

Non-linear regression tutorial

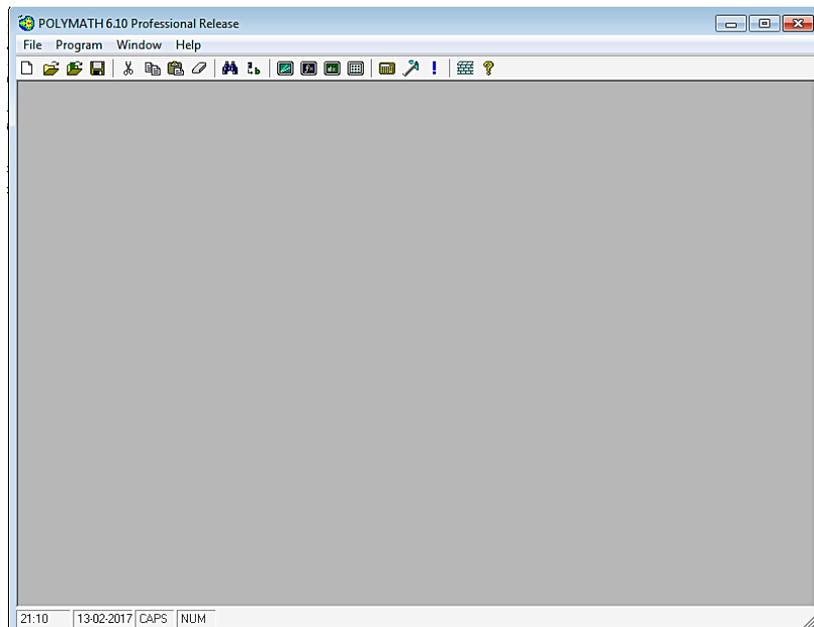
The following table shows the raw data for performing nonlinear regression using Polymath (refer Table E7-4.1, Elements of chemical reaction engineering, 5th edition)

Pco	Ph2	Rate
1.0	1.0	5.2E-03
1.8	1.0	13.2E-03
4.08	1.0	30.0E-03
1.0	0.1	4.95E-03
1.0	0.5	7.42E-03
1.0	4.0	5.25E-03

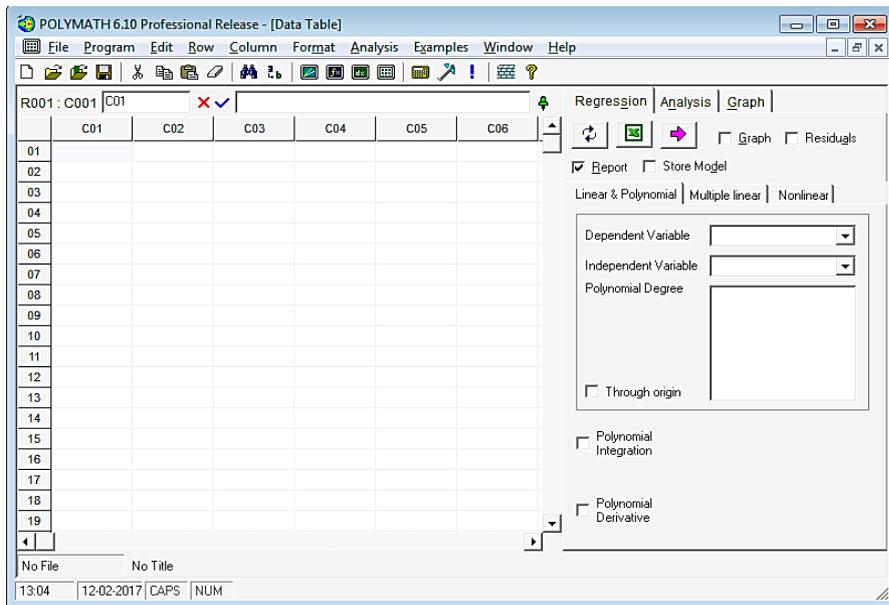
The nonlinear equation is given by

$$\text{Rate} = \frac{a P_{CO} P_{H_2}^{\text{Beta}1}}{1 + b P_{H_2}^{\text{Beta}2}}$$

