

Polymath tutorial for Calculating Conversion with Catalyst Decay in Batch Reactors

(Example 10-4)

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

$$\frac{dX}{dt} = k * (1 - X)$$
$$\frac{dX_d}{dt} = k * \frac{(1 - X_d)}{(1 + k_d t)}$$

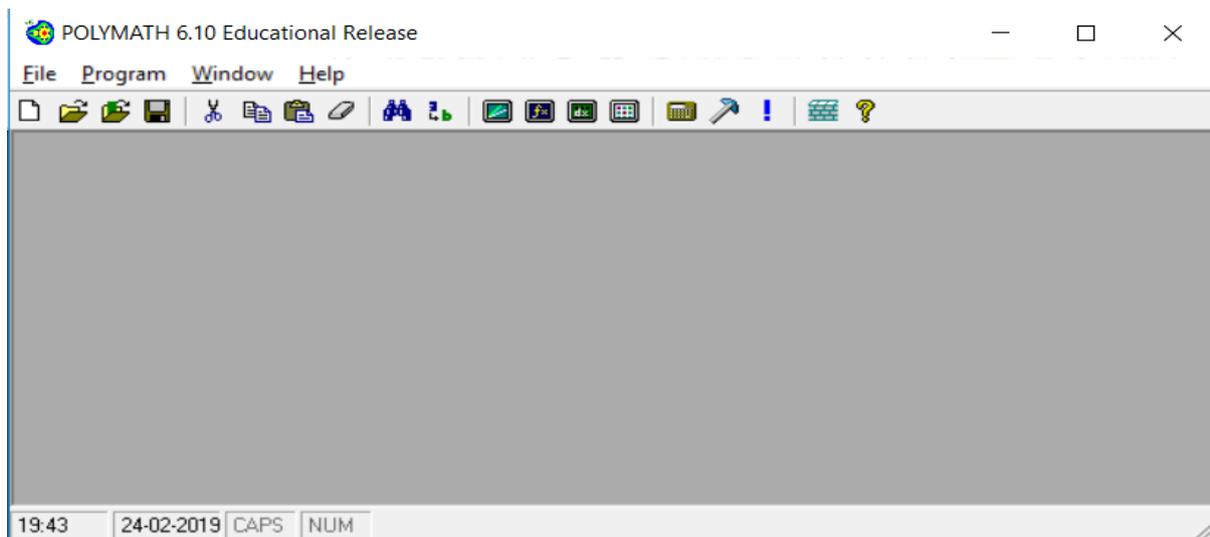
Where,

$$k = 0.01 \text{ and } k_d = 0.1$$

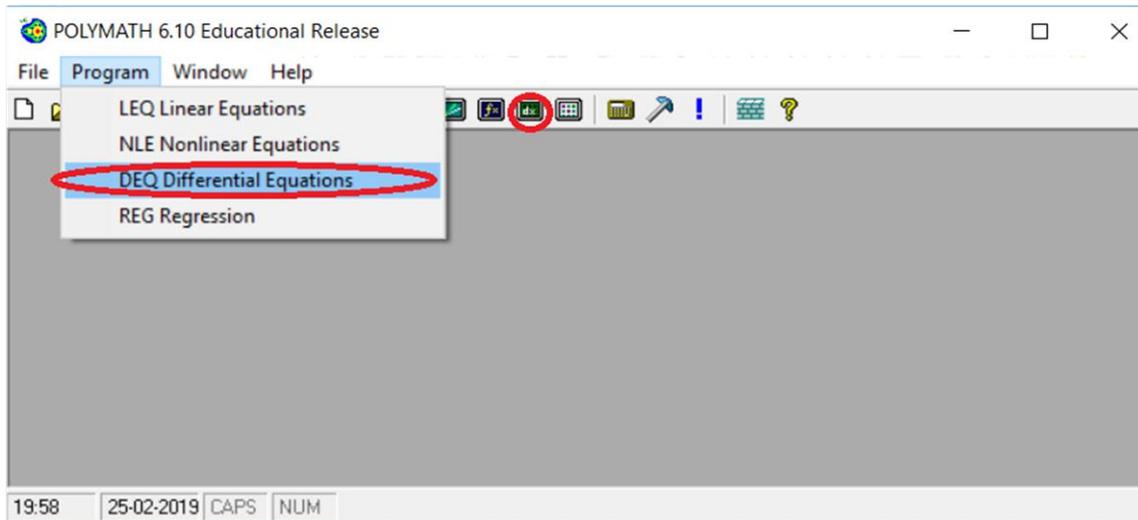
and integration time span is $t = 0$ to $t = 500$

Step 1: First make sure you have polymath installed. If you don't have it then refer to the installation instruction present on <http://www.umich.edu/~elements/5e/software/polymath.html>

