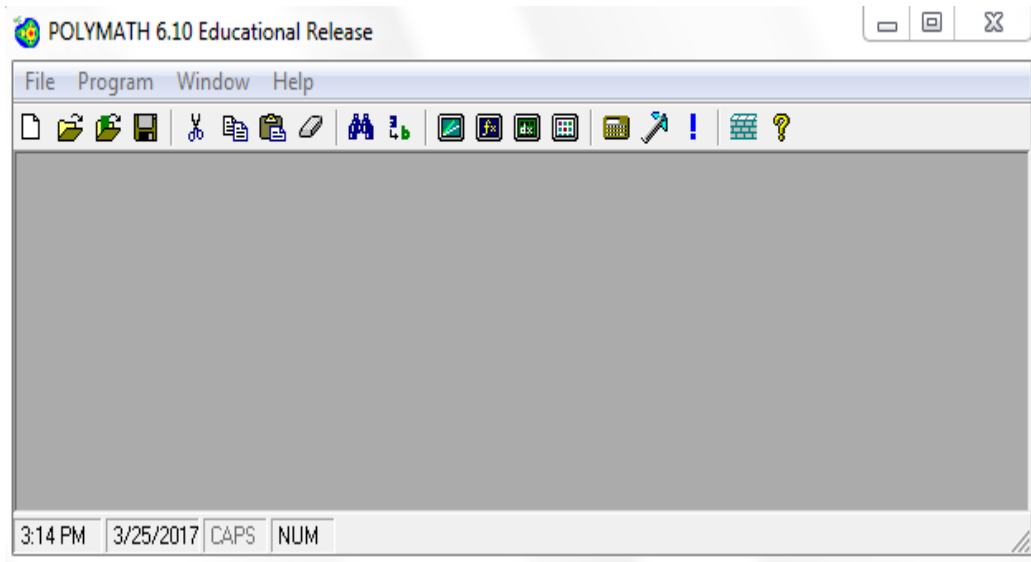


Polymath Tutorial to solve numerically unstable systems (Example-13-6)

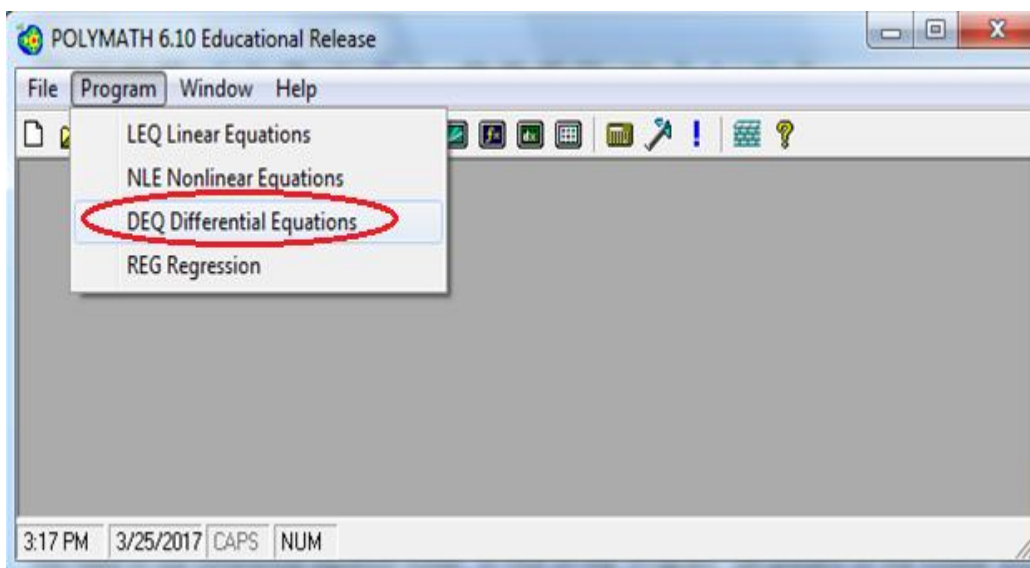
In this tutorial, you will learn how to solve ODE's which involve rapid change of temperature or pressure. This type of system can become numerically unstable and generate error or incorrect results

Step 1: Open the Polymath software. If you don't have it, then refer to the installation instruction available at <http://www.umich.edu/~elements/5e/software/polymath.html>

You will see the following window when you open Polymath



Step 2: Here, we need to use the Differential equation solver, so click on the "Program" tab present on the toolbar and select DEQ Differential Equations. You can also refer to the step-by-step Polymath tutorial for solving DEQ present at <http://www.umich.edu/~elements/5e/software/polymath.html>



Step 3: To prevent ordinary differential equations from becoming numerically unstable, we will use a function called “software switch (SW1)”. We will multiply all the differential equations with SW1, which will set all derivatives to zero when the equations become unstable, i.e. the value of the variables will become constant.