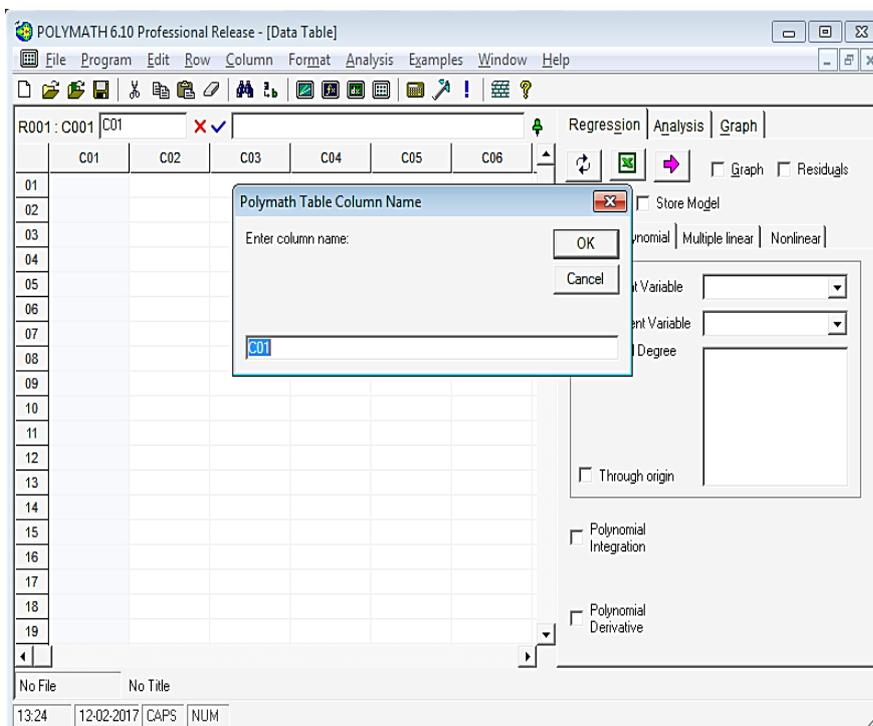
To do the nonlinear regression of the above data, first open Polymath. Your window would appear like this



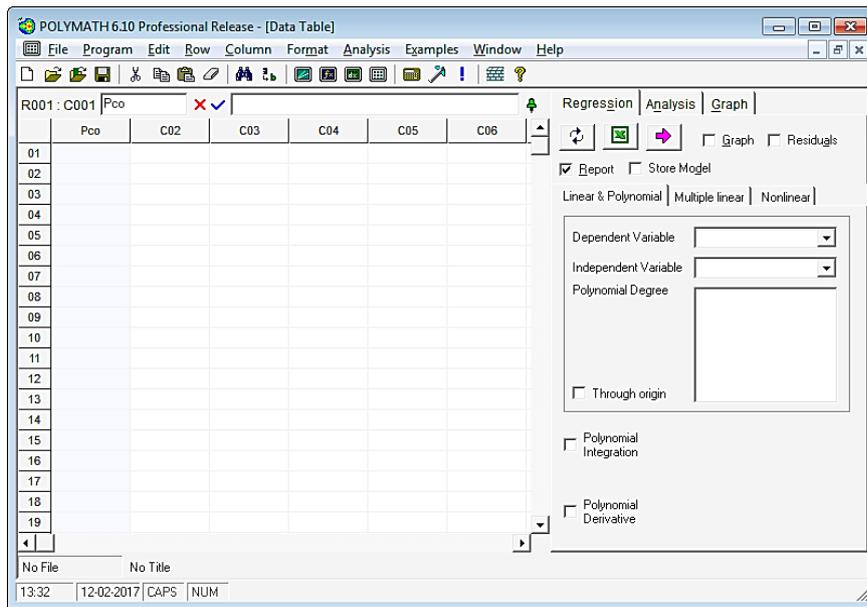
Now, click on the Regression button on the toolbar (). The following window will appear