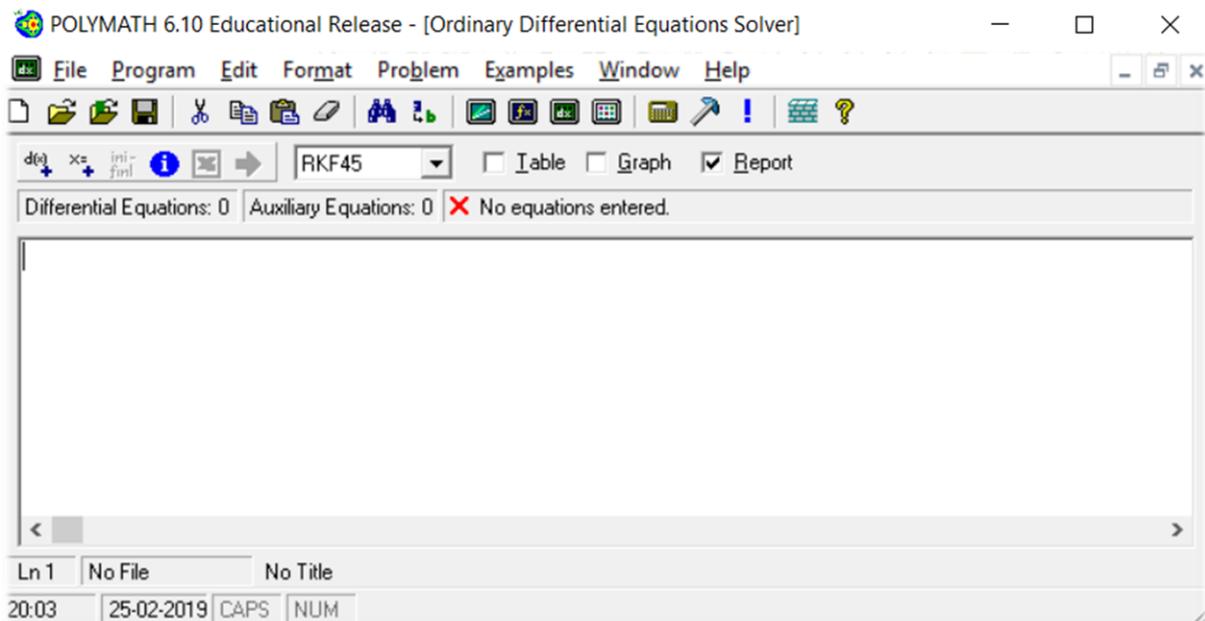
When you open Polymath, following window would appear



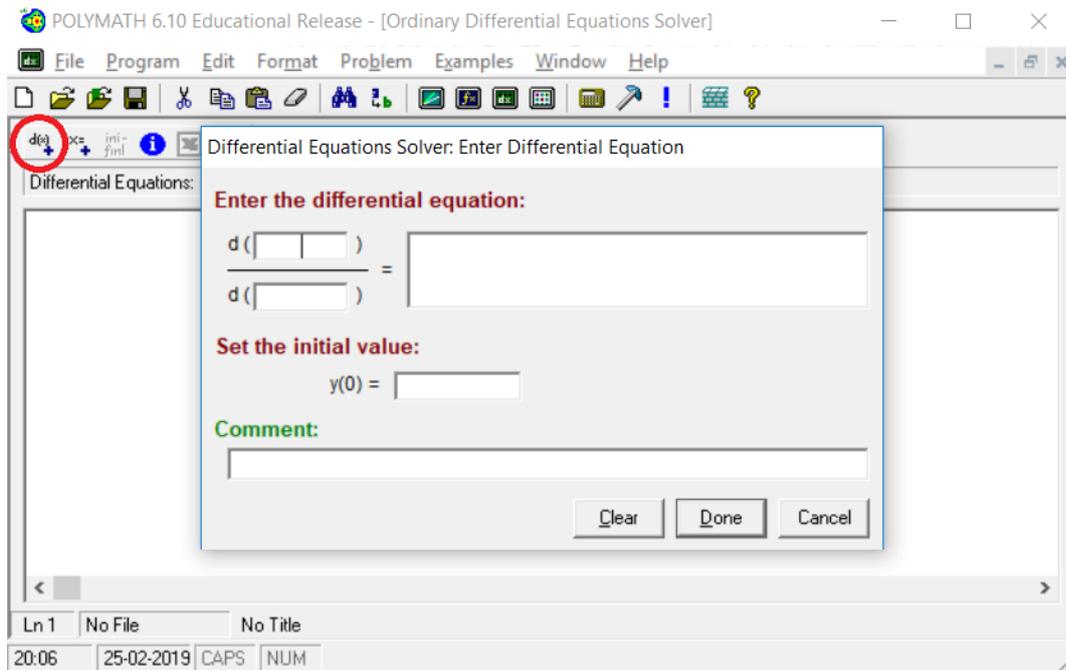
Step 2: To use the ODE solver in Polymath, first click on the “Program” tab present on the toolbar. This will bring up a list of options from which you need to select. In this case we need to solve differential equations so select "DEQ Differential Equations". The shortcut button “dx” for differential 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.



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.

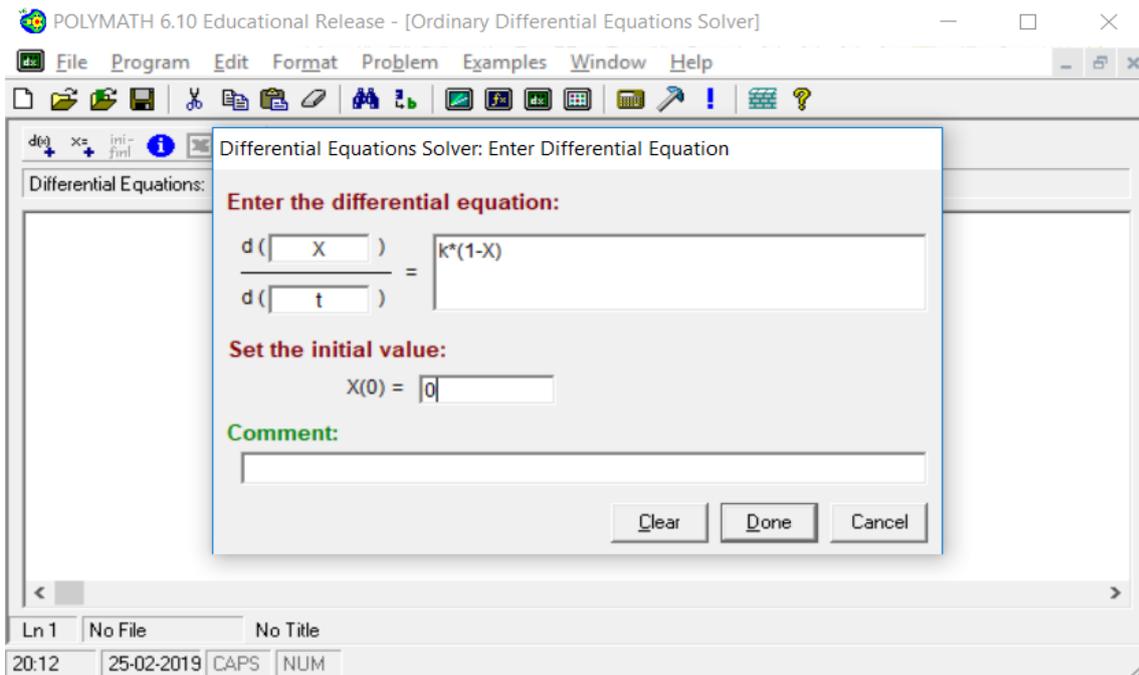


In the above dialogue box, only one differential equation can be entered at one time

