Polymath tutorial to find the Rate-Law parameters (*Example 7-3*)

The following table shows the raw data for performing nonlinear regression to determine model parameters (refer Table E7-1.1, Elements of chemical reaction engineering, 5th edition)

C_A(mol/dm^3)	t (min)
0.05	0
0.038	50
0.0306	100
0.0256	150
0.0222	200
0.0195	250
0.0174	300

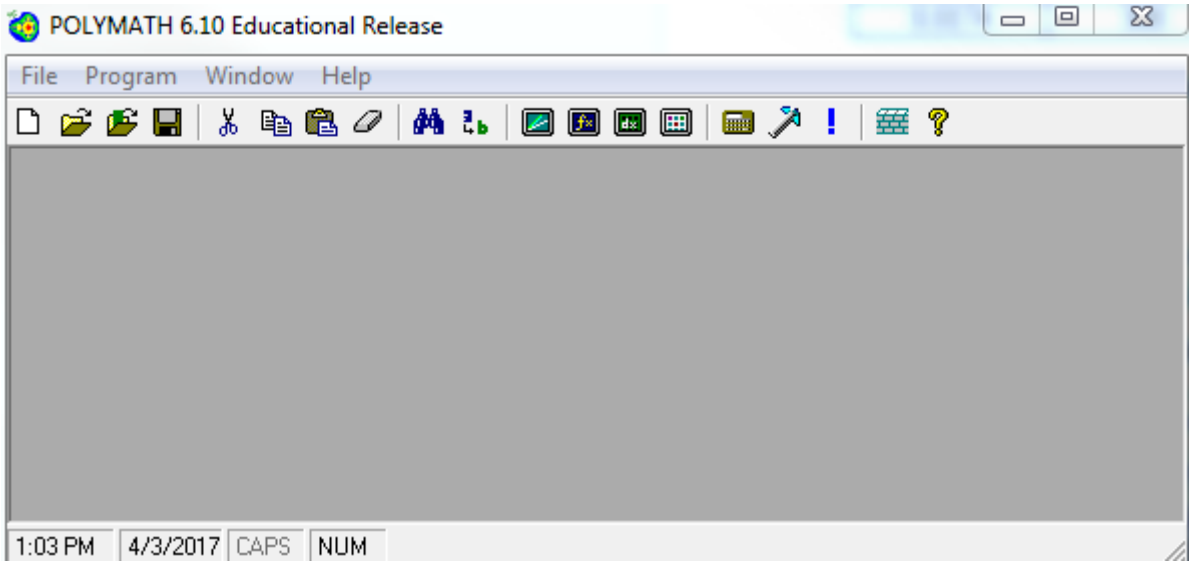
The nonlinear equation is given by

$$t = \frac{1}{k'}\frac{(0.05)^{(1-\alpha)} - C_A^{(1-\alpha)}}{(1-\alpha)}$$

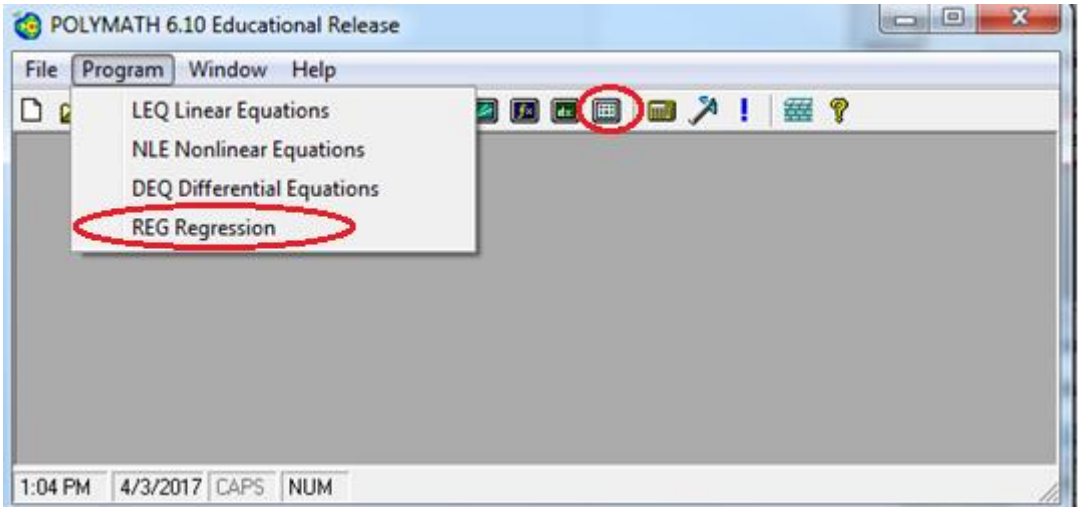
Perform first regression to obtain the value of k' and α and then round off α value to nearest integer. Perform second regression to determine the value of k', keeping the value of α constant (as obtained from first regression).

