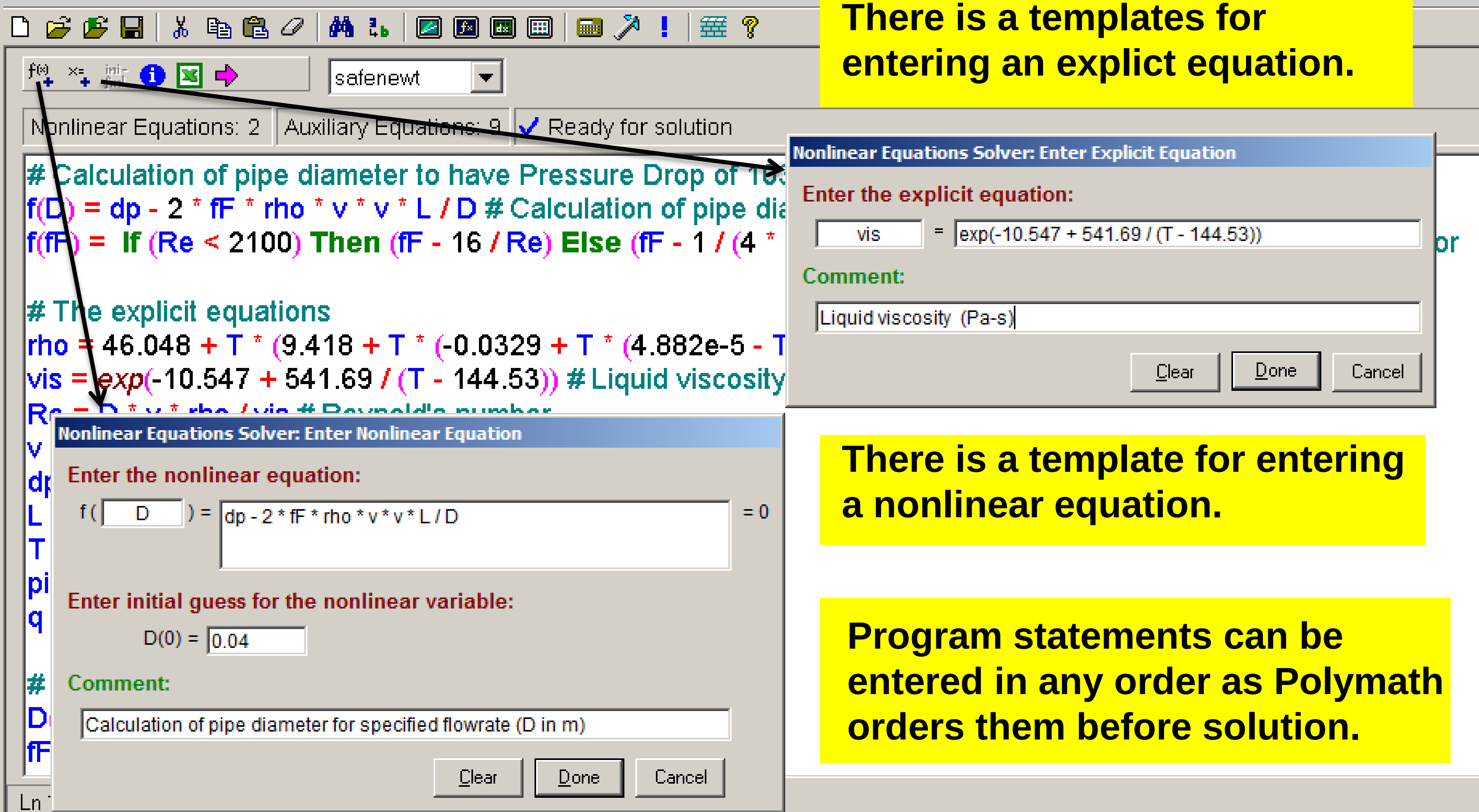
Nonlinear Equations: 2 | Auxiliary Equations: 9 | ✓ Ready for solution

```
# 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 – Pressure Drop Calculation for Pipe Flow Two Nonlinear Equations – Simultaneous Solution with If··· Then··· Else··· Statement



There is a templates for entering an explict equation.

There is a template for entering a nonlinear equation.

Program statements can be entered in any order as Polymath orders them before solution.

Problem 3 – Pressure Drop Calculation for Pipe Flow Two Nonlinear Equations – Simultaneous Solution with If… Then… Else… Statement

The solution is possible when the arrow turns to a red color and is clicked with the mouse.

safenewt

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

```
# Calculation of pipe diameter to have Pressure Drop of 103000 Pa
f(D) = dp - 2 * fF * rho * v * v * L / D # Calculation of pipe diameter fo
f(fF) =  If (Re < 2100) Then (fF - 16 / Re) Else (fF - 1 / (4 * log(Re *
                                                                    actor

# The explicit equations
rho = 46.048 + T * (9.418 + T * (-0.0329 + T * (4.882e-5 - T * 2.895
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 le
T = 25 + 273.15
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
```

Ln 18 | NonLinearEquation02.pol | Calculation of Pipe Diameter

Here is a partial Polymath solution of this problem

Nonlinear Equations Solution #0

File Edit Help

POLYMATH Report | Calculation of Pipe Diameter
Nonlinear Equations | 29-Sep-2013

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

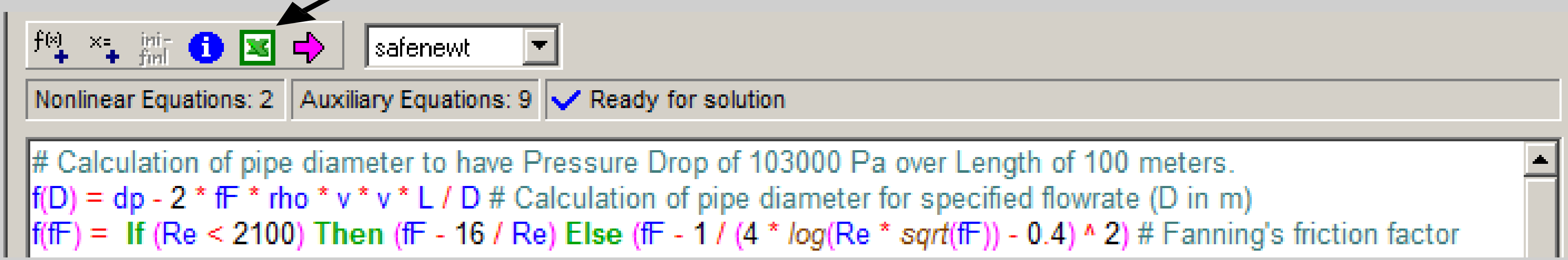
	Variable	Value
1	dp	1.03E+05
2	L	100.
3	pi	3.1416
4	q	0.0025
5	Re	9.097E+04
6	rho	994.5715
7	T	298.15
8	v	2.096491
9	vis	0.0008931

No File | POLYMATH Report

Problem 3 – Pressure Drop Calculation for Pipe Flow

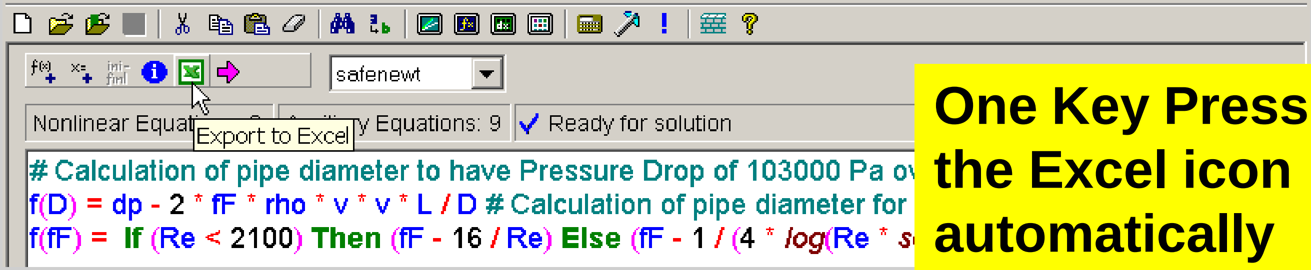
Excel Solution for Two Nonlinear Equations – Simultaneous Solution with If… Then… Else… Logic

Polymath Software has the option of automatically sending a problem to Excel by clicking on the Excel icon where the problem is ready to be solved. For Nonlinear Equations, you will use the Solver Add-In to obtain Excel solution. Excel must be open on your computer.

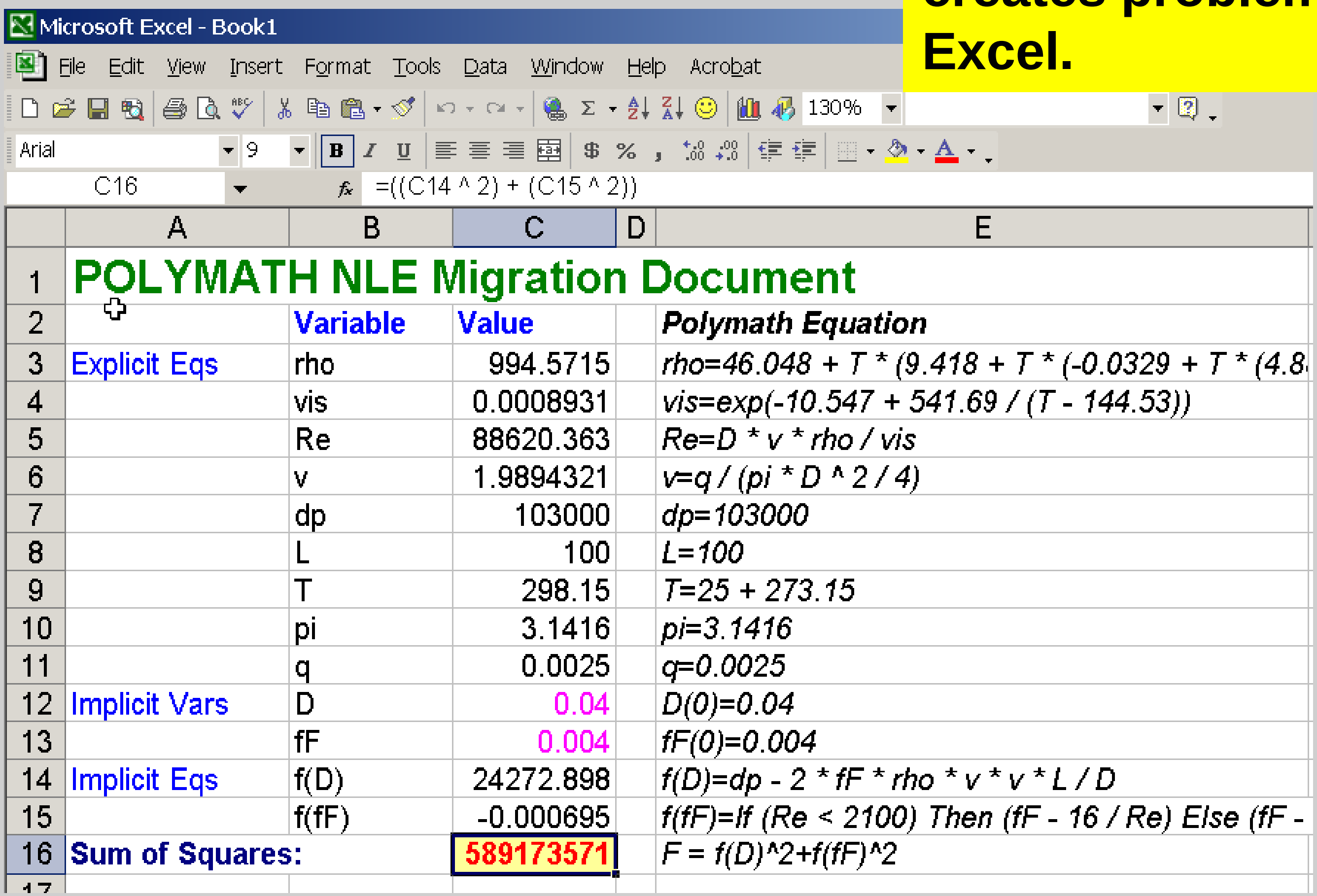


Problem 3 – Pressure Drop Calculation for Pipe Flow

From Polymath



To Excel



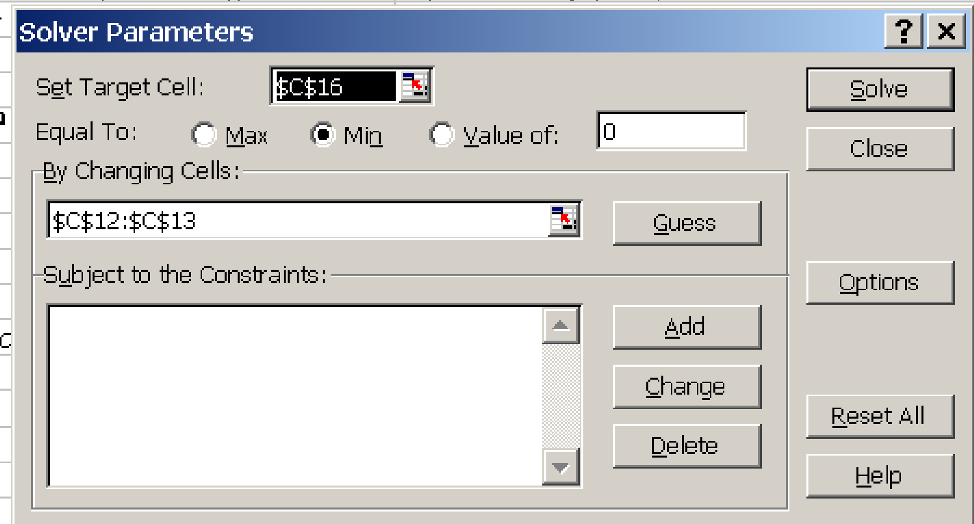
	A	B	C	D	E
1	POLYMATH NLE Migration Document				
2		Variable	Value		Polymath Equation
3	Explicit Eqs	rho	994.5715		rho=46.048 + T * (9.418 + T * (-0.0329 + T * (4.8
4		vis	0.0008931		vis=exp(-10.547 + 541.69 / (T - 144.53))
5		Re	88620.363		Re=D * v * rho / vis
6		v	1.9894321		v=q / (pi * D ^ 2 / 4)
7		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

One Key Press on the Excel icon automatically creates problem in Excel.

