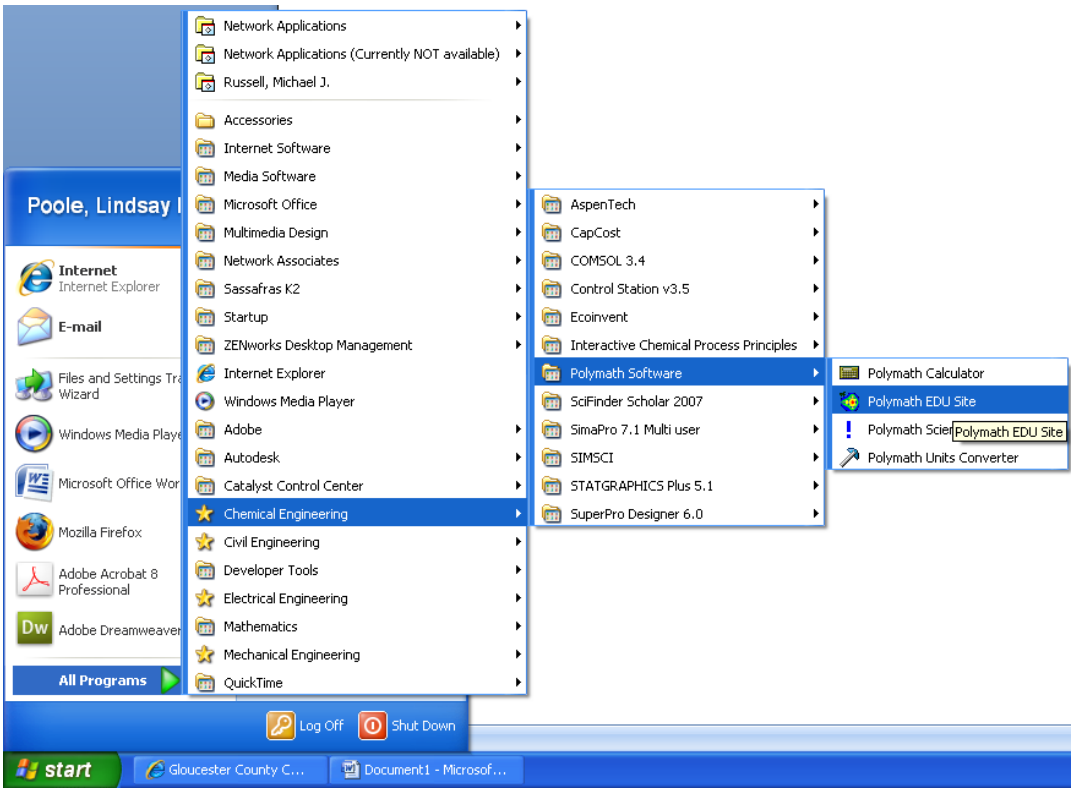
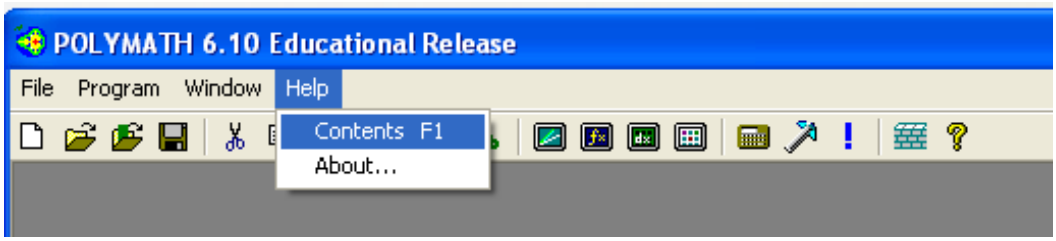
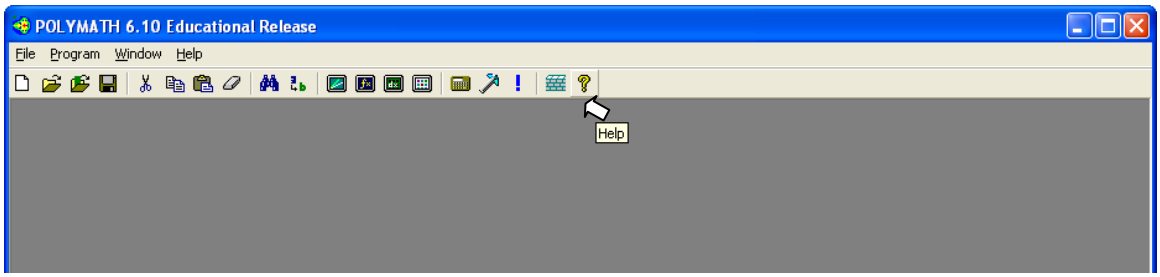
1. Open polymath:

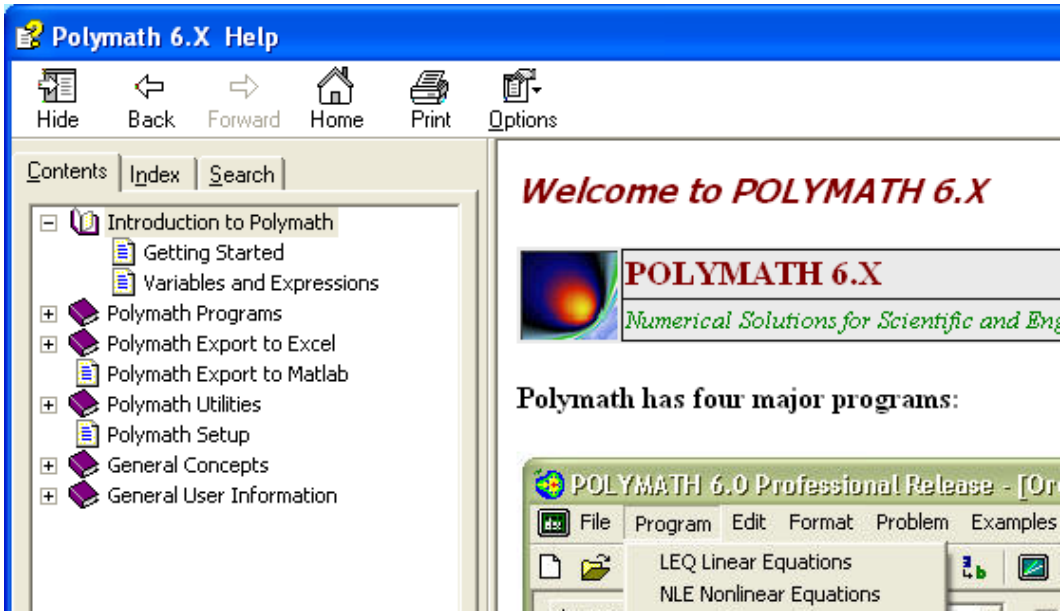


2. Go to Help, Contents F1 or Press F1

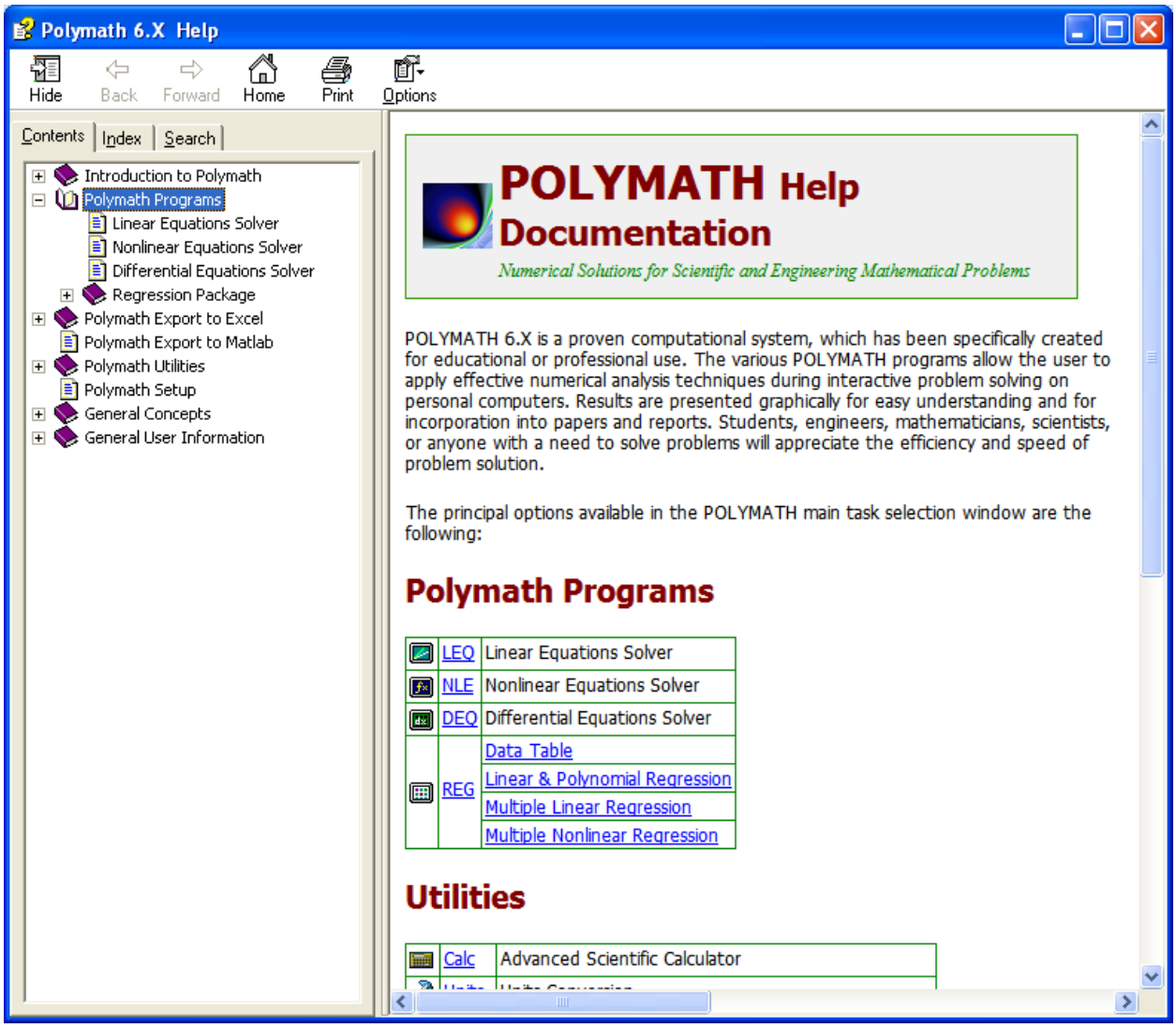




3. Read the section titled *Introduction to Polymath* both getting started and Variables and expressions and answer the following questions typed into a word document to be submitted at the end of the tutorial:



1. How many simultaneous ordinary differential equations can be simultaneously solved using the educational version of POLYMATH?
2. How many explicit equations can be solved using the POLYMATH ode solver?
3. What does NLE represent?
4. What symbol on the tool bar represents the unit conversion calculator? Using the polymath unit conversion calculator convert 1 hp (international) to J/s. (AS OF 1/23/08 first floor lab computers had problems with this portion.)
5. What symbol on the tool bar represents the polymath scientific constants menu? Give the value of pi to an accuracy of 12 digits using polymath scientific constants.
6. How would you have polymath give you the absolute value of a number?
7. Have polymath, using the calculator give you the cosine of 30 degrees. What did you type?