As per the problem statement, the reactor vessel fails when temperature T becomes higher than 600 K or the pressure exceeds 45 atm. So the value of SW1 will be 1 for T < 600 K and P < 45 atm, and the value of SW1 will be 0 when T > 600 K or P > 45 atm.

The Software Switch is therefore an indicator that the vessel has failed. When the vessel fails, the software switch becomes zero and the slopes of the differential equations become zero

Numerically, SW1 can be defined as

SW1 = if (T > 600 or P > 45) then (0) else (1)

So, the differential equation for CA becomes

$$\frac{dCA}{dt} = SW1 * r1A$$

For T < 600 and P < 45

$$\frac{dCA}{dt} = 1 * r1A$$

For T > 600 or P > 45

$$\frac{dCA}{dt} = 0 * r1A$$

Similarly, other differential equations will be defined as

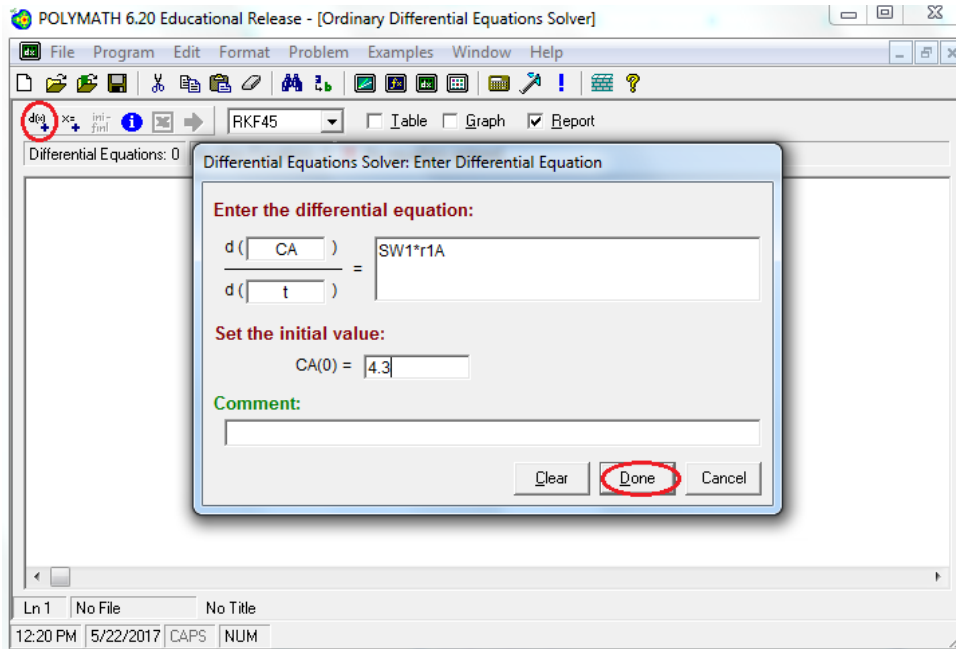
$$\frac{dCB}{dt} = SW1 * r1A$$

$$\frac{dCS}{dt} = SW1 * r2S$$

$$\frac{dP}{dt} = SW1 * ((FD - Fvent) * 0.082 * T / VH)$$

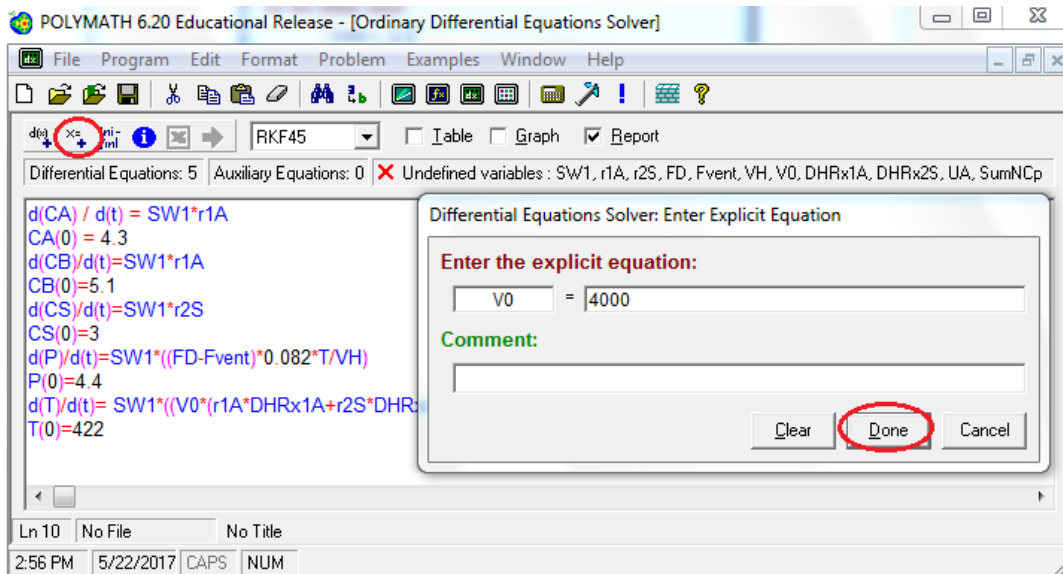
$$\frac{dT}{dt} = SW1 * ((V0 * (r1A * DHRx1A + r2S * DHRx2S) - UA * (T - 373.15)) / SumNCp)$$

