

Polymath tutorial on Ordinary Differential Equation Solver

The following is the differential equation we want to solve using Polymath

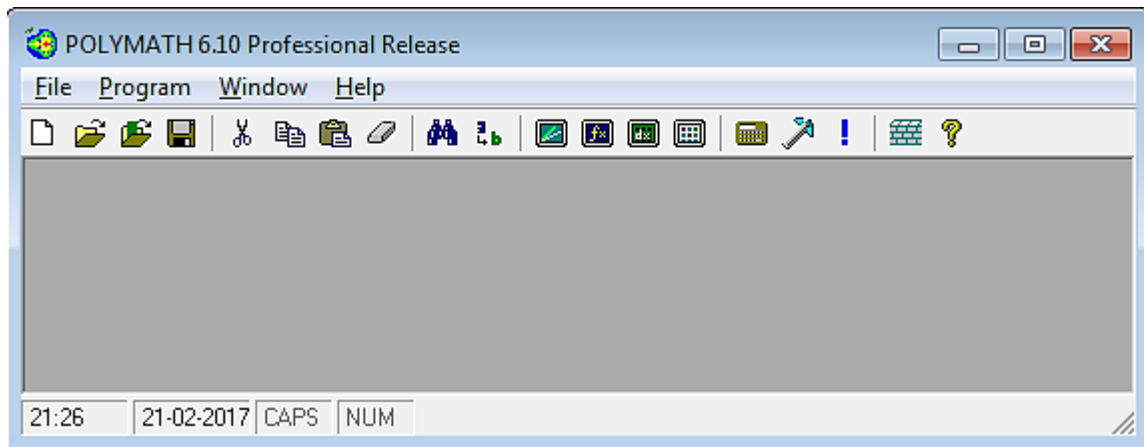
$$\frac{dCa}{dt} = -k_1 Ca Cb$$


$$\frac{dCb}{dt} = -k_1 Ca Cb$$

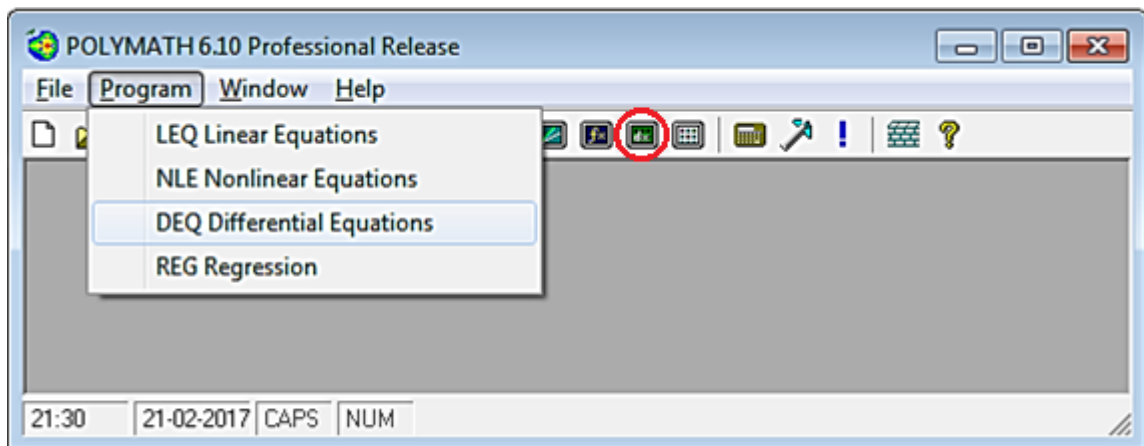
At $t=0$, $Ca = 0.5$ and $Cb = 0.5$

and integration time span is $t= 0$ to $t=30$

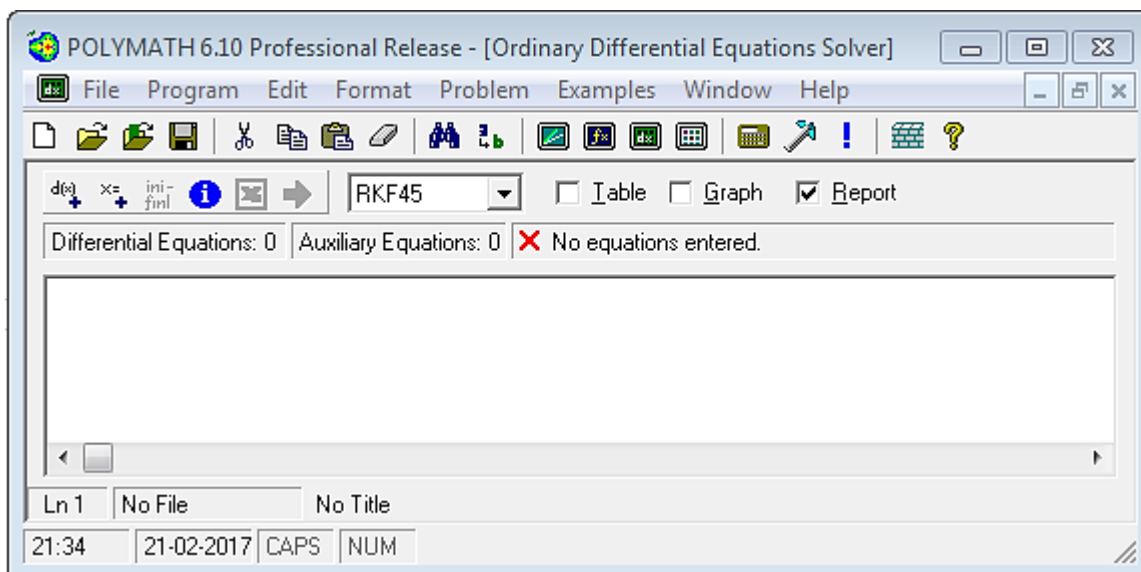
First, launch Polymath which you can download from <http://www.polymath-software.com>. You will see a window that looks like this.