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

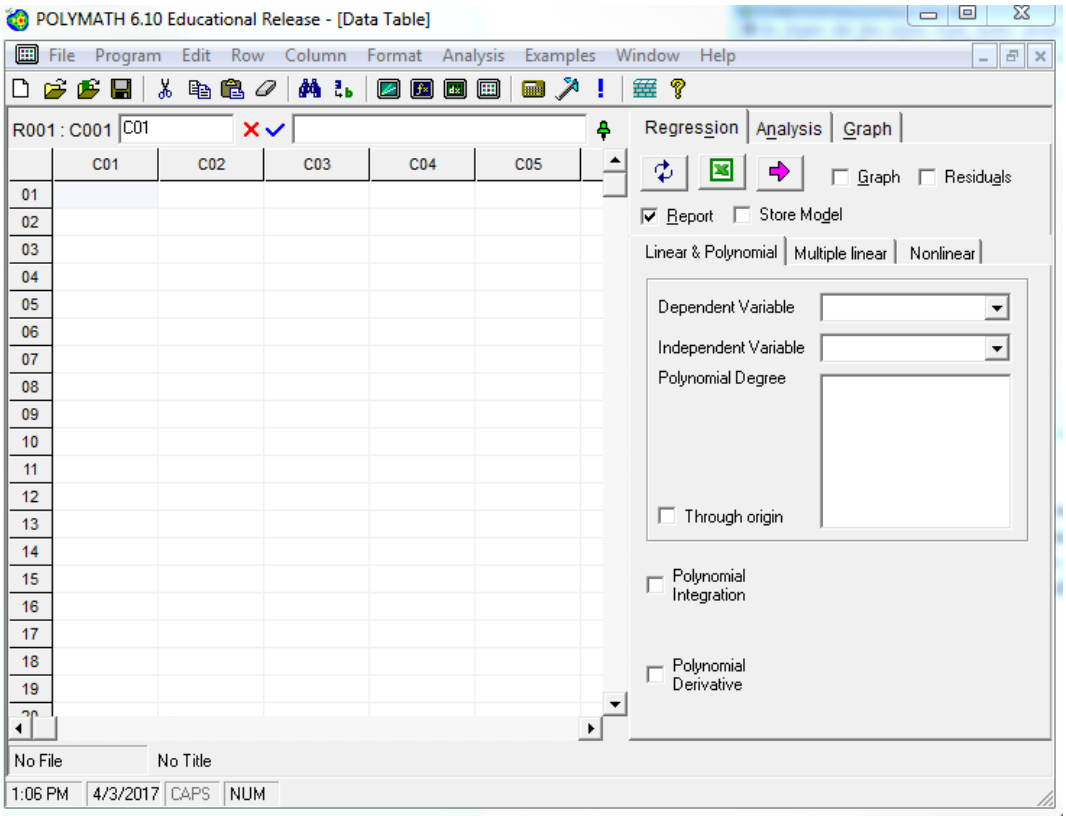
When you open Polymath, following window would appear



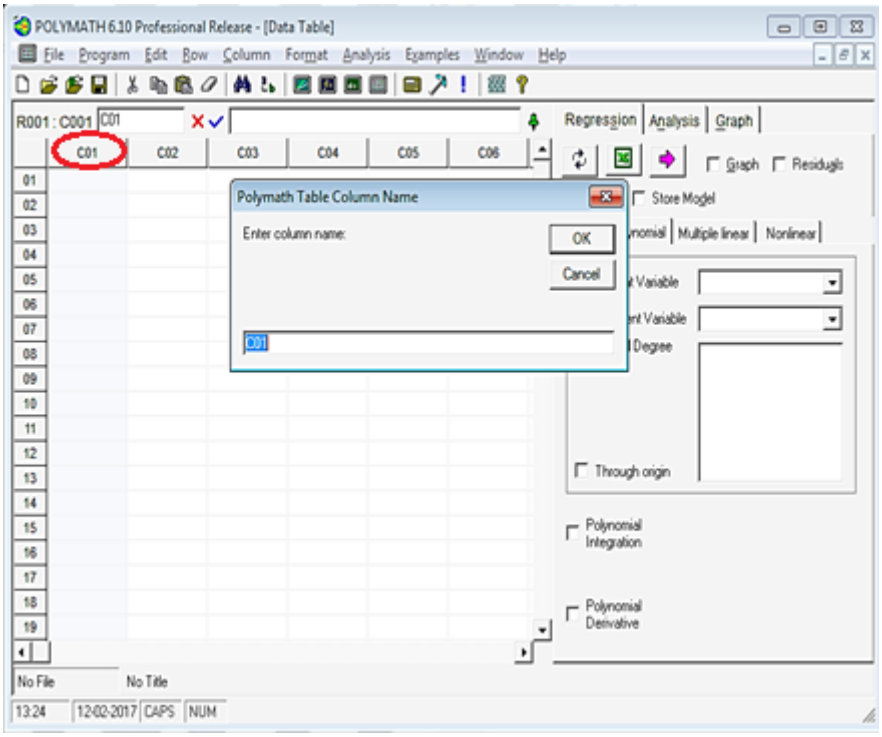
Step 2: To use the nonlinear regression solver in Polymath, first click on the “Program” tab present on the toolbar and select "REG Regression". The shortcut button for nonlinear equation solver is also present on the menu bar as shown by red circle in below screenshot



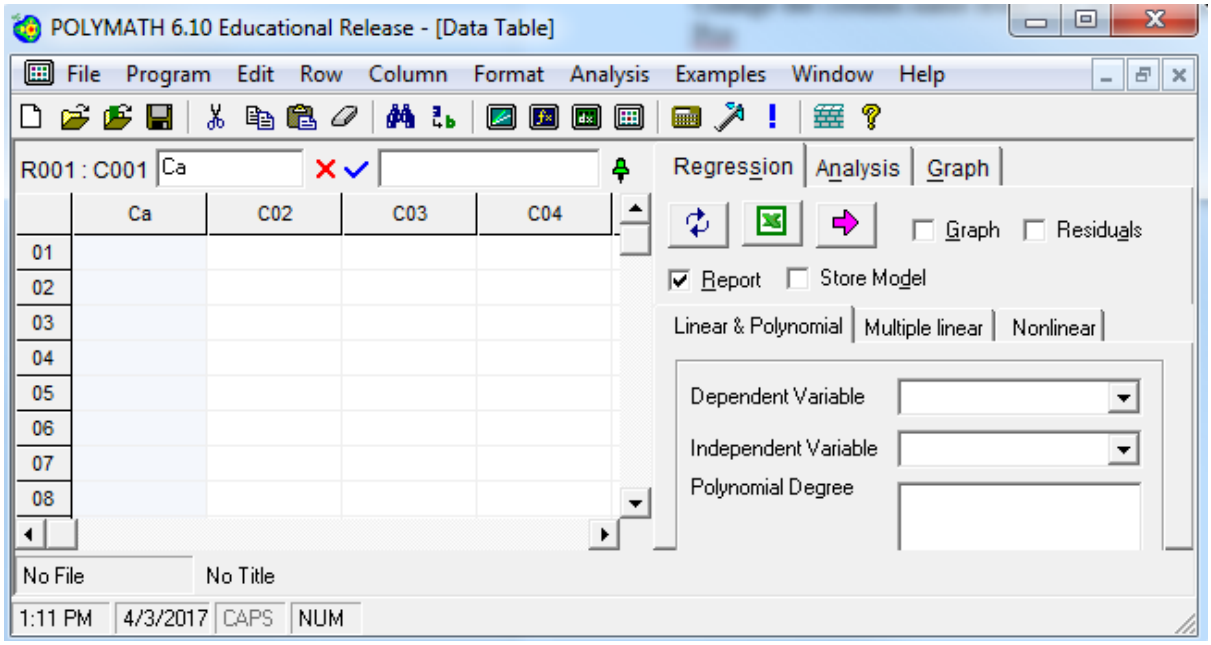
This will open up another window, which looks like this.



