Polymath Tutorial

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?



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

🥹 P	OLYMATH	5.10 Educational Release
File	Program	ndow Help
		· Equations 🙀 🛃 🔟 🔟 💷 📖 🎾 📜 🧱 🦿
	DEQ Diff REG Reg	ential Equations
		Polymath 6.X Help
		12 ← ⇔ CL ← Orint Control for the Back Forward Home Print Options
		Contents Index Search ● Introduction to Polymath ● Object to Polymath ● Polymath Programs ● Linear Equations Solver ● Nonlinear Equations Solver ● Solverath Expand All Collapse All ● Polymath Expand to Expand ● Overview

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...

🤫 POLYMATH 6	.10	Educati	onal Rele	ease - [O	rdinary Di	
🔝 File 🛛 Program	Edit	Format	Problem	Examples	Window I	
🗅 💣 🏂 🔚	Ur	ndo			Ctrl+Z	
$\begin{array}{c} deq & \times_{\bullet} & fm \\ \hline \\ Differential Equation \\ d(A) / d(t) = -k1 \\ d(C) / d(t) = k2^{-1} \\ d(B) / d(t) = k1^{-1} \\ k2 = 2 \ \# \ React \\ k1 = 1 \ \# \ React \\ k1 = 1 \ \# \ React \\ A(0) = 1 \\ C(0) = 0 \\ t(0) = 0 \\ t(f) = 3 \\ B(0) = 0 \end{array}$	Pa Cl Fil Re Ac Ac	opy easte ear elect All nd eplace dd Differe dd Explicit		Ctrl+A Ctrl+F Ctrl+H		
Polymath						
Enter problem title.			el	[OK Cancel	
Concentration Profile of Series Reaction						

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

🤏 POLYMATH 6.10 Educational Release - [Ordinary Differential Equations Solver]	
🕅 File Program Edit Format Problem Examples Window Help	_ 8 ×
D 📂 🗗 📕 🐰 🖻 🛍 🖉 🛤 🏞 🖉 🖾 📾 📾 📾 🎾 ! 🚟 💡	
deg 😋 👬 🚯 🗷 🔶 RKF45 💽 🗖 Iable 🔽 Graph 🔽 Report	
Differential Equations: 3 Auxiliary Equations: 2 🗸 Ready for solution	
Ln 11 No File No Title	
3:55 PM 1/22/2008 CAPS NUM	11.

- 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

Graph Properties						
Curves Titles X,Yaxis Fonts Scale & Marg						
🔽 Connected 🛛 🔽 Auto Scale						
🗖 Sort 📄 Draw Markers						
Curves Width Border Width						
Marker Size 70						
P						



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)

POLYMATH Report Ordinary Differential Equations

Concentration Profile of Series Reaction 22-Jan-2008

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	А	1.	0.0497871	1.	0.0497871
2	В	0	0	0.2499865	0.0473083
3	С	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



Concentration Profile of Series Reaction

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 Program				nta. nni 43, 30tu	tion #4]	
ን 🚅		Edit Row Co	olumn Format	Analysis E>	amples Window I	Help	_ 7
	F 🖻 🔛 🛛	Cut	Ctrl+X		🔲 🖬 🌂 !	# ?	
2004	: C001 C01	Сору	Ctrl+C				Regression Analysis Graph
1	. 0001 [001	Paste Clear	Ctrl+V				
	t				k2	k1 _	🗕 🗘 🔳 🕩 🗖 🖸 🖾 Residuals
1		Copy With H	eaders		Construction		Report T Store Model
2	0766135	Enter Probler	m Title	38312	Copy with		
3	0.1005187	0.0040002		0.036486	Headers		hear & Polynomial Multiple linear Nonlinear
4	0.1245187	0.8829217	0.0137073	0.103370			
5	0.172518	0.8415426	0.0251088	0.1333487	2.	1.	Dependent Variable A
6	0.1965187	Linr	oer left Co	rner	2.	1.	Independent Variable t
7	0.2205187			mer	2.	1.	Polynomial Degree 1 Linear
9	0.2925187	Sele	ects all		2.		2
10	0.2925167	0.7286814	0.0736138	0.1977048	2.	1.	3
10	0.3405187	0.7200014	0.0736136	0.2053095	2.	1.	5
12	0.3645187	0.6945308	0.0933114	0.2033033	2.	1.	
13	0.4125187	0.6619808	0.0303114	0.2121377	2.	1.	Through origin
14	0.4365187	0.6462824	0.1251161	0.2286015	2.	1.	
15	0.4605187	0.6309563	0.1361933	0.2328505	2.	1.	- Polynomial
16	0.4845187	0.6159936	0.1474609	0.2365455	2.	1.	Integration
17	0.5325187	0.5871243	0.1704663	0.2424094	2.	1.	
18	0.5565187	0.5732011	0.1821573	0.2446416	2.	1.	- Polynomial
19	0.5805187	0.559608	0.1939451	0.2464469	2.	1.	Derivative
20	0.6045187	0.5463373	0.2058098	0.2478529	2.	1.	
21	0.6525187	0.5207326	0.2296973	0 2495702	2	1	

- 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.