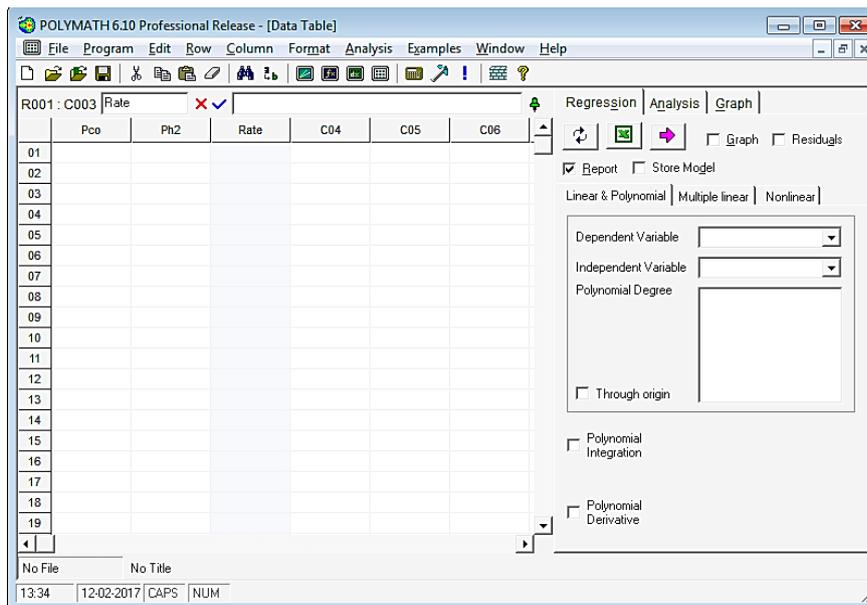
Before inserting the data into the spreadsheet, it is recommended to change the column name with the name of the variable mentioned in the data table. This would make it easy to comprehend the polymath output. To change the column name of C01, double click on the column name “C01” or right click on C01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



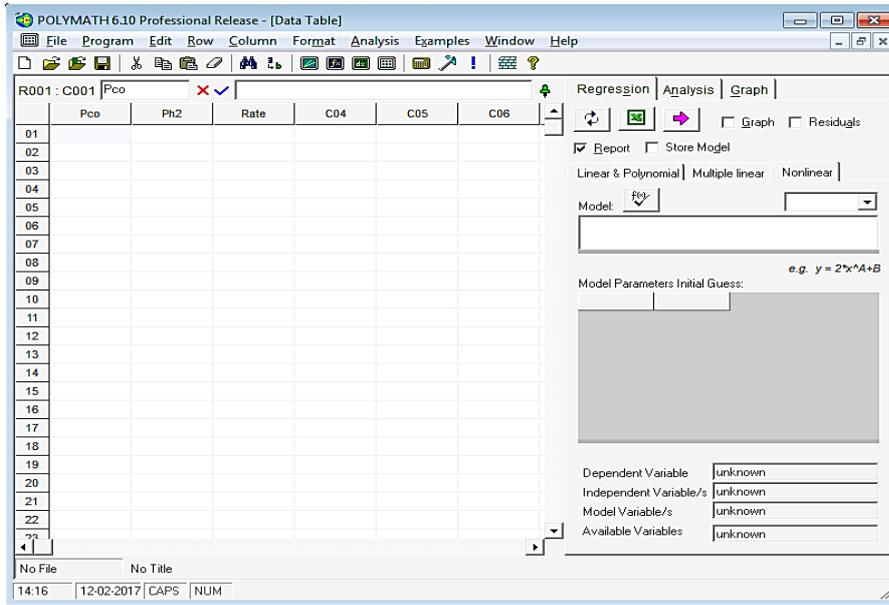
Change the column name from C01 to Pco and press Ok. You will find that column name is changed to Pco



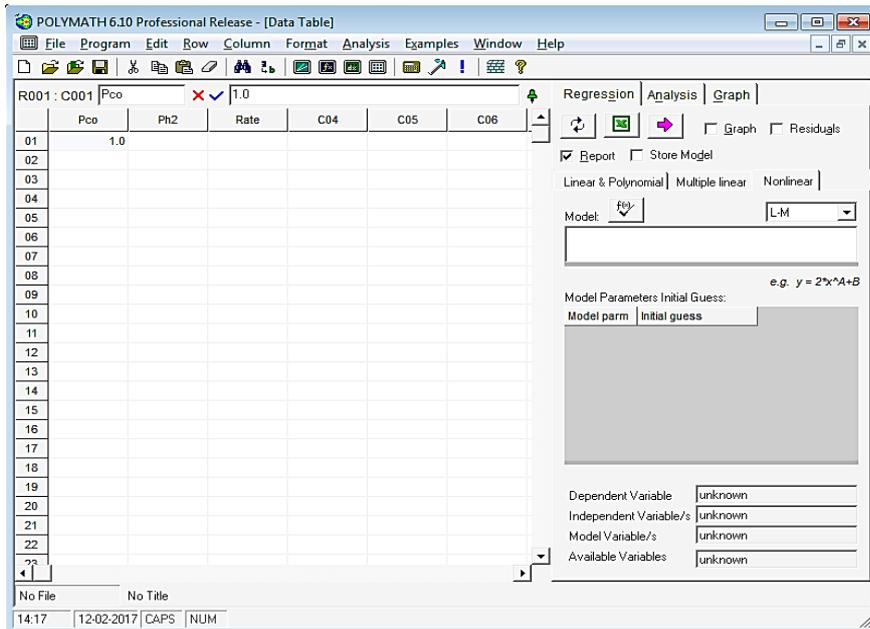
Similarly, rename C02 to Ph2 and C03 to Rate as shown below



