

Tutorial to fool Polymath to generate G(T) and R(T) Curve (Example 12-6)

In this tutorial, we will generate a figure of the $G(T)$ and $R(T)$ as a function of temperature for Example 12-6 (*Multiple Reactions in a CSTR*)

The equations are

$$G(T) = \left[-\frac{\Delta H_{Rx1A} \tau k_1}{1 + \tau k_1} - \frac{\tau k_1 \tau k_2 \Delta H_{Rx2B}}{(1 + \tau k_1)(1 + \tau k_2)} \right]$$

$$R(T) = C_{pA}(1 + \kappa)[T - T_c]$$

$$k_1 = 3.3 \exp\left(\left(\frac{E_1}{1.987}\right) * \left(\frac{1}{300} - \frac{1}{T}\right)\right)$$

$$k_2 = 4.58 \left(\frac{E_2}{1.987}\right) * \left(\frac{1}{500} - \frac{1}{T}\right)$$

$$Ca = Cao/(1 + \tau k_1)$$

$$\kappa = UA/(v_o Cao)/C_p$$

$$T_c = (T_o + \kappa T_a)/(1 + \kappa)$$

The parameter values are

$$C_p = 200, Cao = 0.3, T_o = 283, \tau = 0.01$$

$$\Delta H_{Rx1A} = -55000, \Delta H_{Rx2B} = -71500$$

$$v_o = 1000, E_1 = 9900, E_2 = 27000$$

$$UA = 40000, T_a = 330$$

To get $G(T)$ and $R(T)$ at different temperature, we need to vary temperature in the above equations. We do this by “**fooling**” Polymath by using a dummy independent variable “ t ” i.e.

$$\frac{dT}{dt} = 2$$

Now, you can vary temperature by varying the value of t . Let's plot $G(T)$ and $R(T)$ for temperature ranging from 273 K to 723 K. So initial value of T is

$$T(0) = 273 \text{ K}$$

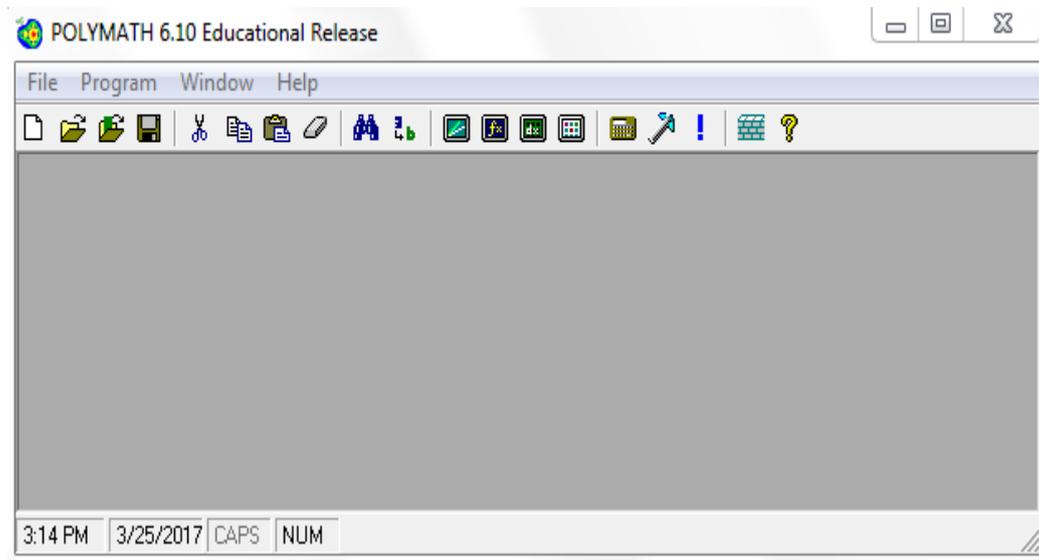
For the final value of $T = 723 \text{ K}$, the integration time span will vary from

$$t_{initial} = 0 \text{ and } t_{final} = 225$$

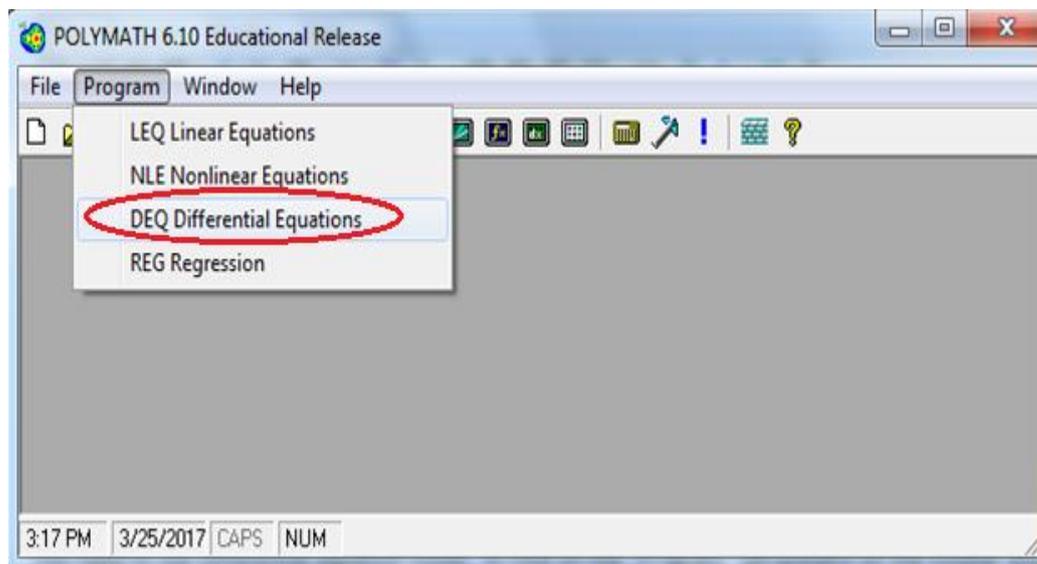
Now, the above problem becomes an ordinary differential equation which can be easily solved using Polymath. Next we change variables in plotting program to make T as the independent variable and $G(T)$ and $R(T)$ as the dependent variables to obtain the desired graph