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

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*

Note - The Solver display, options, and results vary with the Excel version being used.

Problem 3 – Pressure Drop Calculation for Pipe Flow Two Nonlinear Equations – Simultaneous Solution with If… Then… Else… Statement

Refer to the previously presented Polymath Solution and the Export and Solution of Same Problem in Excel to solve this problem with Polymath and Excel.

First Let's Open an Excel Worksheet

Please open Excel and have Solver Add-In available. This file is Excel.xls

Let's Solve Polymath Problem, Export to Excel, and Solve in Excel

POLYMATH – This file is NonLinearEquation02.pol

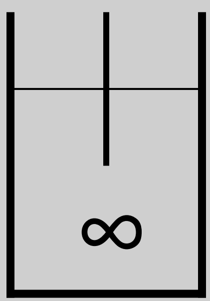
Excel – Ready for Solution file is NonLinearEquation02.xls

Problem 4 – Batch Reactor Kinetics

Differential Equations – Simultaneous ODEs

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

Consider a Batch Reactor that initially has only reactant A



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

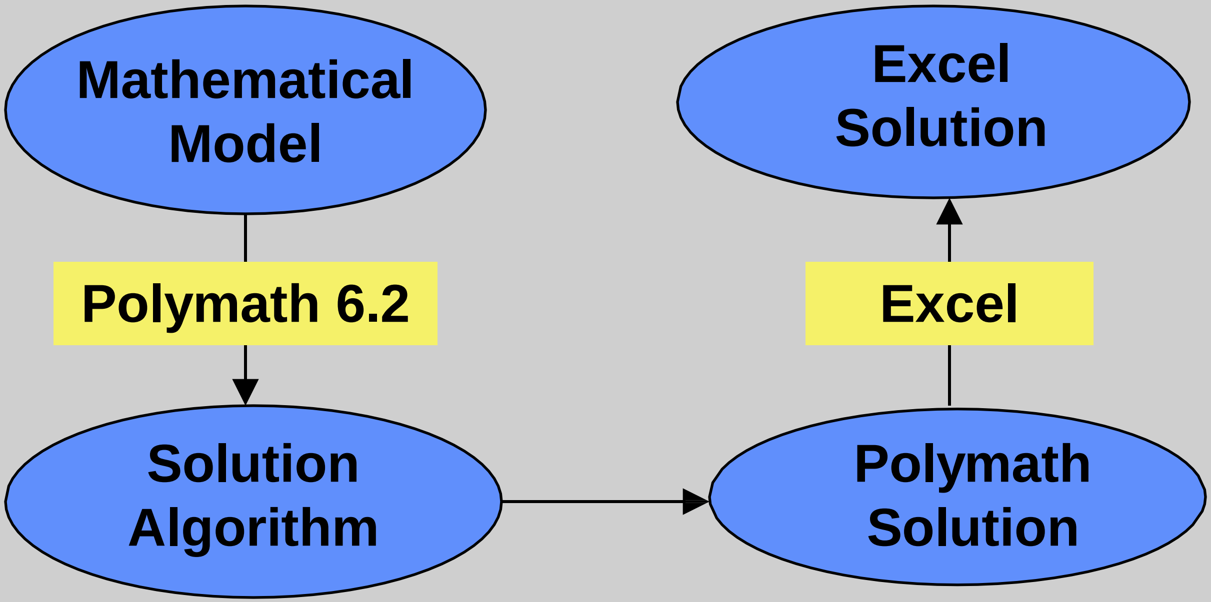
$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B \qquad \text{I. C. } C_B\big|_{t=0} = 0$$

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

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

POLYMATH – This file is DifferentialEquation01.pol

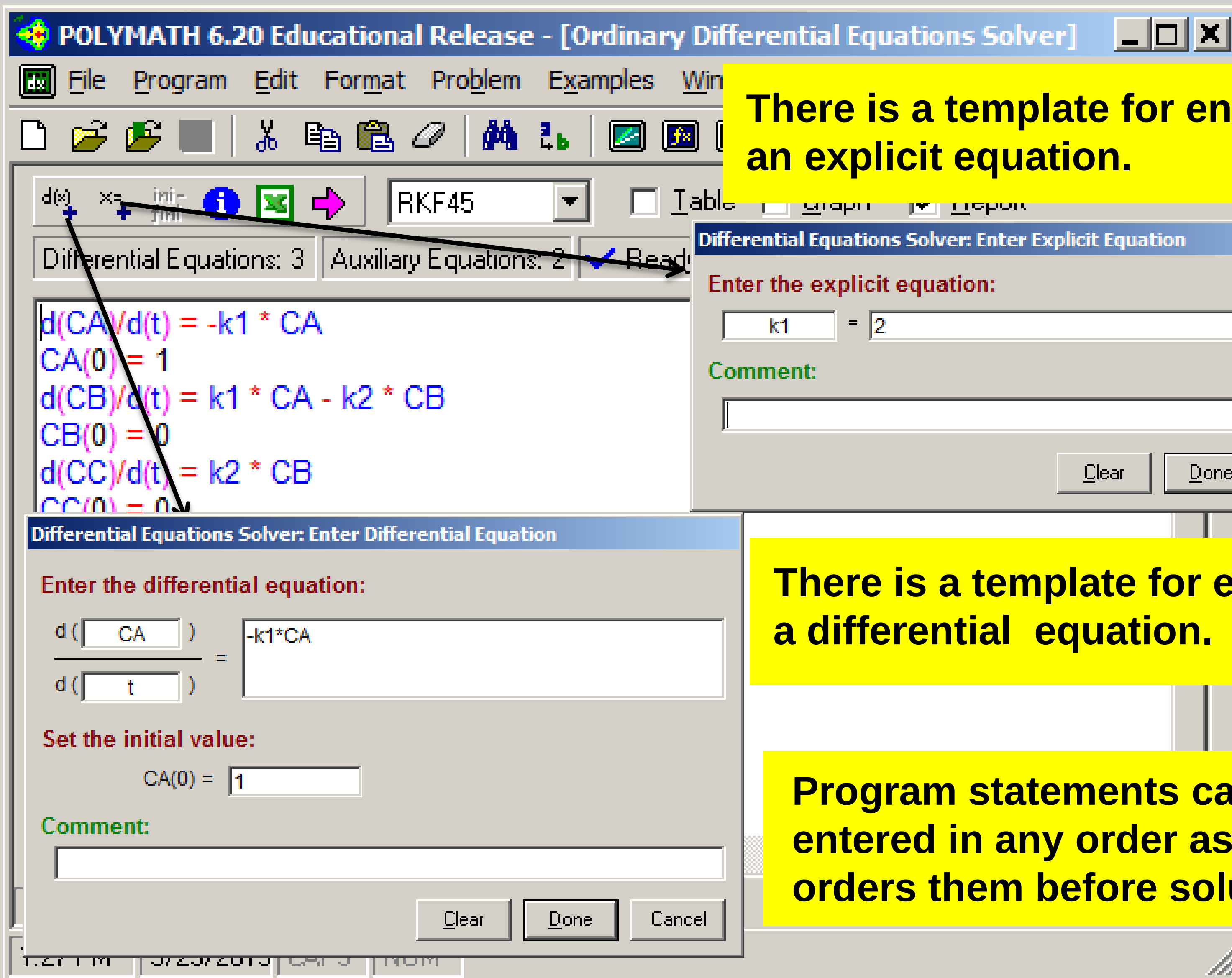
Problem 4 – Batch Reactor Kinetics Differential Equations – Simultaneous ODEs



Let's Enter and Solve this Problem in POLYMATH

POLYMATH – The solution file is DifferentialEquation01.pol. Please check for the Graph and the Report to be given during the solution.