To enter the above differential equation in Polymath, press the "d(x)+" button present on the menu bar (shown by the red circle in the screenshot below). This will bring up a dialogue box in which you can enter your differential equation. You will also need to specify an initial value for the differential variable. Enter the differential equation for CA and click "Done" button

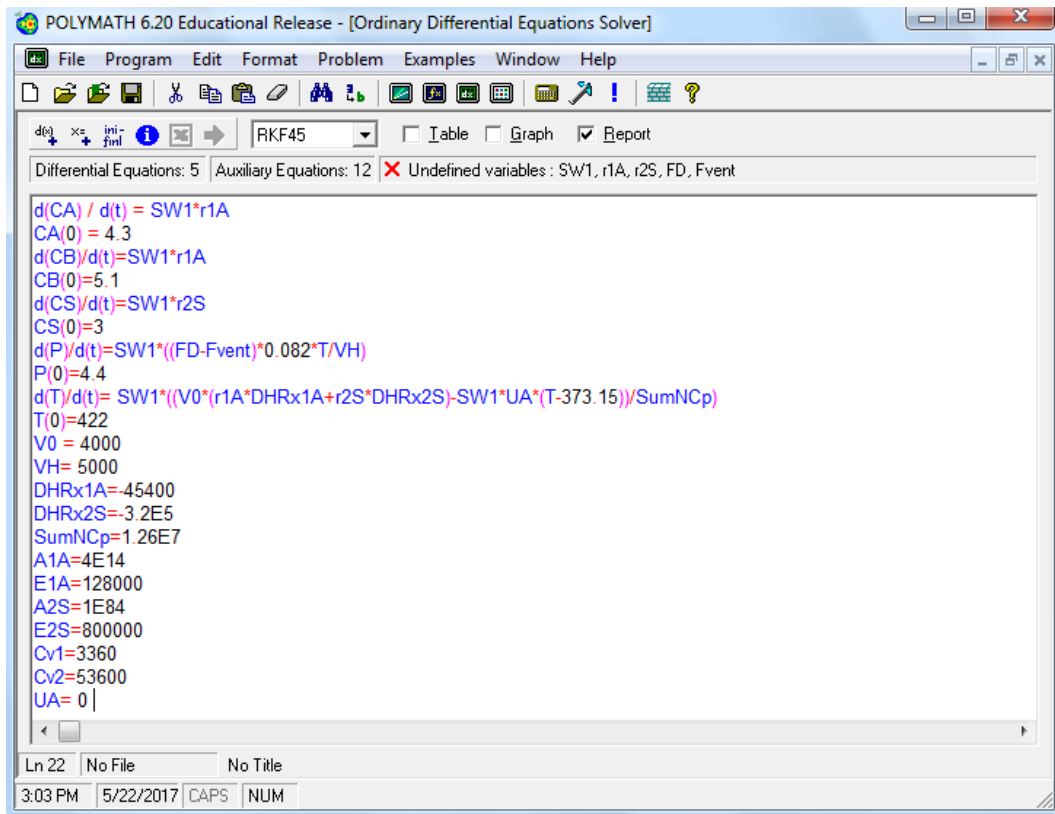


Step 4: You will find that your differential equation is entered in the main window. Similarly enter all the other differential equations. Make sure to multiply each differential equation by SW1