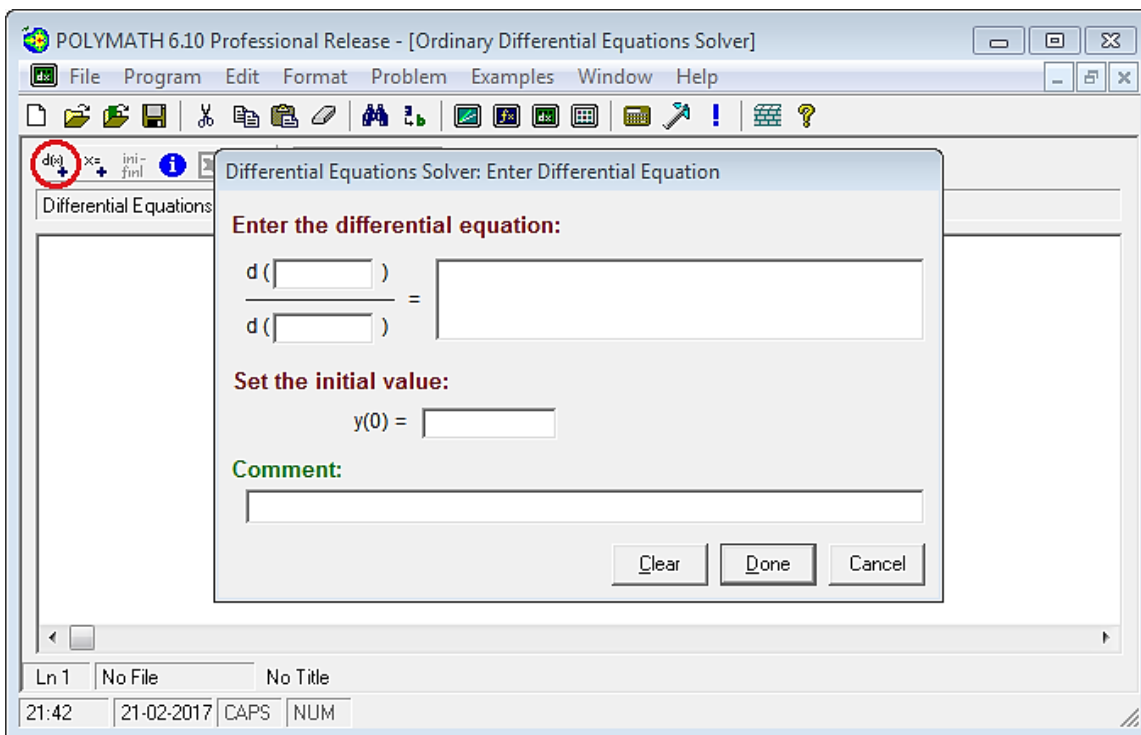
To use the ODE solver in Polymath, first click on the “Program” tab present on the toolbar. This will bring up a list of options from which you need to select. In this case we need to solve differential equations so select "DEQ Differential Equations". The shortcut button “dx” for differential equation solver is also present on the menu bar () as shown by red circle in below screenshot



This will open up another window, which looks like this.



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.

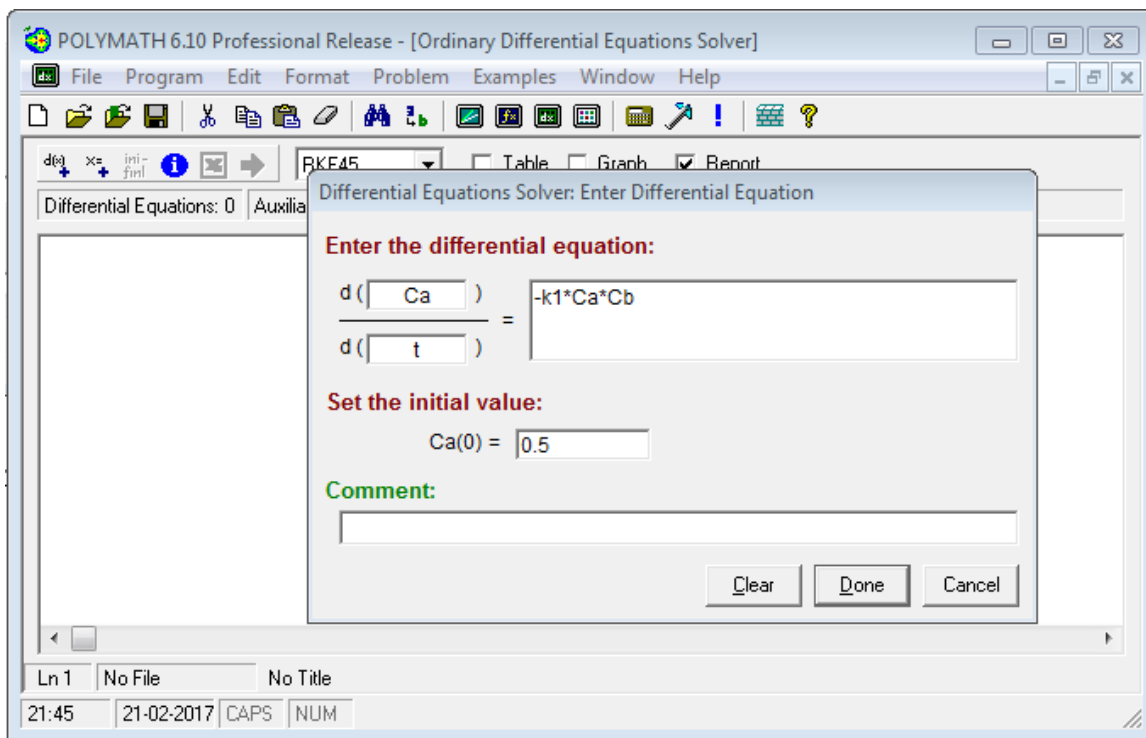


In the above dialogue box, only one differential equation can be entered at one time