Problem 4 – Batch Reactor Kinetics
Differential Equations – Simultaneous ODEs

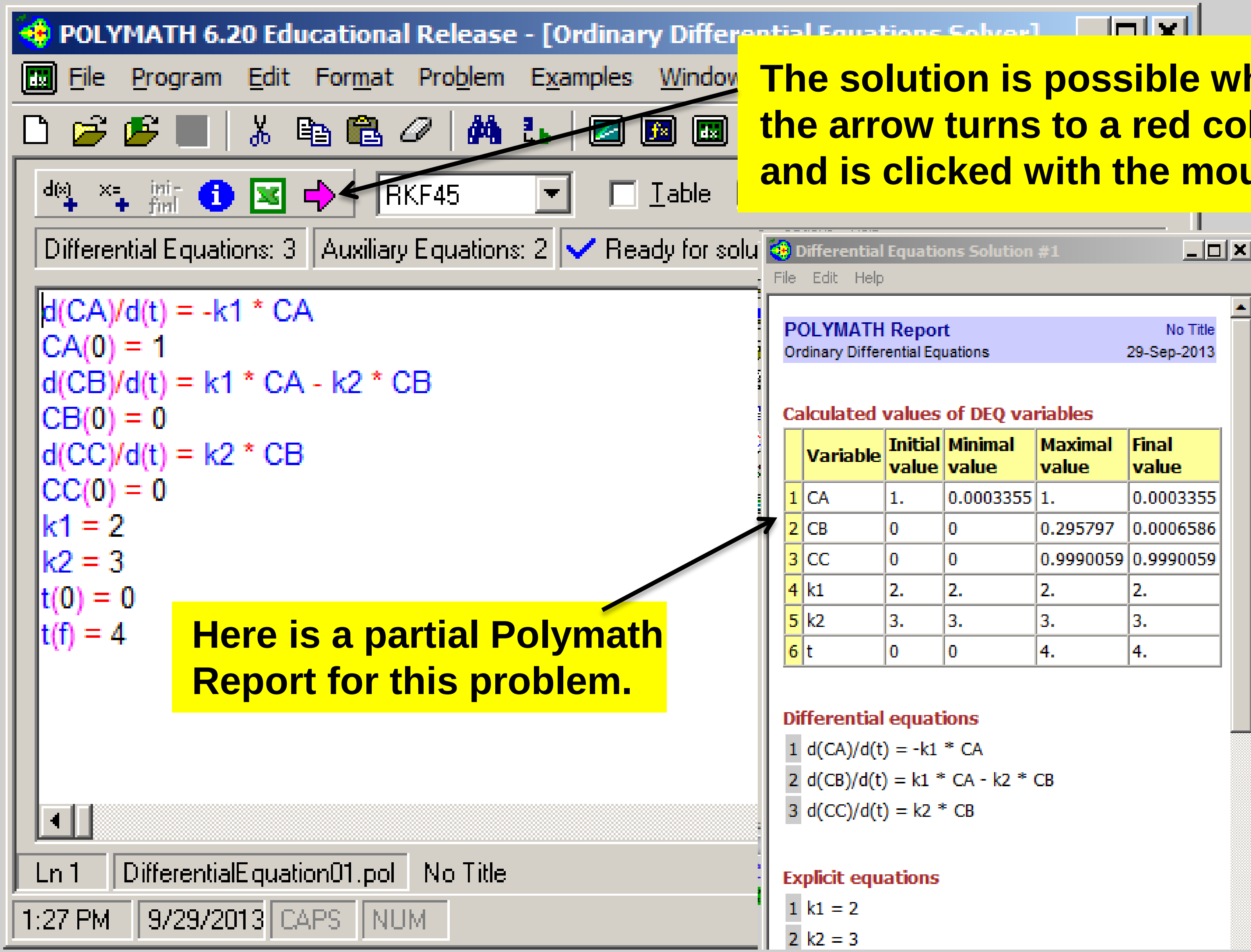


There is a template for entering an explicit equation.

There is a template for entering a differential equation.

Program statements can be entered in any order as Polymath orders them before solution.

Problem 4 – Batch Reactor Kinetics
Differential Equations – Simultaneous ODEs



	Variable	Initial value	Minimal value	Maximal value	Final value
1	CA	1.	0.0003355	1.	0.0003355
2	CB	0	0	0.295797	0.0006586
3	CC	0	0	0.9990059	0.9990059
4	k1	2.	2.	2.	2.
5	k2	3.	3.	3.	3.
6	t	0	0	4.	4.

Differential equations

1 d(CA)/d(t) = -k1 * CA
2 d(CB)/d(t) = k1 * CA - k2 * CB
3 d(CC)/d(t) = k2 * CB

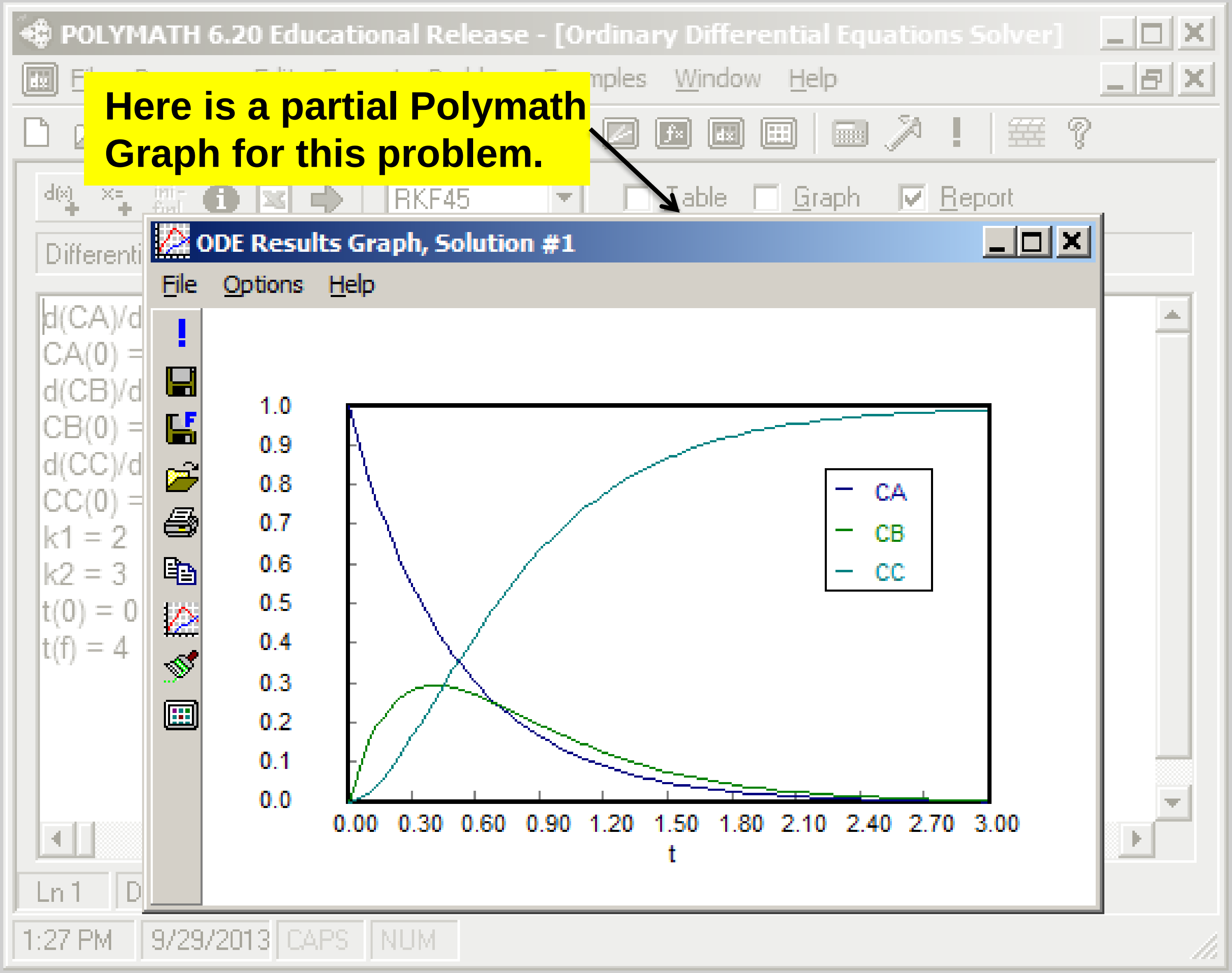
Explicit equations

1 k1 = 2
2 k2 = 3

The solution is possible when the arrow turns to a red color and is clicked with the mouse.

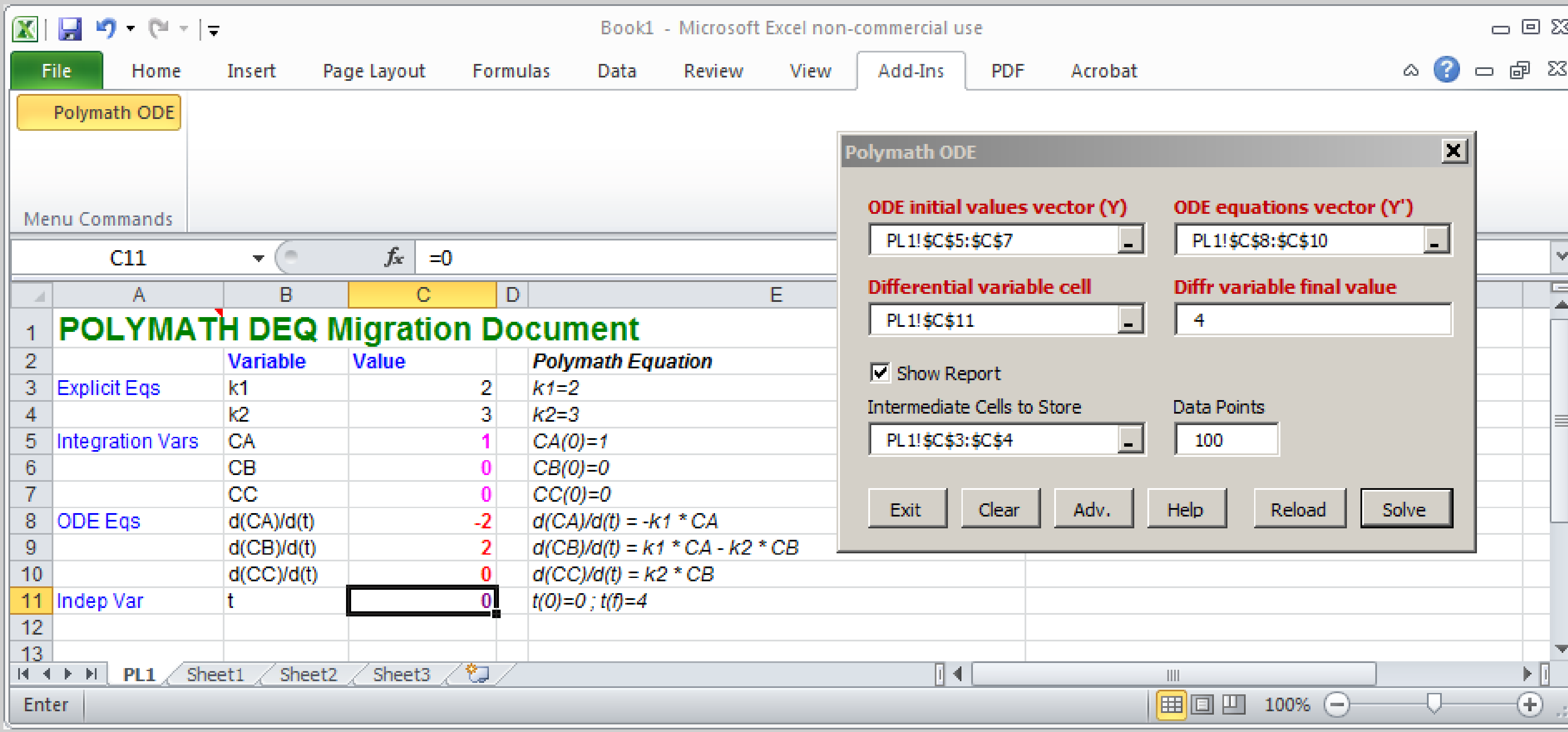
Here is a partial Polymath Report for this problem.

Problem 4 – Batch Reactor Kinetics Differential Equations – Simultaneous ODEs



Problem 4 – Batch Reactor Kinetics
Differential Equations – Simultaneous ODEs

Let's Open Excel and Export Problem to Excel by pressing the Excel icon. Polymath ODE_Solver should be available on Add-Ins sheet at top left and press to bring up Polymath ODE control box.



POLYMATH – The solution file is DifferentialEquation01.pol. Open Excel before export from Polymath or open DifferentialEquation01.xls for solution.

Problem 4 – Batch Reactor Kinetics
Differential Equations – Simultaneous ODEs

Solve using the ODE_Solver and look at the created sheet.
Keep the solution and look at sheet DEQ Solution.