Step 1: Now 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>

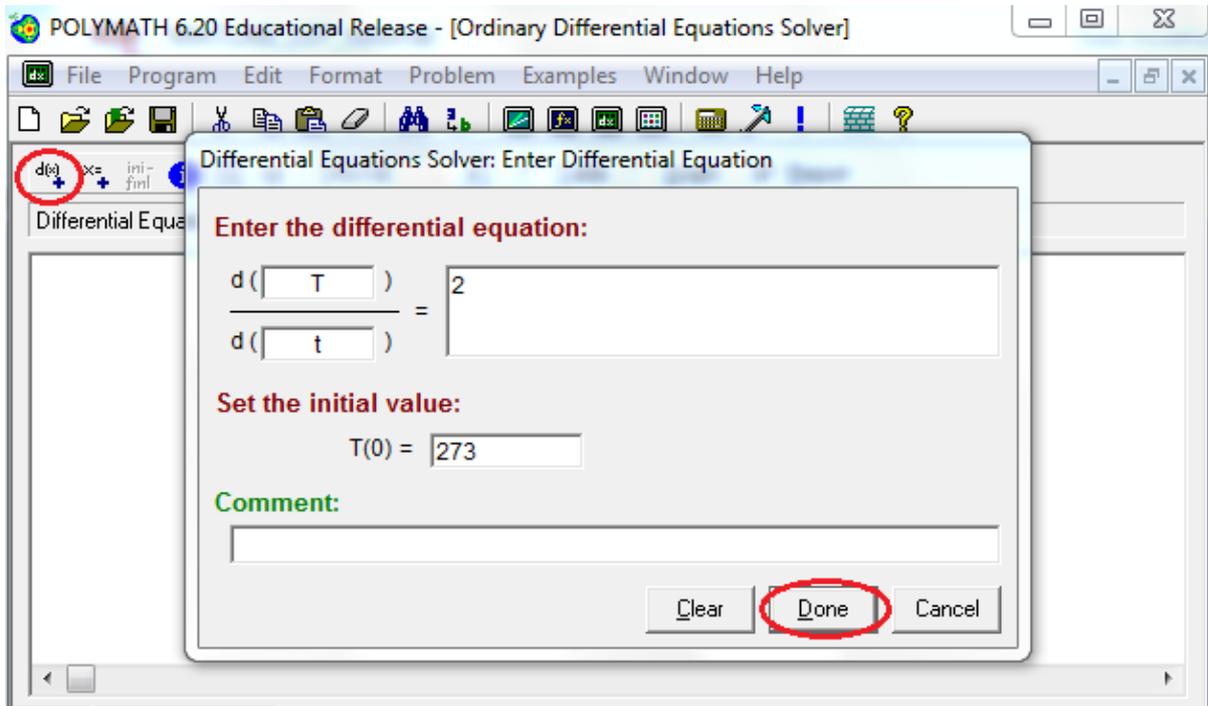
You will see the following window when you open the polymath



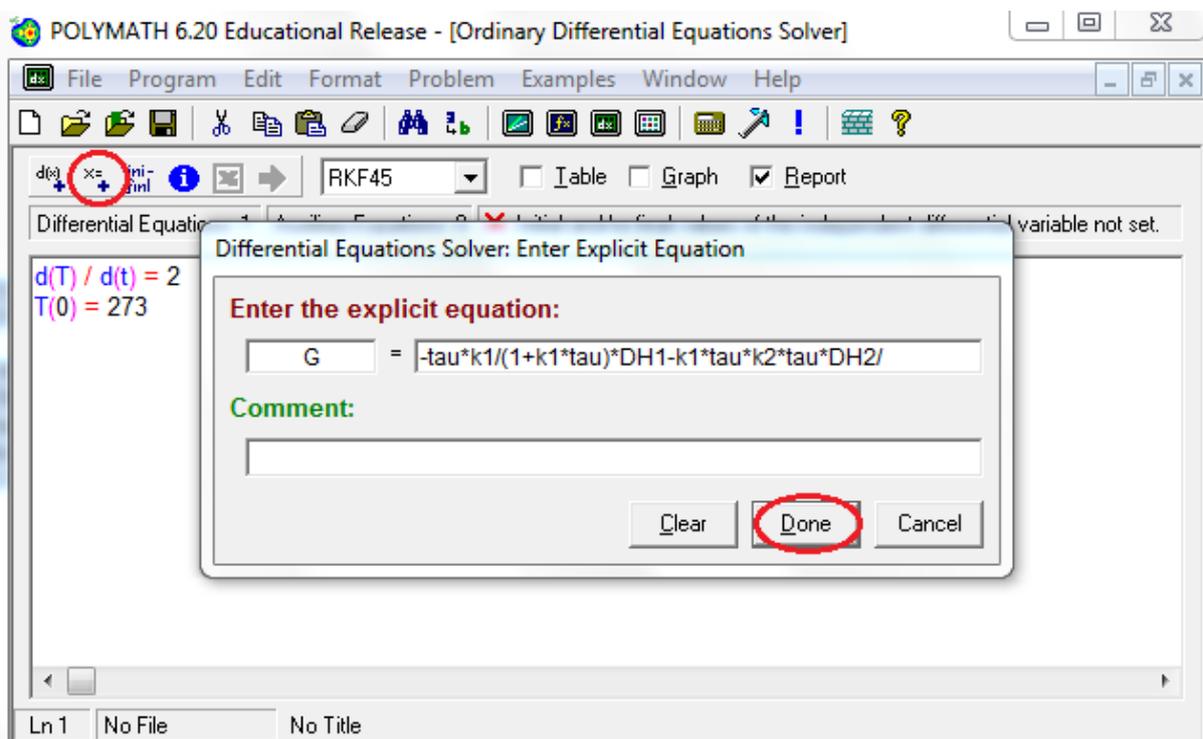
Step 2: Here, we need to use Differential equation solver, so click on the “Program” tab present on the toolbar and select DEQ Differential Equations. You can also refer to step-by-step Polymath tutorial for solving DEQ present at <http://www.umich.edu/~elements/5e/software/polymath.html>