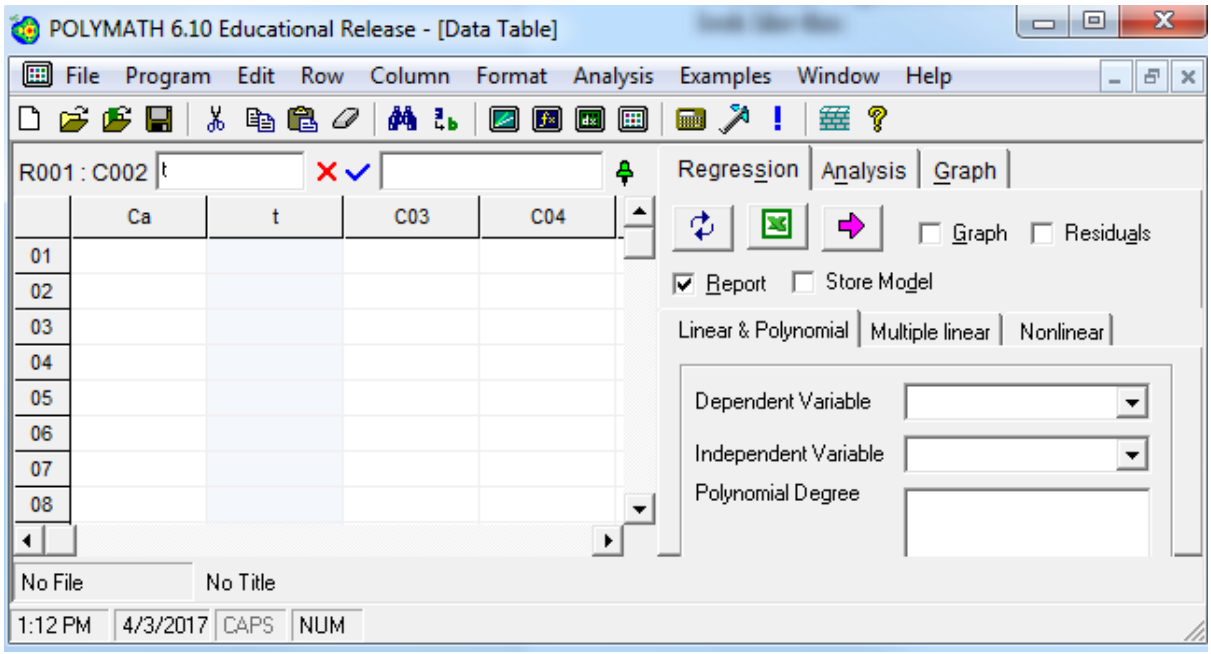
Step 3: Before inserting the data into the spreadsheet, it is recommended to change the column name with the name of the variable mentioned in the data table. This would make it easy to comprehend the polymath output. To change the column name of C01, double click on the column name "C01" or right click on C01 and select "Column Name…" A dialog box will appear where column name can be changed



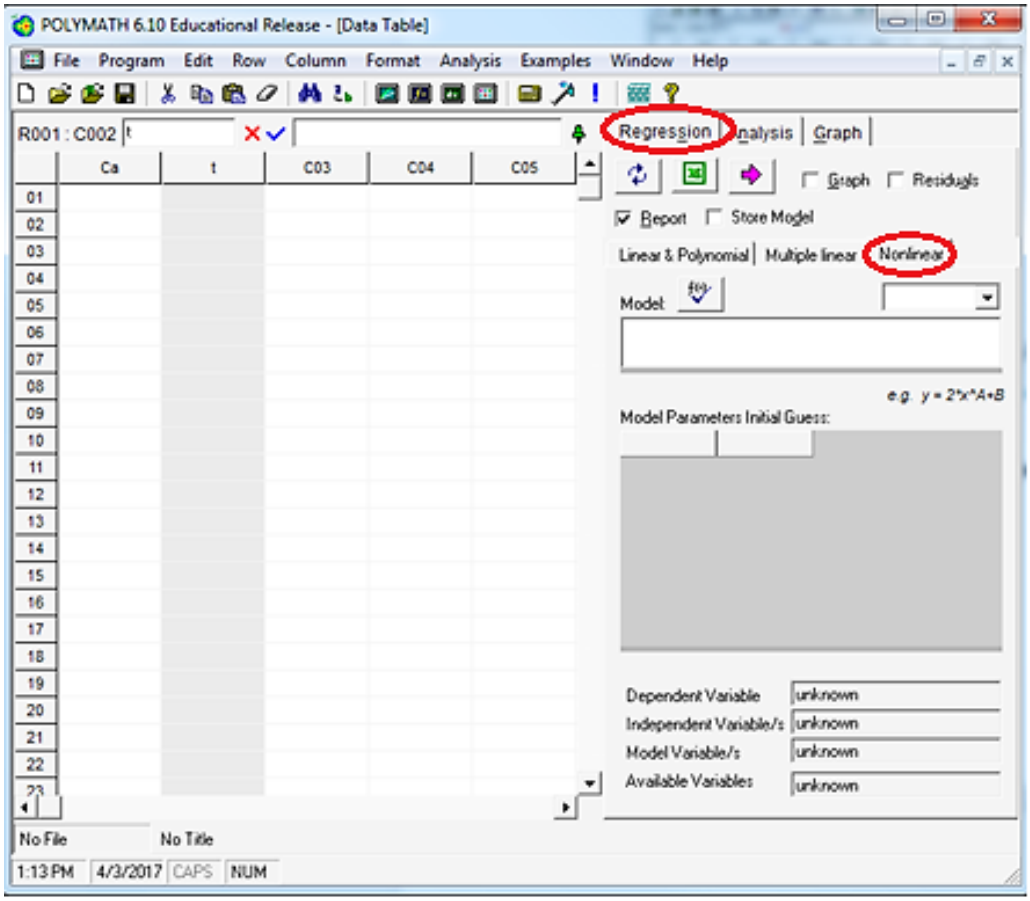
Change the column name from C01 to Ca and click Ok. You will find that 1st column name is changed to Ca



