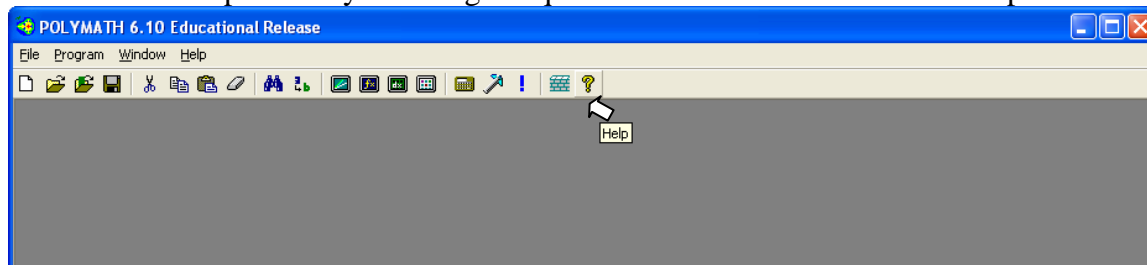
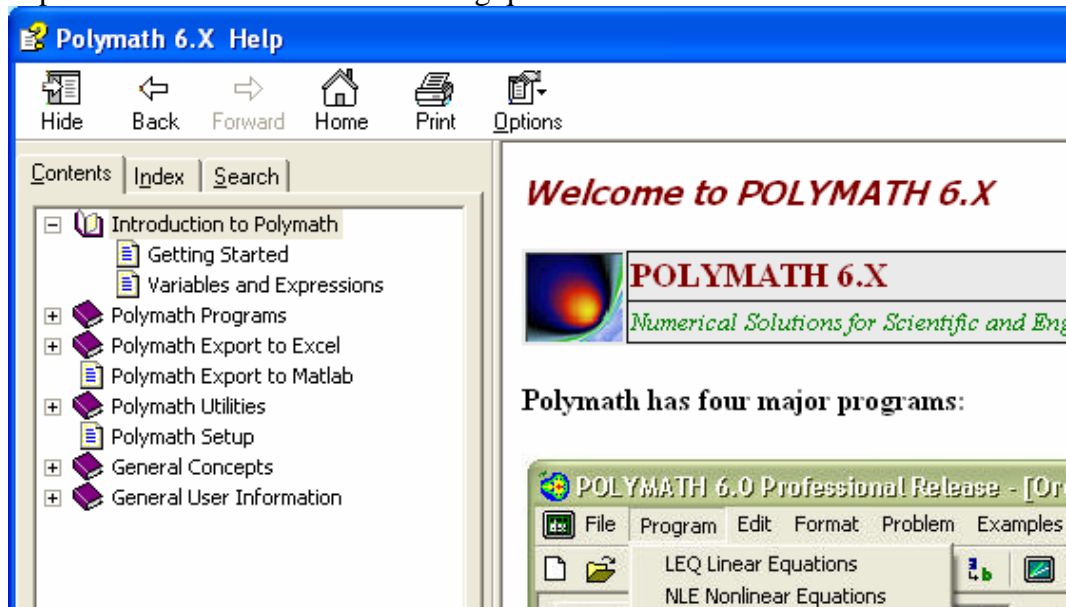


This tutorial will introduce you to the basics of Polymath. Start the tutorial by opening the POLYMATH program which is usually found from the Chemical Apps section of the Start, Programs menu. Select the Polymath program “Polymath EDU site”.

Examine the Help menu by selecting the question mark or the word menu Help.

