Tutorial to fool Polymath (*Example 11-4*)

In this tutorial, we will generate a figure of the equilibrium conversion (X_e and X_{EB}) as a function of temperature for Example 11-4 (*Calculating the Adiabatic Equilibrium temperature*)

The equations are

$$K_e = K_{e2} \exp\left[\frac{\Delta H_{Rx}}{R}\left(\frac{1}{T2} - \frac{1}{T}\right)\right]$$

$$X_e = \frac{K_e}{1 + K_e}$$

$$X_{EB} = \left(C_{P_A} + \theta_I C_{P_I}\right)(T - T_0)$$

Where,

$K_{e2} = 75{,}000$ at $T_2 = 298\ K$

$\Delta H_{RX} = -14{,}000\ cal/mol,\ \ \theta_I = 1$

$C_{P_A} = 25\ \frac{cal}{mol.K},\ \ C_{P_I} = 50\ \frac{cal}{mol.K}$

To get equilibrium conversion 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.

$$\frac{dT}{dt} = 1$$

Now, you can vary temperature by varying the value of t .Let's plot X_e and X_{EB} for temperature ranging from 300 K to 800 K. So initial value of T is

T(0)=300 K

For the final value of T=800 K, the integration time span will vary from

$t_{initial} = 0$ and $t_{final} = 500$

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 X_e and X_{EB} 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
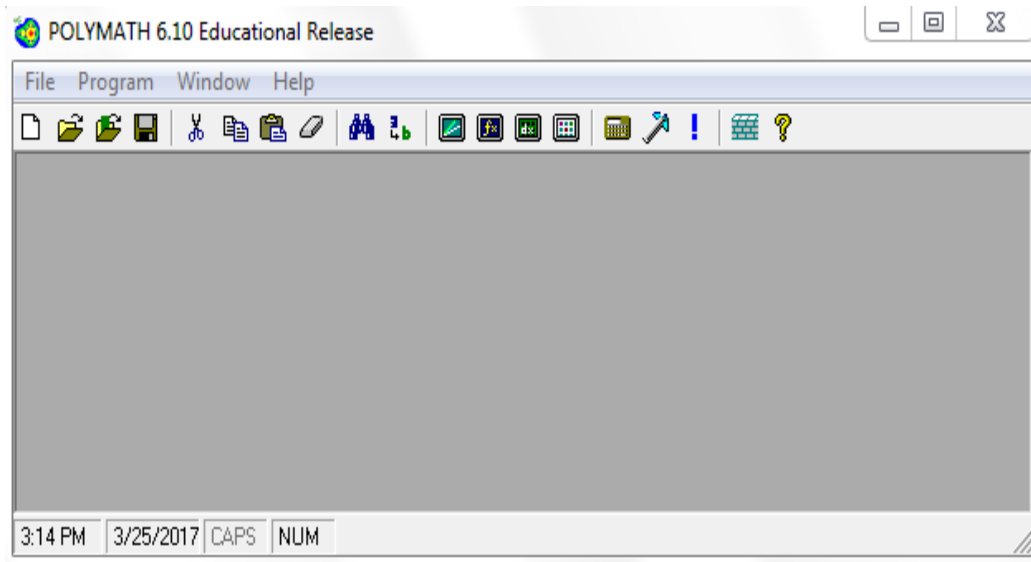
Step 2: Here, we need to use Differential equation solver, so click on the "Program" tab present on the toolbar and select DEQ Differential Equations. You can also refer to step-by-step Polymath tutorial for solving DEQ present at http://www.umich.edu/~elements/5e/software/polymath.html
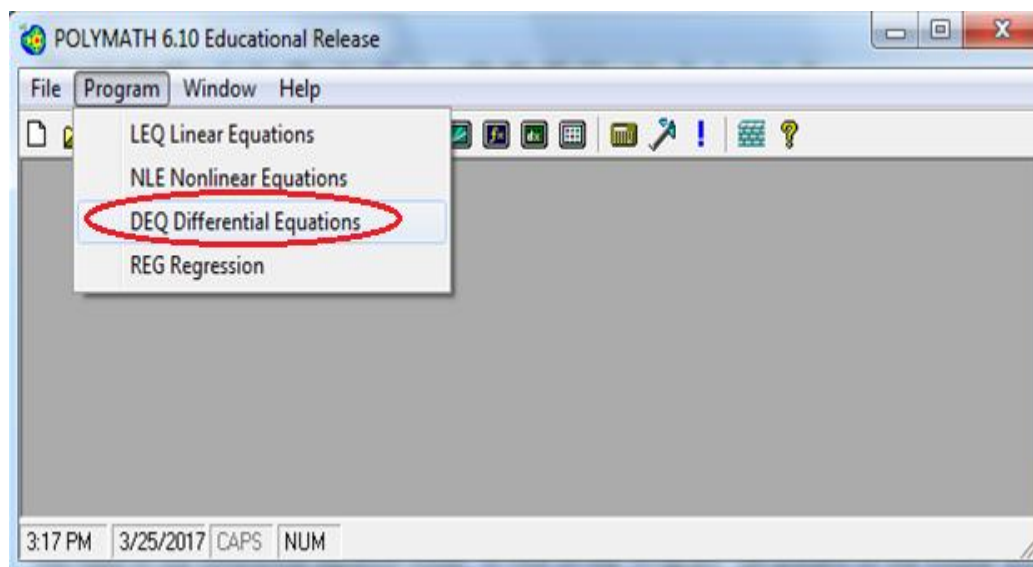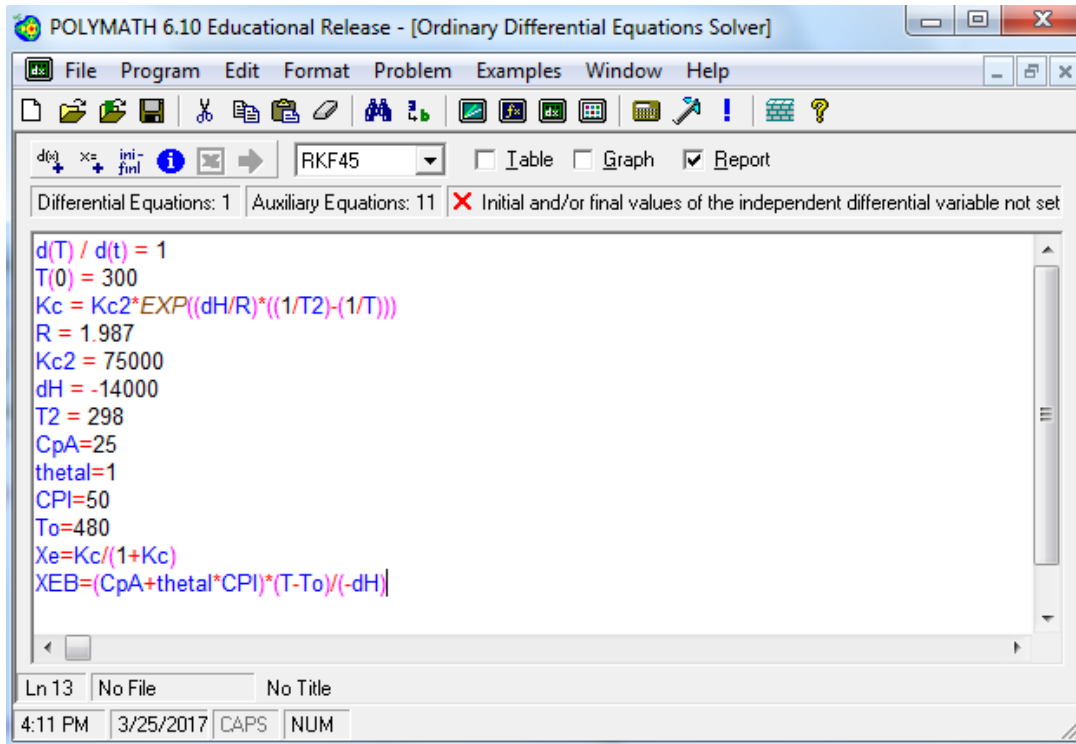
Step 3: To enter the differential equations, press the "**d(x)₊**" button present on the menu bar (shown by red circle in the below screenshot). This will bring up a dialogue box in which you can enter your differential equation. You will also need to specify an initial value for the differential variable. Enter the differential equation for T and click "Done" button
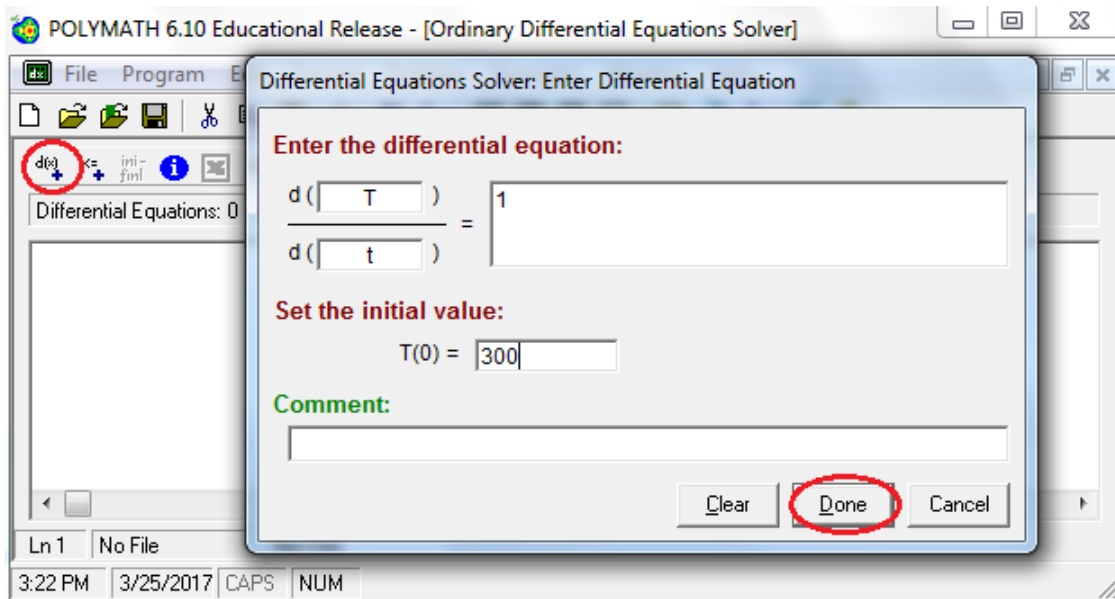