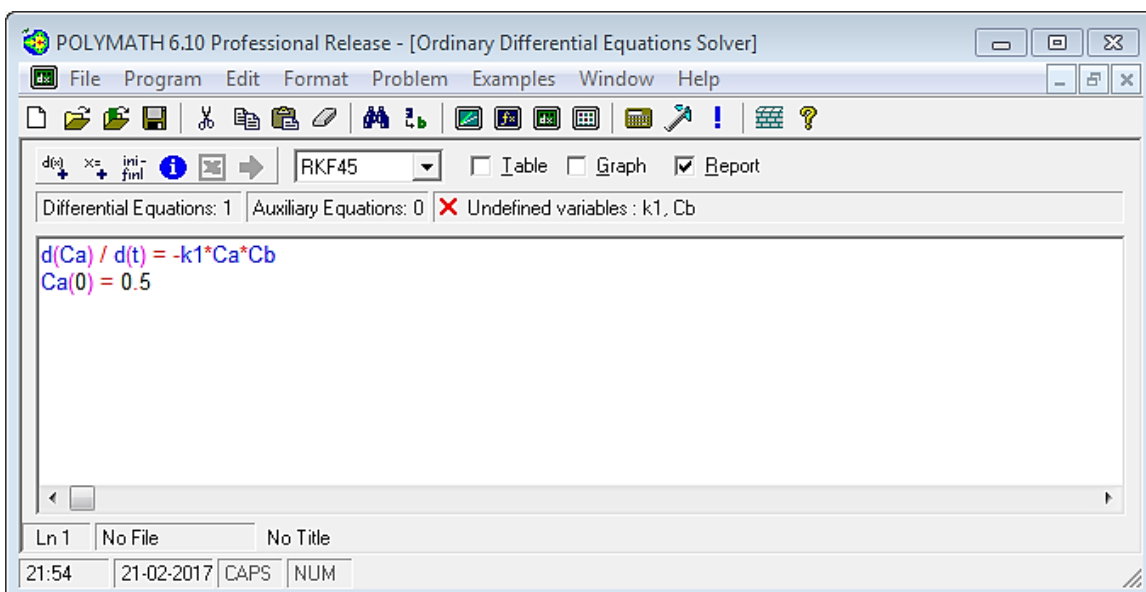
First differential equation is

$$\frac{dCa}{dt} = -k_1 * Ca * Cb \text{ and } Ca(0) = 0.5$$

Enter the above equation and initial value in the space provided in the rectangular box as shown below.

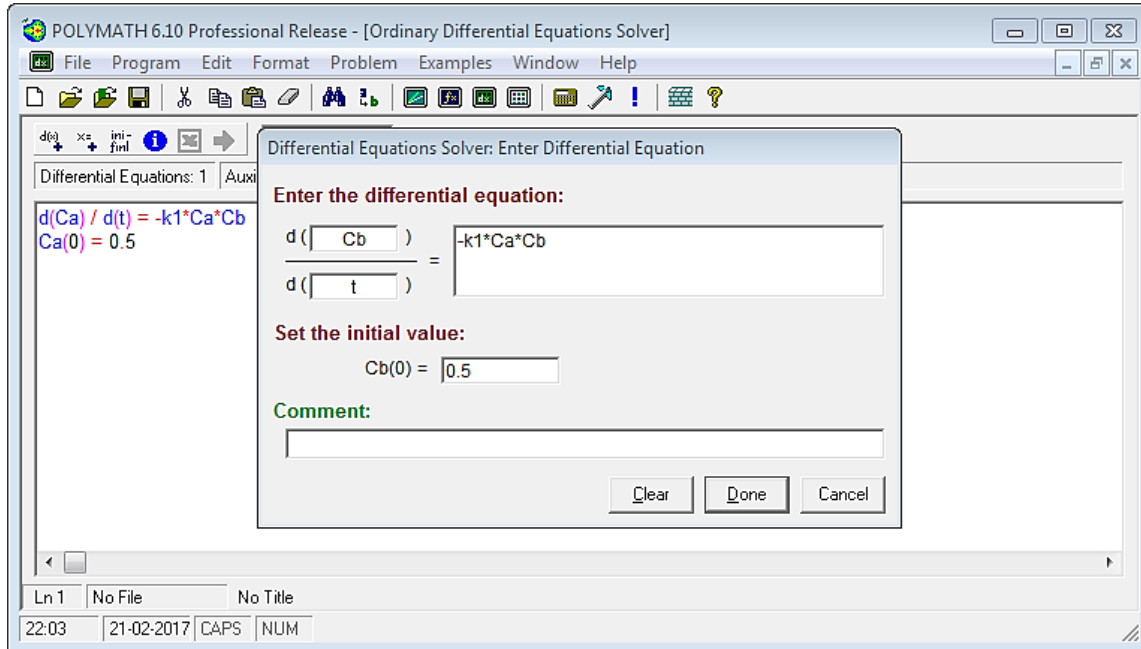


Now, press Done button. You will find that your equations are entered in the main window