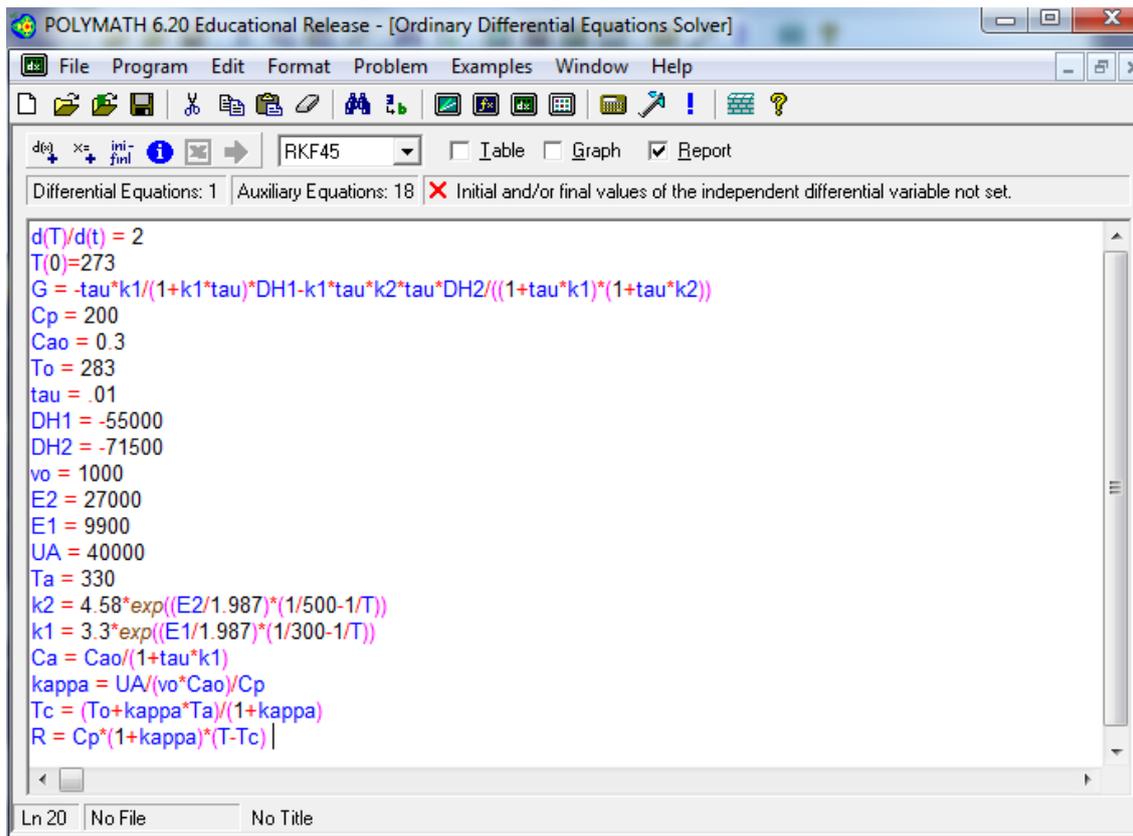
Step 3: To enter the differential equations, press the "d(x)+" button present on the menu bar (shown by red circle in the below screenshot). This will bring up a dialogue box in which you can enter your differential equation. You will also need to specify an initial value for the differential variable. Enter the differential equation for T and click "Done" button