Step 4: You will find that your differential equation is entered in the main window. Now press "**x=₊**" button to enter all the explicit equation and parameter values. Enter the expression for Kc and click "Done" as shown below
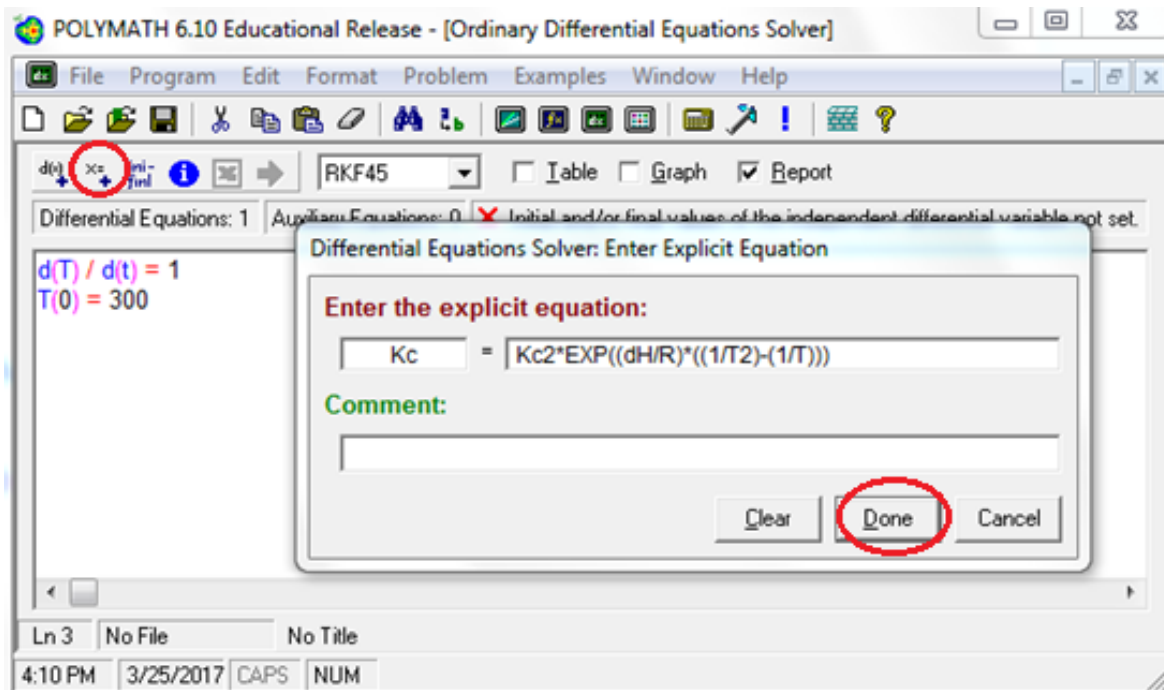
Step 5: Similarly enter all other explicit equations and parameter values in the window