1	**POLYMATH Report DEQ**					
2	Ordinary Differential Equations (RKF45).					
3						
4	**Calculated values of DEQ variables**					
5		Variable	Initial	Minimal	Maximal	Final
6	1	t	0	0	4	4
7	2	CA	1	0.000335	1	0.000335
8	3	CB	0	0	0.296062	0.000659
9	4	CC	0	0	0.999006	0.999006
10	5	k1	2	2	2	2
11	6	k2	3	3	3	3

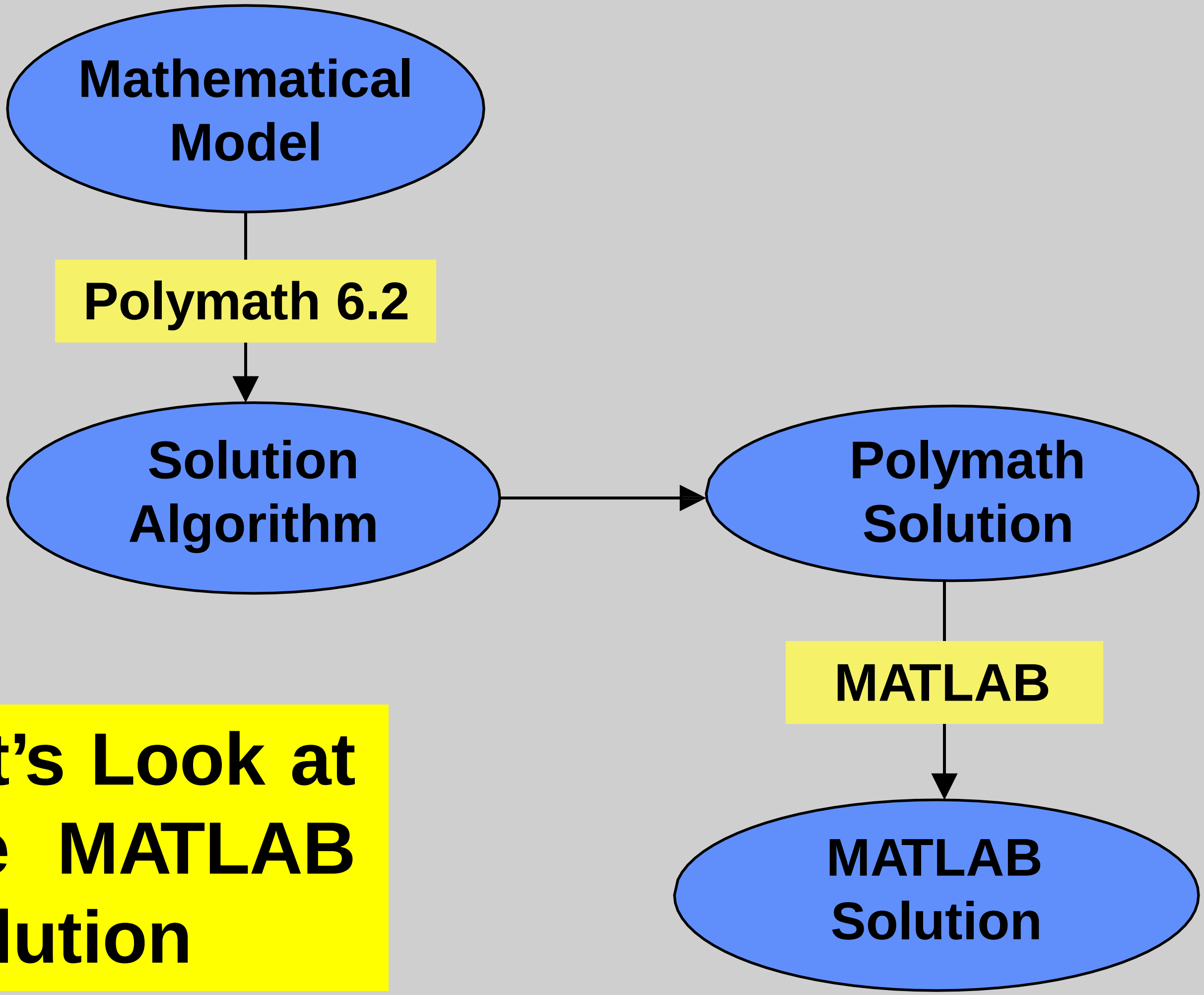
27	**Intermediate data points**				
28		t	CA	CB	CC
29	1	0	1	0	0
30	2	0.082463	0.847957	0.134239	0.017804
31	3	0.133428	0.765783	0.191308	0.04291
32	4	0.162938	0.721894	0.217083	0.061023
33	5	0.212227	0.654127	0.250163	0.09571
34	6	0.248472	0.608388	0.2677	0.123912
35	7	0.287481	0.562726	0.281193	0.156081
36	8	0.329327	0.517547	0.29044	0.192013
37	9	0.374102	0.473216	0.295375	0.231409
38	10	0.421921	0.430055	0.296062	0.273883
39	11	0.446763	0.40921	0.294881	0.295909
40	12	0.497562	0.369677	0.289819	0.340504

The problem variables names can be added to the results that is similar to the Polymath report.

The problem variables can be added to the Intermediate data points and plotted using Excel graphics.

Solution is on DifferentialEquation01.xls on sheet DEQ Solution (1).

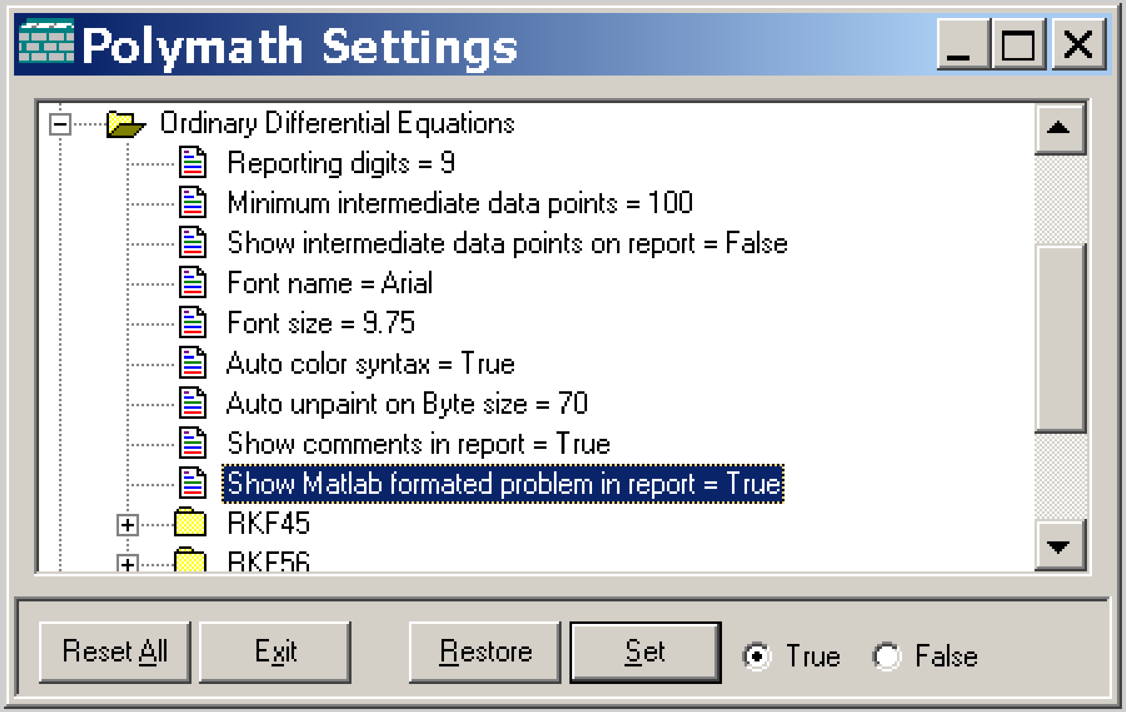
Problem 4 – Batch Reactor Kinetics
Differential Equations – Simultaneous ODEs



Let's Look at the MATLAB Solution