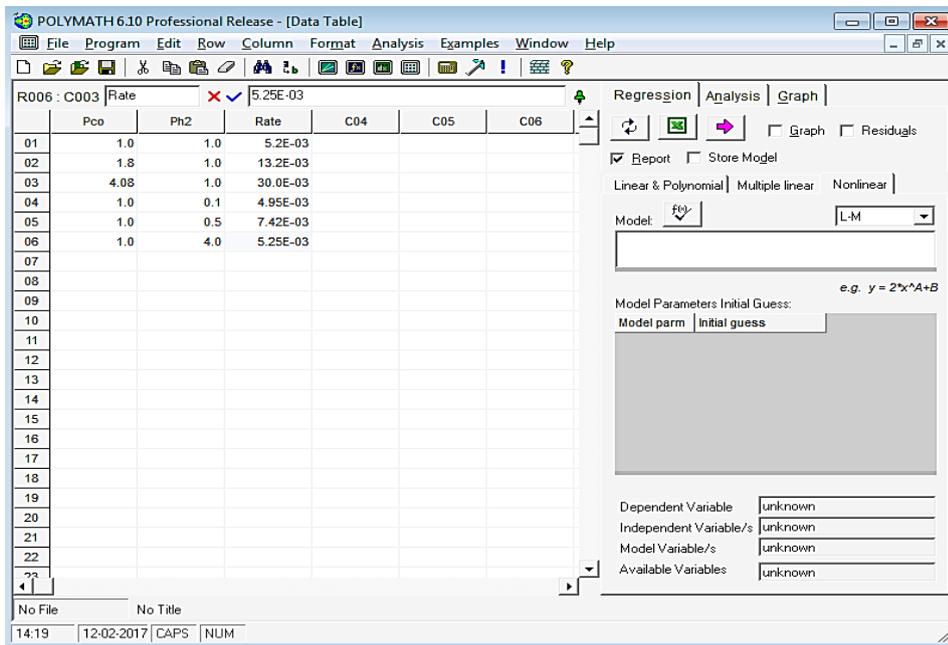
For nonlinear regression, click on the Regression tab on the right side of the window, and select the "Nonlinear" regression tab under the "Report" and "Store Model" check boxes. The window should look like this:



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

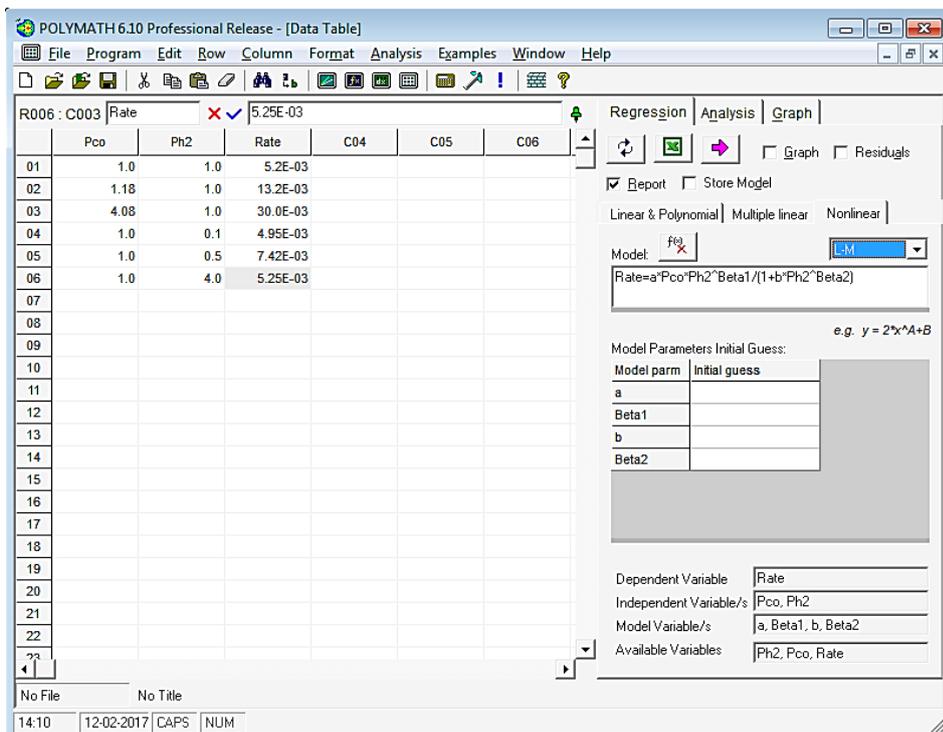


Similarly, enter the remaining data of Pco in subsequent rows. Repeat this procedure to input the data for Ph2 and Rate. After entering the data, the spreadsheet would look like this:

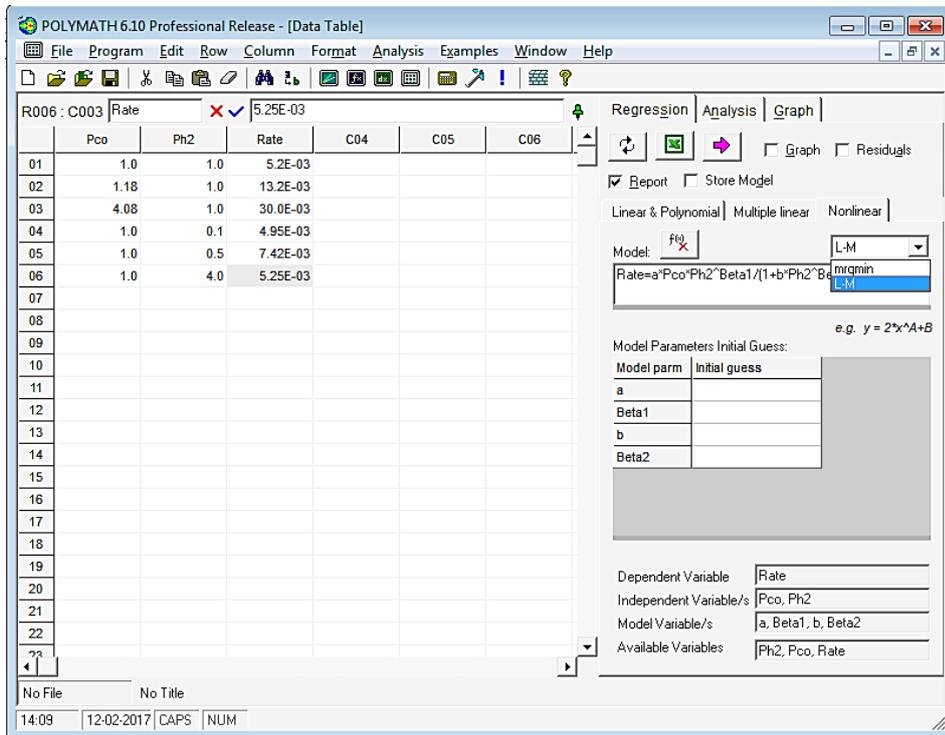


Now, you need to input the model form you wish your equation to match. In this case, the form is $\text{Rate} = a \cdot \text{Pco} \cdot \text{Ph2}^{\text{Beta1}} / (1 + b \cdot \text{Ph2}^{\text{Beta2}})$, where Pco, Ph2 and rate are columns in the data table that we are using.