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=500 and then press Ok
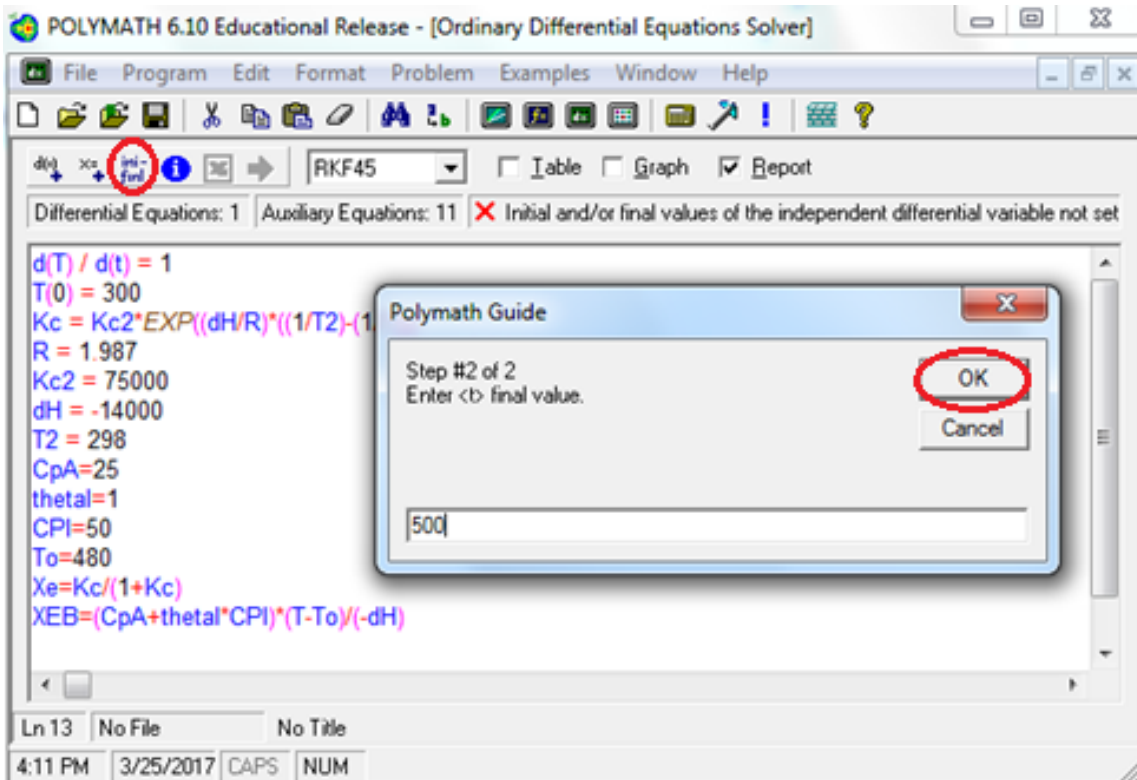
Step 7: When all of the necessary information has been specified, the screen will look like this. Check the box corresponding to graph option to generate the graph in addition to report. Next click on the pink arrow ➡ to have Polymath perform the integration.
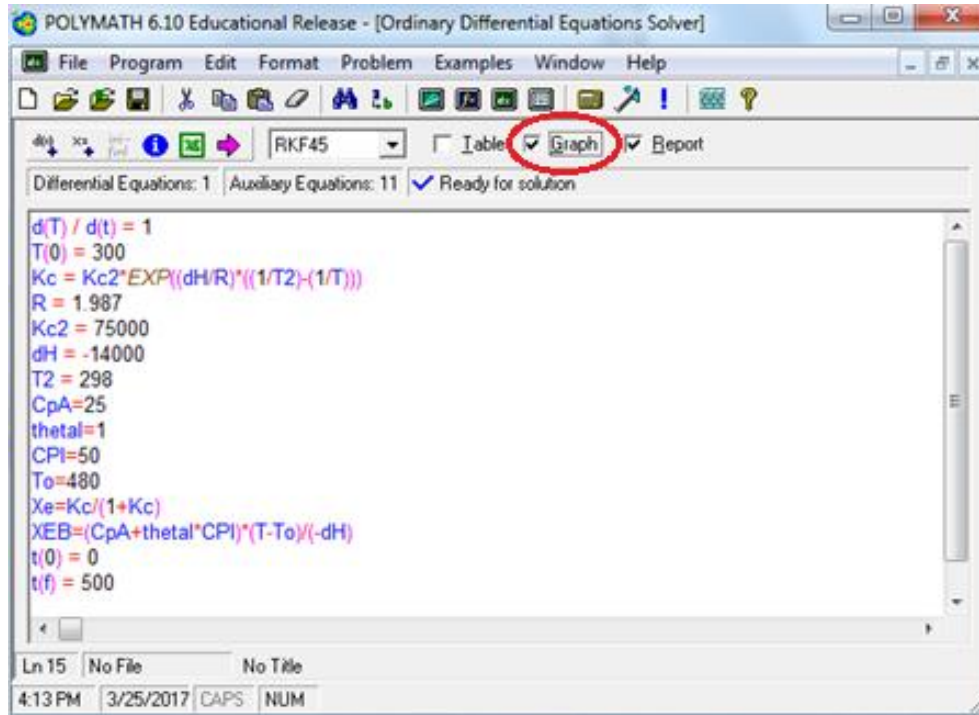