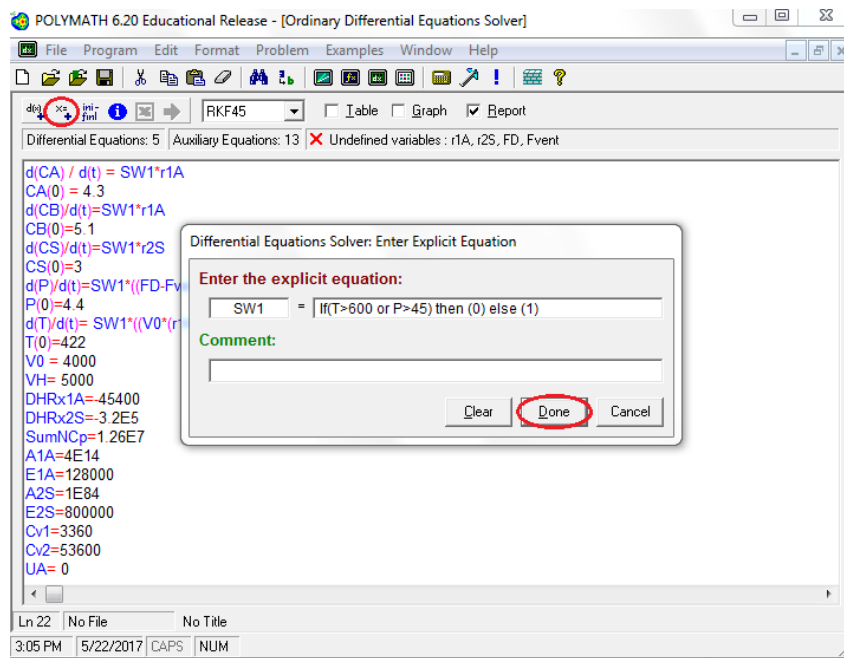
After you have entered all the differential equations, press "x+=" button to enter all the explicit equation and parameter values. Enter the expression for V0 and click "Done" as shown below