Problem 4 – Batch Reactor Kinetics Differential Equations – Simultaneous ODEs

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



Problem 4 – Batch Reactor Kinetics Differential Equations – Simultaneous ODEs

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

```
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];
```

Differential Equations – Simultaneous ODEs

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
```

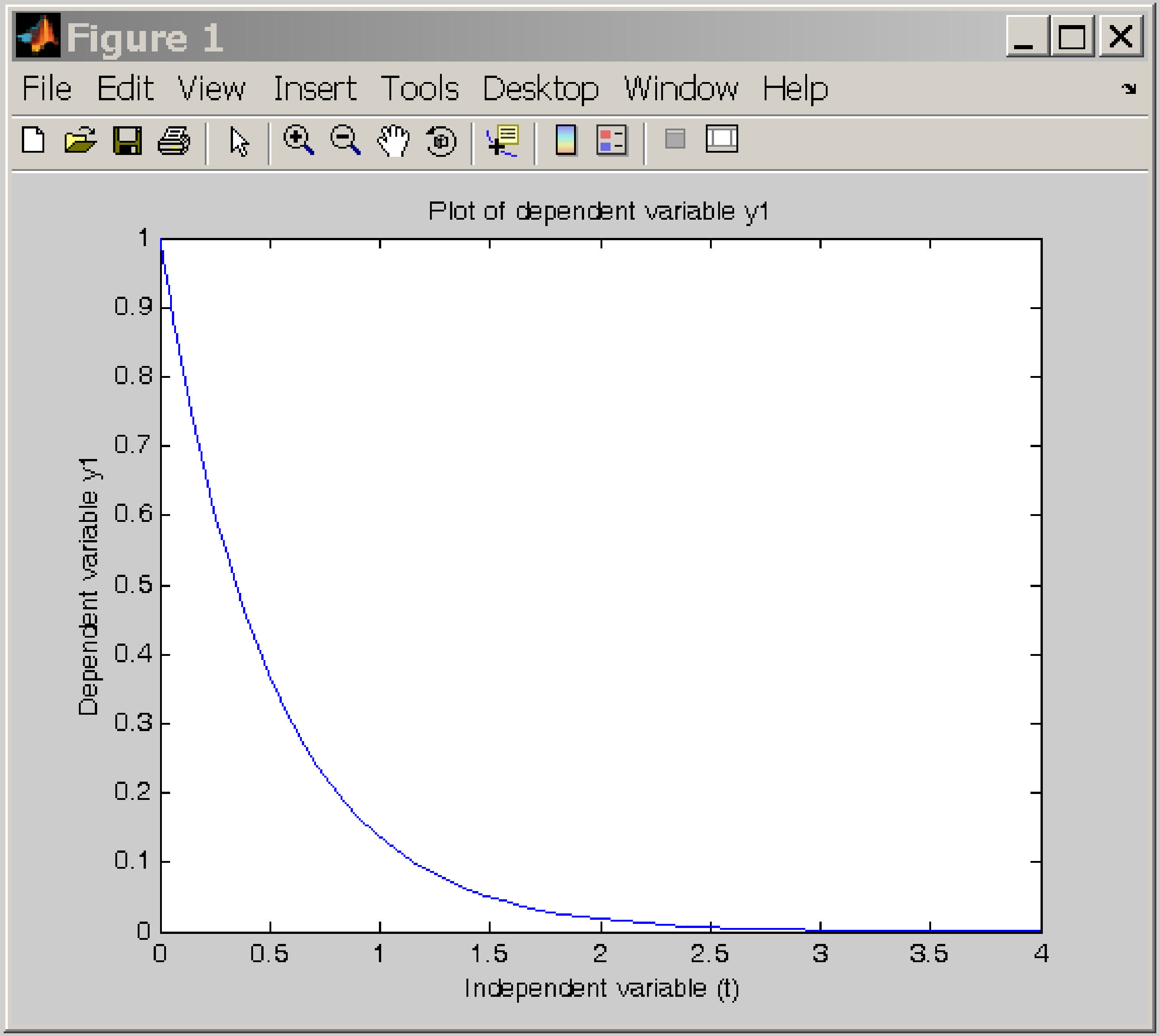
Differential Equations – Simultaneous ODEs

```
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 is entered into template

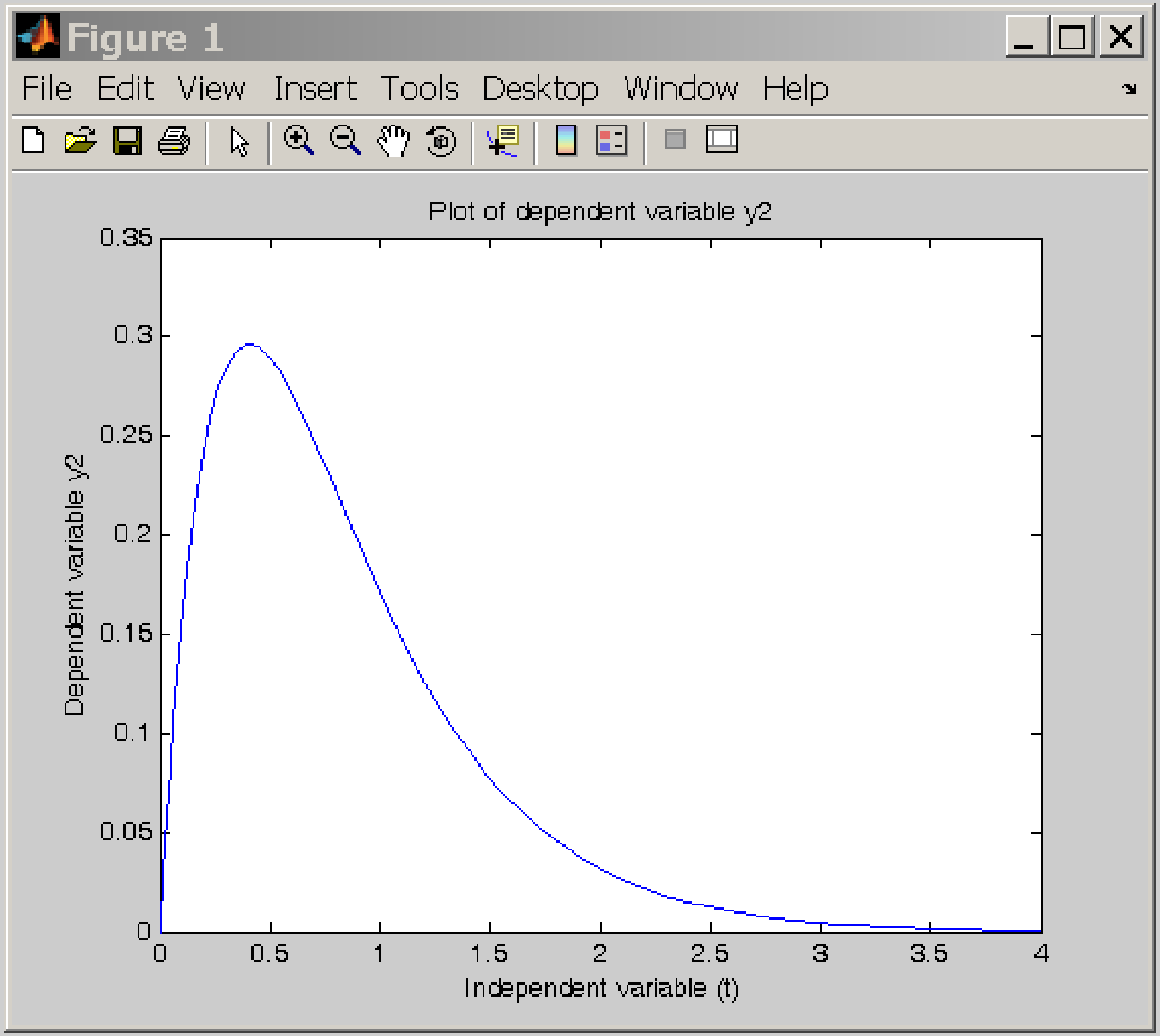
Differential Equations – Simultaneous ODEs

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



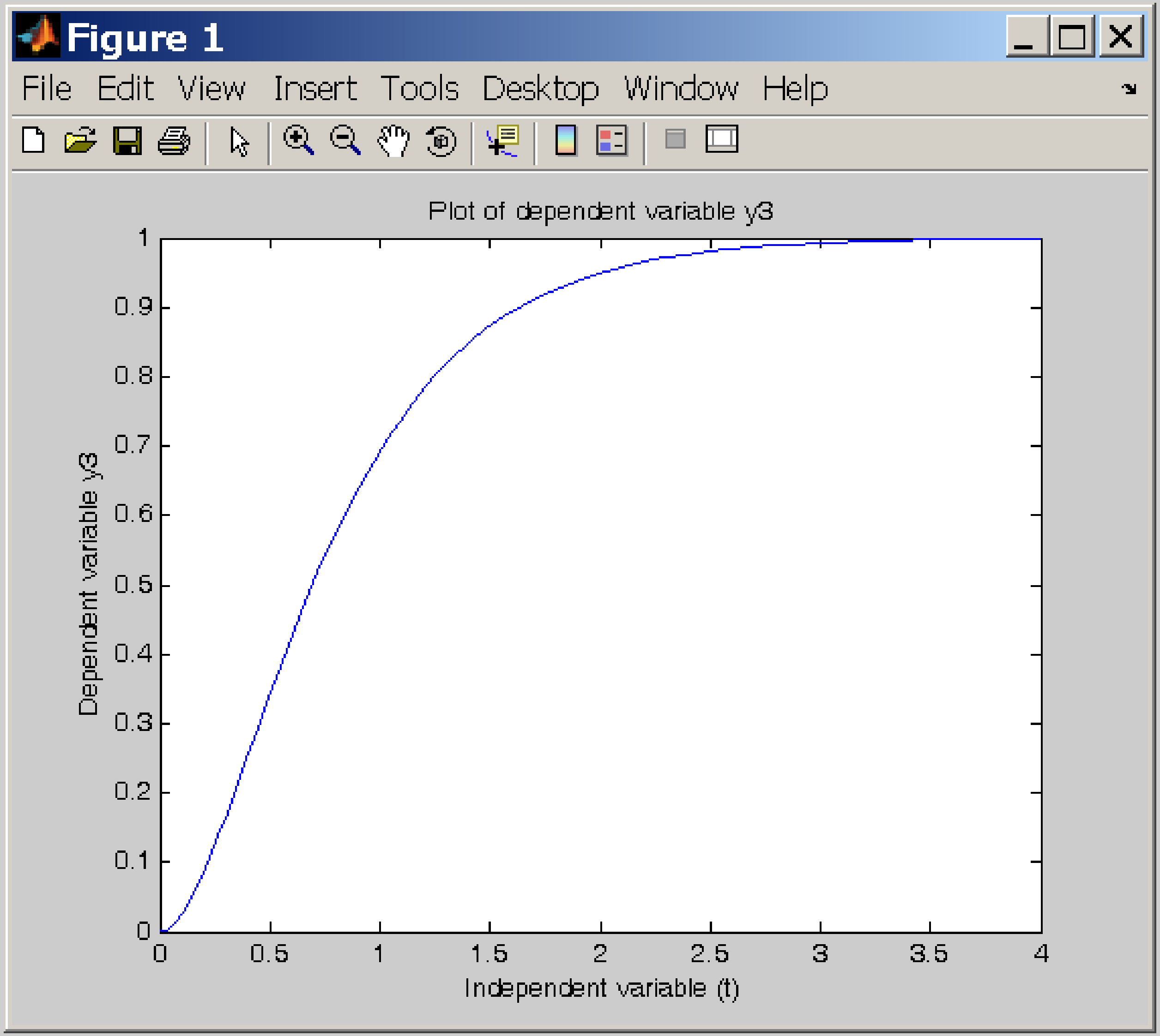
Differential Equations – Simultaneous ODEs

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



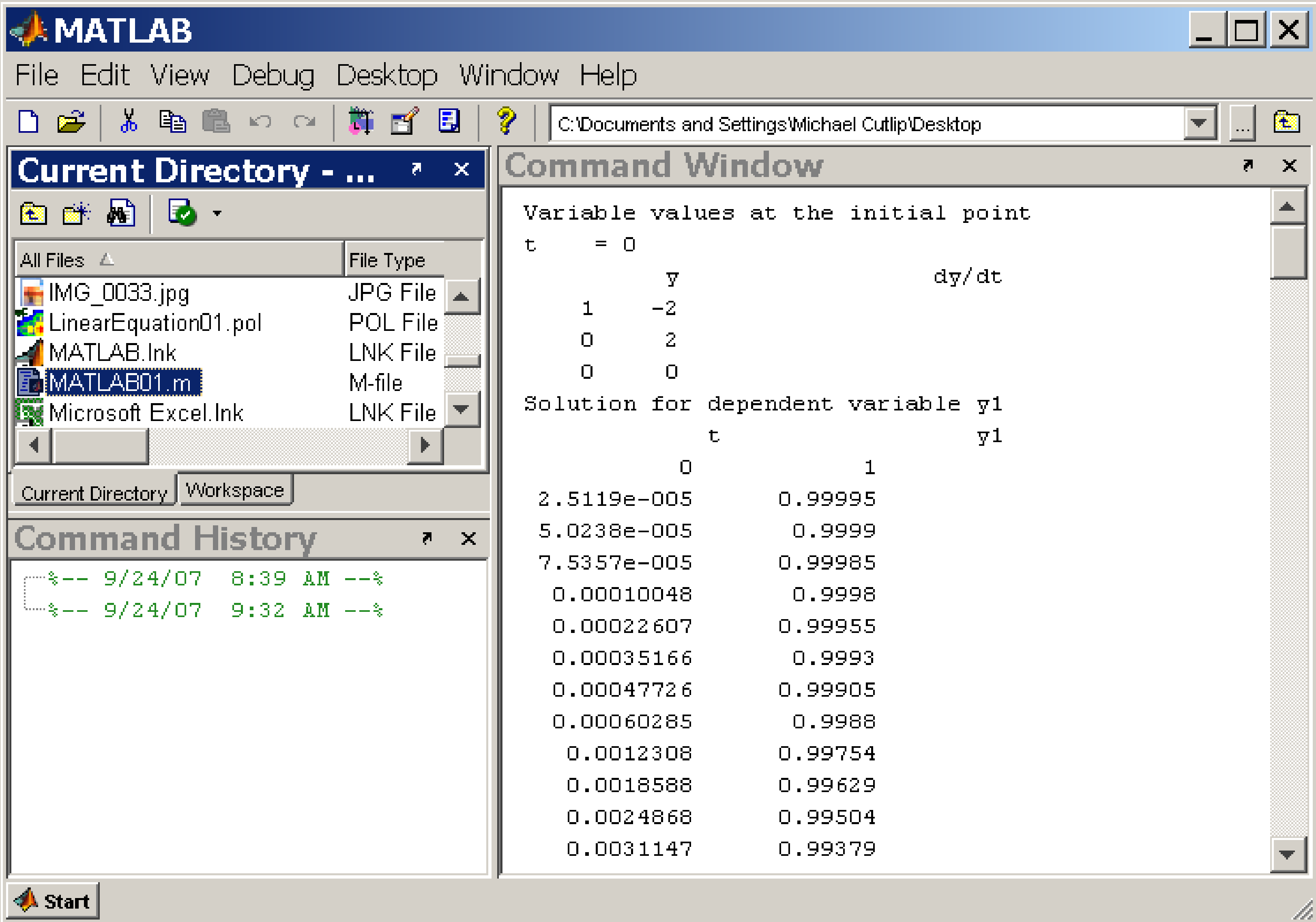
Differential Equations – Simultaneous ODEs

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



Differential Equations – Simultaneous ODEs

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



Problem 4 – Batch Reactor Kinetics
Differential Equations – Simultaneous ODEs

This optional demonstration requires the use of MATLAB program on your PC.

Let's Go to the POLYMATH Problem, Solve the Problem, and Generate MATLAB Code!