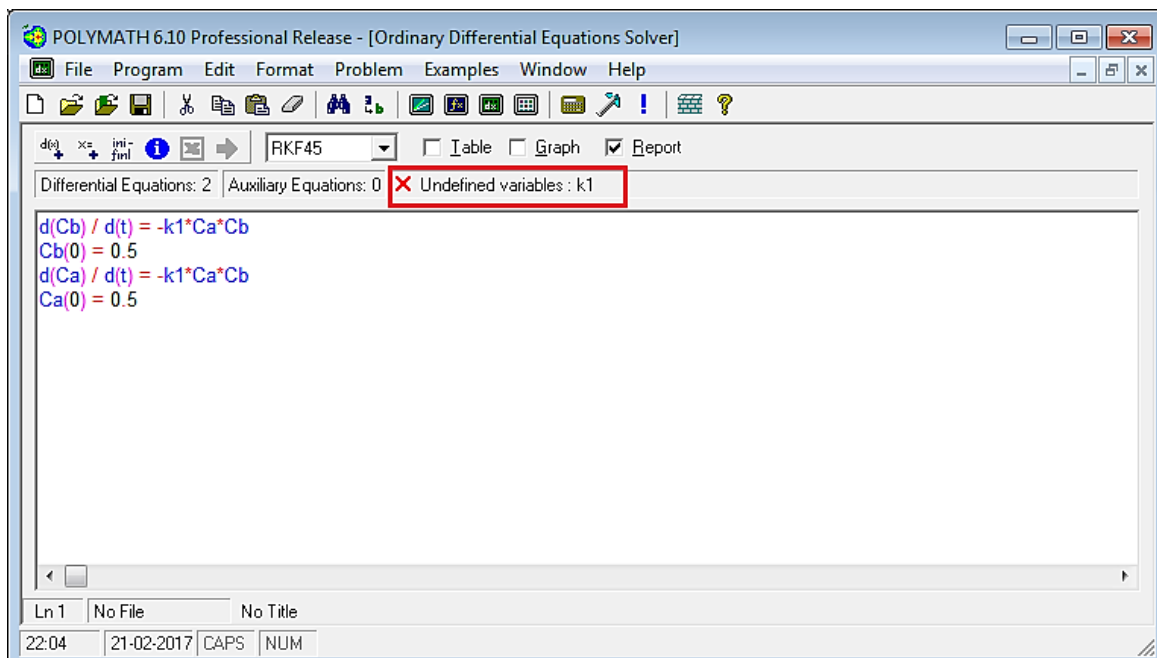


Repeat the similar exercise to enter the equations for 2nd differential equation

$$\frac{dCb}{dt} = -k_1 * Ca * Cb \text{ and } Cb(0) = 0.5$$

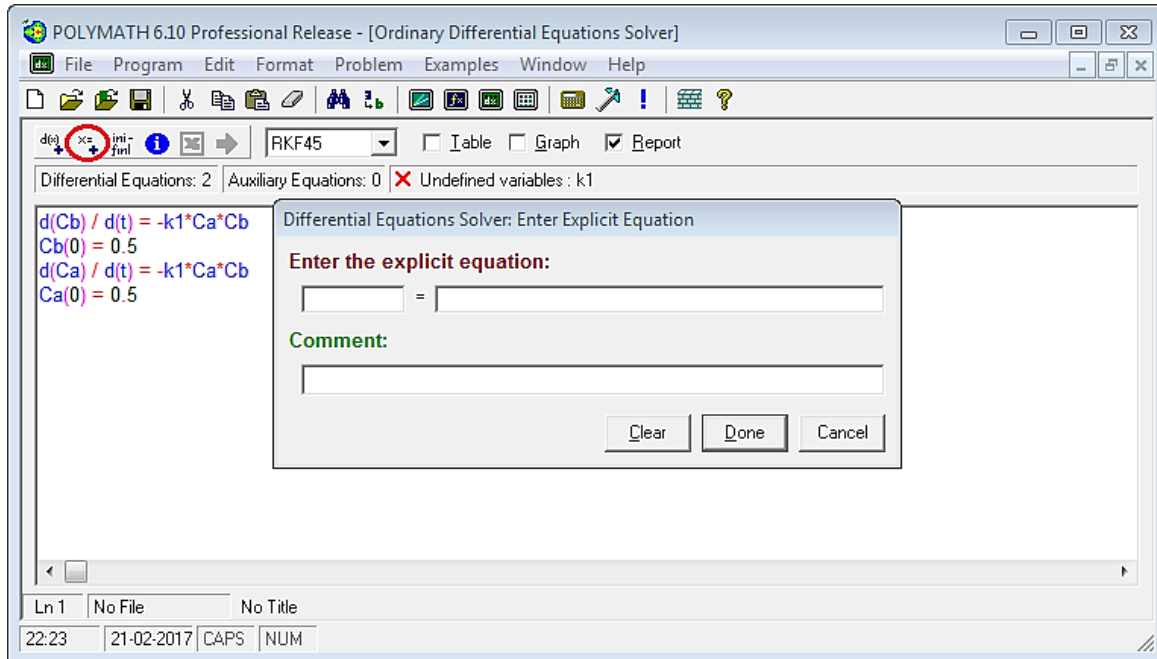


After pressing Done, your main window will look like this



In the window above, there is a variable that has not been specified, as indicated by the red **X**. The information following the **X** will tell you what variables have not been specified. Here, it shows that k1 is an undefined variable.

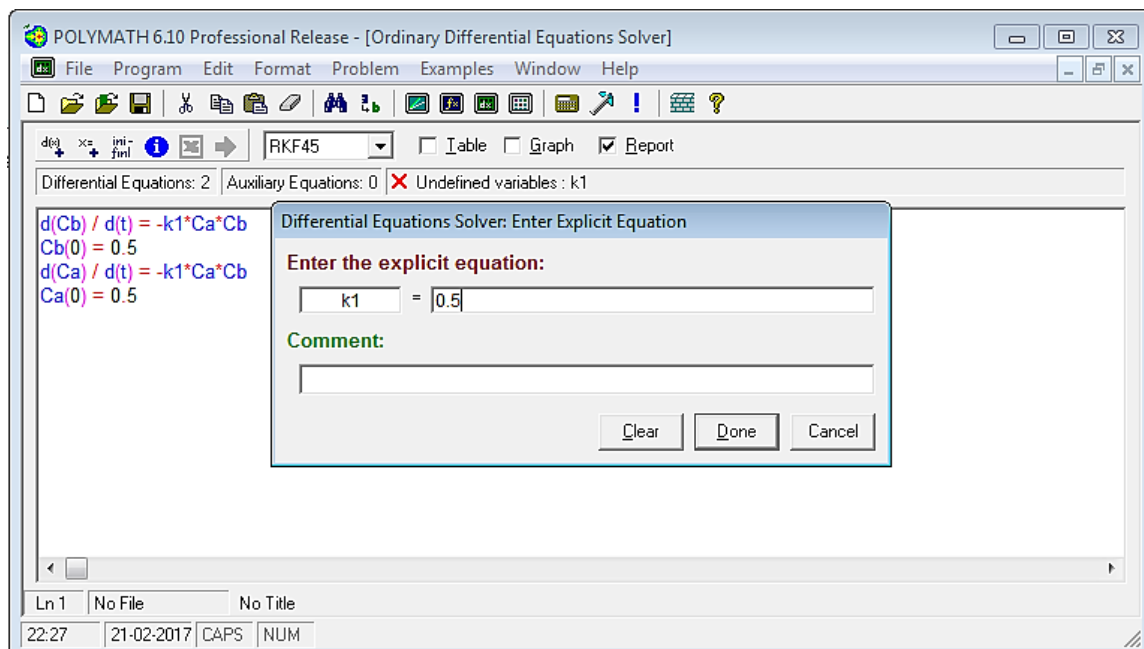
Now, to specify the value of k_1 , press "x=" button (shown by red circle in below screen). Pressing this button brings up a different dialogue box in which you can specify explicit equations in your system.