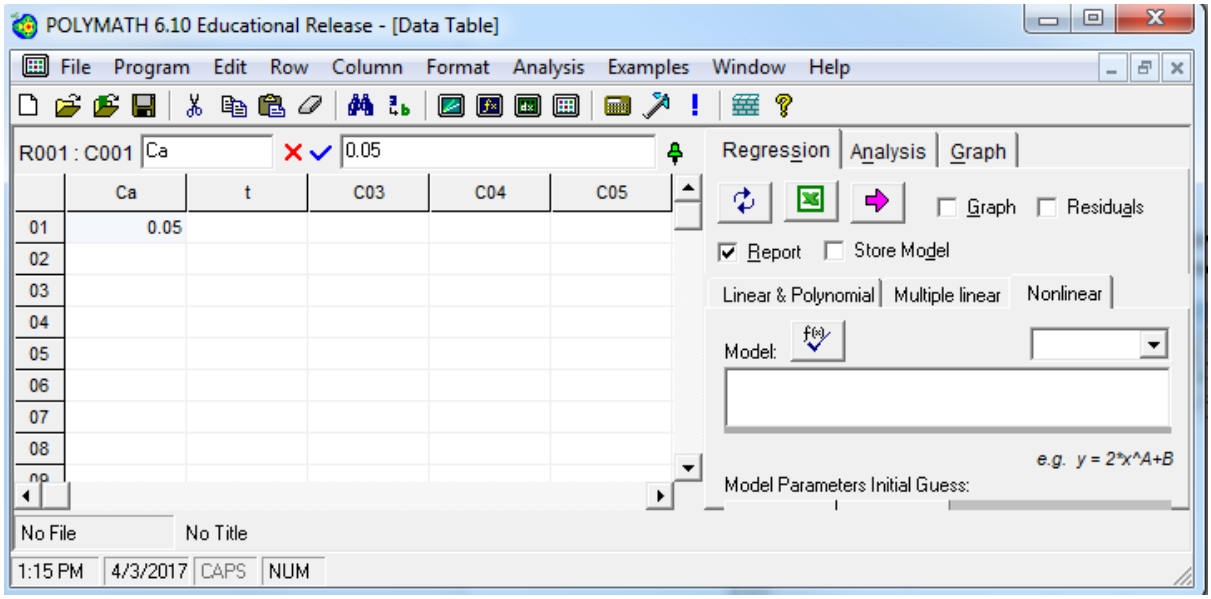
Similarly, rename C02 to t as shown below



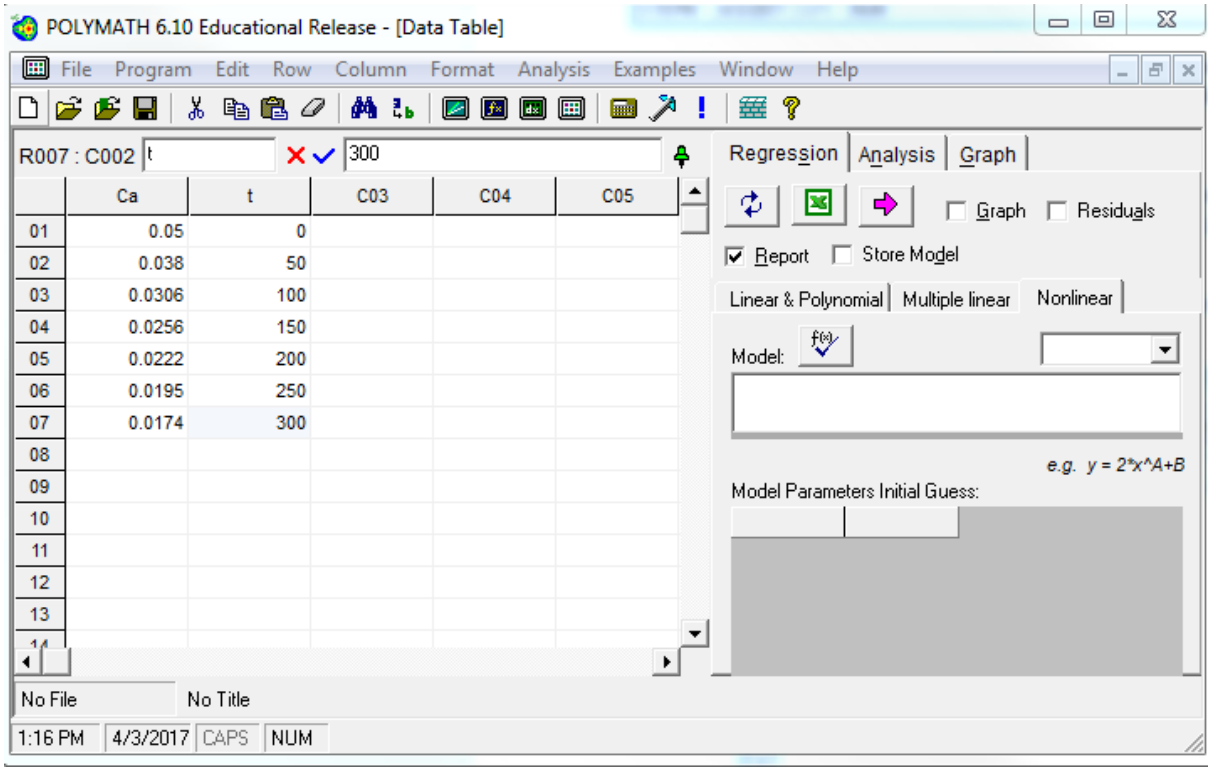
Step 4: For using nonlinear regression solver, click on the Regression tab on the right side of the window, and select the "Nonlinear" regression tab under the "Report" and "Store Model" check boxes. The window should look like this:



Step 5: To input the data for Ca, select the first cell (row 01, column Ca) and enter the first data as shown below:



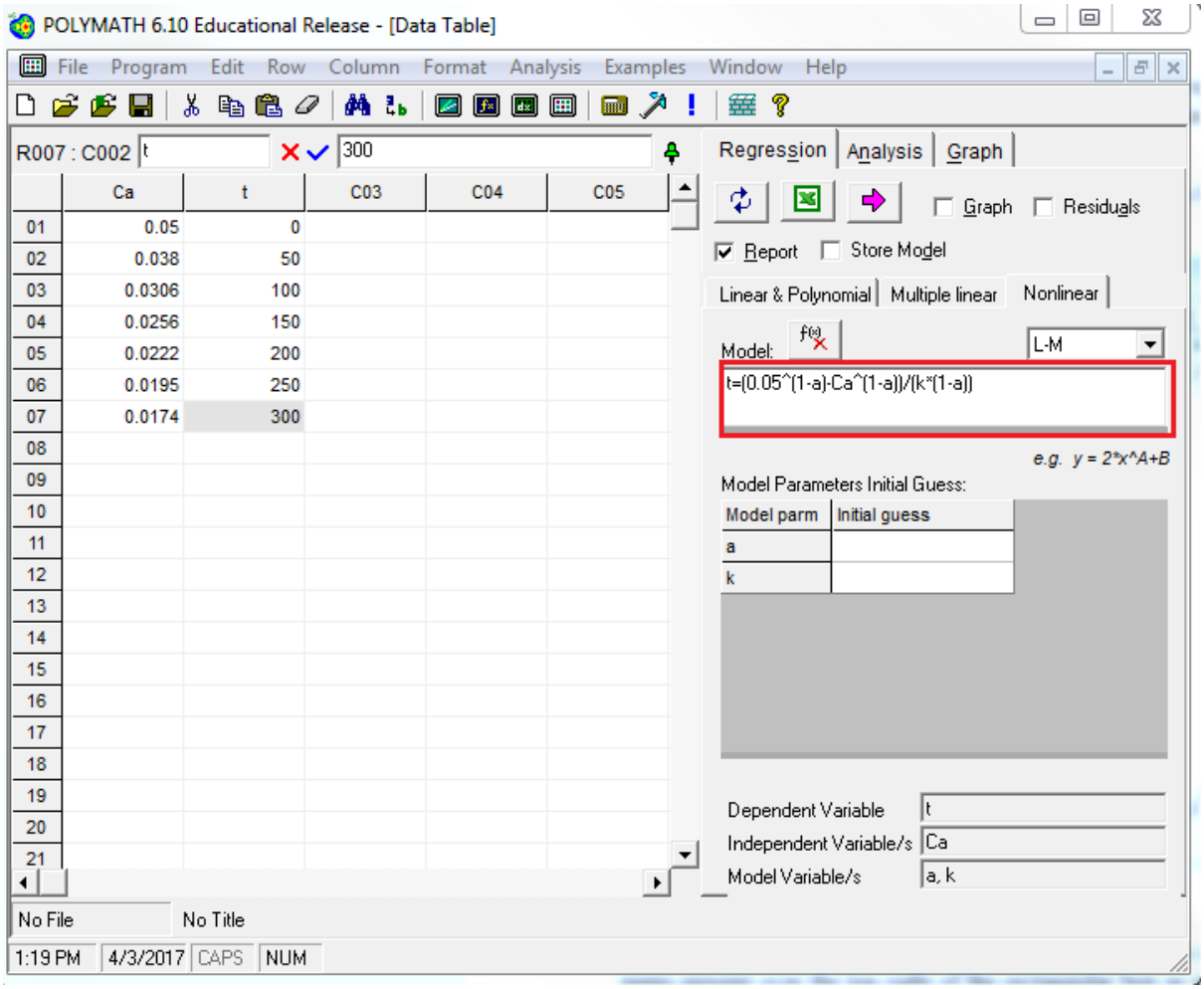
Similarly, enter the remaining data of Ca in subsequent rows. Repeat this procedure to input the data for t. After entering the data, the spreadsheet would look like this:



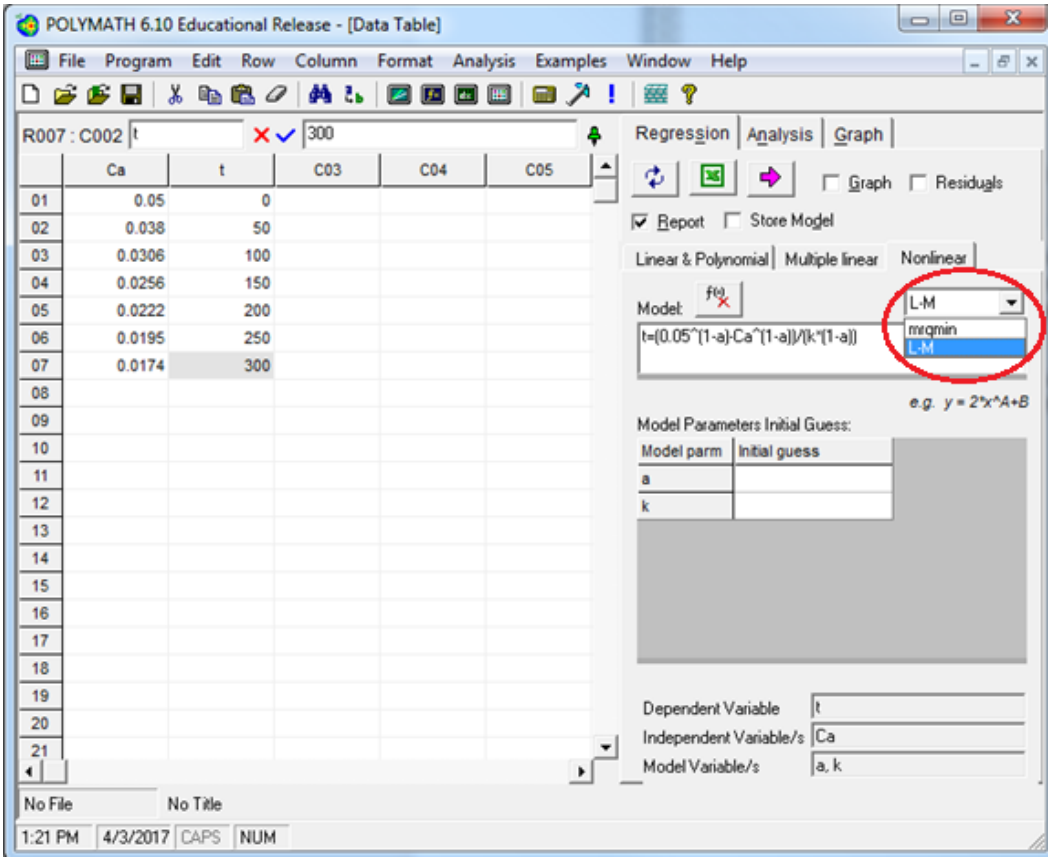
First Regression

Step 6: Now, you need to input the model form you wish your equation to match. In this case, the form is t= (0.05^(1-a)-Ca^(1-a))/(k*(1-a))), where Ca and t are columns in the data table that we are using. a and k are the model parameters which you need to fit

To input the model, place the cursor in the rectangular box below "Model:" and type the equation as shown in the below screen shot.

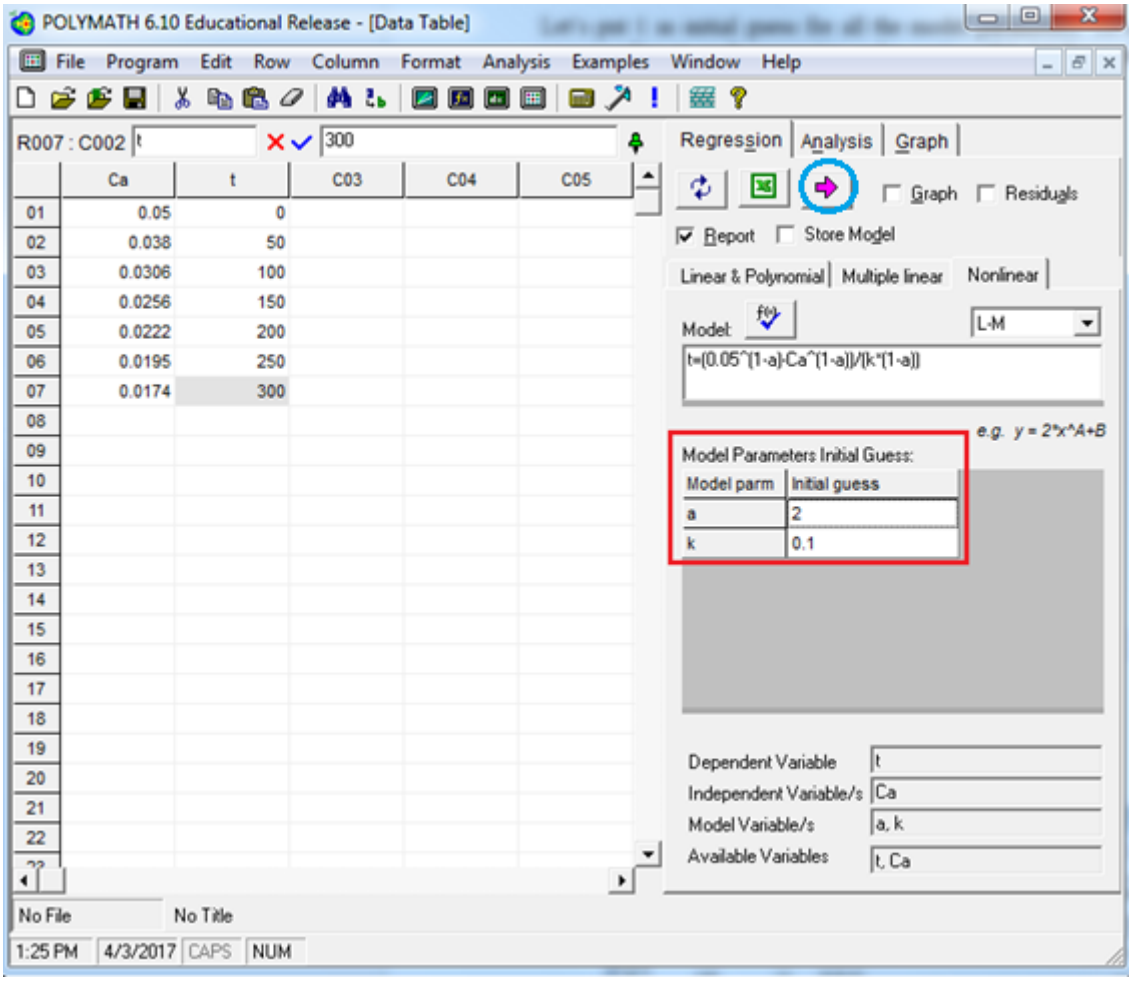


Step 7: Next we need to select an appropriate regression analysis routine. To select, click on the drop down menu present over the top right of the rectangular box as shown and select the regression method. In this case, choose "L-M" as regression method