POLYMATH – This file is DifferentialEquation01.pol

Let's Open MATLAB with Template for Multiple Differential Equations, Insert Generated Code, and Solve in MATLAB

Template File is MultipleDEQtemplate.m **Solution File is MATLAB01.m**

Problem 5 – Regression of Hardening of Concrete

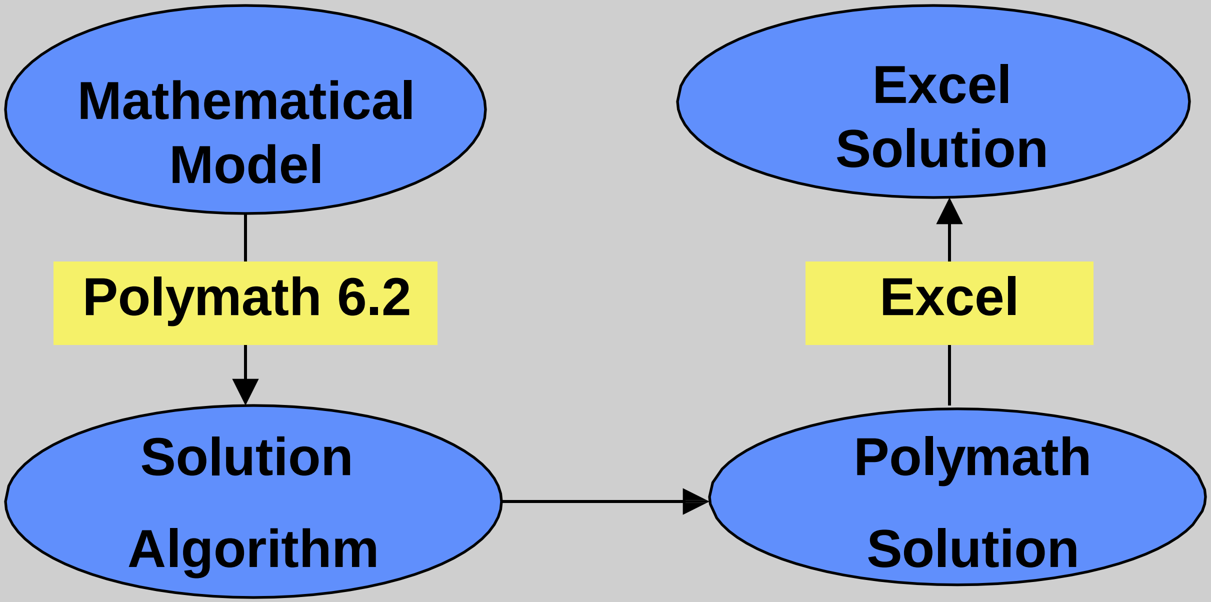
Regression – Multiple Linear

Consider laboratory data for the hardening of cement with four components.

	Wpc1	Wpc2	Wpc3	Wpc4	hard_heat
01	7	26	6	60	78.7
02	1	29	15	52	74.3
03	11	56	8	20	104.3
04	11	31	8	47	87.6
05	7	52	6	33	95.9
06	11	55	9	22	109.2
07	3	71	17	6	102.7
08	1	31	22	44	72.5
09	2	54	18	22	93.1
10	21	47	4	26	115.9
11	1	40	23	34	83.8
12	11	66	9	12	113.3
13	10	68	8	12	109.4

Problem 5 – Regression of Hardening of Concrete

Regression – Multiple Linear



Problem 5 – Regression of Hardening of Concrete

Regression – Multiple Linear

Use Multiple Linear Regression to correlate the hardening of cement with four components.

This Polymath option will fit a linear function of the form:

$$y(x_1, x_2, ..., x_n) = a_0 + a_1 * x_1 + a_2 * x_2 + ... + a_n * x_n$$

where a_0, a_1, ..., a_n are regression parameters, to a set of N tabulated values of x_1, x_2, ..., x_n (independent variables) versus y (dependent variable). Note that the number of data points must be greater than n+1 (thus N >= n+1). The program calculates the coefficients a_0, a_1, ..., a_n by minimizing the sum of squares of the deviations between the calculated and the data for y.

Problem 5 – Regression of Hardening of Concrete

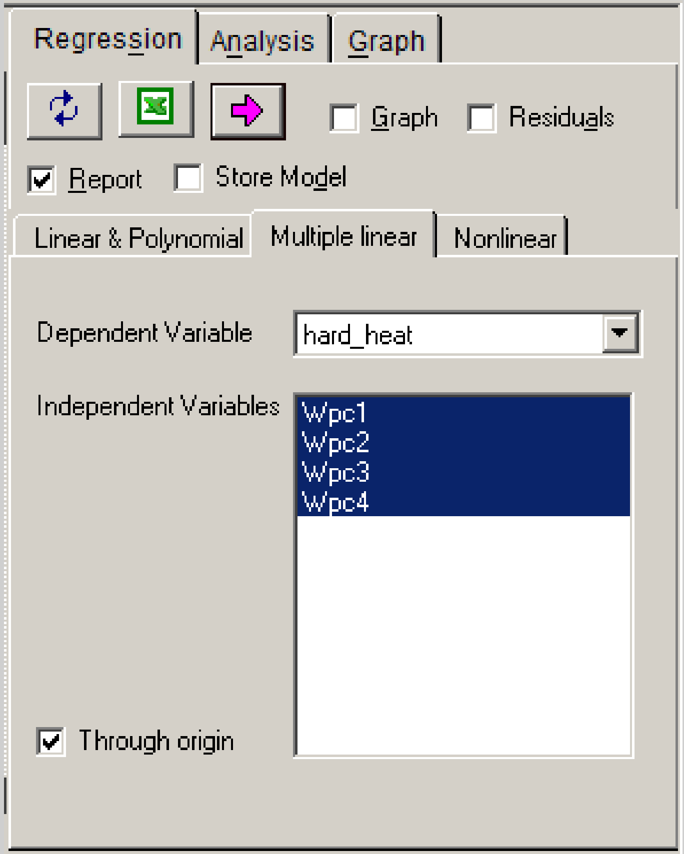
Regression – Multiple Linear

Live Demonstration of the Polymath Solution

Let's Go to POLYMATH and Generate the Problem Solution

POLYMATH – This file is Regression01.pol

Use the Regression Program to carry out a Multiple Linear Regression using the variables indicated where the holding down the Ctrl key allows all independent variables to be selected. This case yields the lowest variance.



Problem 5 – Regression of Hardening of Concrete

Regression – Multiple Linear

POLYMATH Multiple Linear Problem Report (through the origin)

Multiple Linear Report, Solution #2

File Edit Help

POLYMATH Report Heat of hardening of portland cement

Multiple linear regression 29-Sep-2013

Model: hard_heat = a1*Wpc1 + a2*Wpc2 + a3*Wpc3 + a4*Wpc4

Variable	Value	95% confidence
a1	2.189177	0.4182687
a2	1.154136	0.1082325
a3	0.7532949	0.3601112
a4	0.4885452	0.093483

General

Number of independent variables = 4
Regression not including a free parameter
Number of observations = 13

Statistics

R^2	0.9806563
R^2adj	0.9742084
Rmsd	0.5568439
Variance	5.822523

Source data points and calculated data points

	Wpc1	Wpc2	Wpc3	Wpc4	hard_heat	hard_heat calc	Delta hard_heat
1	7	26	6	60	78.7	79.16424	-0.4642423
2	1	29	15	52	74.3	72.36288	1.937117

No File POLYMATH Report

Problem 5 – Regression of Hardening of Concrete
Regression – Multiple Linear

Live Demonstration of the Polymath Solution and Solution of Same Problem in Excel

Let's Open Excel and Export Polymath Problem to Excel.

Excel – The Solution file is Regression01.xls

POLYMATH Multiple Linear Regression Migration Docume

								Multiple Linear Regression. No free parameter.				
Wpc1	Wpc2	Wpc3	Wpc4	hard_heat	hard_heat	hard_heat	hard_heat residual ^2		a4	a3	a2	a1
7	26	6	60	78.7	79.16424	0.464242	0.215521	Coefficients	0.488545	0.753295	1.154136	2.189177
1	29	15	52	74.3	72.36288	-1.93712	3.752422	Std.dev.s	0.041328	0.1592	0.047848	0.184911
11	56	8	20	104.3	104.5098	0.209802	0.044017	R2, SE (y)	0.999567	2.41299	#N/A	#N/A
11	31	8	47	87.6	88.84713	1.24713	1.555333	95% conf. int.	0.093483	0.360111	0.108233	0.418269
7	52	6	33	95.9	95.98105	0.08105	0.006569	Variance	5.822523			
11	55	9	22	109.2	105.0861	-4.11395	16.92457	Sum of Squares	52.40271			
3	71	17	6	102.7	104.2484	1.548447	2.397688	Model	hard_heat = a4 * Wpc1 + a3 * Wpc2 + a2 * Wpc3 + a1 * Wpc4			
1	31	22	44	72.5	76.03586	3.535858	12.50229					
2	54	18	22	93.1	91.00898	-2.09102	4.372358					
21	47	4	26	115.9	115.9324	0.032439	0.001052					
1	40	23	34	83.8	82.29092	-1.50908	2.277316					
11	66	9	12	113.3	112.8961	-0.40391	0.163141					
10	68	8	12	109.4	112.2619	2.861893	8.190429					

The Excel result compares very nicely to the Polymath result.

Problem 6 – 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.

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

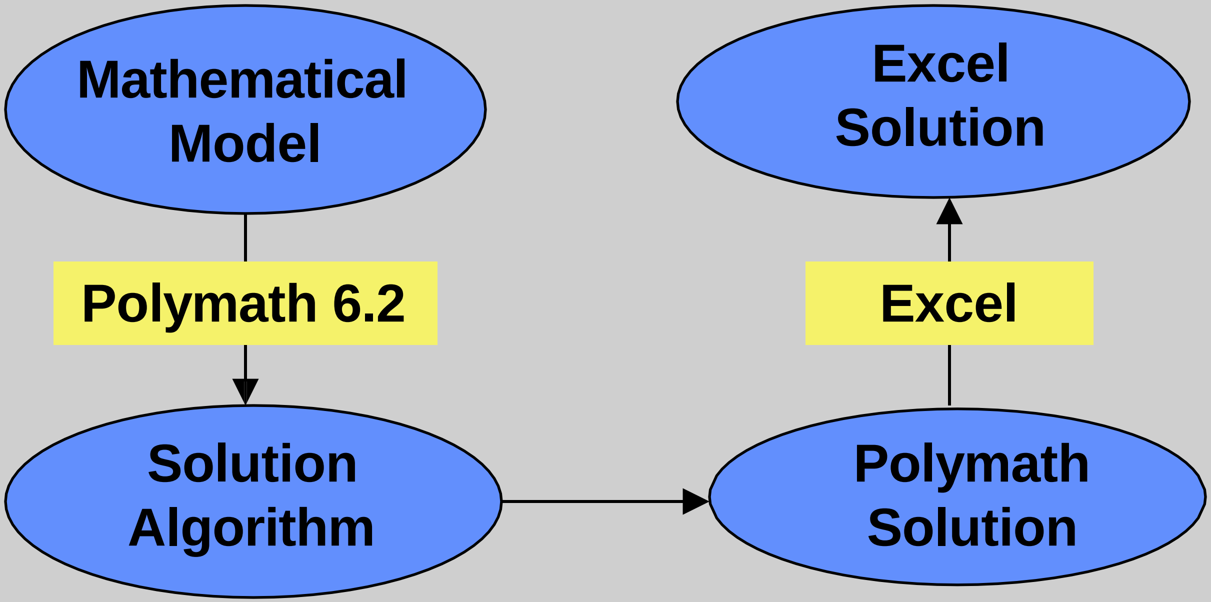
Determine the values of D and E for the Clapeyron equation and the values of A, B, and C for the Antoine equation using the data given below. Compare these correlations.