Similarly enter all other parameter values as shown below

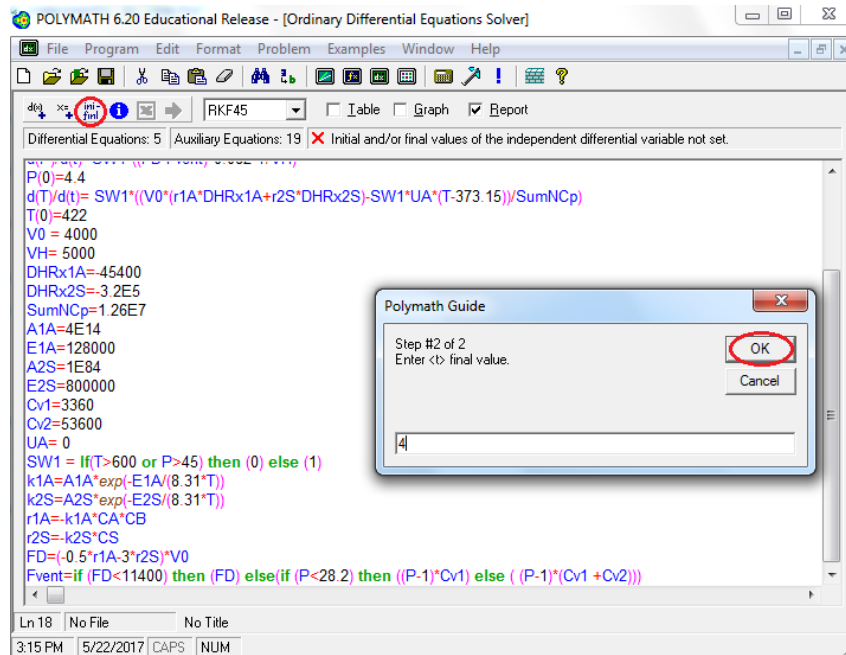



Step 5: Now enter the expression for SW1 as shown below

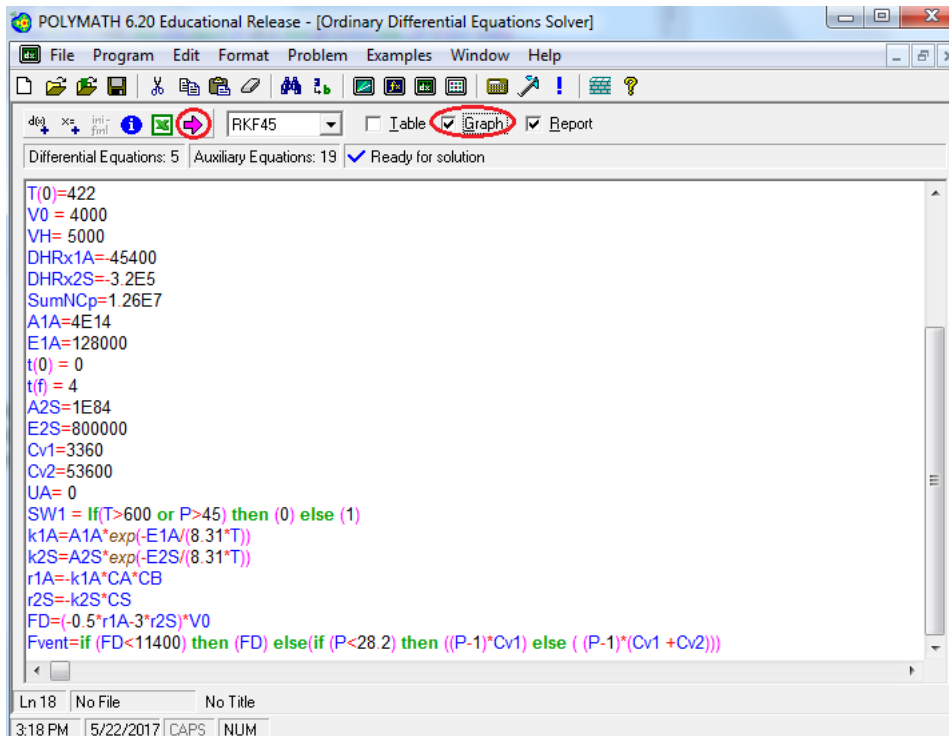


Similarly enter all the remaining equations in Polymath

Step 6: You have now entered both the differential equations and the explicit equations. Now you need to set the time span for which you want to perform the integration. To specify the initial and final values of t, click the "ini-finl" button present on the menu bar. A dialogue box will appear again. Enter the initial and final value of t in the space provided. In this case t initial =0 and t final=4. Then press OK



Step 7: When all of the necessary information has been specified, the screen will look like this. Check the box corresponding to Graph option to generate the graph in addition to the report. Next click on the pink arrow  to have Polymath perform the integration.



Step 8: The following report will be generated which gives initial and final values of every variable present, the minimum and maximum values of the variables in the given interval, and the equations you entered. Click on “X” to close the report and obtain the graph

Differential Equations Solution #5

File Edit Help

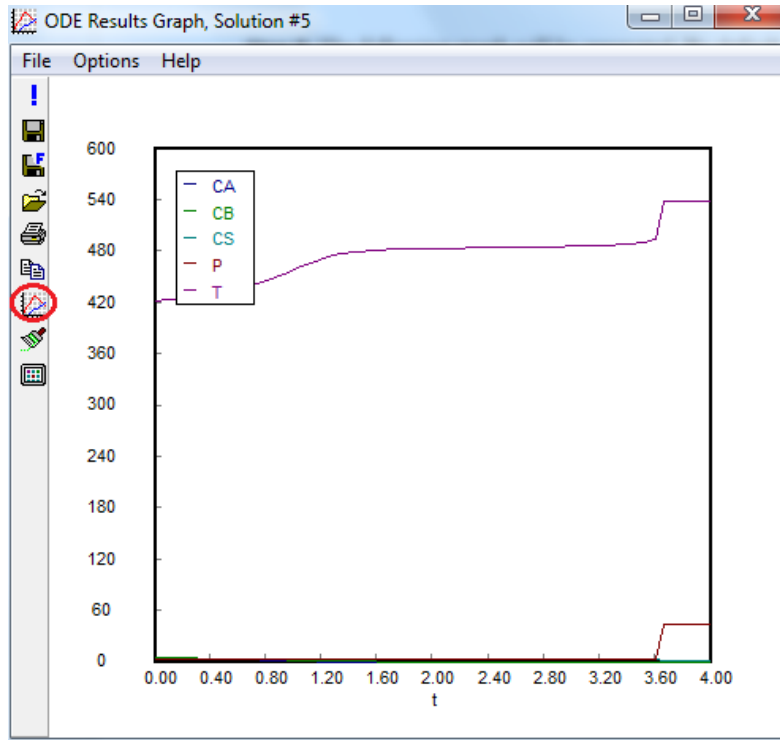
POLYMATH Report
Ordinary Differential Equations 22-May-2017