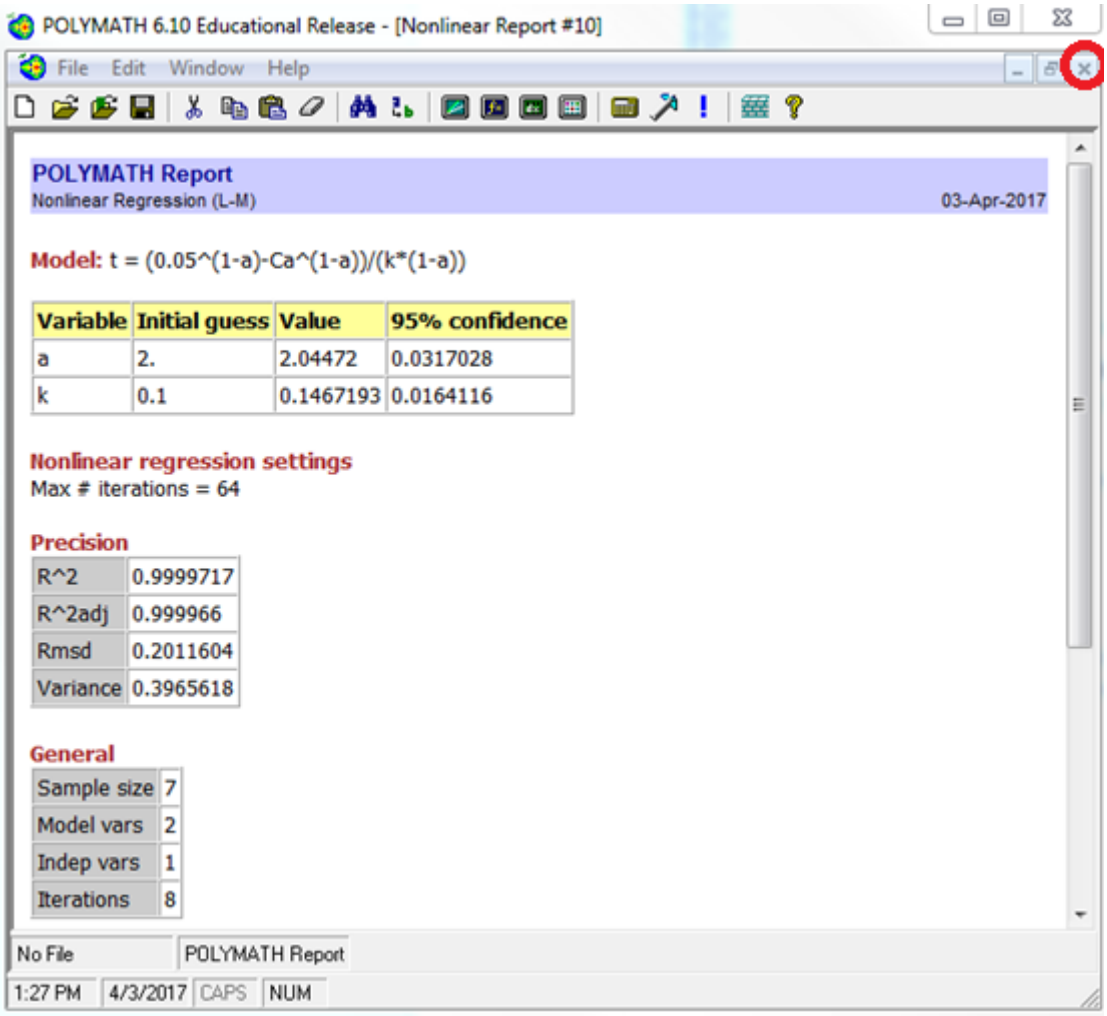
Step 8: Next, you need to provide initial guesses for the parameters in your model, in this case, a and k (Note: The solution Polymath provides may be very sensitive to the initial value guesses, so if the first regression solution is not very good, you may want to change the initial guesses and rerun the regression).

Let's put 2 as initial guess for a and 0.1 as initial guess for k. To input the initial guess, select the cell corresponding to each parameter under section "Model Parameters Initial Guess" and then enter the guess value



Now select what you want polymath to output by checking the boxes on the upper right side of the window. The options are Graph, Residuals, Report, and Store Model. Click on the pink arrow  to have Polymath perform the regression.

Step 9: If you checked the box for "Report" you will see a screen like this that details the statistics from the regression analysis. The R^2 value obtained is 0.999 which indicates a very good fit