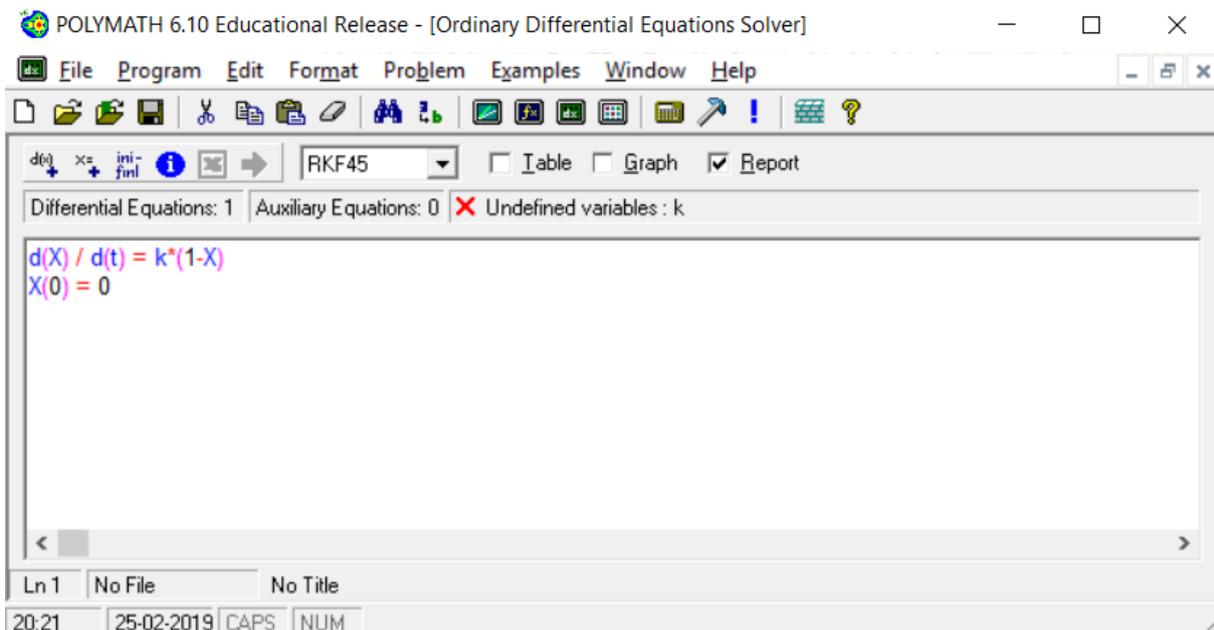
First differential equation is

$$\frac{dX}{dt} = k * (1 - X) \text{ and } X(0) = 0$$

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



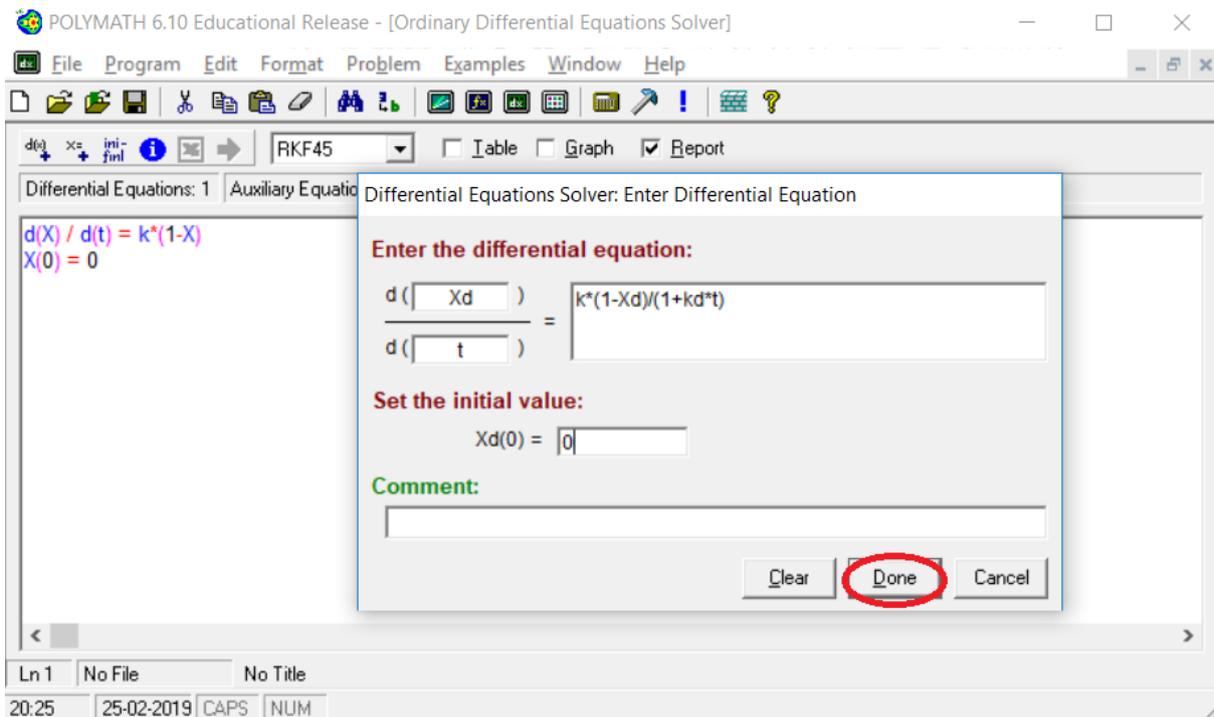
Now, press Done button. You will find that your equations are entered in the main window