Step 8: The following report will be generated which gives initial and final values of every variable present, the minimum and maximum values of the variables in the given interval, and the equations you entered. Click on "X" to close the report and obtain graph
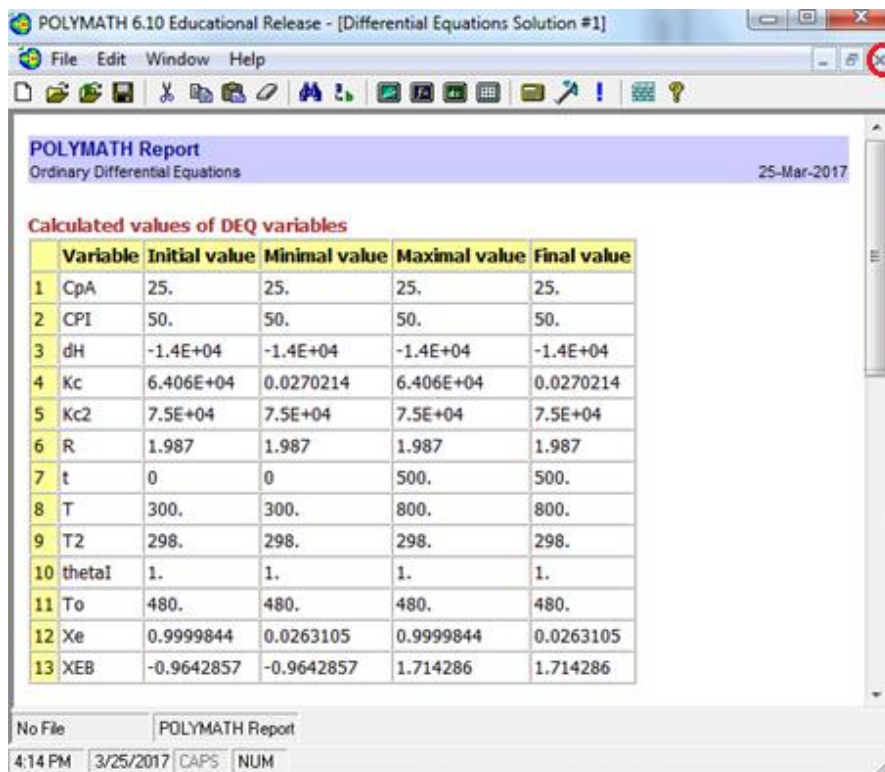
Step 9: The following graph will be generated. By default, polymath plots all dependent variable on Y axis and independent variable on X axis. In this case, dependent variable is *T* and independent variable is *t*. To select the variable you want to plot, double click on the graph or click on graph button present on left panel (shown below). This will open up a dialogue box.
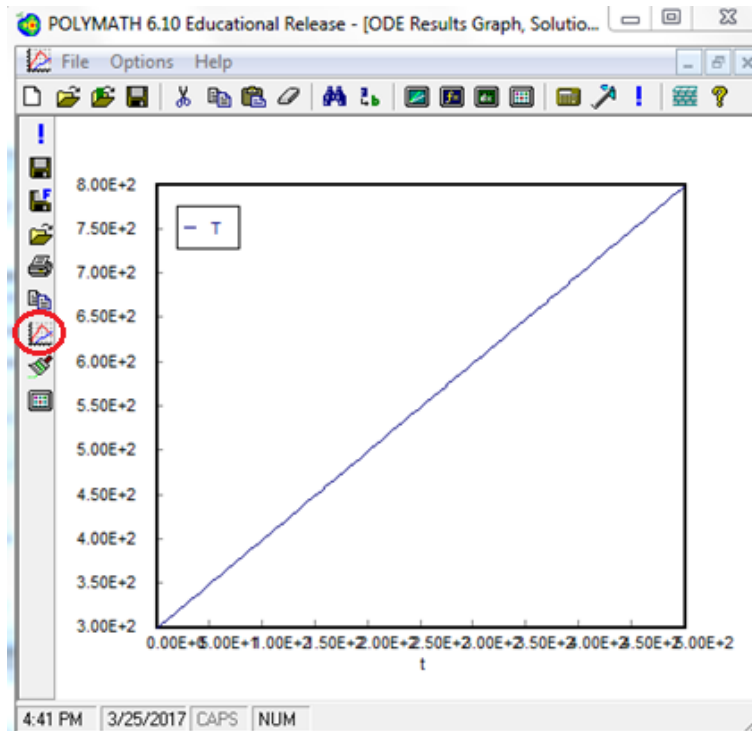