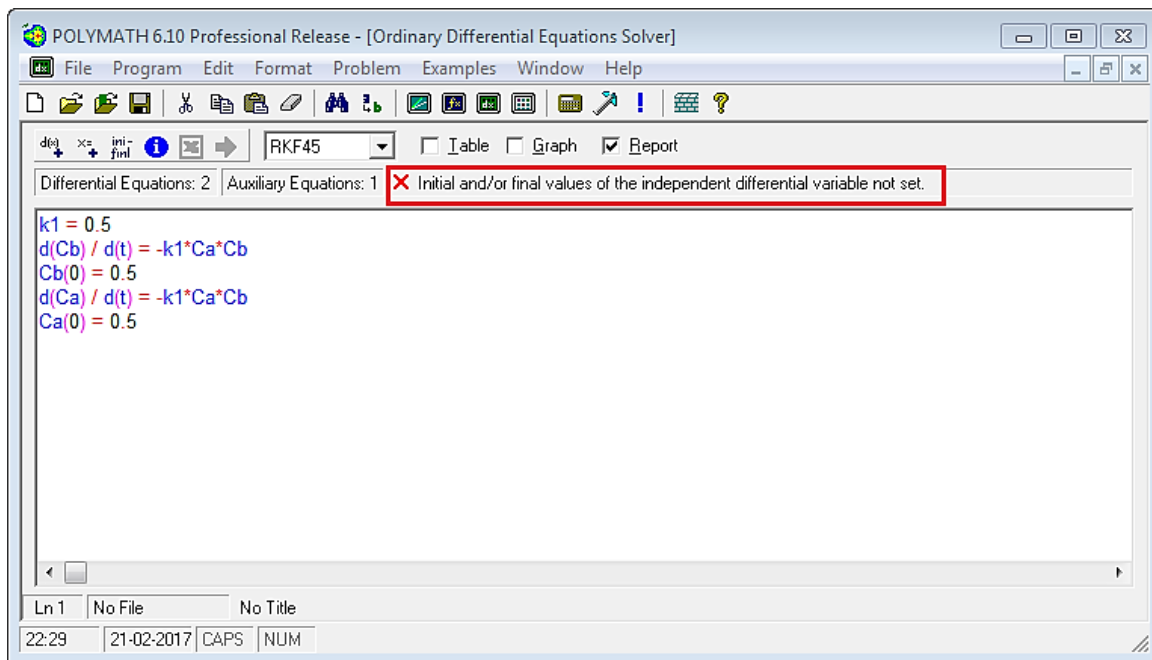
In this case, we only have one variable i.e.

$$k_1 = 0.5$$

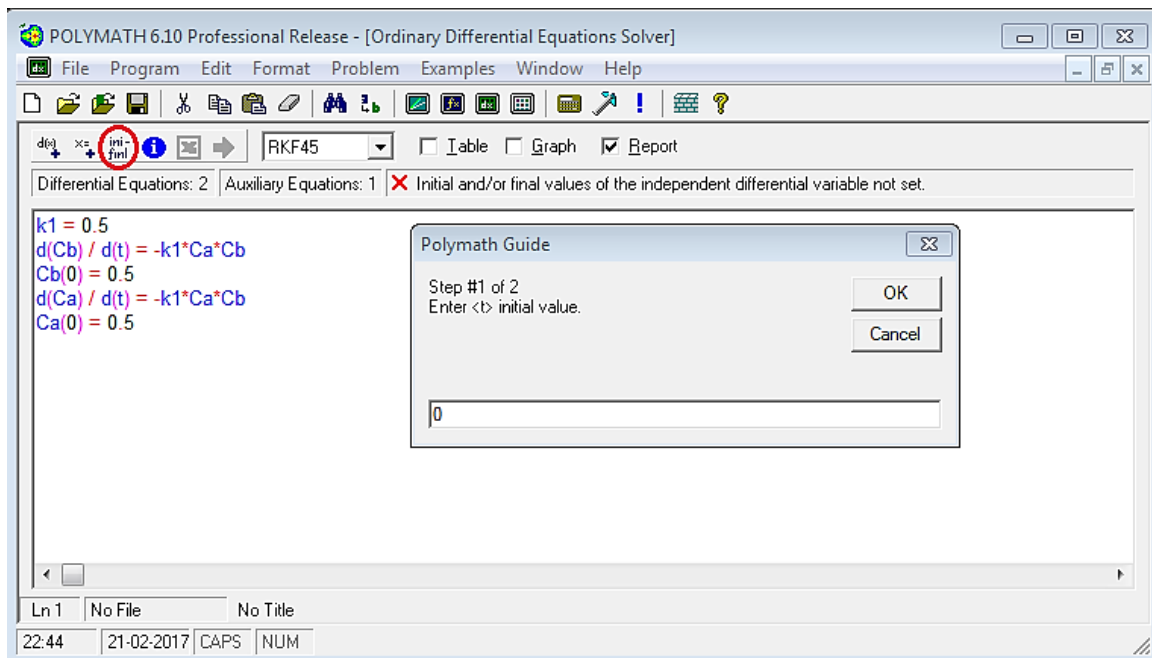
Enter the value of k_1 in the space provided in the rectangular box as shown below