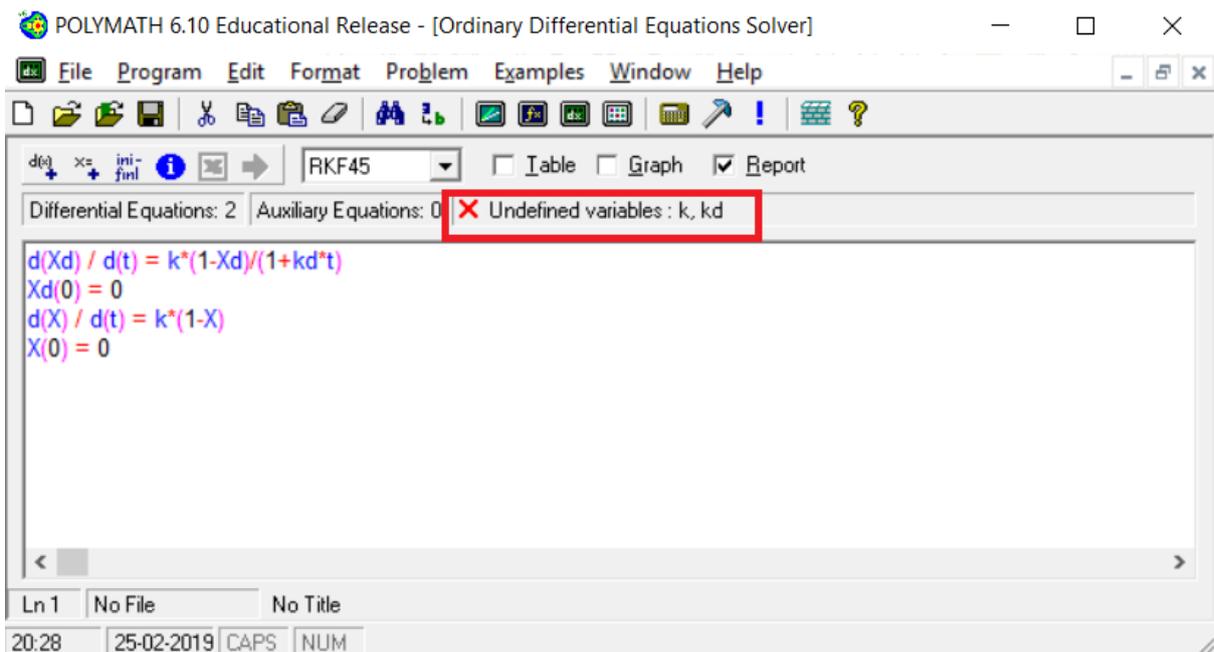
Repeat the similar exercise to enter the equations for 2nd differential equation

$$\frac{dX_d}{dt} = k * \frac{(1 - X_d)}{(1 + k_d t)}, X_d(0) = 0$$

Enter the differential equation as shown below and press Done button.

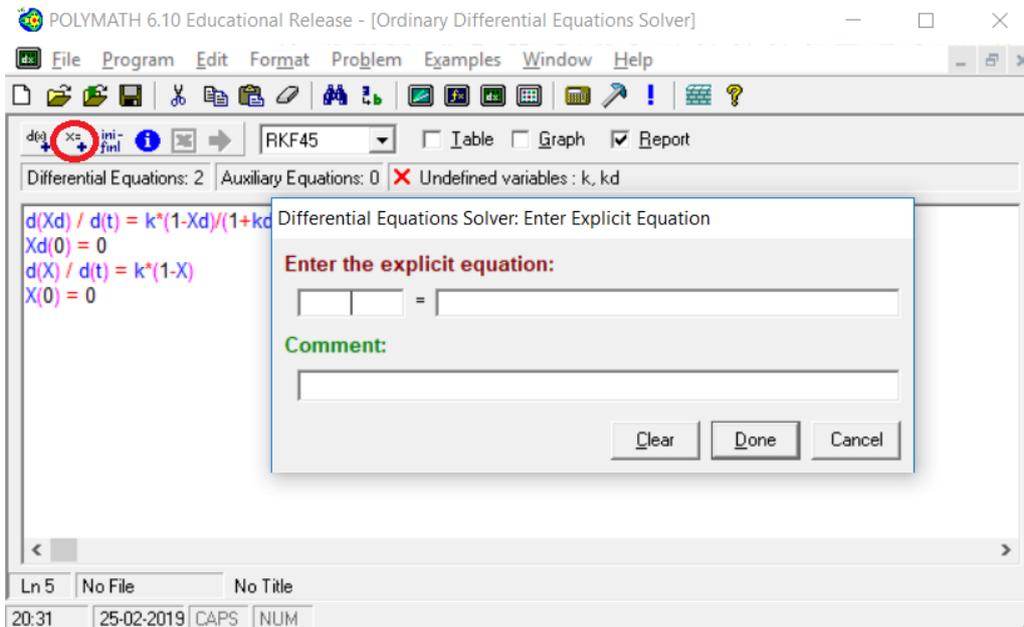


After pressing Done, your main window will look like this



Step 4: In the window above, there are variables that have 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 k and kd are undefined variables.