Step 10: You can now select independent variable from drop- down menu and dependent variable by checking/unchecking the boxes next to the variable name. In this case, you want to plot X and XEB as a function of Temperature. So select independent variable as T. Check the boxes corresponding to Xe and XEB and uncheck the box for T. After you are done, hit Close button
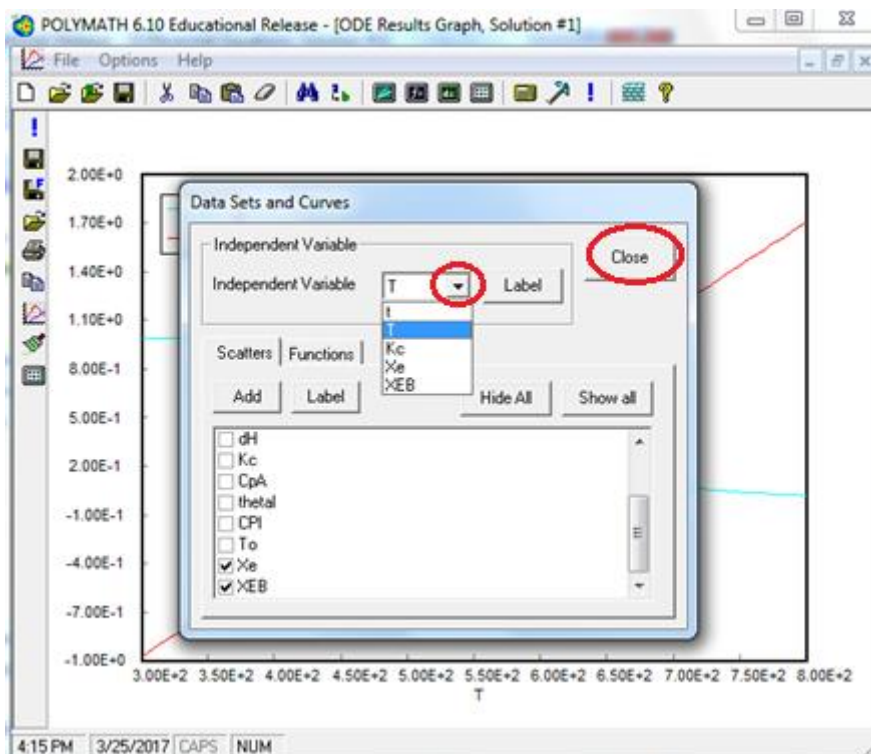
Step 11: Now your graph will change as shown. The axis mark up and scaling is not very convenient to read. So let's edit graph properties. Right click on graph and select "Format" or click on brush button present on the left panel.
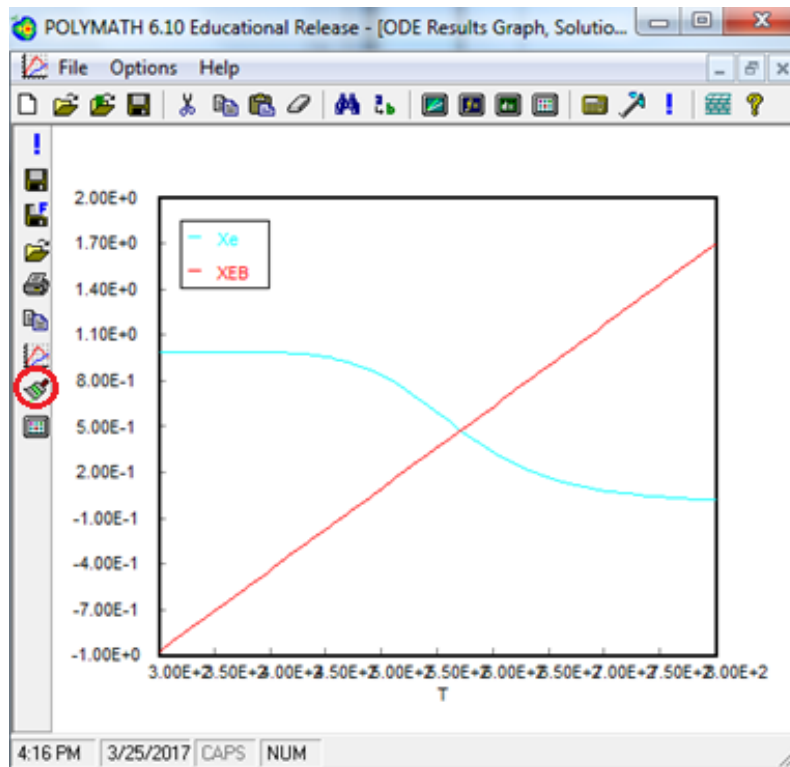