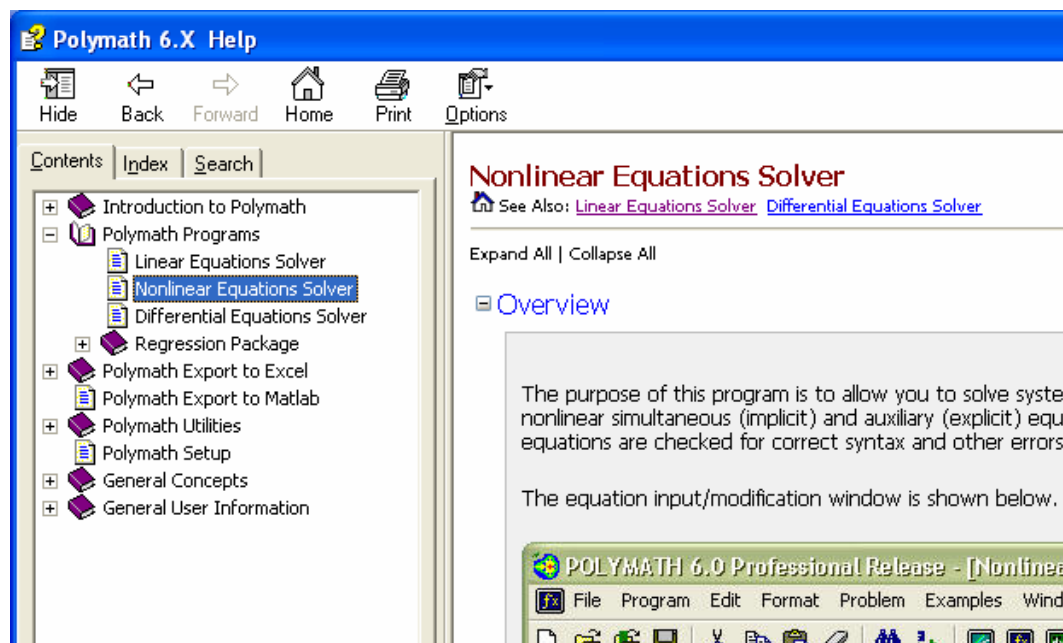


Read the section titled *Introduction to Polymath* both getting started and Variables and expressions and answer the following questions:



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.
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?

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

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

Where

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

And

$$b = \frac{RT_c}{8P_c} \quad (3)$$

The variables are defined as:

P = pressure in atm

V = molar volume in L/gmol

T = temperature in K

$R = 0.08206 \text{ atm L/(gmol K)}$

$T_c = 405.5 \text{ K}$ for ammonia

$P_c = 111.3 \text{ atm}$ for ammonia

The reduced pressure is defined as

$$P_r = \frac{P}{P_c} \quad (4)$$

And the compressibility factor is given by

$$Z = \frac{PV}{RT} \quad (5)$$

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: and produce the printout found on the following page:

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.

POLYMATH Report	1.1(a) Molar Volume and Compress... Van Der Waals Equation
Nonlinear Equation	16-Jan-2007

Calculated values of NLE variables

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

	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 $T_c = 405.5$
- 5 $P_c = 111.3$
- 6 $P_r = P/P_c$
- 7 $a = 27 \cdot (R^2 \cdot T_c^2 / P_c) / 64$
- 8 $b = R \cdot T_c / (8 \cdot P_c)$
- 9 $Z = P \cdot V / (R \cdot T)$

General Settings

Total number of equations	10
Number of implicit equations	1
Number of explicit equations	9
Elapsed time	0.0000 sec
Solution method	SAFENEWT
Max iterations	150
Tolerance F	0.0000001
Tolerance X	0.0000001
Tolerance min	0.0000001