Polymath 6.X Help
Hide
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Contents
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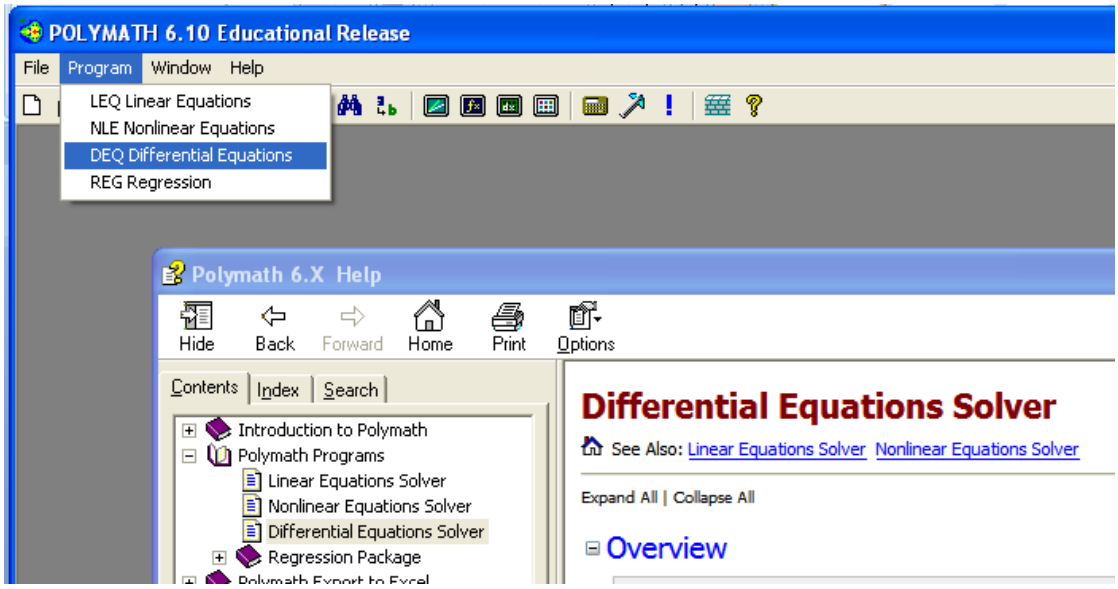
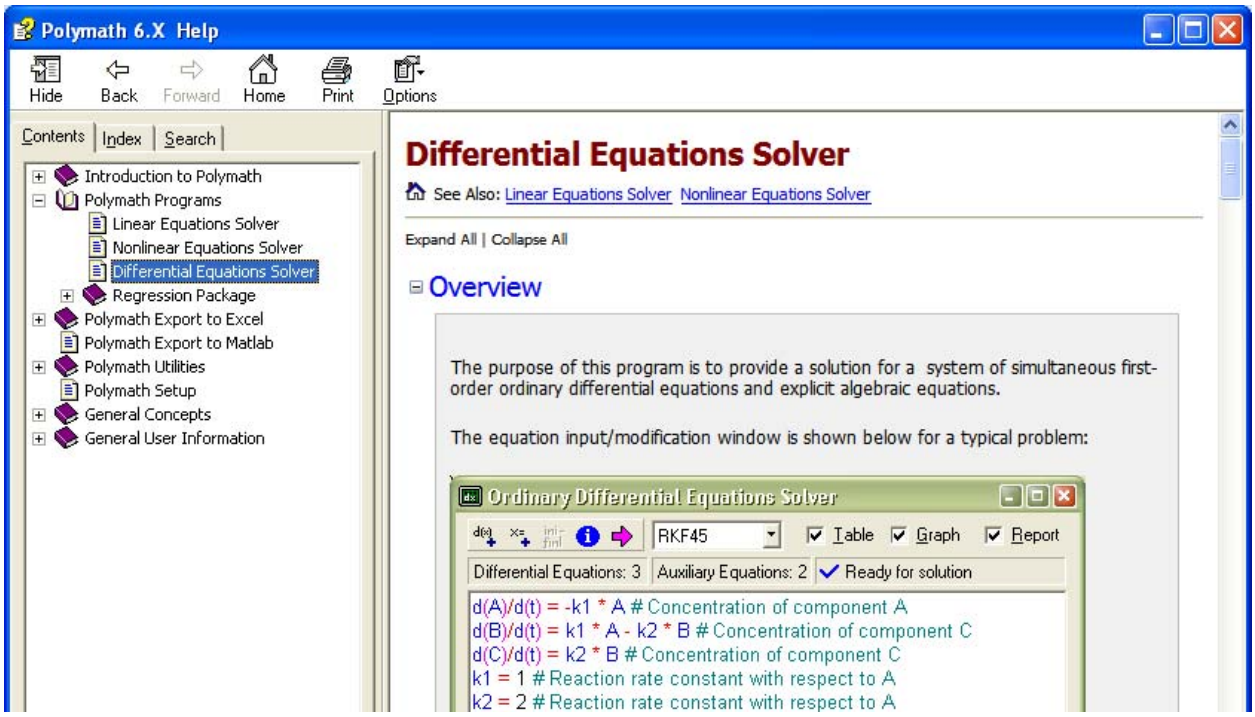
Introduction to Polymath
Polymath Programs
Linear Equations Solver
Nonlinear Equations Solver
Differential Equations Solver
Regression Package
Polymath Export to Excel
Polymath Export to Matlab
Polymath Utilities
Polymath Setup
General Concepts
General User Information
POLYMATH Help Documentation
Numerical Solutions for Scientific and Engineering Mathematical Problems
POLYMATH 6.X is a proven computational system, which has been specifically created for educational or professional use. The various POLYMATH programs allow the user to apply effective numerical analysis techniques during interactive problem solving on personal computers. Results are presented graphically for easy understanding and for incorporation into papers and reports. Students, engineers, mathematicians, scientists, or anyone with a need to solve problems will appreciate the efficiency and speed of problem solution.
The principal options available in the POLYMATH main task selection window are the following:
Polymath Programs
LEQ Linear Equations Solver
NLE Nonlinear Equations Solver
DEQ Differential Equations Solver
REG Data Table
Linear & Polynomial Regression
Multiple Linear Regression
Multiple Nonlinear Regression
Utilities
Calc Advanced Scientific Calculator

4. Start the Differential Equations Solver by selecting Program, DEQ Differential Equations and keep the help window open