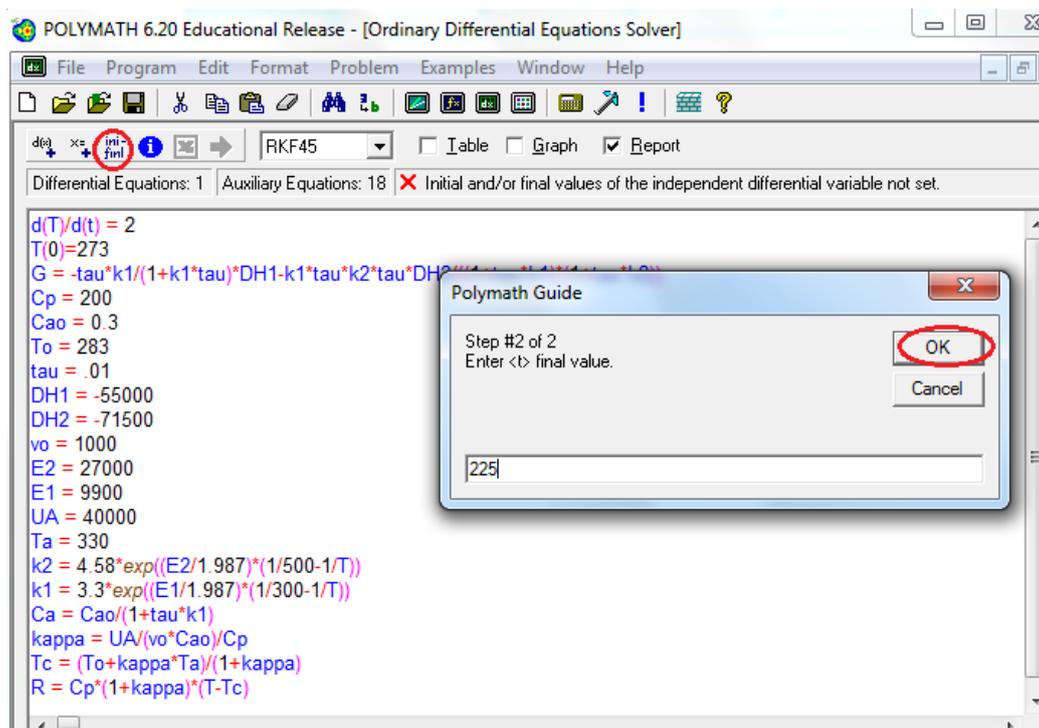
Step 4: You will find that your differential equation is entered in the main window. Now press "x=+" button to enter the explicit equation and parameter values. Enter the expression for G and click "Done" as shown below



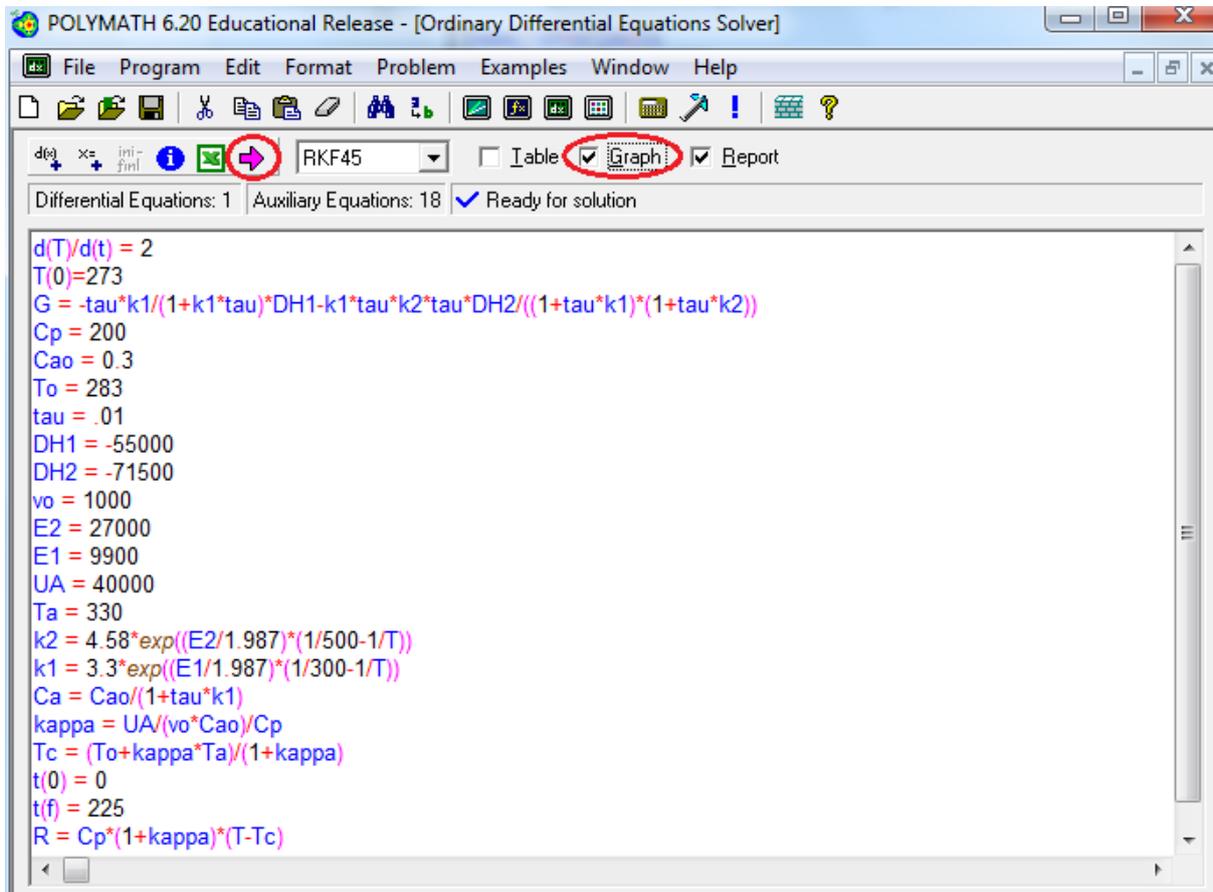
Step 5: Similarly enter all other explicit equations and parameter values in the window



Step 6: You have now entered both the differential equations and the explicit equation. 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=225 and 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 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.