Calculated values of DEQ variables

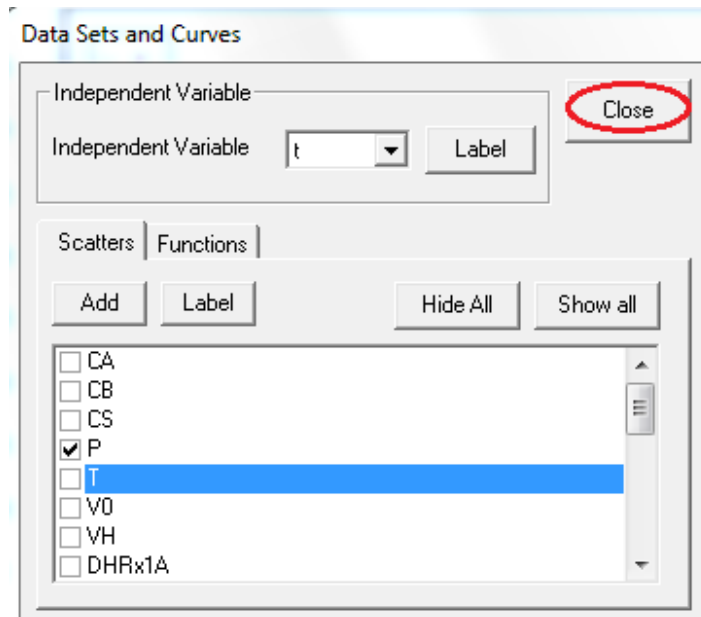
	Variable	Initial value	Minimal value	Maximal value	Final value
1	A1A	4.0E+14	4.0E+14	4.0E+14	4.0E+14
2	A2S	1.0E+84	1.0E+84	1.0E+84	1.0E+84
3	CA	4.3	9.919E-07	4.3	9.919E-07
4	CB	5.1	0.800001	5.1	0.800001
5	CS	3.	2.460265	3.	2.460265
6	Cv1	3360.	3360.	3360.	3360.
7	Cv2	5.36E+04	5.36E+04	5.36E+04	5.36E+04
8	DHRx1A	-4.54E+04	-4.54E+04	-4.54E+04	-4.54E+04
9	DHRx2S	-3.2E+05	-3.2E+05	-3.2E+05	-3.2E+05
10	E1A	1.28E+05	1.28E+05	1.28E+05	1.28E+05
11	E2S	8.0E+05	8.0E+05	8.0E+05	8.0E+05
12	FD	2467.445	253.5832	7.477E+10	7.477E+10
13	Fvent	2467.445	253.5832	2.507E+06	2.507E+06
14	k1A	0.0562573	0.0562573	153.6843	153.6843
15	k2S	8.428E-16	8.428E-16	2.533E+06	2.533E+06
16	P	4.4	4.4	45.01004	45.01004
17	r1A	-1.233723	-4.707609	-1.318E-05	-0.000122
18	r2S	-2.529E-15	-6.231E+06	-2.529E-15	-6.231E+06
19	SumNCp	1.26E+07	1.26E+07	1.26E+07	1.26E+07
20	SW1	1.	0	1.	0
21	t	0	0	4.	4.
22	T	422.	422.	538.8048	538.8048
23	UA	0	0	0	0
24	V0	4000.	4000.	4000.	4000.
25	VH	5000.	5000.	5000.	5000.

No File POLYMATH Report

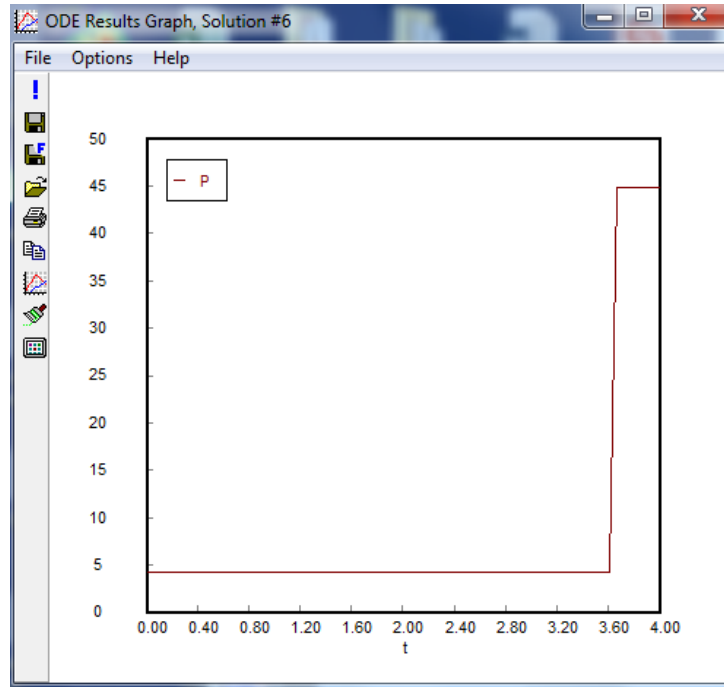
Step 9: The following graph will be generated. By default, polymath plots all dependent variables on Y axis and independent variable on X axis. In this case, dependent variables are CA, CB, CS, P, and T and independent variable is t . To select the variable you want to plot, double click on the graph or click on graph button present on left panel (shown below). This will open up a dialogue box.