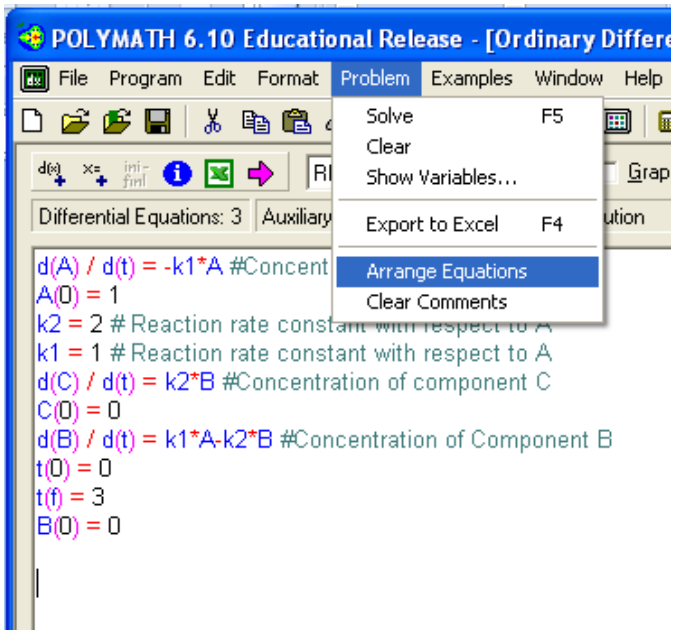


5. Choose the Differential Equations solver in the help menu

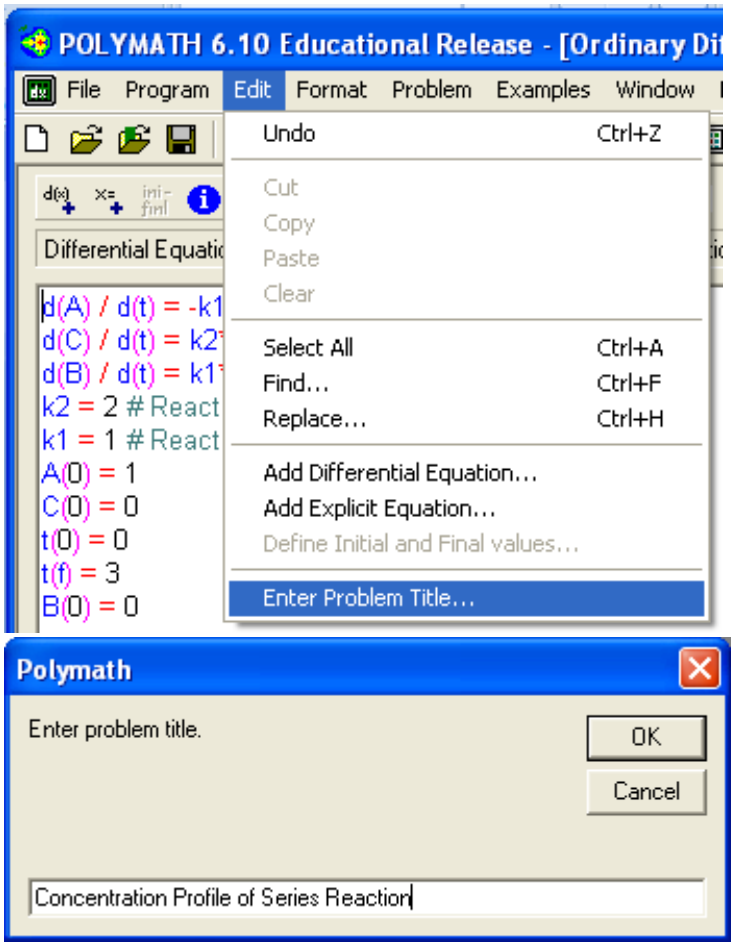


6. Enter the 3 differential Equations and supporting explicit algebraic equations. To do this and learn about POLYMATH, I suggest that you read through the POLYMATH help file starting with the Overview section. After entering the equations and running the program return to step 7.

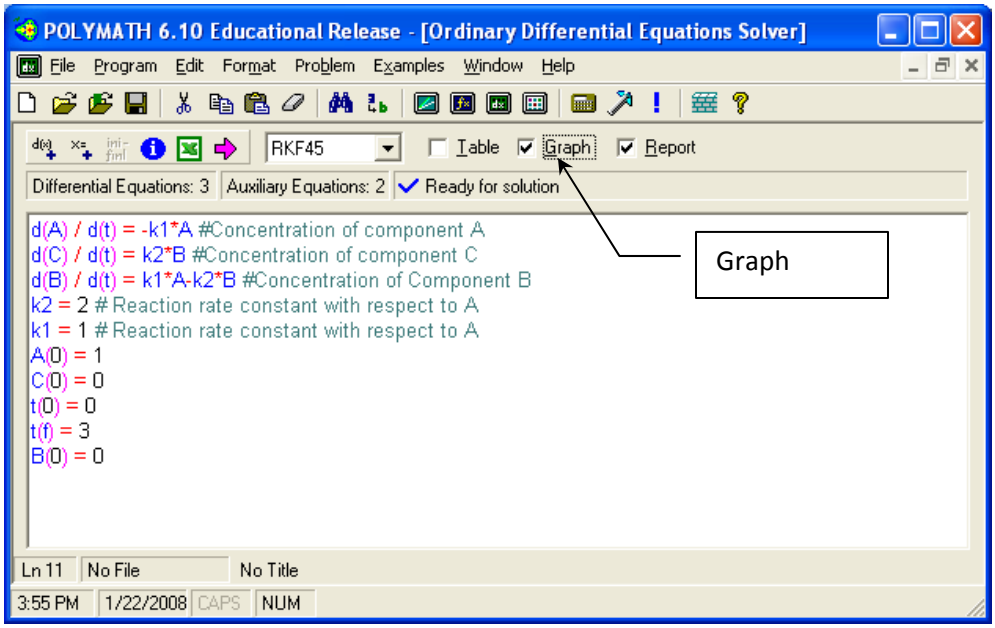
7. Sort the equation by using the button



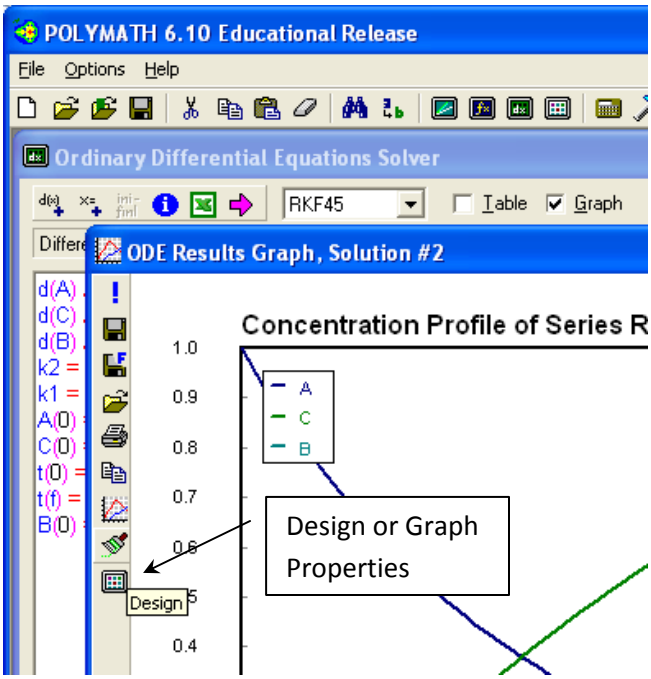
8. Now enter a problem title by selecting Edit, Enter Problem Title…