POLYMATH Report
Ordinary Differential Equations 05-Jun-2017

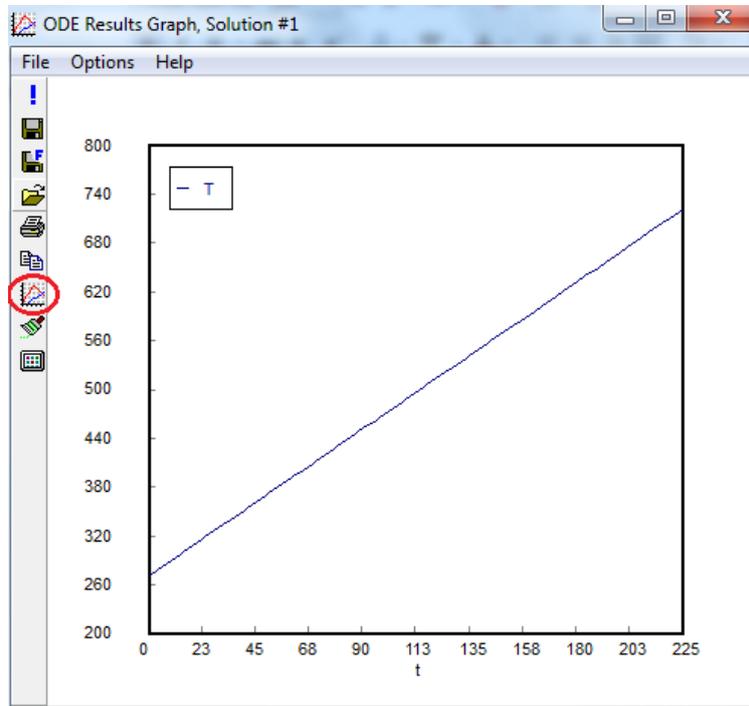
Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	Ca	0.2980966	0.0005469	0.2980966	0.0005469
2	Cao	0.3	0.3	0.3	0.3
3	Cp	200.	200.	200.	200.
4	DH1	-5.5E+04	-5.5E+04	-5.5E+04	-5.5E+04
5	DH2	-7.15E+04	-7.15E+04	-7.15E+04	-7.15E+04
6	E1	9900.	9900.	9900.	9900.
7	E2	2.7E+04	2.7E+04	2.7E+04	2.7E+04
8	G	348.9509	348.9509	1.259E+05	1.259E+05
9	k1	0.6385073	0.6385073	5.475E+04	5.475E+04
10	k2	7.03E-10	7.03E-10	2.001E+04	2.001E+04
11	kappa	0.6666667	0.6666667	0.6666667	0.6666667
12	R	-9600.	-9600.	1.404E+05	1.404E+05
13	t	0	0	225.	225.
14	T	273.	273.	723.	723.
15	Ta	330.	330.	330.	330.
16	tau	0.01	0.01	0.01	0.01
17	Tc	301.8	301.8	301.8	301.8
18	To	283.	283.	283.	283.
19	UA	4.0E+04	4.0E+04	4.0E+04	4.0E+04
20	vo	1000.	1000.	1000.	1000.