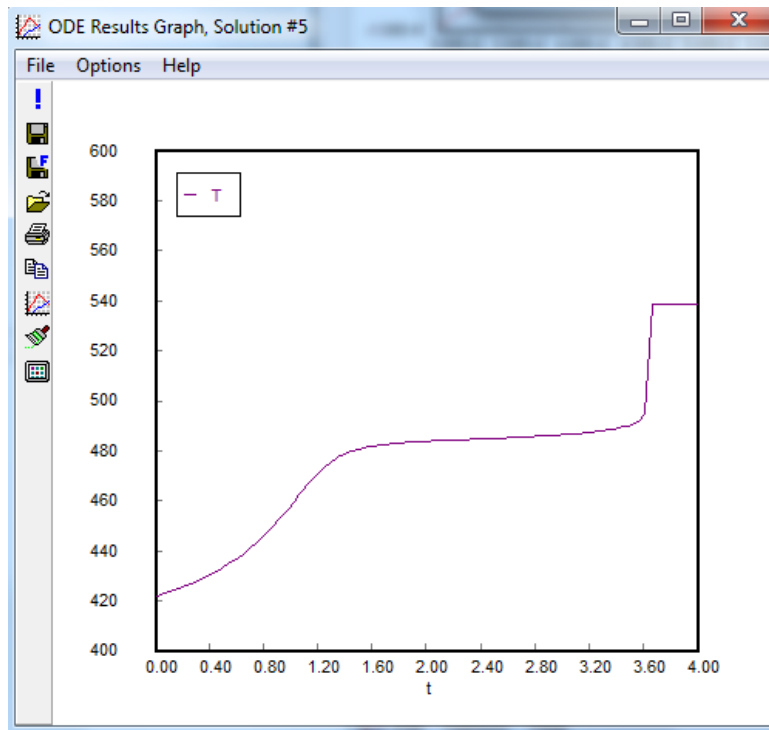
Step 10: You can now select the dependent variable by checking/unchecking the boxes next to the variable name. In this case, you want to plot P as a function of time. So uncheck the boxes corresponding to CA, CB, CS, and T. After you are done, click on the Close button



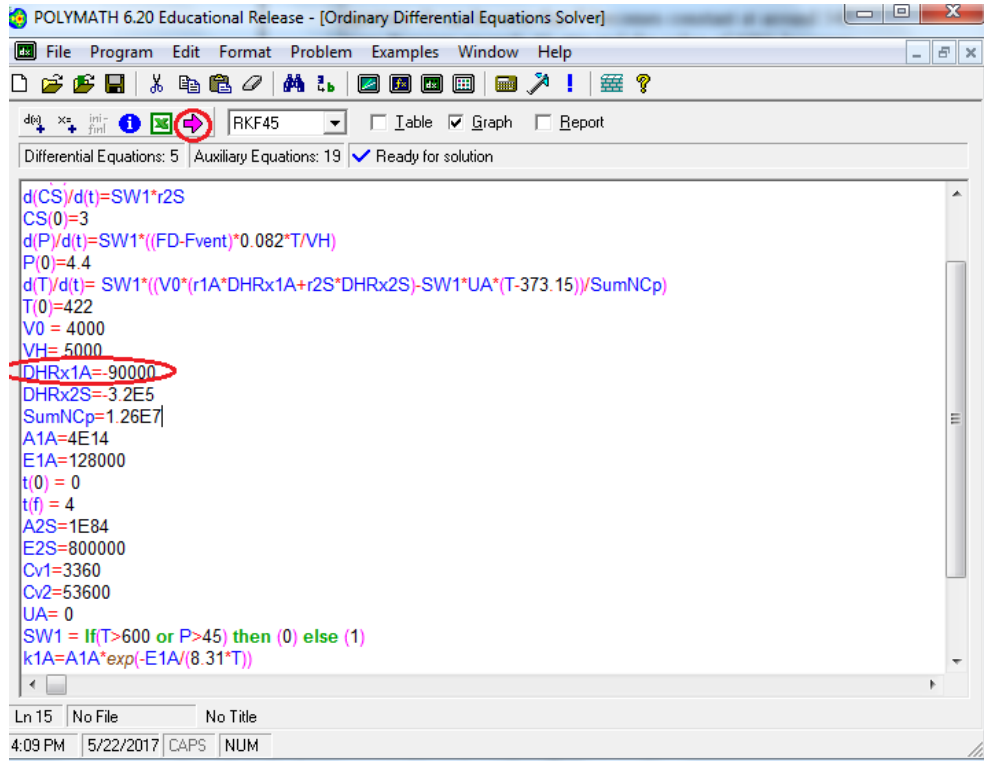
Step 11: Now your graph will change as shown. The graph below shows the Pressure trajectory. It can be seen that the pressure becomes constant after 45 atm. This is because the value of Software switch (SW1) becomes zero at $P > 45$ atm and this sets $d(P)/d(t)=0$ after this point