From the above report,

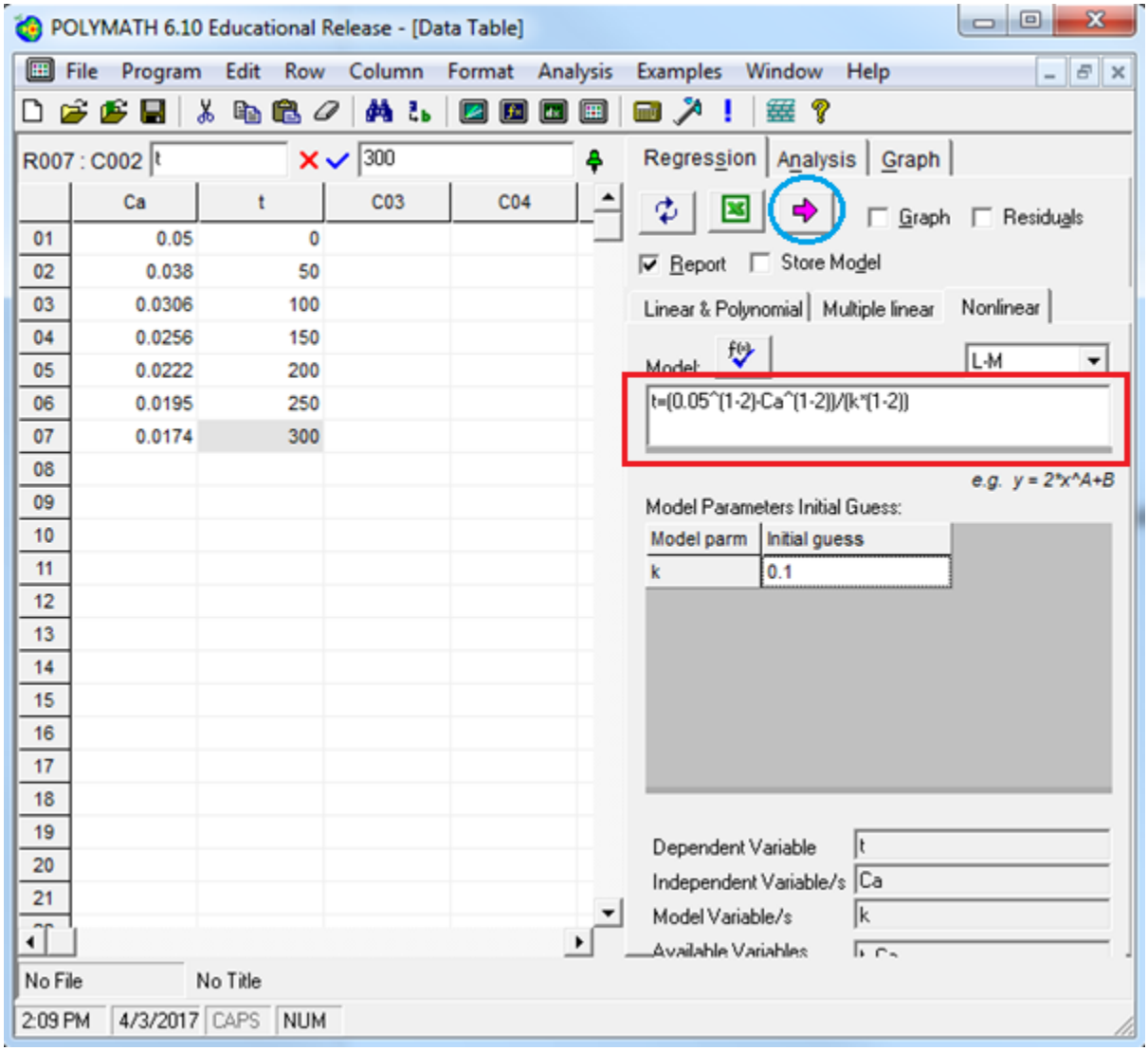
$$\alpha = 2.04$$

$$k' = 0.147$$

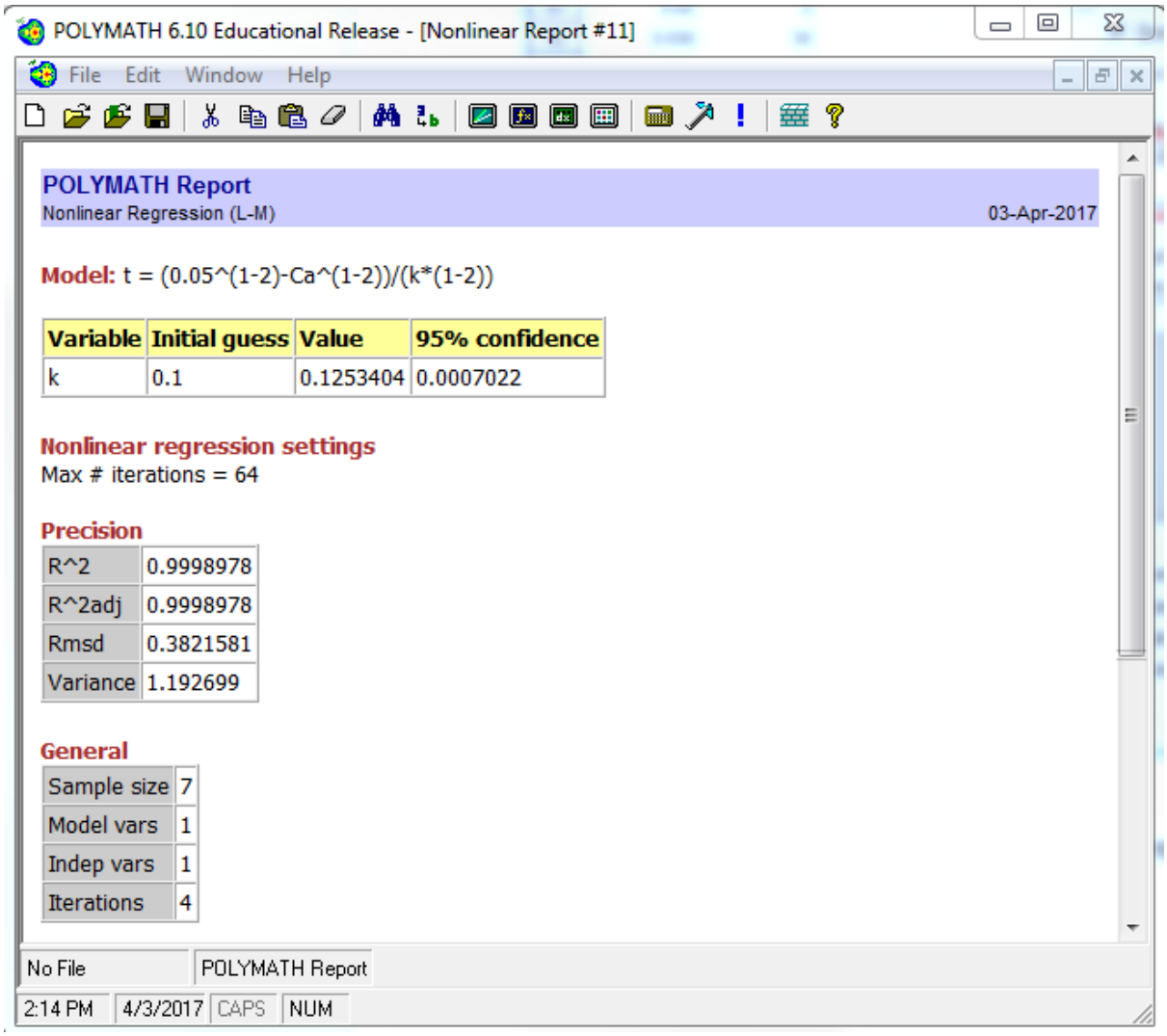
The first regression gives $\alpha = 2.04$. Round off α to the value of 2. Now, we will do second regression to find k', keeping α fixed at 2

Second Regression

Step 10: Close the report window by clicking on X button as shown in above screenshot. This will take you to **Step 8.** Now, in the model equation replace parameter "a" by 2 as shown below. You will also find that parameter a is removed from the Initial guess box. Enter the initial guess of k as 0.1



Step 11: Click on the pink arrow  to have Polymath perform the regression.



From the above report, the second regression gives

$$k' = 0.125$$