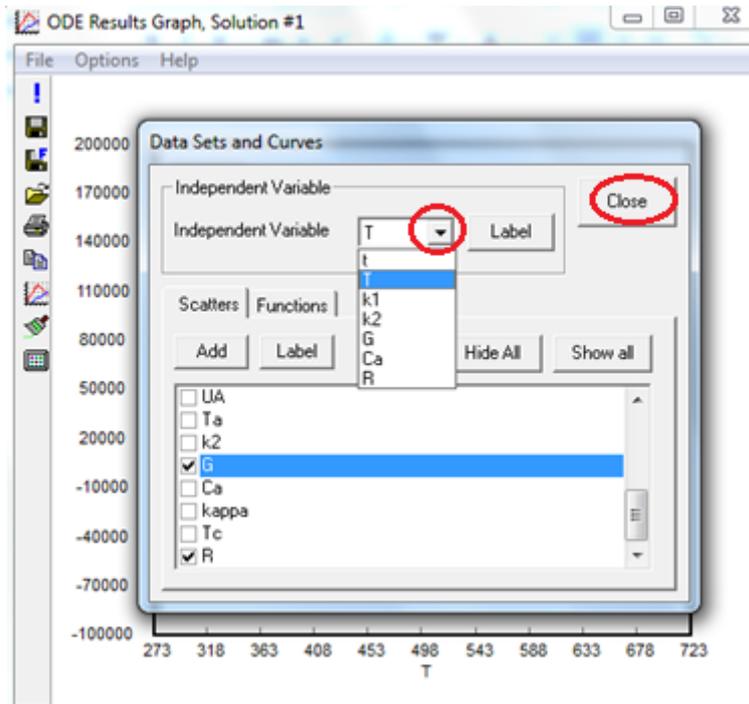
Differential equations

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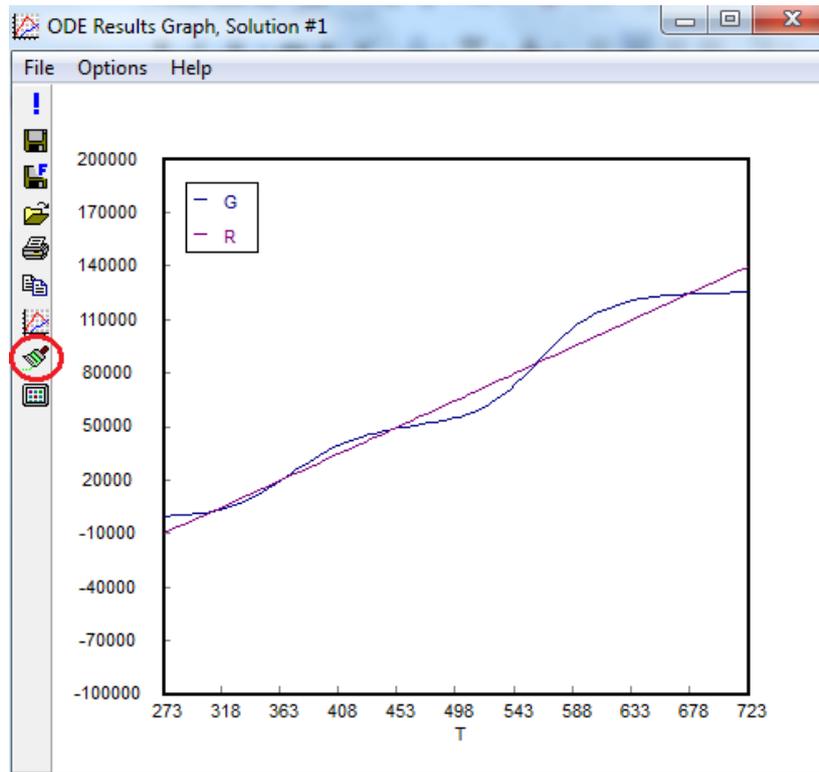
Step 9: The following graph will be generated. By default, polymath plots all dependent variable on Y axis and independent variable on X axis. In this case, dependent variable is T and independent variable is t . To select the variable you want to plot, double click on the graph or click on graph button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



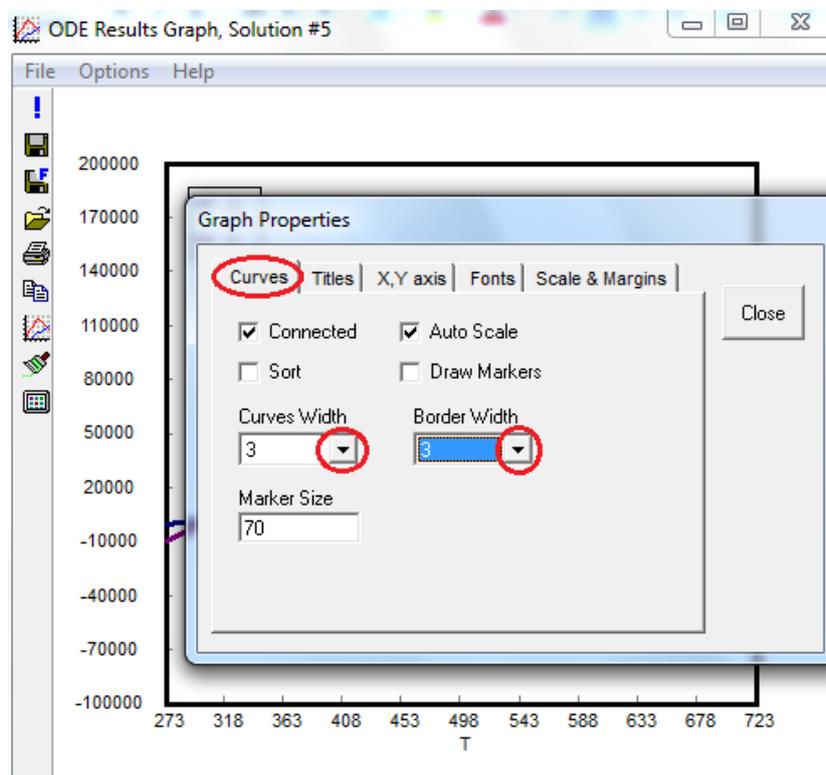
Step 10: You can now select independent variable from drop-down menu and dependent variable by checking/unchecking the boxes next to the variable name. In this case, you want to plot G and R as a function of Temperature. So select independent variable as T . Check the boxes corresponding to G and R and uncheck the box for T . After you are done, hit Close button



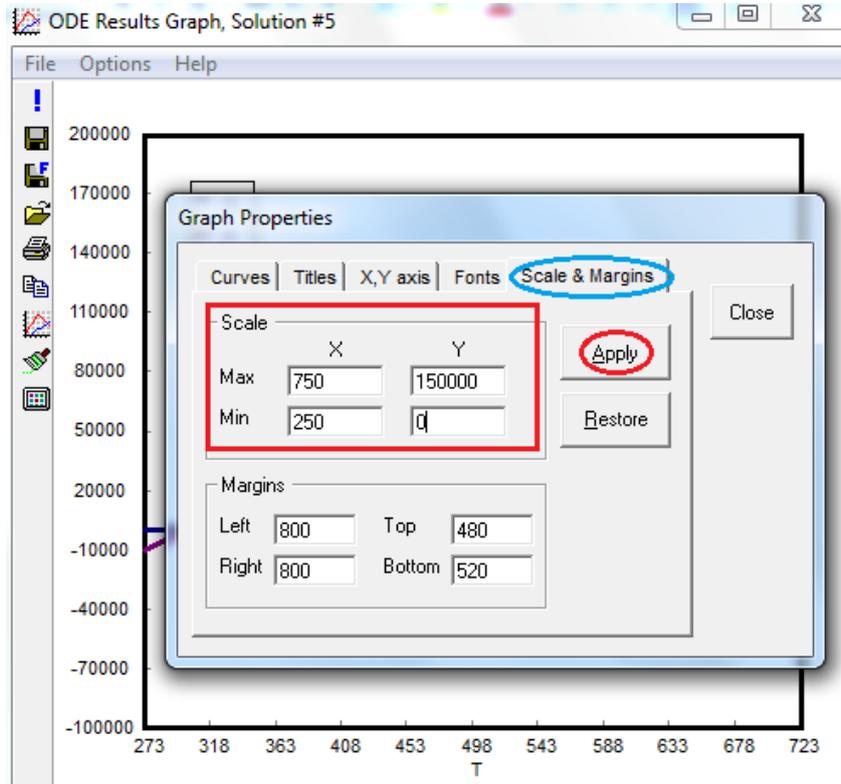
Step 11: Your graph will change as shown. Now, we will edit some of the graph properties. Right click on graph and select “Format” or click on brush button present on the left panel.