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 6 – Regressions - Vapor Pressure Data

Regressions – Linear and Nonlinear



Problem 6 – Regressions – Vapor Pressure Data

POLYMATH Clapeyron Equation Linear Regression EXERCISE

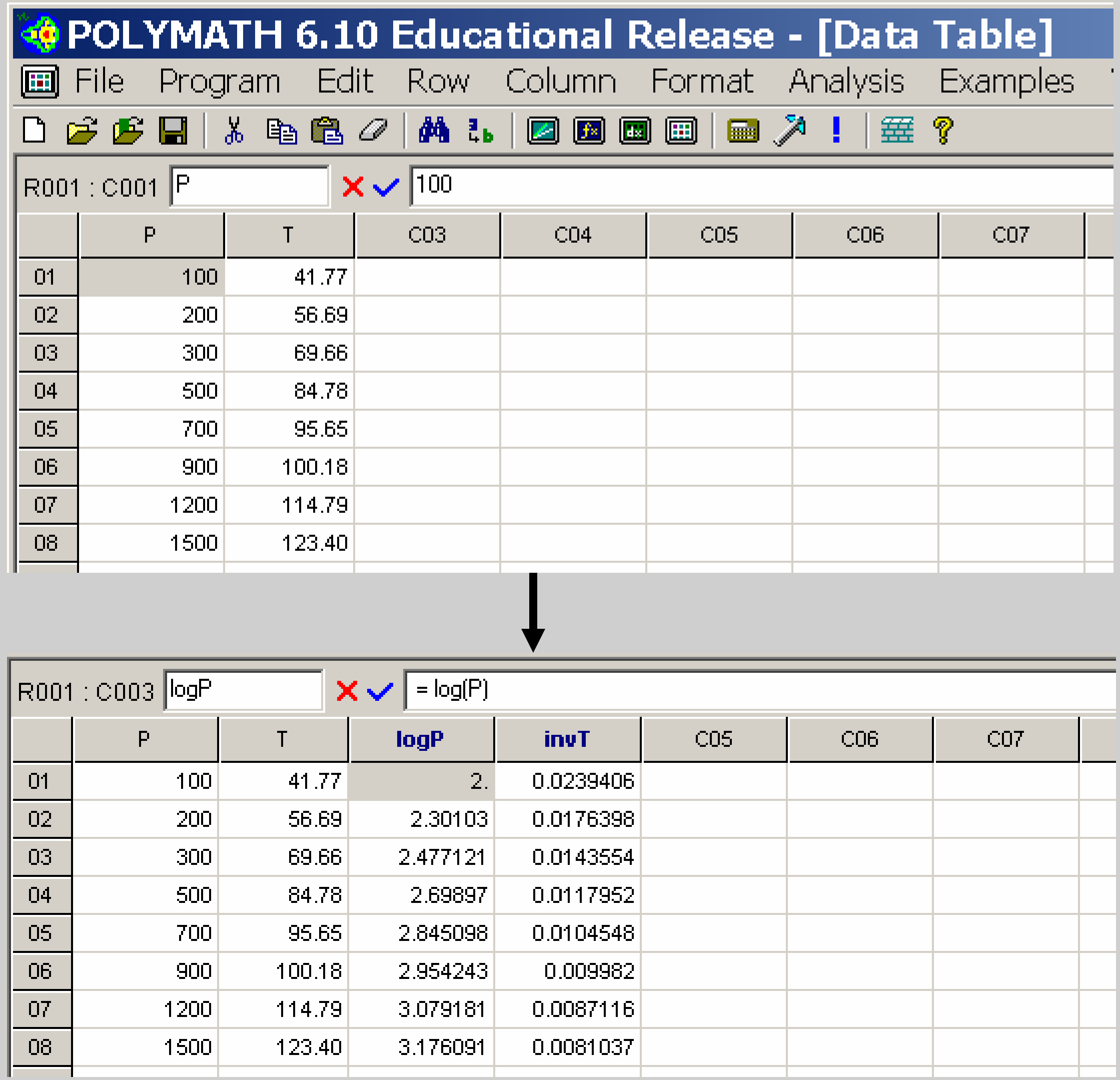
Utilize the Polymath Regression Program to input the data to the Data Table.

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



	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					

	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 6 – Regressions – Vapor Pressure Data POLYMATH/Excel Solution EXERCISE

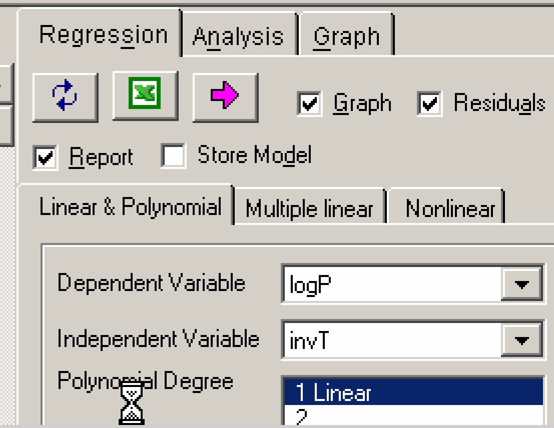
Utilize the Polymath Regression Program to make a Linear Regression of logP versus invTK to yield the parameters D and E of the Clapeyron equation.

E = a0 = 3.658

D = a1 = -73.61

R013 : C001 P

	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

Use the Polymath Problem Data File

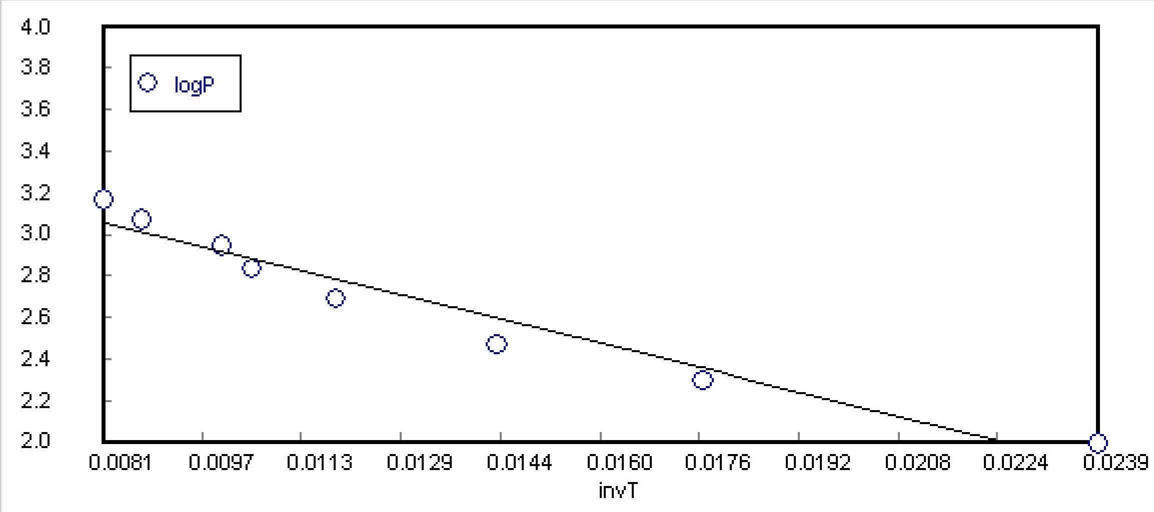
OR

Use the Polymath Solution File

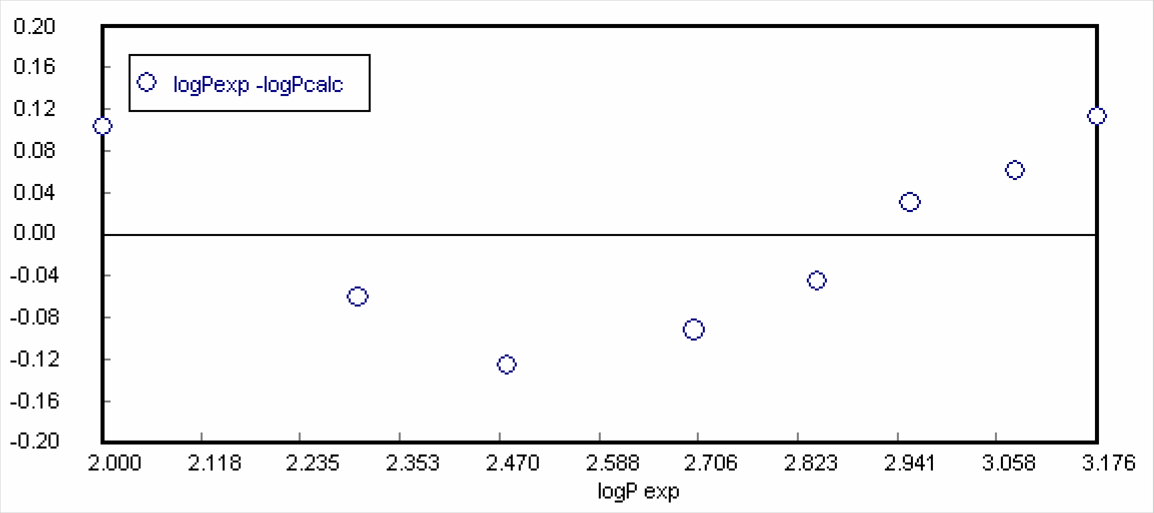
Polymath Data File is RegressionData02.pol **Polymath Solution File is Regression02.pol**

Problem 6 – 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 6 – 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									

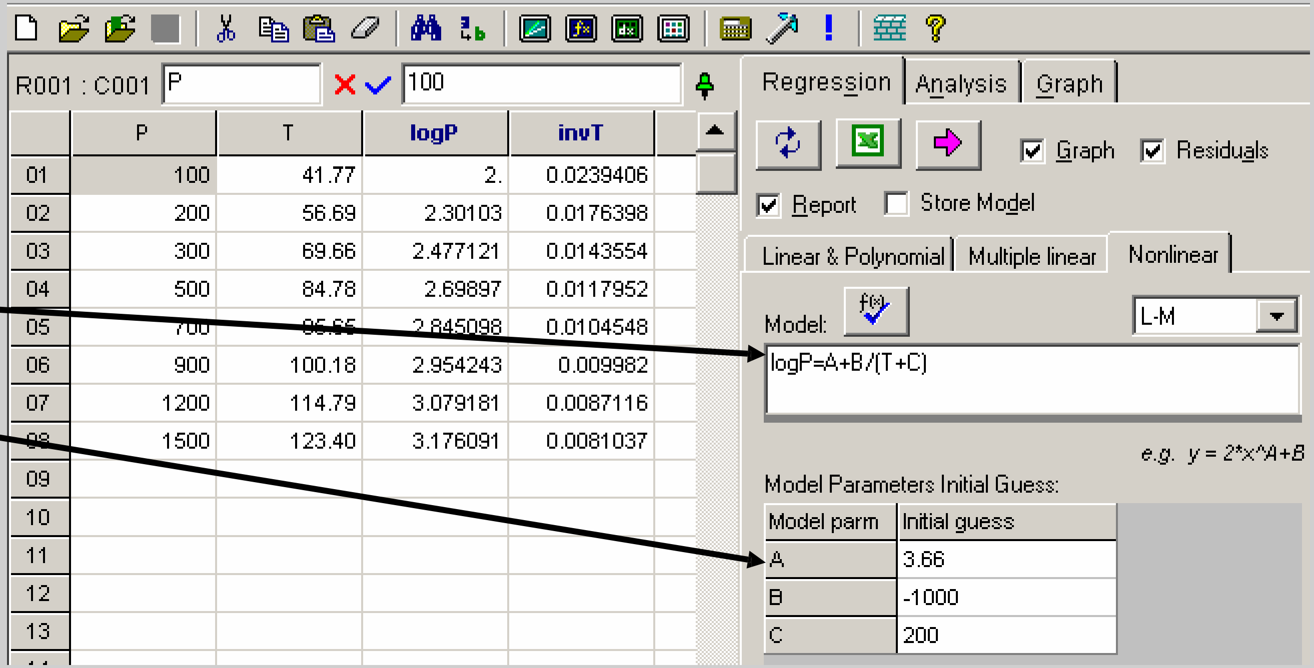
You may the EXCEL Problem Solution File

(for those who need it)

File is Regression02.xls

Problem 6 – 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.