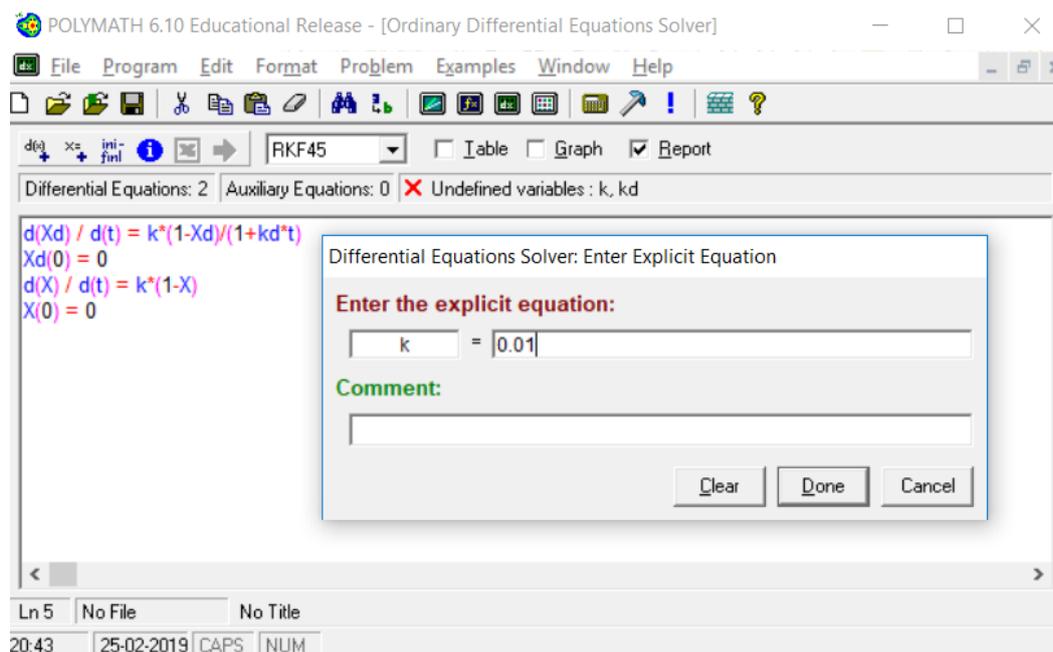
Now, to specify the value of variables, press "x=+" button (shown by red circle in below screen). Pressing this button brings up a dialogue box where you can specify explicit equations in your system. Only 1 equation can be entered at a time.



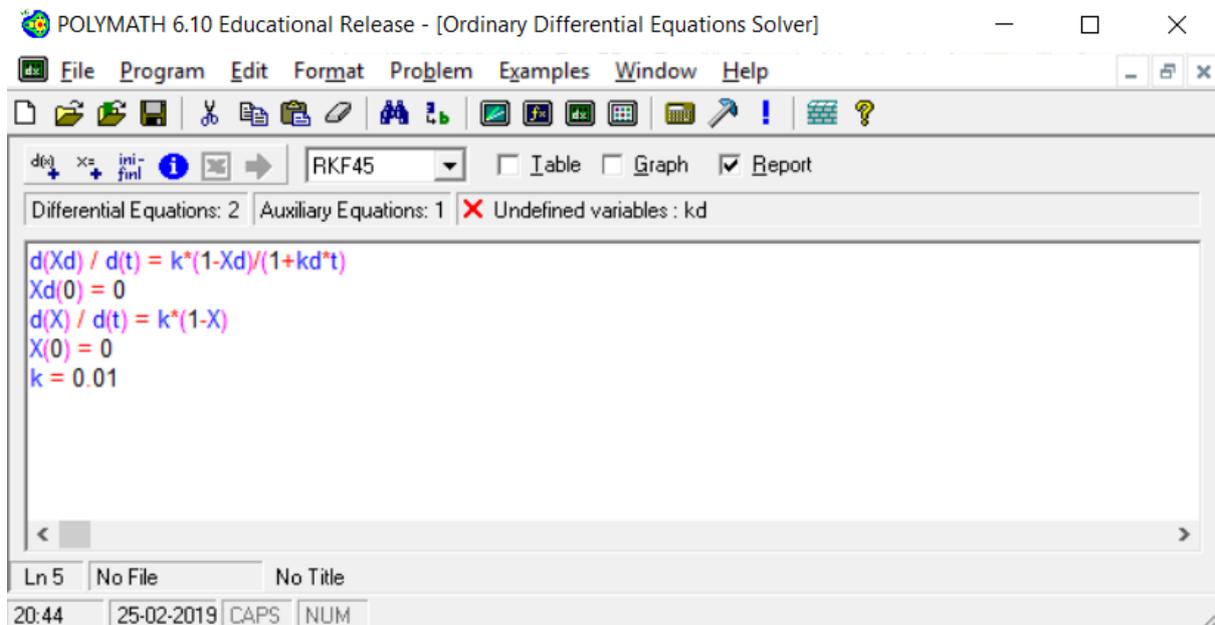
In this case, we have two variables i.e. k and kd

$$k = 0.01 \text{ and } kd=0.1$$

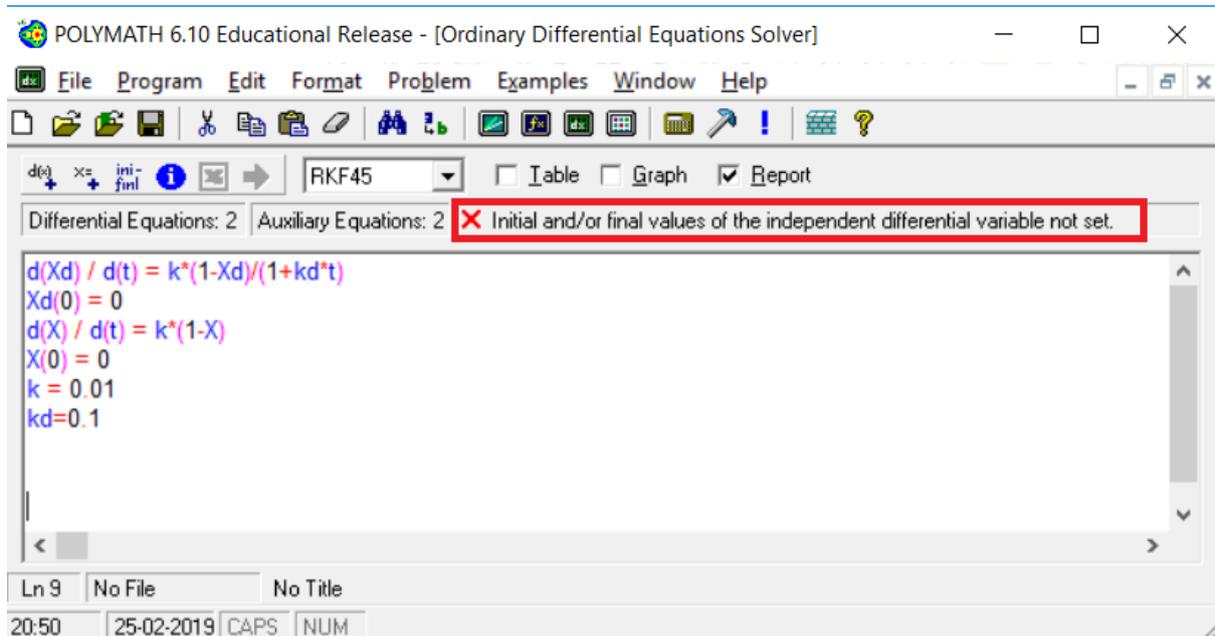
Enter the value of k in the space provided in the rectangular box as shown below