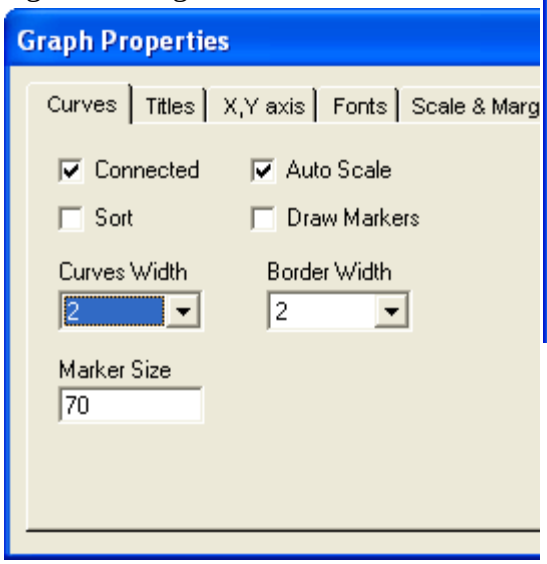


9. Add a graph to the output by clicking the box and rerun the program

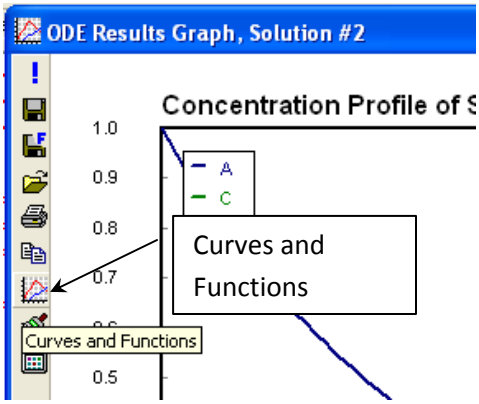


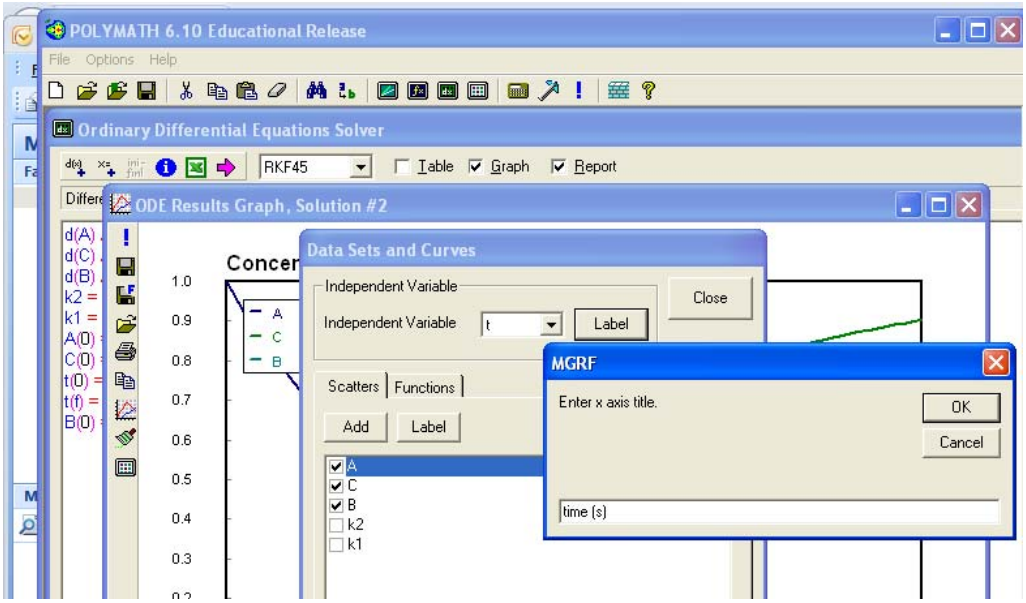
10. Edit the POLYMATH produced graph by doing the following:
    a. Open the Design or Graph properties window by clicking on the paint brush Increase the width of the lines to a 2
    b. Add a title
    c. Change the x,y axis to a decimal with 2 digits showing





d. Open the Curves and Functions menu and edit the x-axis by selecting the Label button. The x-axis should have a label: time (s). Always give units on labels. Please note that the SI abbreviation for seconds is s.





e. The only part missing is the y-axis which will be entered later. You can do this either by writing on the paper or adding text as shown next.

11. Now prepare this polymath program results to be handed in for a homework assignment. This is what you will do for all homework assignments involving POLYMATH.
    a. Select the "Differential Equations Solution" output screen, click on the text and then choose Edit, Select All. Then paste this into a word document.
    b. Copy the graph (you can use the copy button, Ctrl + C etc.)
    c. In word select the graph and use text wrapping so that the output will fit on one page.
    d. Now add a y-axis using the textbox tool. Concentration (mol/m^3)

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	A	1.	0.0497871	1.	0.0497871
2	B	0	0	0.2499865	0.0473083
3	C	0	0	0.9029046	0.9029046
4	k1	1.	1.	1.	1.
5	k2	2.	2.	2.	2.
6	t	0	0	3.	3.

Differential equations

1 d(A)/d(t) = -k1*A

Concentration of component A

2 d(C)/d(t) = k2*B

Concentration of component C

3 d(B)/d(t) = k1*A-k2*B

Concentration of Component B

Explicit equations

1 k2 = 2

Reaction rate constant with respect to A

2 k1 = 1

Reaction rate constant with respect to A

General

Total number of equations	5
Number of differential equations	3
Number of explicit equations	2
Elapsed time	0.000 sec
Solution method	RKF_45
Step size guess. h	0.000001
Truncation error tolerance. eps	0.000001