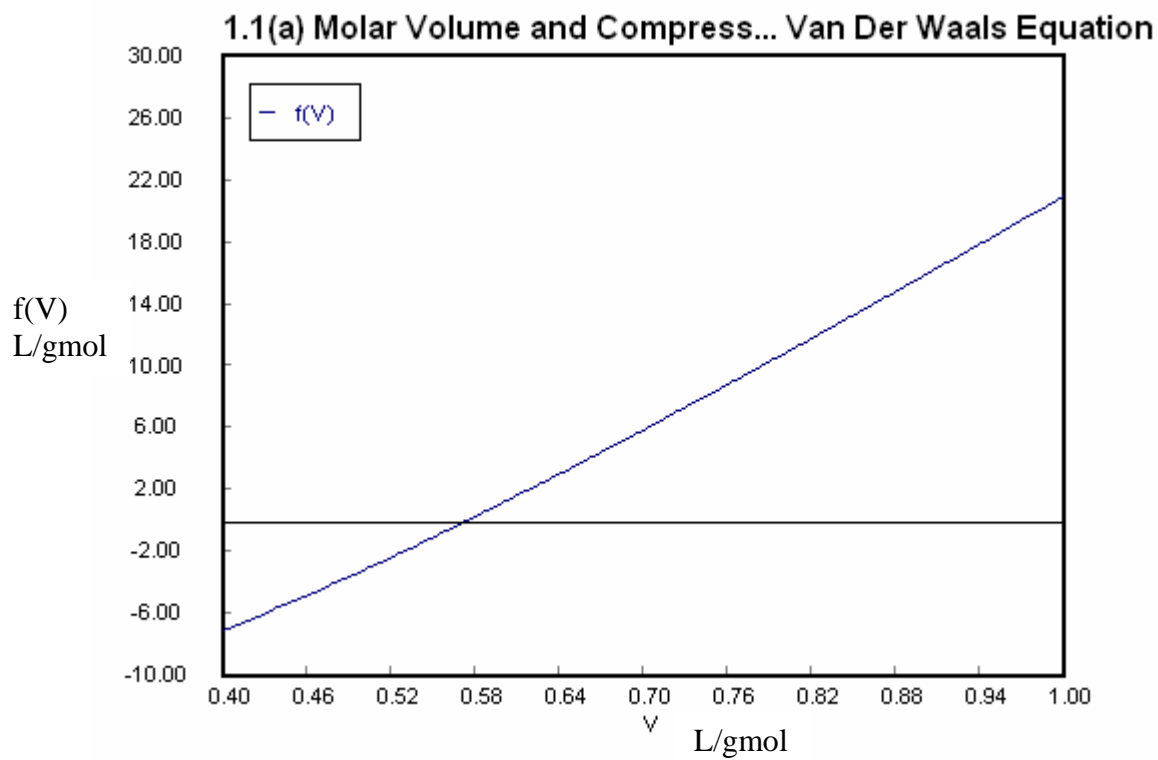
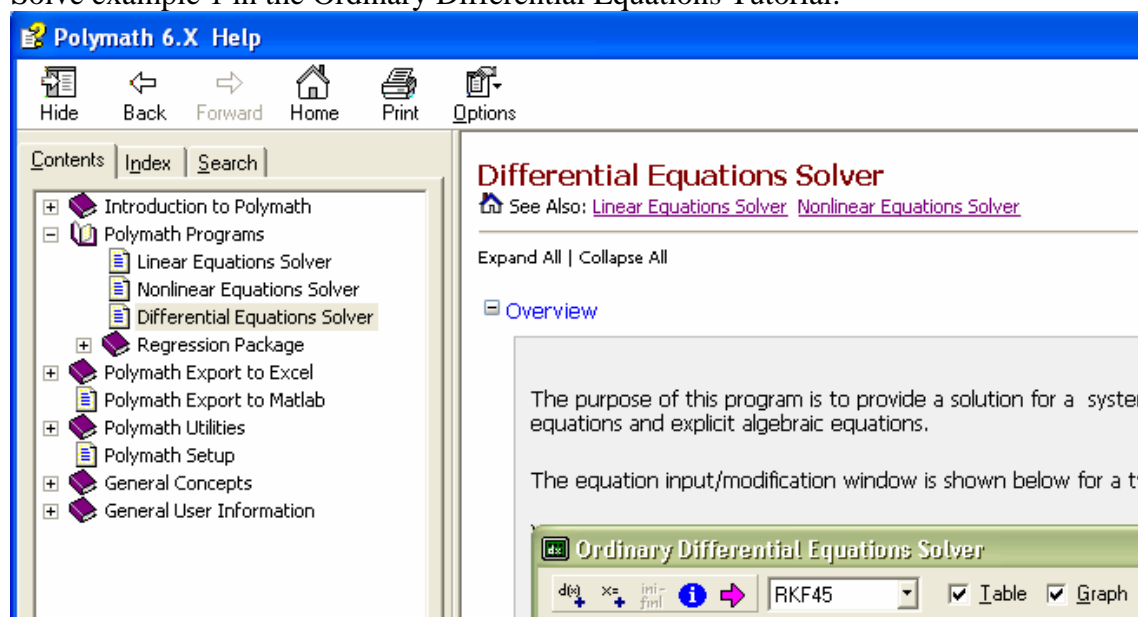


Figure 1: Polymath Plot for Van der Waals Problem

Solve example 1 in the Ordinary Differential Equations Tutorial:



In presenting the solution do the following and produce the printout found on the following page:

8. Write the program.
9. Write the calculation for the rate of change in A, B and C. In many homework problems this calculation can be based on the initial values. For this problem assume that the units of A, B and C are concentration with units mol/L and the units of each of the k's are s⁻¹.

$$d(A)/d(t) = -k_1A$$
 using an initial value of A

$$d(B)/d(t) = k_1A - k_2B$$
, using assumed values of A and B

$$d(C)/d(t) = k_2B$$
, using assumed values of B
 Show all of the necessary units.
10. Select the option to produce a table and a graph.
11. Solve the program using POLYMATH.
12. Then use select all and cut and paste the POLYMATH report into a word document as shown below as well as the graph.
13. 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.