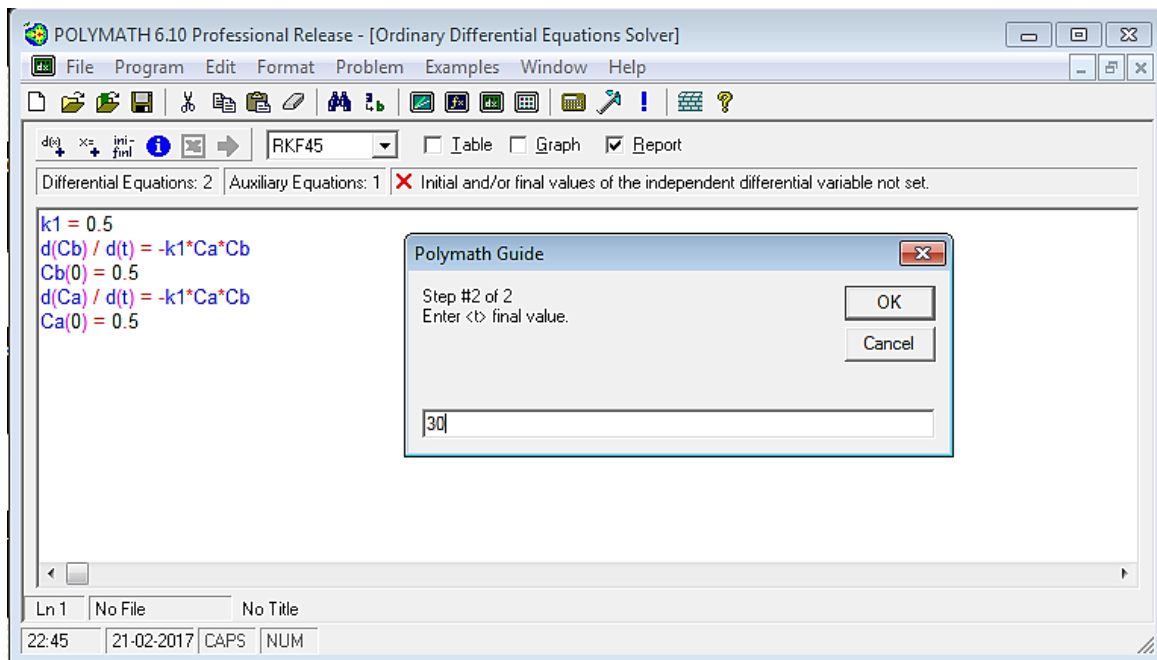
After you press Done, your window will appear like this



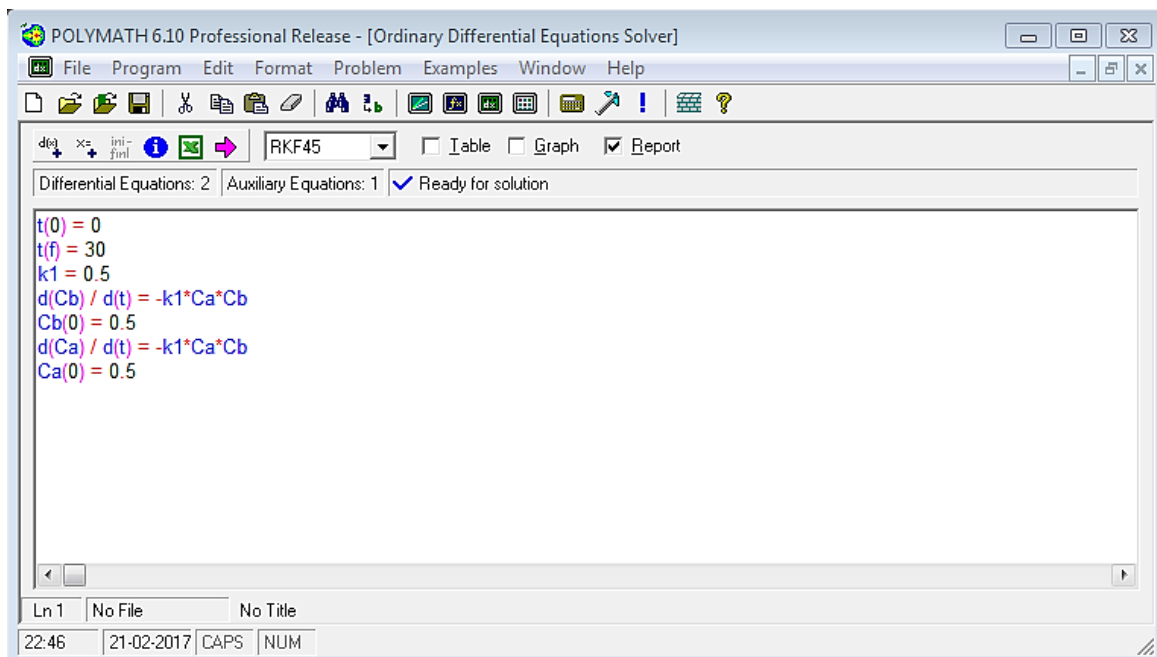
You have now entered both the differential equations and the explicit equation. Now you need to set the time span for which you want to perform the integration. This is a required input and can be seen from the comment following the **X**. To specify the initial and final values of t , click the "**ini-finl**" button present on the menu bar (shown by red circle in below screenshot). A dialogue box will appear again. Enter the initial value of t in the space provided. In this case t initial = 0