Step 12: This will open up a dialogue box where you can edit graph properties. Click on "Titles" tab to add title to the graph. Enter the title as "Xe and XEB as a function of T"
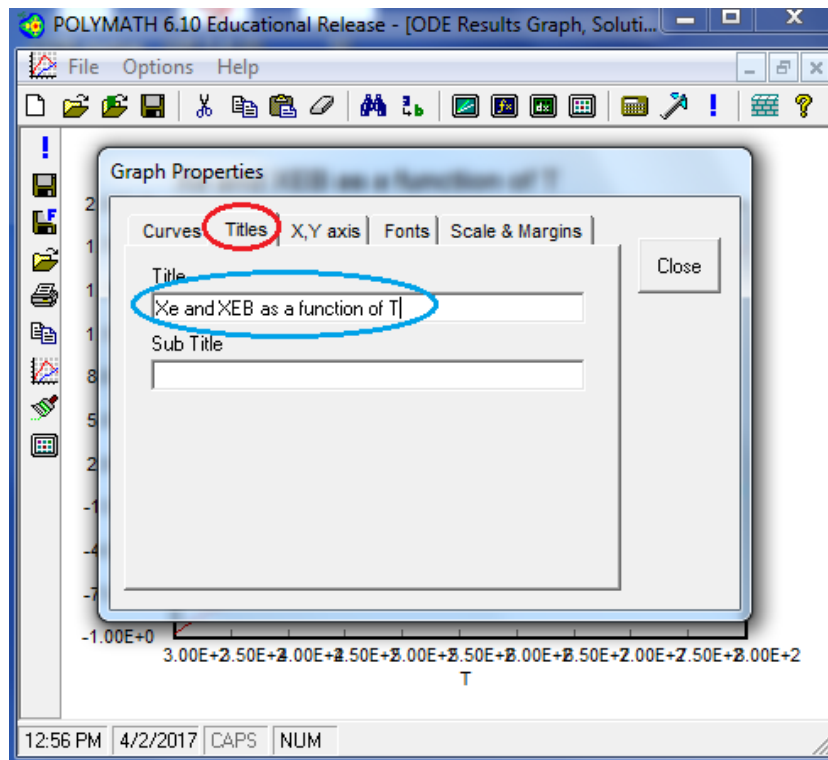
Step 13: Now, Click on "X, Y" axis tab to change the decimal point of axis numbers. From the drop down menu, select 0 for X Axis and 0.0 for Y axis
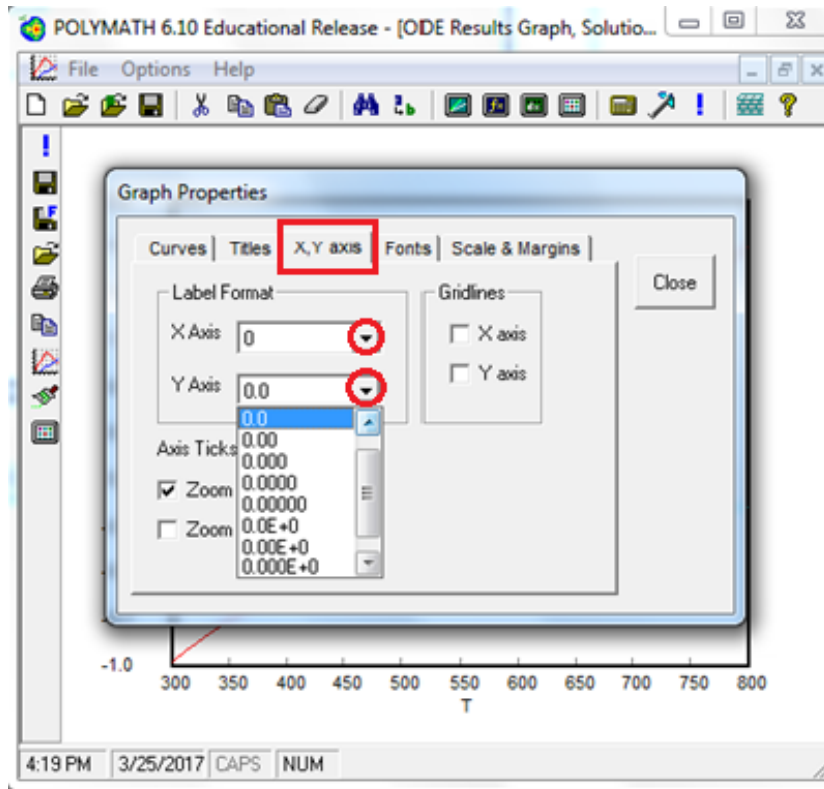
Step 14: Next, click on "Scale and Margins" tab to change the axis range. Under Y header, enter the value of Max=1 and Min=0. This defines the range of Y axis. Now click "Apply" Button
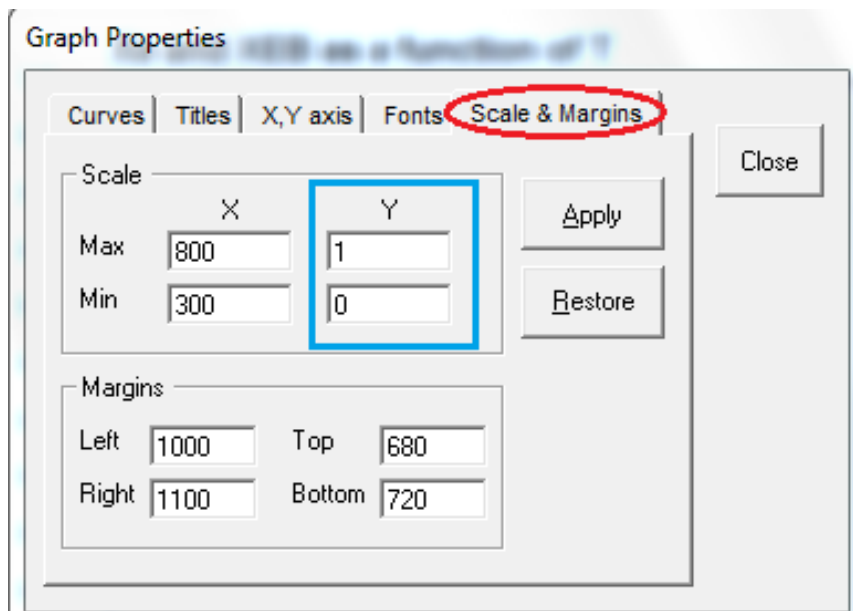