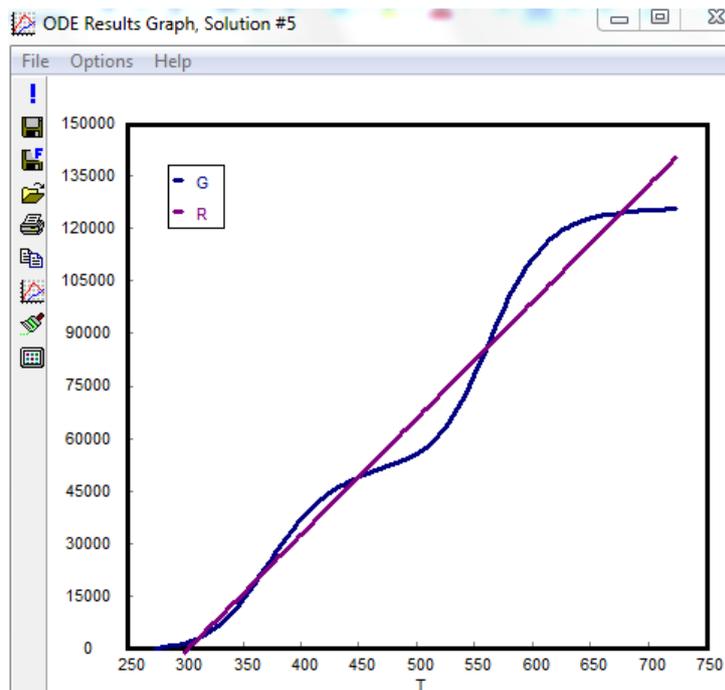
Step 12: This will open up a dialogue box where you can edit graph properties. The first tab is “Curves”. Let’s select Curve width and border width as 3 using drop down menu as shown below.



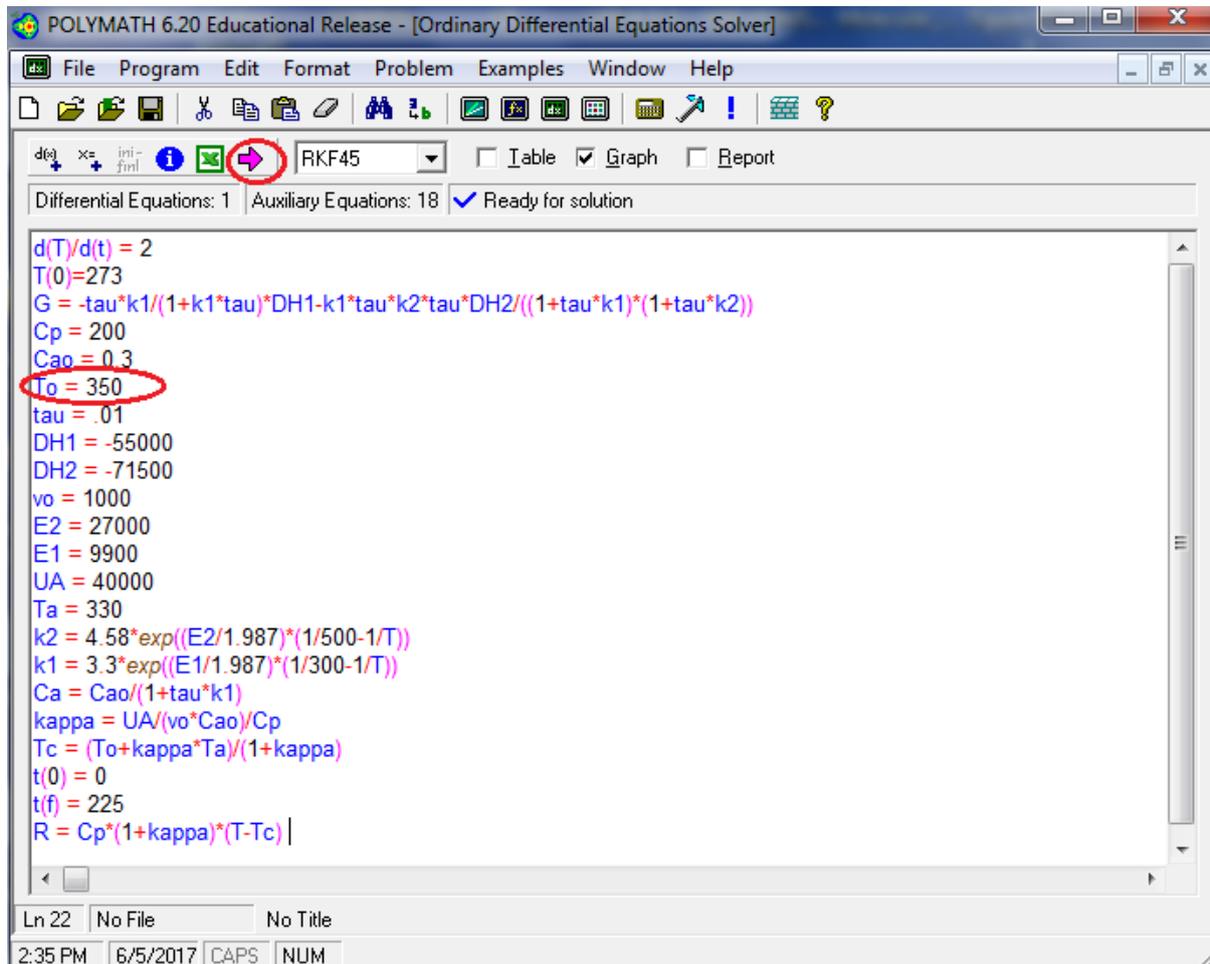
Step 13: Next, click on “Scale and Margins” tab to change the axis range. Under X header, enter the value of Max=750 and Min=250 to define the range of X axis. Under Y header, enter the value of Max=150000 and Min=0. This defines the range of Y axis. Now click “Apply” Button