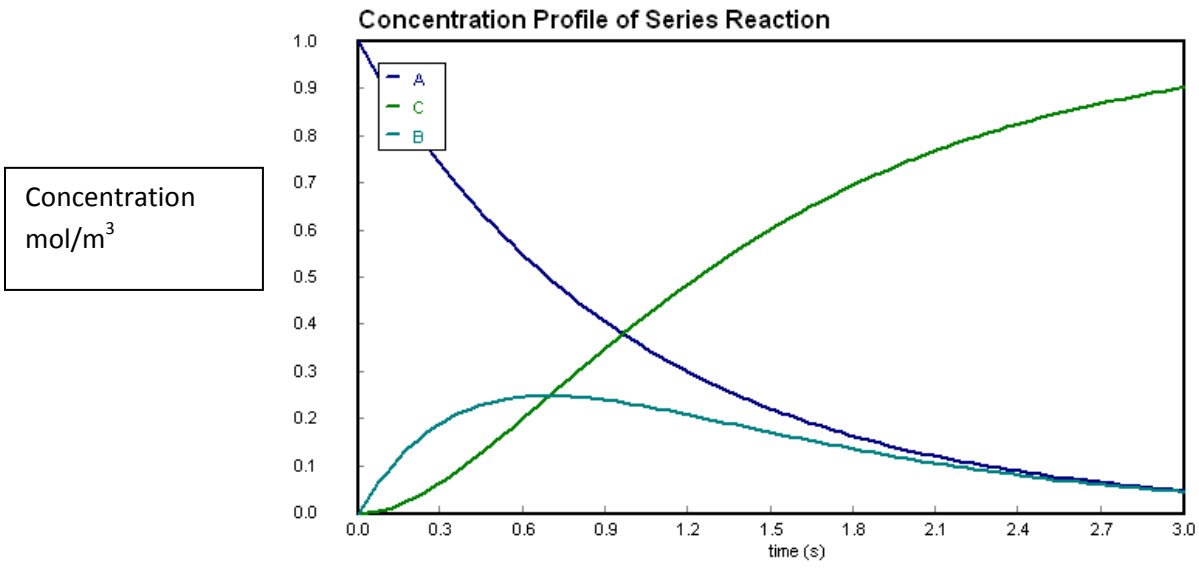
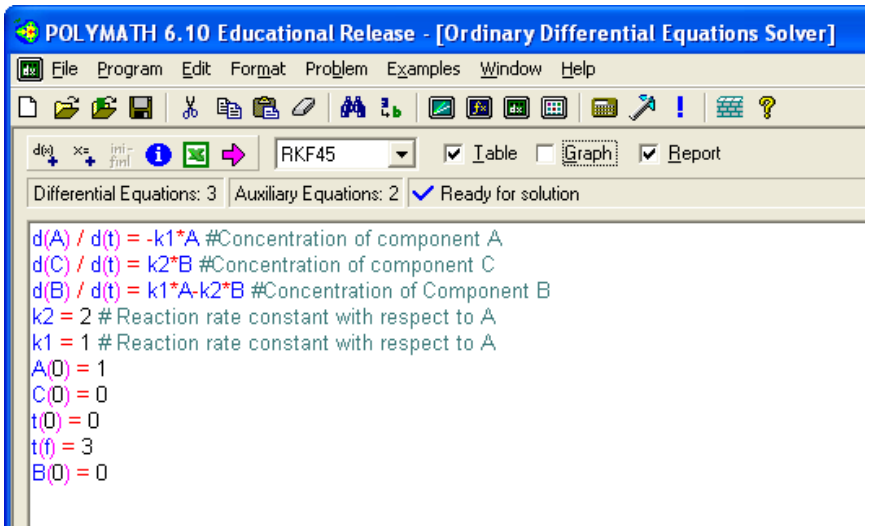
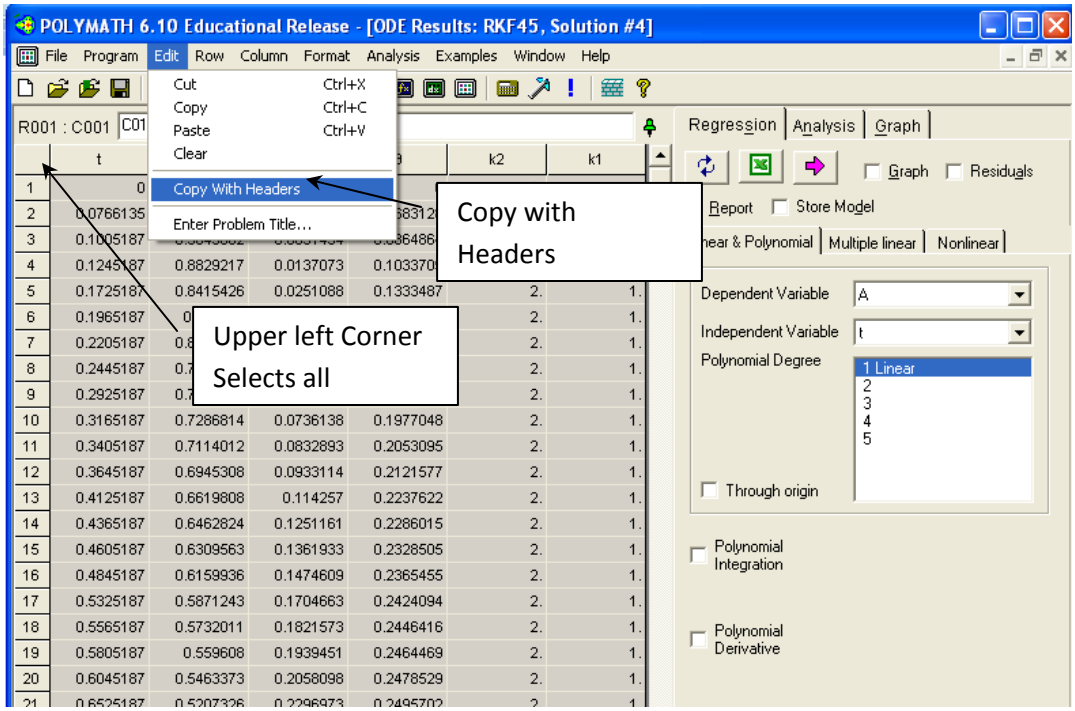


Figure 1: Concentration Profile of a Series Reaction

12. The above was probably too much work for a graph. An alternative method which I prefer is to use excel to produce the graph. In this case you should do the following
    a. Select the Table output button



    b. Run the program again
    c. Select the table
    d. Click on the upper left corner of the table (similar to excel)



    e. Then select Edit, Copy With Headers. (This will copy the names of the variables as well as the numbers)
    f. Paste this into an excel spreadsheet and produce a graph with all titles given and labels. Notice that for computer generated data, no markers are used. Draw this data using a line and not markers.

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	A	1.	0.0497871	1.	0.0497871
2	B	0	0	0.2499865	0.0473083
3	C	0	0	0.9029046	0.9029046
4	k1	1.	1.	1.	1.
5	k2	2.	2.	2.	2.
6	t	0	0	3.	3.

Differential equations

1 d(A)/d(t) = -k1*A

Concentration of component A

2 d(C)/d(t) = k2*B

Concentration of component C

3 d(B)/d(t) = k1*A-k2*B

Concentration of Component B

Explicit equations

1 k2 = 2

Reaction rate constant with respect to A

2 k1 = 1

Reaction rate constant with respect to A

General

Total number of equations	5
Number of differential equations	3
Number of explicit equations	2
Elapsed time	0.000 sec
Solution method	RKF_45
Step size guess. h	0.000001
Truncation error tolerance. eps	0.000001