Step 15: After you are done, press Close button. You will see that graph properties have changed as desired. The following graph shows Xe and XEB as a function of Temperature. You can now find the intersection of Xe and XEB to determine adiabatic equilibrium temperature
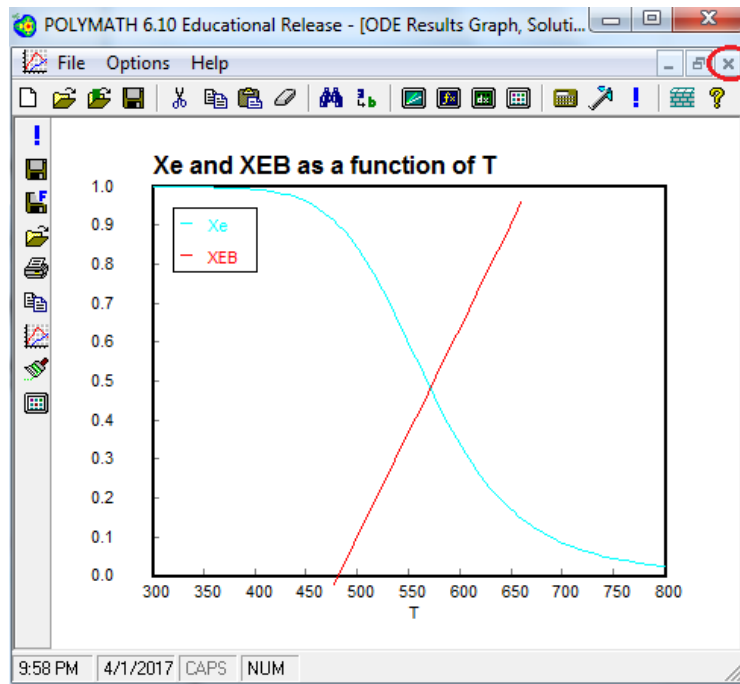
Step 16: Now let's obtain the graph of Xe and XEB for different inlet temperature. Let's evaluate at To=380 K. Close the above graph by clicking on X to go back to **Step 7**. Now change the value of To from 480 to 380 as shown below. Click on pink arrow to run the program

Step 17: You should obtain following report.

Step 18: Close the report to obtain graph. Repeat **Step 9-15** to obtain below graph for To=380 K