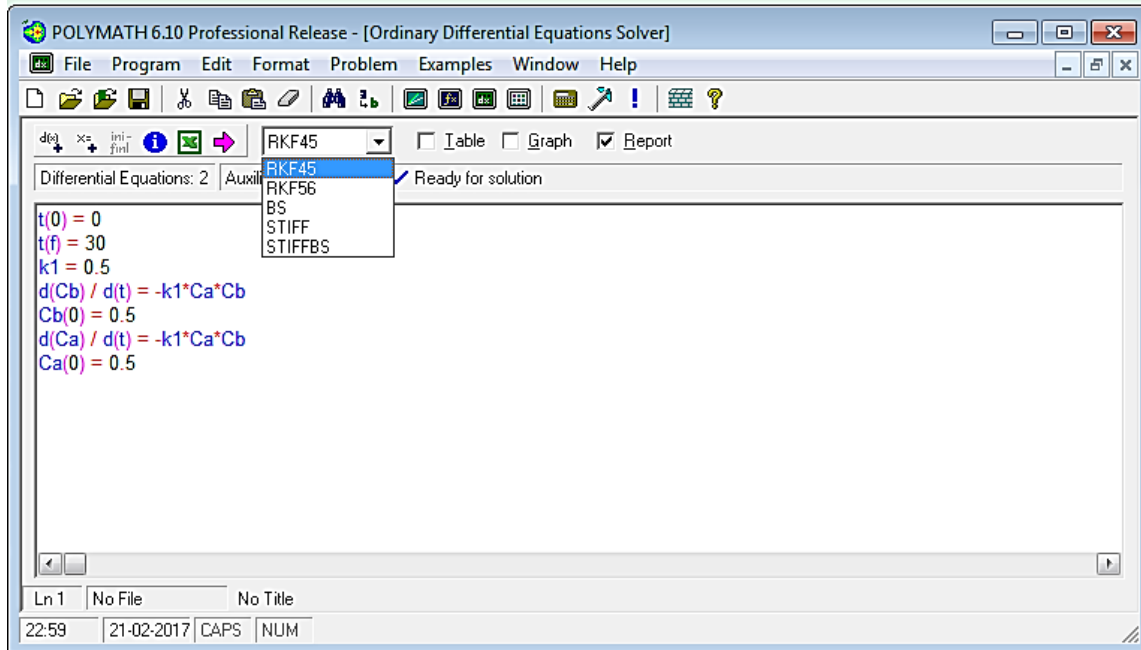
Now, enter the final value of t i.e. t=30




Press OK. When all of the necessary information has been specified, the screen will look like this. You can check that **X** is now replaced by "Ready for solution"

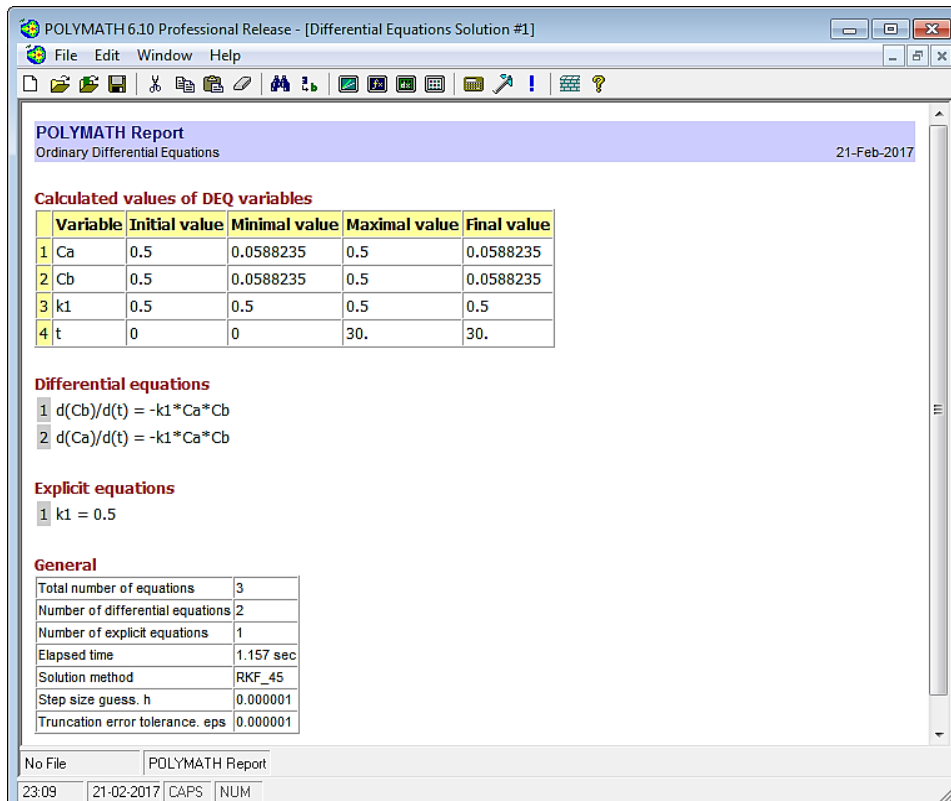


You can choose the method of ODE solver you would like to use by selecting the option from the drop down menu present next to RKF45. By default, polymath uses RKF45 method. In this case, we will choose RKF45



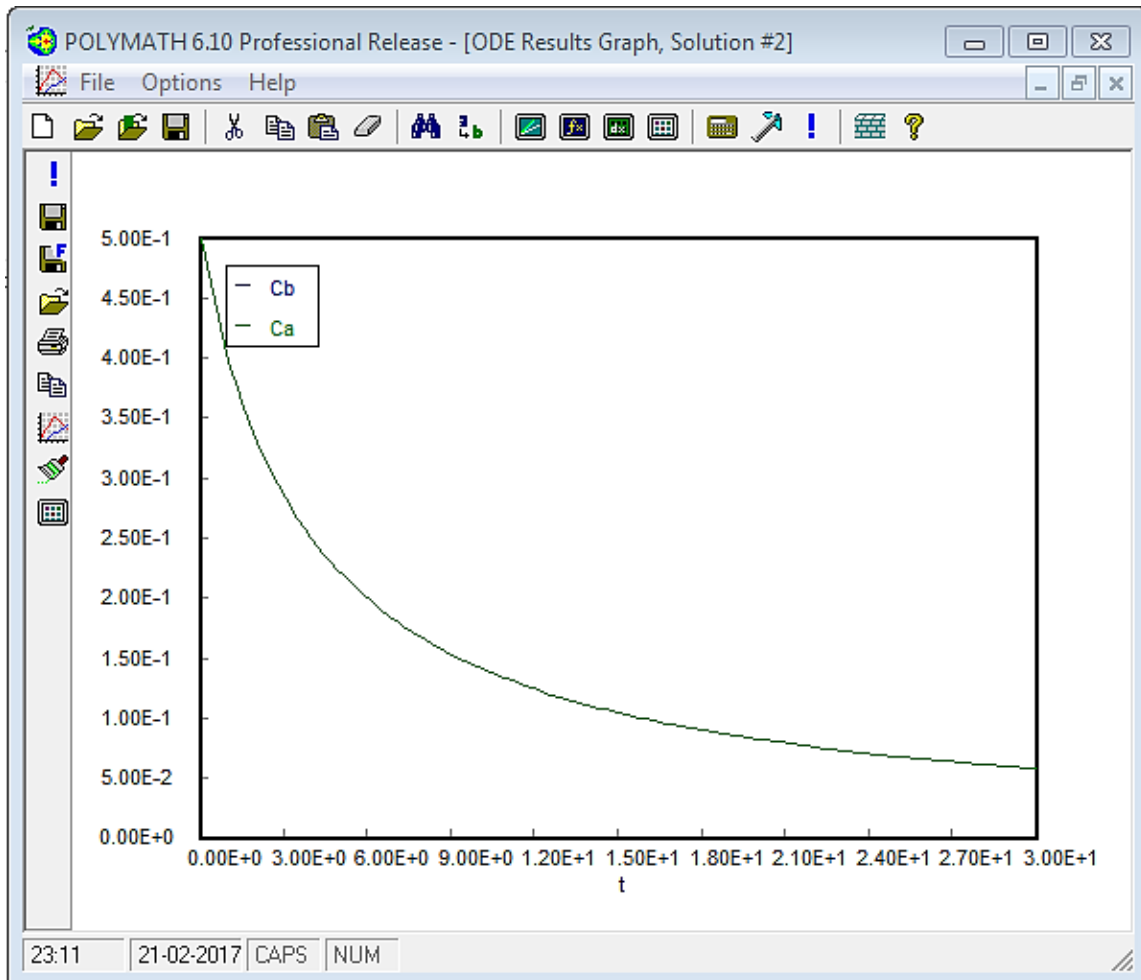
Now select what you want polymath to output by checking the boxes on the right side of the window. The simulation will output results depending on what is selected. The options available are Table, Graph, and Report. Select the appropriate option and then Click on the pink arrow  to have Polymath perform the integration.