You may use the Polymath Problem Data File

File is RegressionData02.pol

OR

You may use the Polymath Solution File

File is Regression03.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

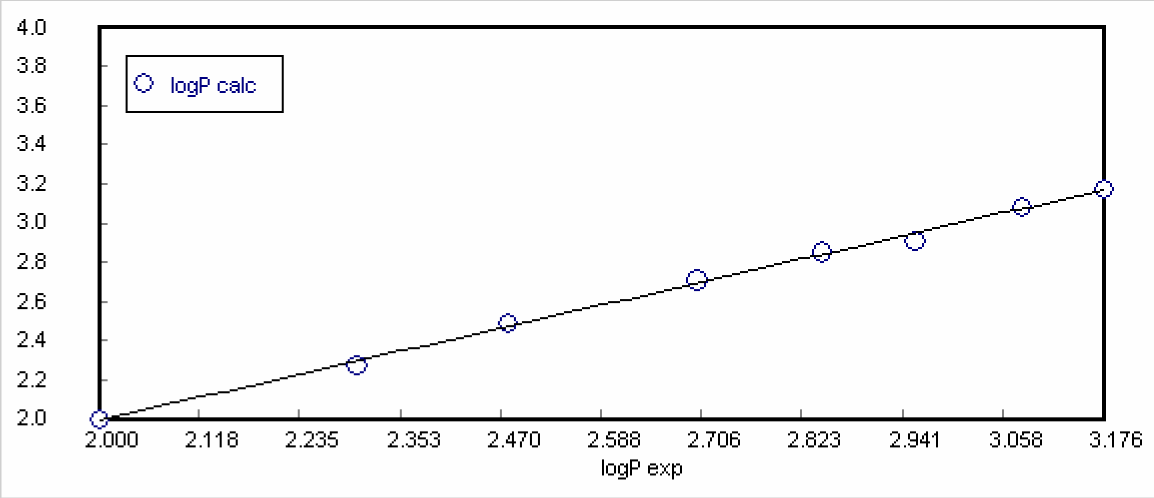
Max # iterations = 64

Precision

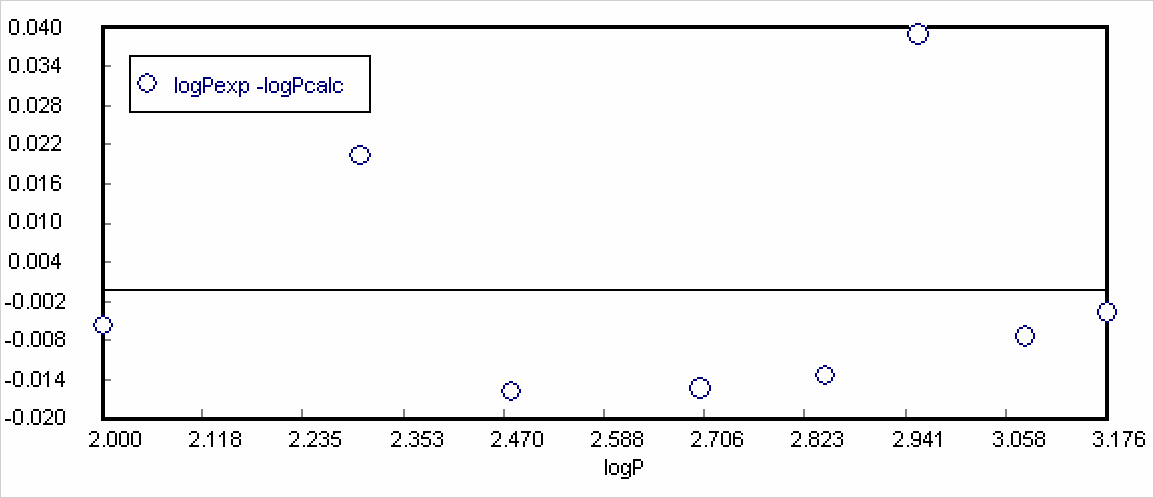
R^2	0.9976599
R^2adj	0.9967238
Rmsd	0.0064969
Variance	0.0005403

Problem 6 – 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.

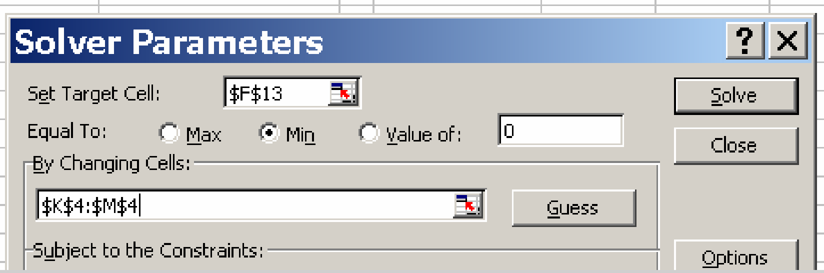


These graphs plus the lower variance for the Antoine equation indicate that the data are well represented.

Problem 6 – 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.

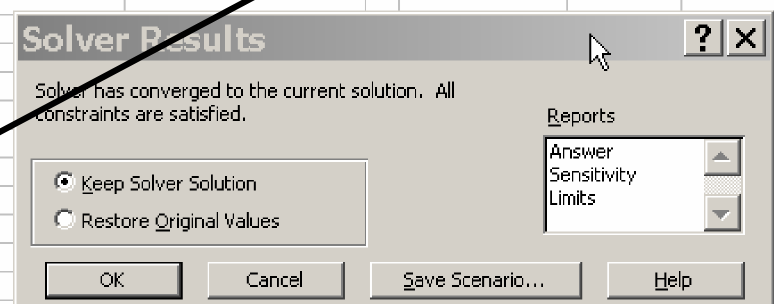
	A	B	C	D	E	F	G	H	I	J	K	L	M
1	POLYMATH Multiple Nonlinear Regression Migration Document												
2										Nonlinear Regression			
3		T	logP	logP calc	logP residual	logP residual ^2	(logP - logPavg)^2	(logPcalc - logPavg)^2			A	B	C
4		41.77	2	-0.476162468	-2.476162468	6.13138057	3.494257976	0.368290014		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					
12													
13					Sum	52.47675925							
14													
15													
16													
17													
18													
19													
20													



Problem 6 – 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.

	A	B	C	D	E	F	G	H	I	J	K	L	M
1	POLYMATH Multiple Nonlinear Regression Migration Document												
2										Nonlinear Regression			
3		T	logP	logP calc	logP residual	logP residual ^2	(logP - logPavg)^2	(logPcalc - logPavg)^2			A	B	C
4		41.77	2	2.006165146	0.006165146	3.8009E-05	0.478129438	0.469641432		Coefficients	6.435009	-1002.14	184.5053
5		56.69	2.30103	2.280127127	-0.020902873	0.00043693	0.152442647	0.169202172		R2, SE (y)	0.997769	0.018384	
6		69.66	2.477121	2.492149822	0.015028822	0.000225865	0.045945084	0.039728152		Variance	0.000338		
7		84.78	2.69897	2.713535931	0.014565931	0.000212166	5.62644E-05	0.000486948		Average logP	2.691469		
8		95.65	2.845098	2.857928733	0.012830733	0.000164628	0.023601856	0.027708828		Model	logP = A+B/(T+C)		
9		100.18	2.954243	2.914848329	-0.039394671	0.00155194	0.069050152	0.049898305					
10		114.79	3.079181	3.086683783	0.007502783	5.62918E-05	0.150320561	0.156194691					
11		123.4	3.176091	3.180313475	0.004222475	1.78293E-05	0.234858441	0.238908878					
12													
13					Sum	0.00270366							

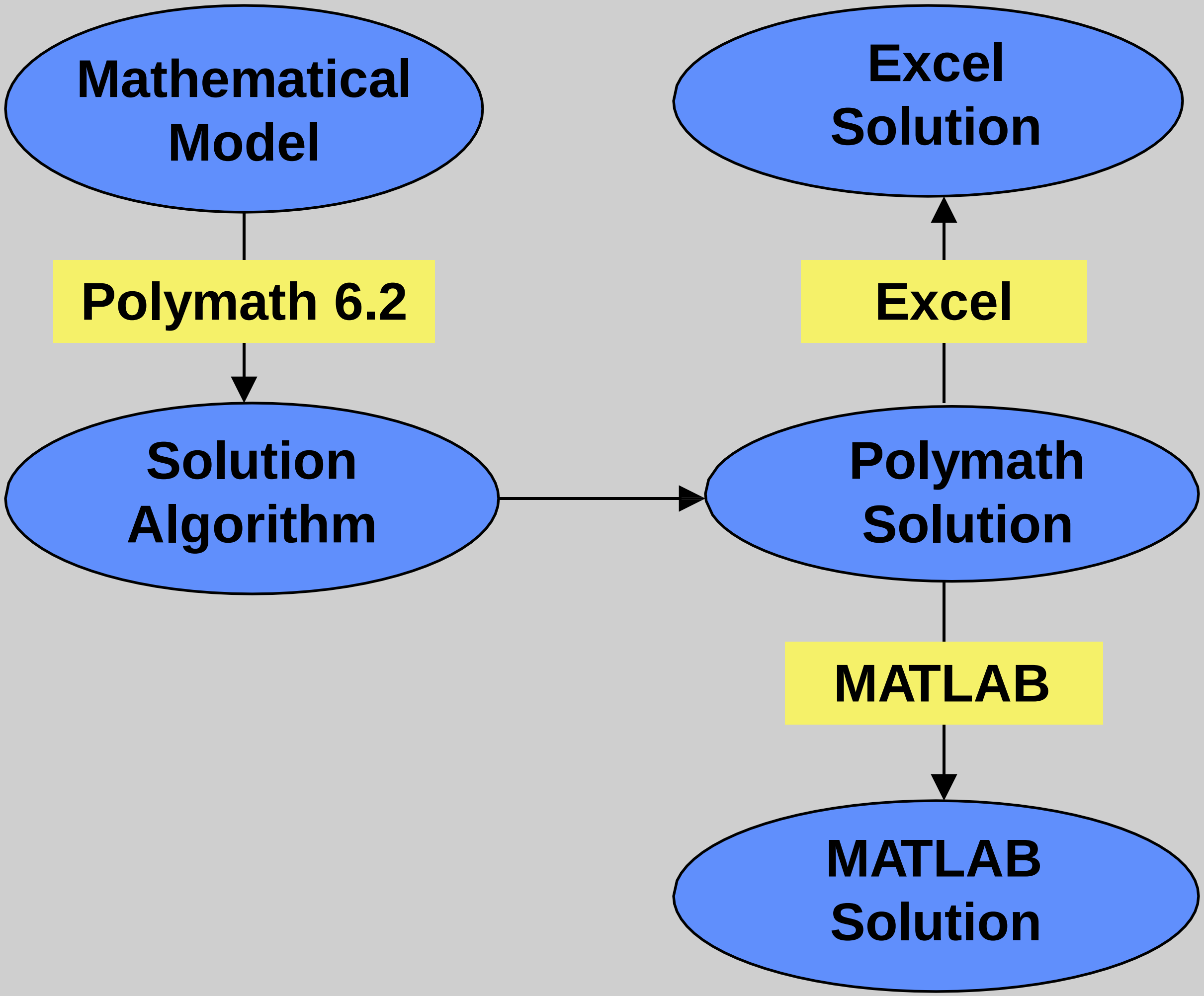


Nonlinear Regression			
	A	B	C
Coefficients	6.435009	-1002.138	184.5053
R2, SE (y)	0.997769	0.018384	
Variance	0.000338		
Average logP	2.691469		
Model	logP = A+B/(T+C)		

You may use the EXCEL Solution File

File is Regression03.xls

SUMMARY - Desktop Problem Solving Involving Polymath, Excel, and MATLAB



Happy Problem Solving!