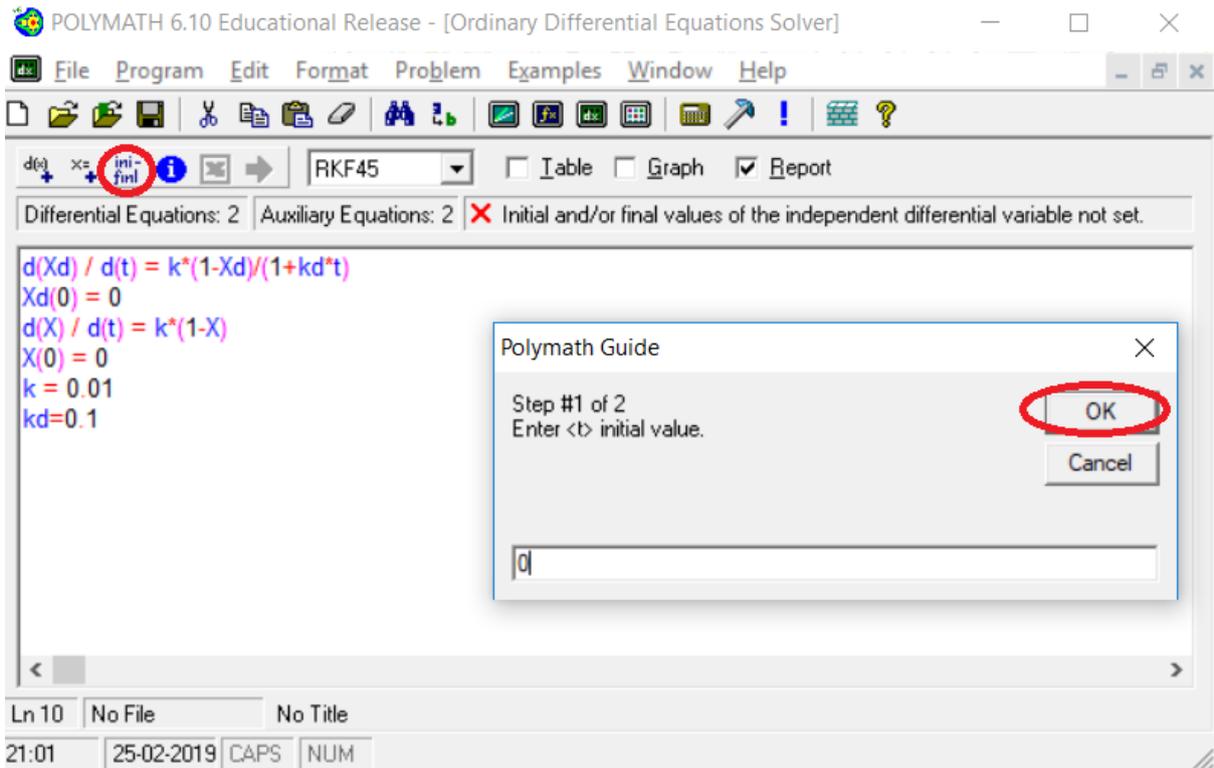
After you press Done, your window will appear like this



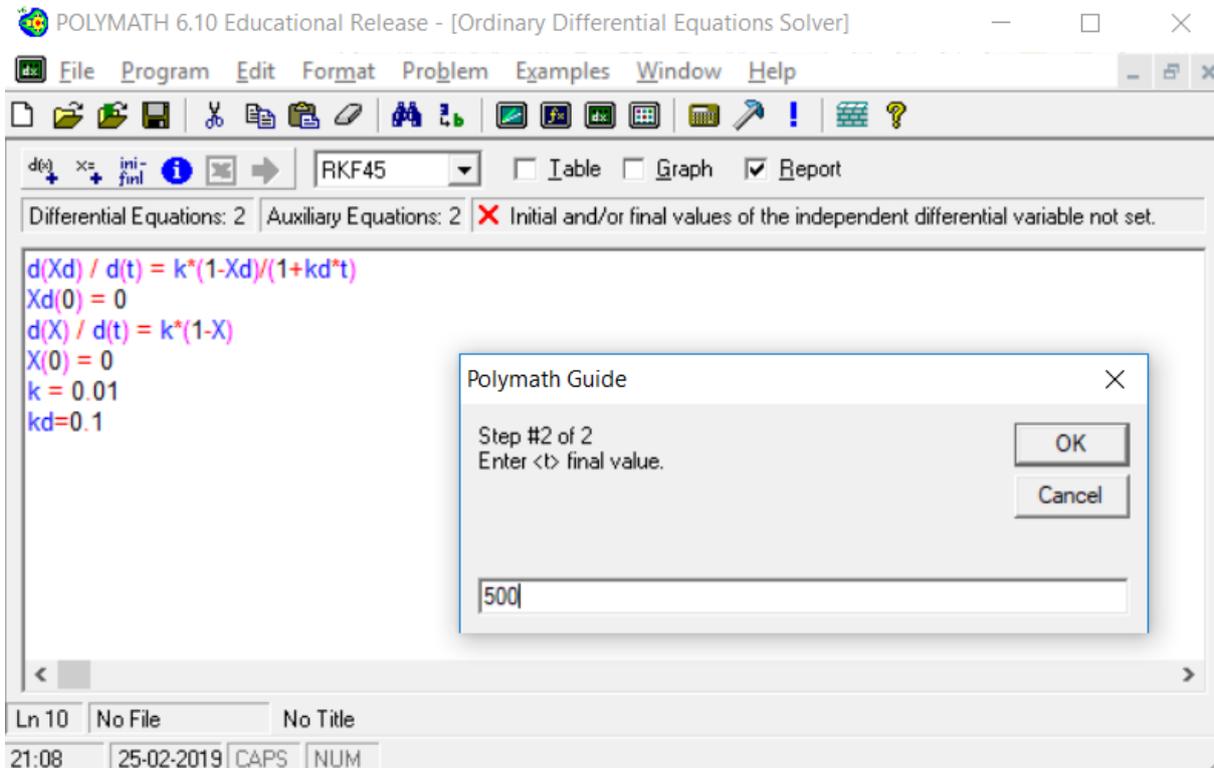
Repeat the similar exercise to enter the equation for kd. After you enter the equations, your screen will appear like this:



Step 5: 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. 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. Press OK after you have entered the initial value.

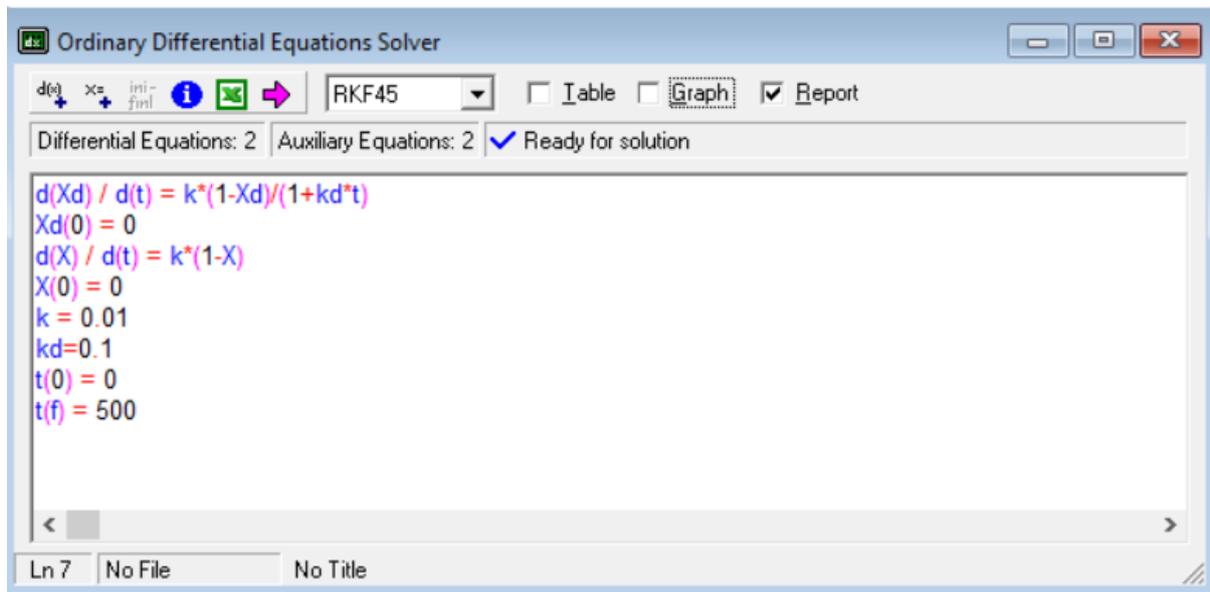


Now, you will be prompted to enter the final value of t i.e. t=500 as shown below