POLYMATH Report Ordinary Differential Equations

-											
	Calculated values of DEQ variables										
	Variable Initial value		Minimal value	Maximal value	Final value						
1	Α	1.	0.0497871	1.	0.0497871						
2	В	0	0	0.2499865	0.0473083						
3	С	0	0	0.9029046	0.9029046						
4	k1	1.	1.	1.	1.						
5 k2 2. 2. 2. 2.											
6	6 t 0 0 3. 3.										
	Differential equations										

L	лп	er	en	tia	n e	qu	ati
						- C	

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



Concentration Profile of Series Reaction 22-Jan-2008 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.

0	0 0 9	- (* -) -			Book2 -	Microsoft E	cel			-	= x
	Home	Insert	Page La	yout Fo	rmulas I	Data Rev	view V	/iew Add-I	ns	0.	- = x
	ste	Calibri BJJU Calibri C	* 11 * * A A A * 5		₽ ₽ ₽	General → \$ → % → \$.00 →.00 Number	Styles	Gran Insert ▼ Cells	Fi	ort & Find & lter * Select *	
	C1	•	0	∫ _x C							*
	Α	В	С	D	E	F	G	Н	1	J	K
1	t	А	С	В	k2	k1					
2	0	1	NO.	0	2	1					- I and
3	0.076614	0.926248	0.005439	0.068313	2	1					
4	0.100519	0.904368	0.009145	0.086486	2	1	1				
5	0.124519	0.882922	0.013707	0.103371	2	1		Co	ncent	ration	Prof
6	0.172519	0.841543	0.025109	0.133349	Listelia	م داد م داد :44		1.2			
7	0.196519	0.821586	0.031832	0.146583		g the shift		1.2			
8	0.220519	0.802103	0.039163	0.158734	key; do	ouble click	on	a 1 b			_
9	0.244519	0.783081	0.047054	0.169865	the lov	ver dark		E			
10	0.292519	0.746381	0.064323	0.189296	black li	ine		0.8			
11	0.316519	0.728681	0.073614	0.197705		-					/
12	0.340519	0.711401	0.083289	0.20531	2	1		Concentration (mol/m ³)	1		
13	0.364519	0.694531	0.093311	0.212158	2	1		0.4		\checkmark	
14	0.412519	0.661981	0.114257	0.223762	2	1		OUO		~	
15		0.646282 eet1 She		0.228602 et3	2	1		8 ₀₂	7		
Rea	dy							⊞□□ 10	0% Θ		

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

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

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) $T_c = 405.5K \text{ for ammonia}$ $P_c = 111.3 \text{ atm for ammonia}$

The reduced pressure is defined as

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

And the compressibility factor is given by

$$Z = \frac{PV}{RT}$$
(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

	Ca	lculated	values of	NLE varia	bles
	1	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!
	ľ	Variable	Value		
Ĩ	1	а	4.196946	'n	
Í	2	b	0.0373712	-	
÷	3		56.	Ξ.	
ĺ	4	Pc	111.3		
	5	Pr	0.5031447		
Ì	6	R	0.08206		
	7	Т	450.	-	
	8	Тс	405.5		
	9	Z	0.8718268		
-	No	onlinear e	equations	1	
	1	f(V) = (P+	-a/(V^2))*((V-b)-R*T :	= 0
	Ех	plicit equ	uations		
	1	P = 56			
ĺ	2	R = 0.082	06		
ĺ	3	T = 450			
ĺ	4	Tc = 405.	5		
ĺ	5	Pc = 111.	3		
j	6	Pr = P/Pc			
j	7	a = 27*(R	2*Tc^2/F	Pc)/64	
Î	8	b = R*Tc/	′(8*Pc)		
	9	$Z = P^*V/($	R*T)		
	Ge	eneral Se	ttings	;	
	Tot	al number o	f equations	10	
	Nu	mber of impl	icit equations	1	
	Nu	mber of expl	icit equations		
	Ela	psed time		1.1574 sec	
	Sol	lution metho	d	SAFENEWT	
	Ma	x iterations		150	
]	Tol	erance F		0.0000001	
- 6		erance X		0.0000001	
[Tol	erance 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)