POLYMATH Report	ODE Tutorial Example 1
Ordinary Differential Equations	17-Jan-2007

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 $d(C)/d(t) = k_2 \cdot B$

concentration of component C in mol/L

2 $d(B)/d(t) = k_1 \cdot A - k_2 \cdot B$

concentration of component B in mol/L

3 $d(A)/d(t) = -k_1 \cdot A$

Concentration of Component A in mol/L

Explicit equations

1 $k_2 = 2$

rate constant with units 1/s

2 $k_1 = 1$

rate constant with units 1/s

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

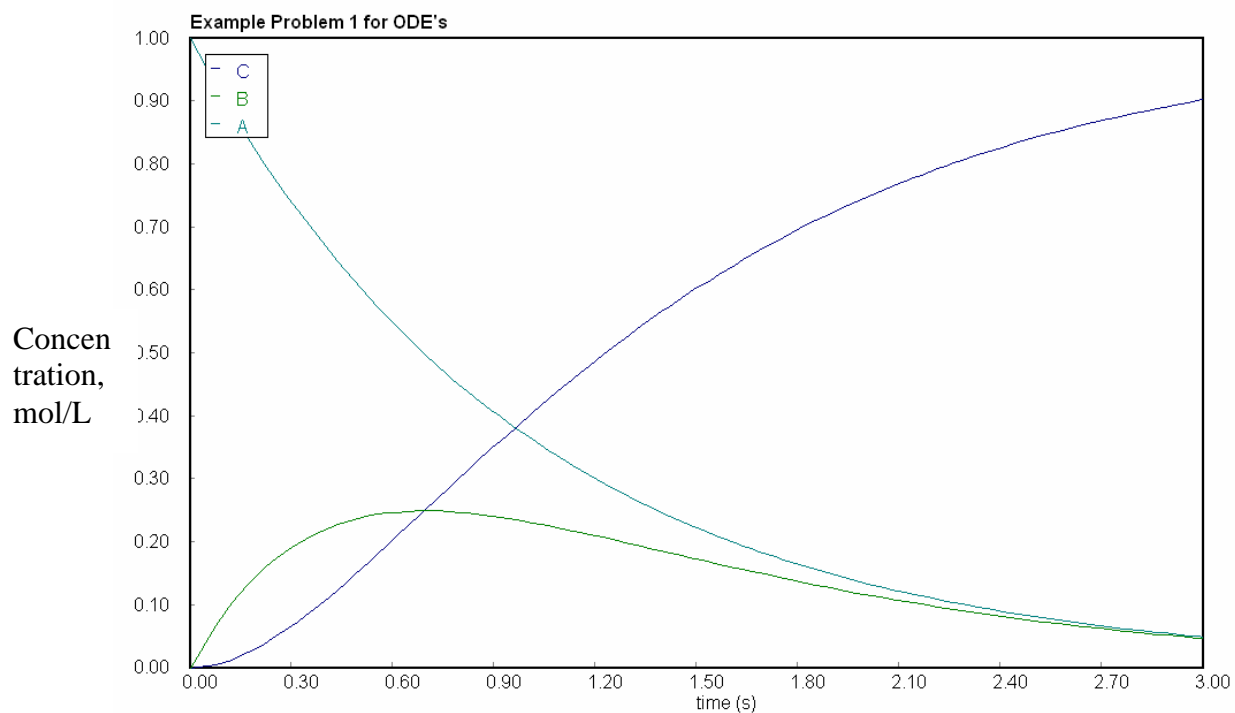


Figure 2: Polymath Plot for ODE Problem

Now produce the same graph using excel. Remember to use the edit copy headers option from the table command:

The screenshot shows the POLYMATH 6.10 Educational Release interface. The main window displays a table of results for 'ODE Results: RK45, Solution #4'. The table has columns for time (t), concentration (C), and other variables (B, A, k2, k1). The data is as follows:

	t	C	B	A	k2	k1
1	0	0	0	1.	2.	1.
2	0.0766135	0.0054394	0.0683128	0.9262478	2.	1.
3	0.1005187	0.0091454	0.0864864	0.9043682	2.	1.
4	0.1245187	0.0137073	0.1033709	0.8829217	2.	1.
5	0.1725187	0.0251088	0.1333487	0.8415426	2.	1.
6	0.1965187	0.0318316	0.1465825	0.821586	2.	1.
7	0.2205187	0.0391634	0.158734	0.8021026	2.	1.
8	0.2445187	0.0470537	0.169865	0.7830813	2.	1.
9	0.2925187	0.0643225	0.1892963	0.7463813	2.	1.
10	0.3165187	0.0736138	0.1977048	0.7286814	2.	1.
11	0.3405187	0.0832893	0.2053095	0.7114012	2.	1.
12	0.3645187	0.0933114	0.2121577	0.6945308	2.	1.
13	0.4125187	0.114257	0.2237622	0.6619808	2.	1.
14	0.4365187	0.1251161	0.2286015	0.6462824	2.	1.
15	0.4605187	0.1361933	0.2328505	0.6309563	2.	1.
16	0.4845187	0.1474609	0.2365455	0.6159936	2.	1.
17	0.5325187	0.1704663	0.2424094	0.5871243	2.	1.

Overlaid on the table is the 'Regression' window. It shows the 'Report' tab selected. The 'Dependent Variable' is 'C' and the 'Independent Variable' is 't'. The 'Polynomial Degree' is set to '1 Linear'. The 'Through origin' checkbox is unchecked. The 'Polynomial Integration' checkbox is also unchecked. The window title is 'ODE Results: RK45, Solution #4'.

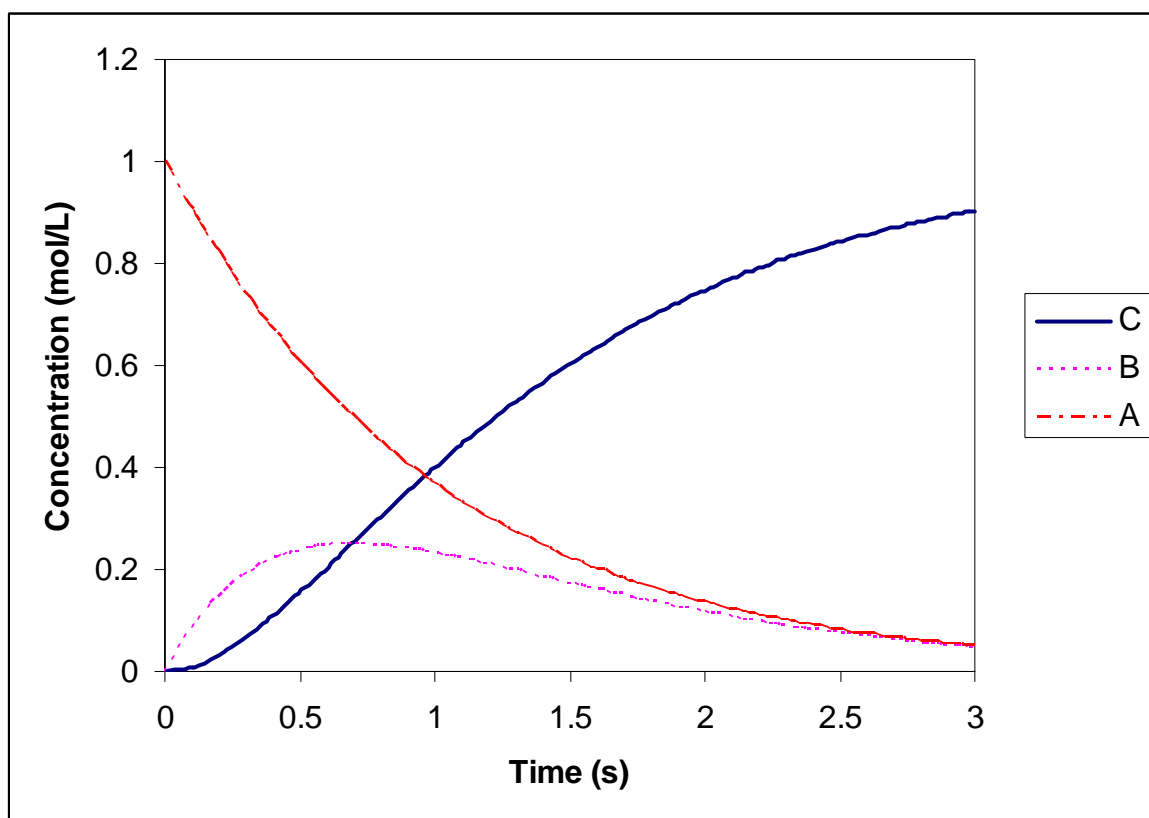


Figure 3: Excel Graph of ODE Example 1