If you selected "Report" then following screen will be displayed.

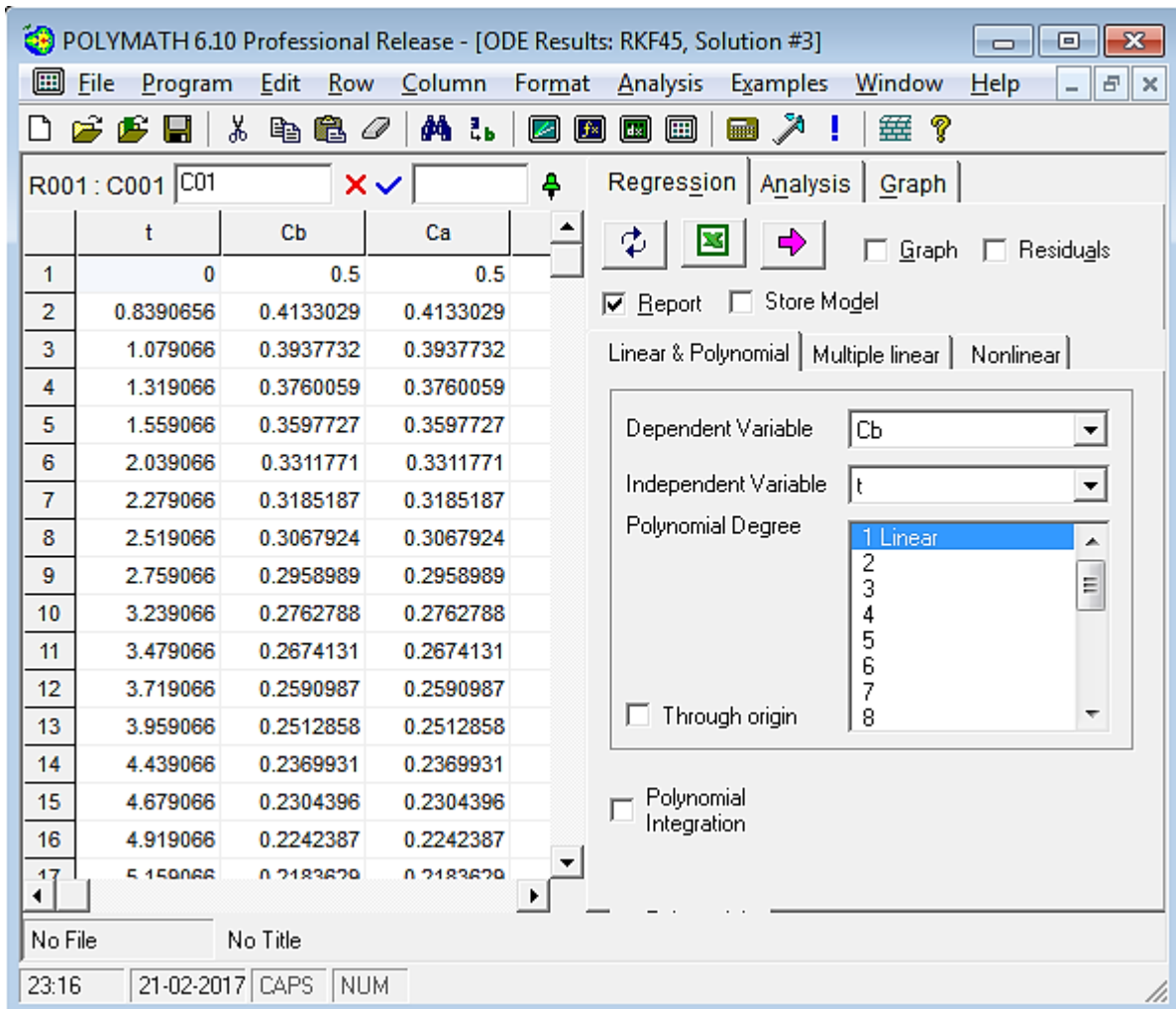


The above report gives various information such as initial and final values of every variable present, the minimum and maximum values of the variables in the given interval, and the equations you entered.

If you selected Graph, you will get a graph of dependent variable as a function of independent variable



Selecting "Table" will cause a data table to be generated. It includes the values of the variables at each different step in the differential variable, in this case, time t.



To get an output that you had not previously selected, you will need to check the corresponding box and rerun the simulation by clicking on the pink arrow.