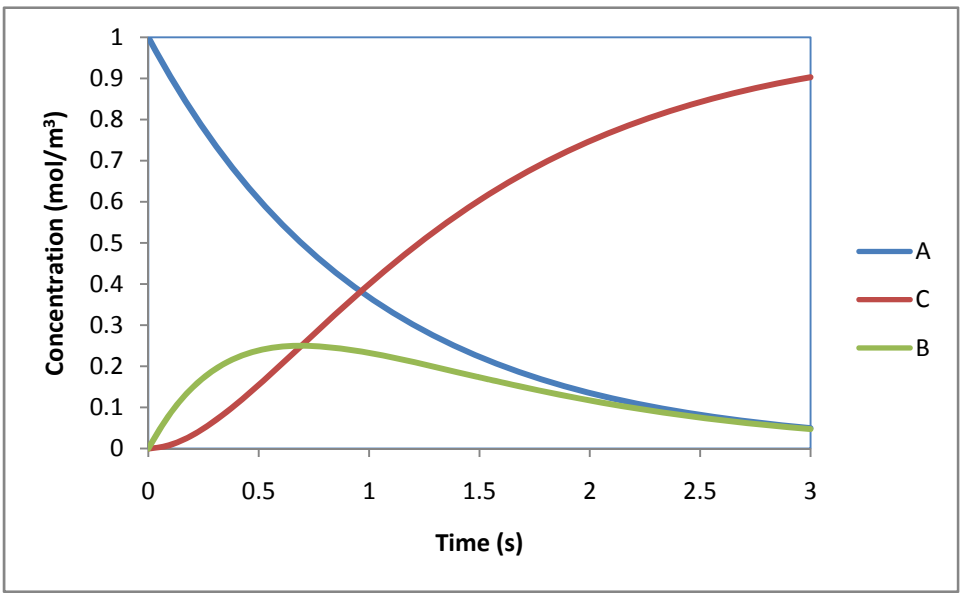
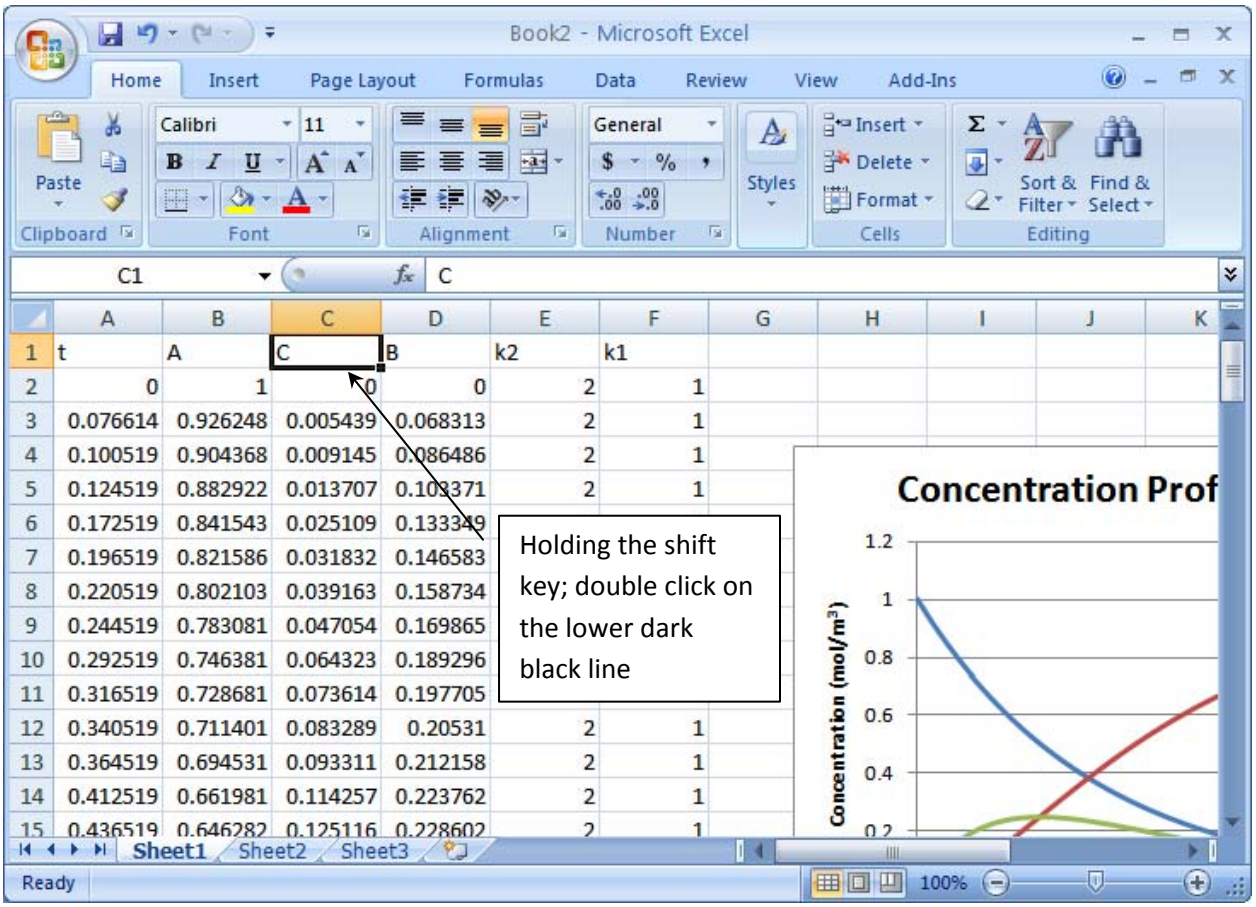


Figure 2: Concentration Profile of a Series Reaction

Excel Hint:

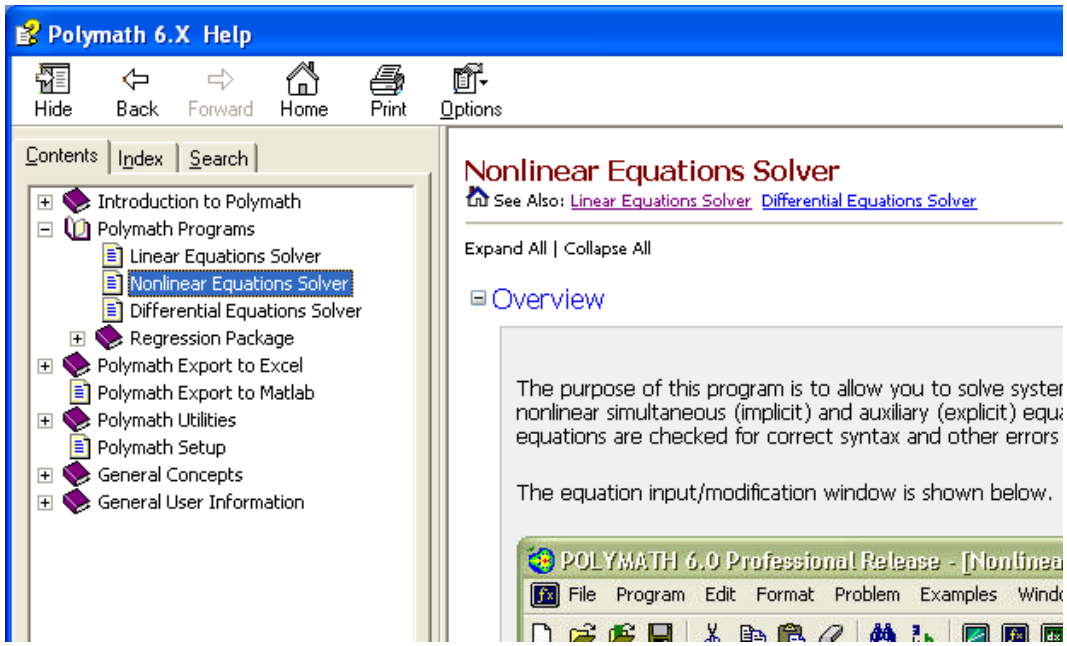
Did you know that one way to select a column of data is to hold the shift key down and double click on the lower line? For example to select the Column C data go to cell C1 and double click on the line between rows 1 and 2 . Similarly if you want to move to the bottom of a data set you can just double click on the lower dark black line without holding the shift key.