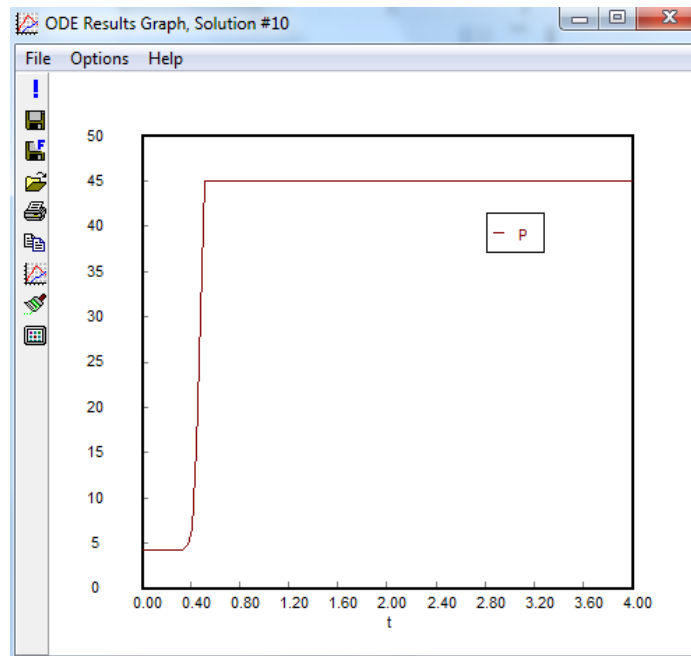
Step 12: Similarly plot the temperature Trajectory. It can be seen that T becomes constant at around 540 K at time $t=3.7$ hr. This is because at this time Pressure exceeds 45 atm and the value of SW1 becomes zero. This sets $dT/dt=0$ after this point



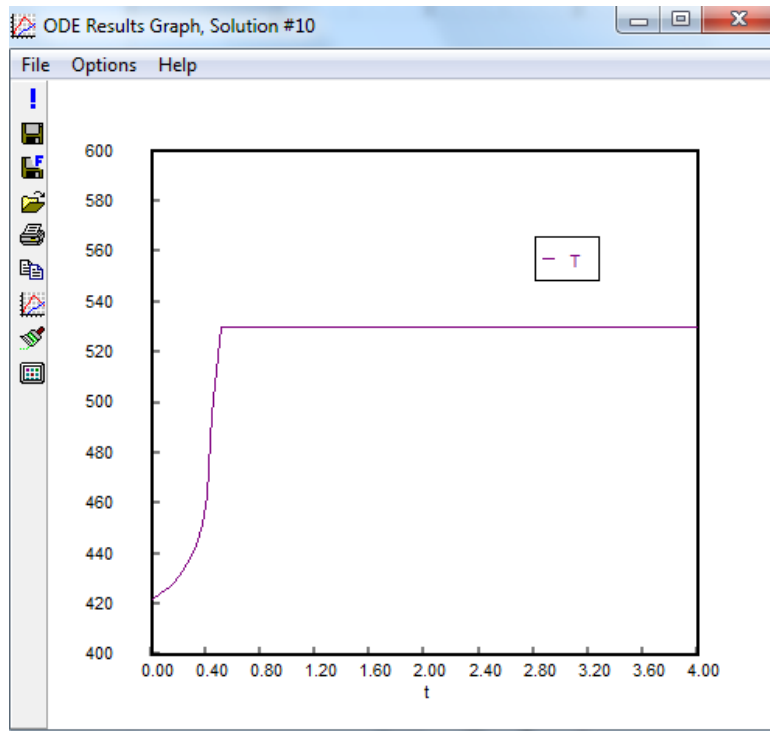
Step 13: Let's change a variable and see the effect on profile. Change DHRx1A from -45400 to -90000 and run the program by clicking on pink arrow.



The following Pressure profile graph will be generated. You can see that with higher DHRx1A, the pressure shoots up rapidly to 45 atm



The following graph will be obtained for Temperature trajectory. Again the temperature shoots up rapidly and becomes constant



Step 14: Similarly, change other parameter values and analyse the change in Pressure and Temperature trajectories