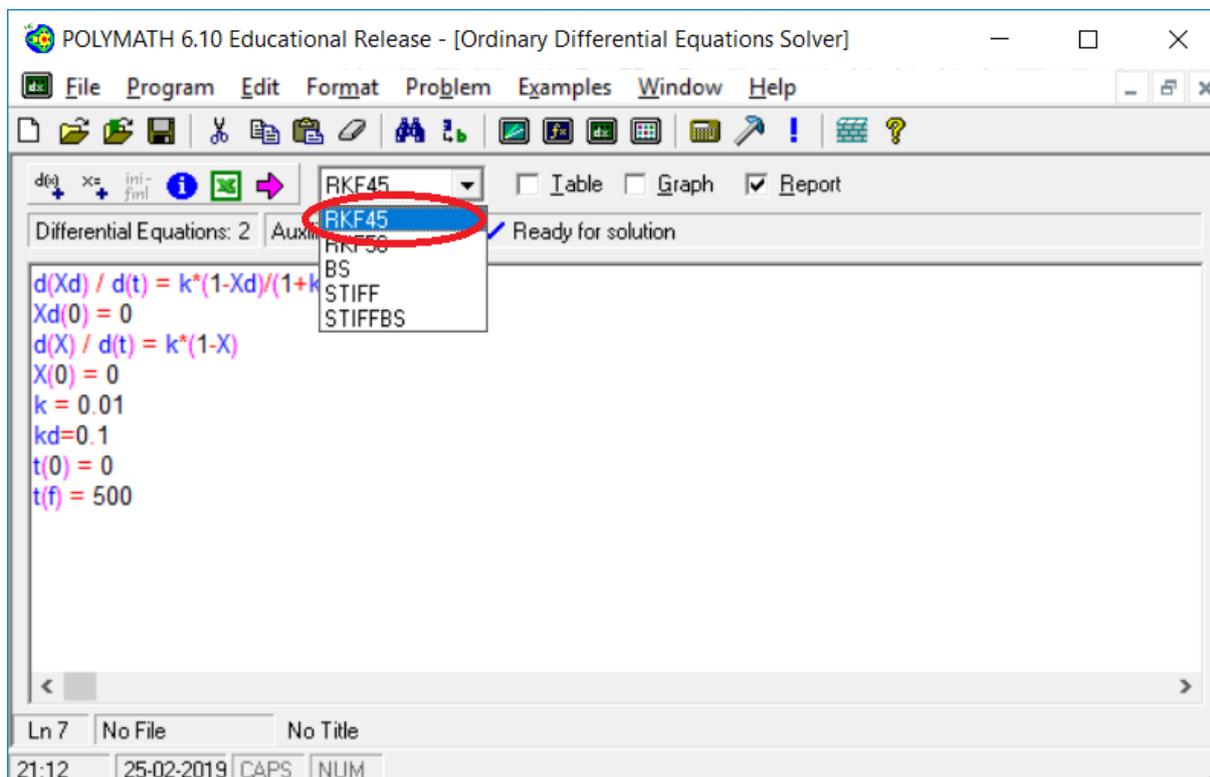


Press OK.

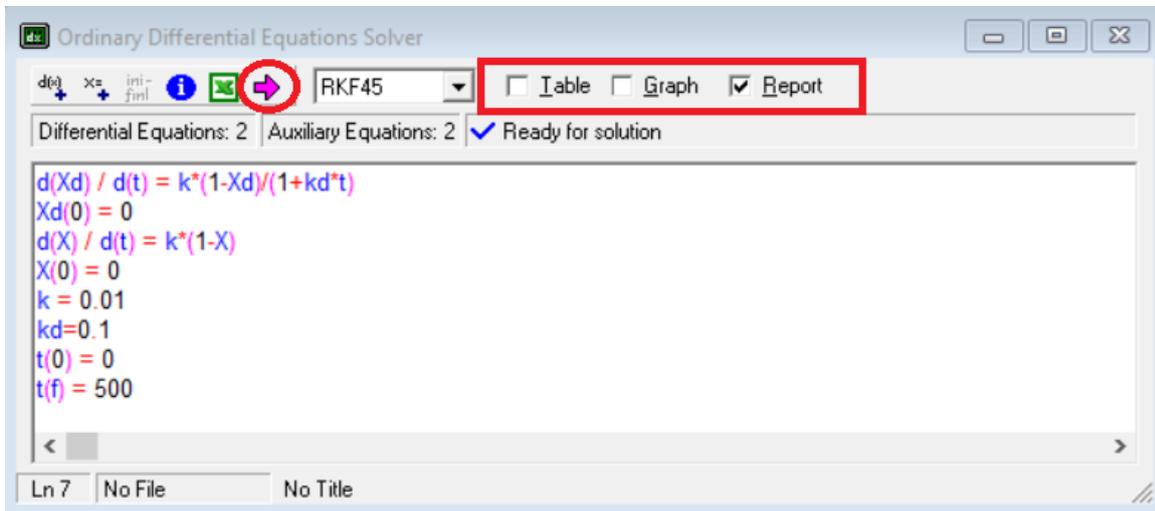
When all of the necessary information has been specified, the screen will look like this. You can check that X is now replaced by “Ready for solution”



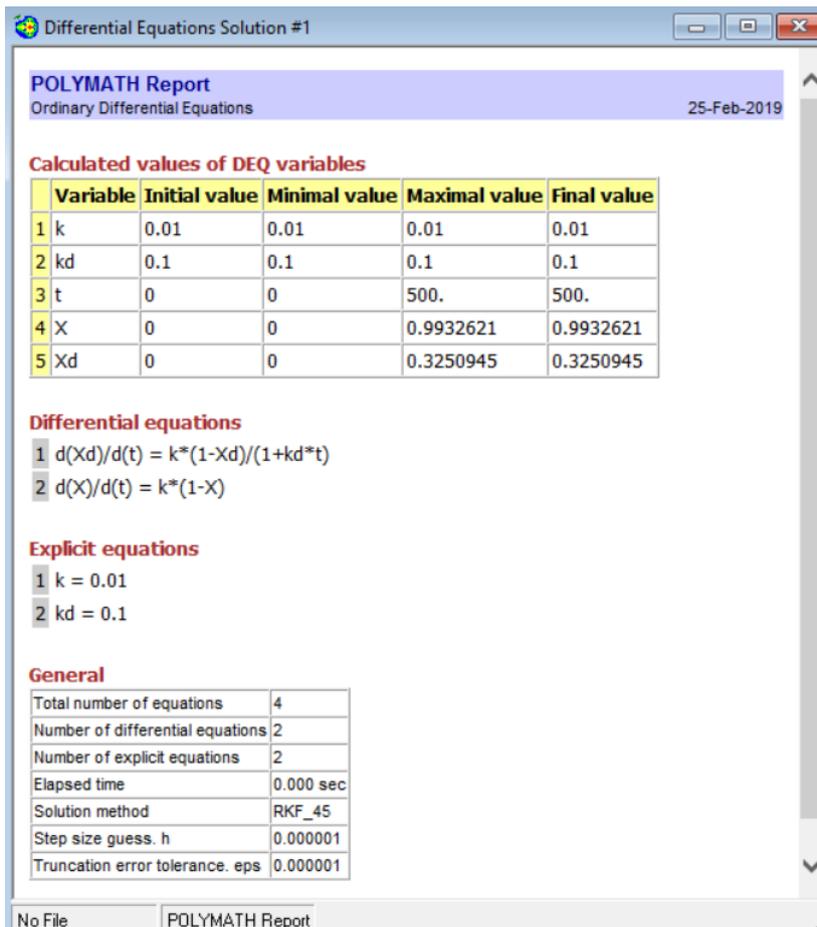
Step 6: You can choose the method of ODE solver you would like to use by selecting the option from the drop-down menu present next to RKF45. By default, polymath uses RKF45 method. In this case, we will choose RKF45.



Step 7: Now select what you want polymath to output by checking the boxes on the right side of the window (shown below). The simulation will output results depending on what is selected. The options available are Table, Graph, and Report. You can check multiple boxes also at the same time. 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