Step 14: After you are done, press Close button. You will see that graph properties have changed as desired. The following graph shows G and R as a function of Temperature. You can now find the number of steady state solutions from the intersection of G and R curve. We can see that 5 steady state solution exists!



Step 15: Now let's obtain the graph of G and R for different inlet temperature. Let's evaluate at $T_0=350$ K. Close the above graph by clicking on X to go back to **Step 7**. Now change the value of T_0 from 283 to 350 as shown below. Click on pink arrow to run the program



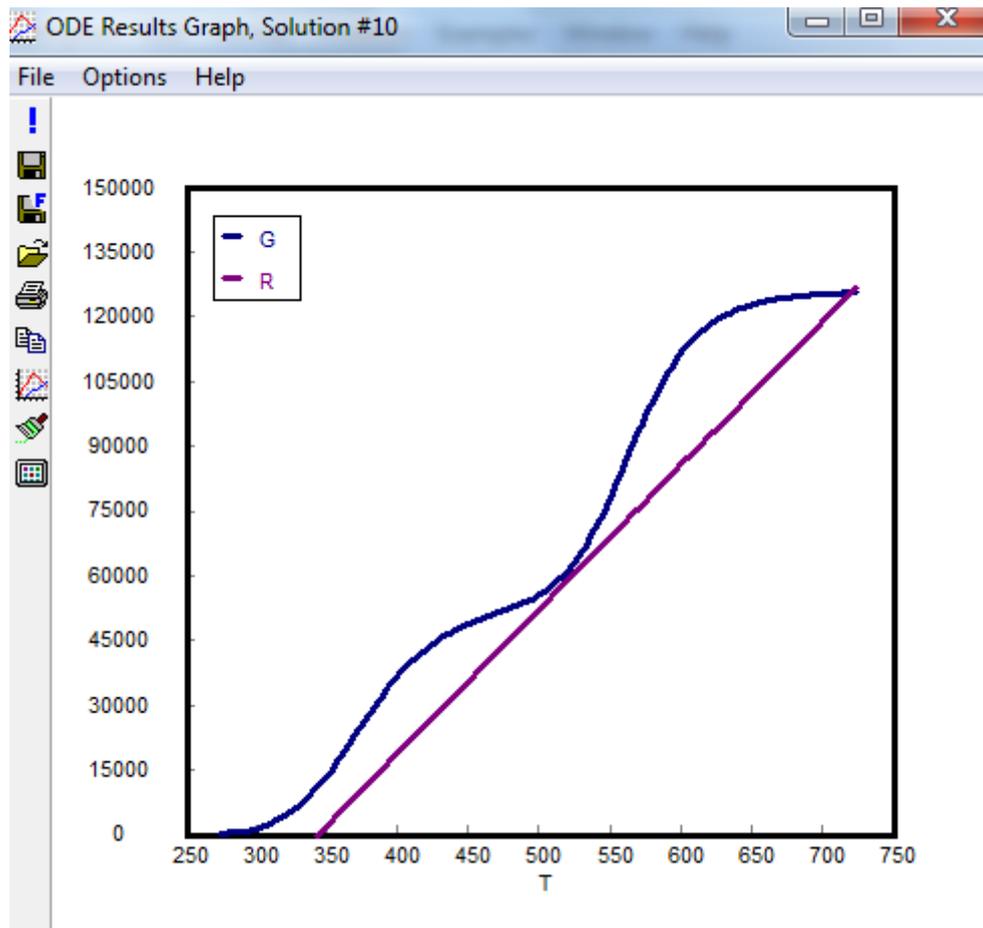
Step 16: You should obtain following report.

POLYMATH Report
Ordinary Differential Equations 05-Jun-2017

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	Ca	0.2980966	0.0005469	0.2980966	0.0005469
2	Cao	0.3	0.3	0.3	0.3
3	Cp	200.	200.	200.	200.
4	DH1	-5.5E+04	-5.5E+04	-5.5E+04	-5.5E+04
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6	E1	9900.	9900.	9900.	9900.
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12	R	-2.3E+04	-2.3E+04	1.27E+05	1.27E+05
13	t	0	0	225.	225.
14	T	273.	273.	723.	723.
15	Ta	330.	330.	330.	330.
16	tau	0.01	0.01	0.01	0.01
17	Tc	342.	342.	342.	342.
18	To	350.	350.	350.	350.
19	UA	4.0E+04	4.0E+04	4.0E+04	4.0E+04
20	vo	1000.	1000.	1000.	1000.

Step 17: Repeat **Step 9-14** to obtain below graph for $T_0=350$ K



From the above figure, you can see that at $T_0=350$ K, only 2 steady state solution exists!

Step 18: Change the various parameters yourself and observe the corresponding change in graph