	A	B	C	D	E	F
1	t	A	C	B	k2	k1
2	0	1	0	0	2	1
3	0.076614	0.926248	0.005439	0.068313	2	1
4	0.100519	0.904368	0.009145	0.086486	2	1
5	0.124519	0.882922	0.013707	0.103371	2	1
6	0.172519	0.841543	0.025109	0.133349		
7	0.196519	0.821586	0.031832	0.146583		
8	0.220519	0.802103	0.039163	0.158734		
9	0.244519	0.783081	0.047054	0.169865		
10	0.292519	0.746381	0.064323	0.189296		
11	0.316519	0.728681	0.073614	0.197705		
12	0.340519	0.711401	0.083289	0.20531	2	1
13	0.364519	0.694531	0.093311	0.212158	2	1
14	0.412519	0.661981	0.114257	0.223762	2	1
15	0.436519	0.646282	0.125116	0.228602	2	1

THE FOLLOWING IS OPTIONAL AND SHOULD NOT BE SUBMITED

Now review the Non linear Equations solver:



Following Example 1 and Example 2 given in the Polymath program tutorial solve the following problem. This is taken from the Cutlip and Shacham text book titled, "Problem solving in Chemical Engineering with Numerical Methods."

The van der Waals equation of state is given by

$$\left(P+\frac{a}{V^2}\right)\left(V-b\right)=RT \tag{1}$$

Where

$$a=\frac{27}{64}\left(\frac{R^2T_c^2}{P_c}\right) \tag{2}$$

And

$$b=\frac{RT_c}{8P_c} \tag{3}$$

The variables are defined as:

P = pressure in atm

V = molar volume in L/gmol

T = temperature in K

$R = 0.08206$ atm L/(gmol K)

$T_c = 405.5K$ for ammonia

$P_c = 111.3$ atm for ammonia

The reduced pressure is defined as

$$P_r = \frac{P}{P_c} \tag{4}$$

And the compressibility factor is given by

$$Z = \frac{PV}{RT} \tag{5}$$

Calculate the molar volume and compressibility factor for gaseous ammonia at a pressure of 56 atm and a temperature of 450 K using the van der Waals equation of state.

In presenting the solution do the following:

1. Write the program.
2. Estimate the volume using the ideal gas law.
3. Write this calculation on engineering paper as well your hand calculations with units for equations 1, 2, 3, and 5. Note that for equation 1, this should be a sample calculation using your initial guess. Show all of the necessary units.
4. Select the option to produce a graph
5. Solve it using POLYMATH.
6. Then use select all and cut and paste the POLYMATH report into a word document as shown below as well as the graph.
7. You will need to edit the graph to label the axis to produce what is shown below. You can either hand write the units to the axis or use the Microsoft drawing tools to add the units.
8. produce the printout found on the following page

POLYMATH Report 2.1(a) MOLAR VOLUME AND COMPRESSIBILITY FACTOR FROM VAN DER WAALS EQUATION
Nonlinear Equation 22-Jan-2008

Calculated values of NLE variables

	Variable	Value	f(x)	Initial Guess
1	V	0.5748919	6.395E-13	*Use the ideal gas law to obtain a good guess! Show this hand calculation on a separate page!*

	Variable	Value
1	a	4.196946
2	b	0.0373712
3	P	56.
4	Pc	111.3
5	Pr	0.5031447
6	R	0.08206
7	T	450.
8	Tc	405.5
9	Z	0.8718268

Nonlinear equations

1 f(V) = (P+a/(V^2))*(V-b)-R*T = 0

Explicit equations

1 P = 56

2 R = 0.08206

3 T = 450

4 Tc = 405.5

5 Pc = 111.3

6 Pr = P/Pc

7 a = 27*(R^2*Tc^2/Pc)/64

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

9 Z = P*V/(R*T)

General Settings

Total number of equations	10
Number of implicit equations	1
Number of explicit equations	9
Elapsed time	1.1574 sec
Solution method	SAFENEWT
Max iterations	150
Tolerance F	0.0000001
Tolerance X	0.0000001
Tolerance min	0.0000001

Data file: k:\heskethdrive\courses\reaction engineering\lectures&examples\p2-01a.pol

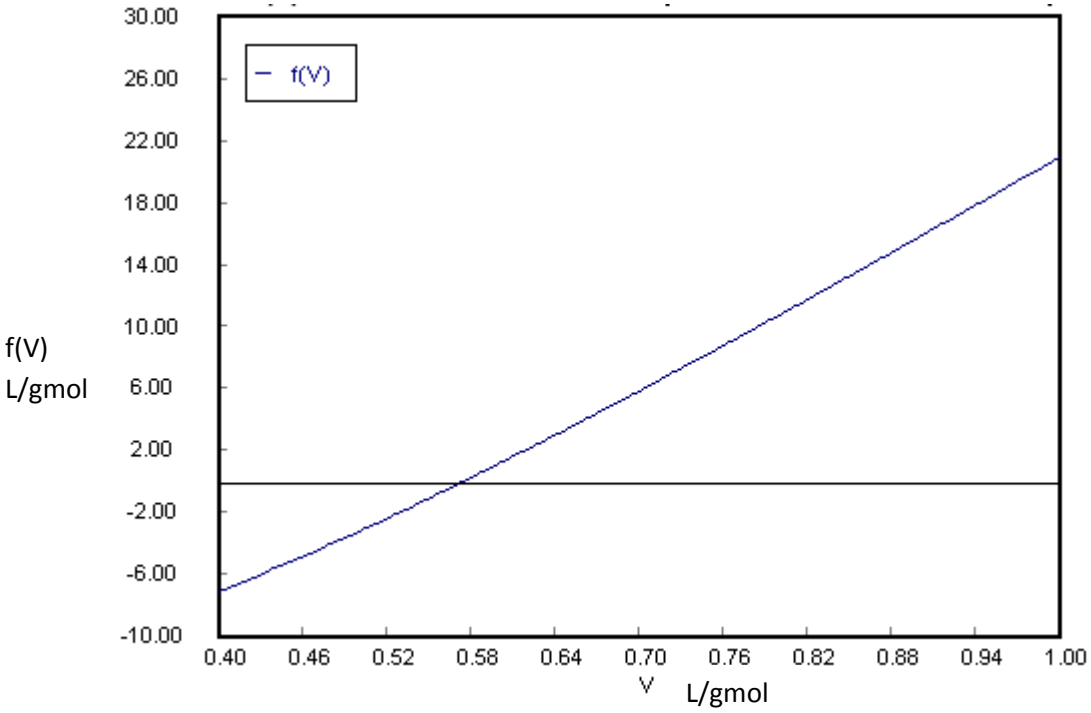


Figure 3 Polymath Plot for Van der Waals Problem in Cutlip and Shacham Book 2.1 (a)