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

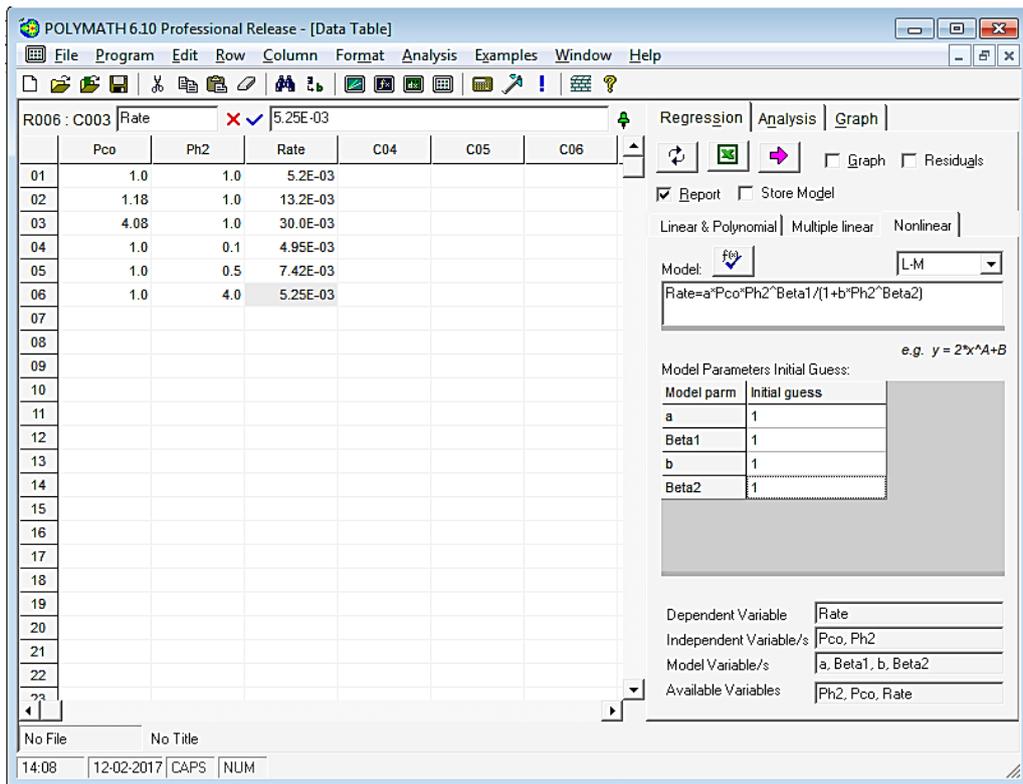


Next we need to select an appropriate regression analysis routine. To select, click on the drop down menu present over the top right of the rectangular box as shown and select the regression method. In this case, we have chosen "L-M".



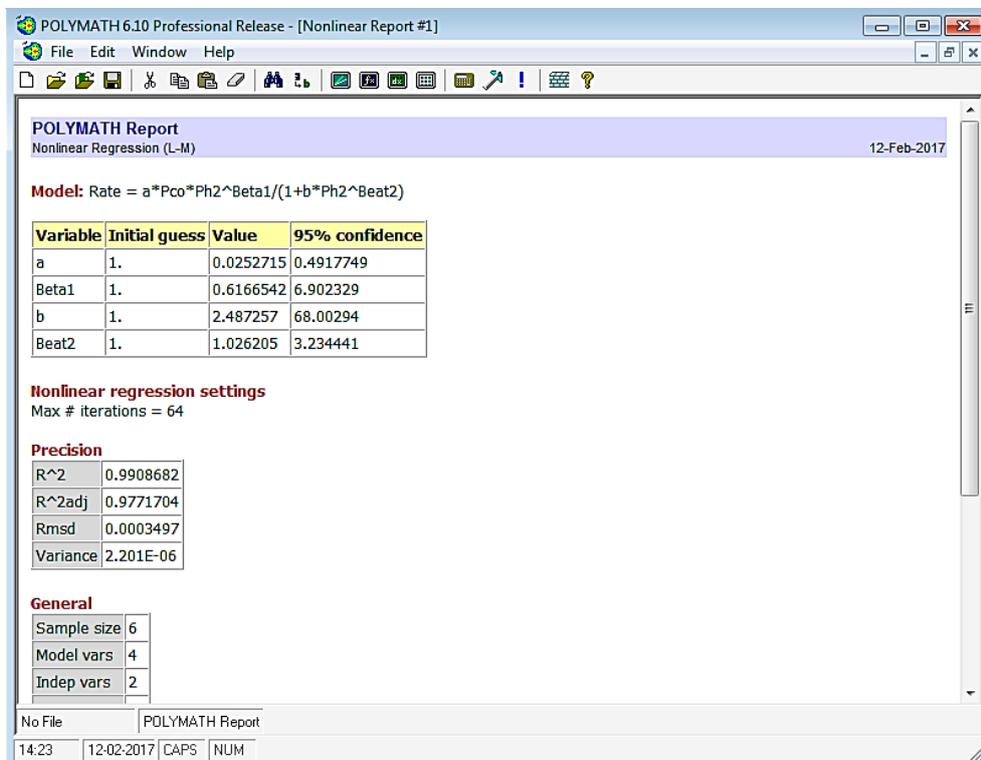
Next, you need to provide initial guesses for the parameters in your model, in this case, a, b, Beta1 and Beta2. (Note: The solution Polymath provides may be very sensitive to the initial value guesses, so if the first regression solution is not very good, you may want to change the initial guesses and rerun the regression).

Let's put 1 as initial guess for all the model parameters. To input the initial guess, select the cell corresponding to each parameter under section "Model Parameters Initial Guess" and then enter the guess value

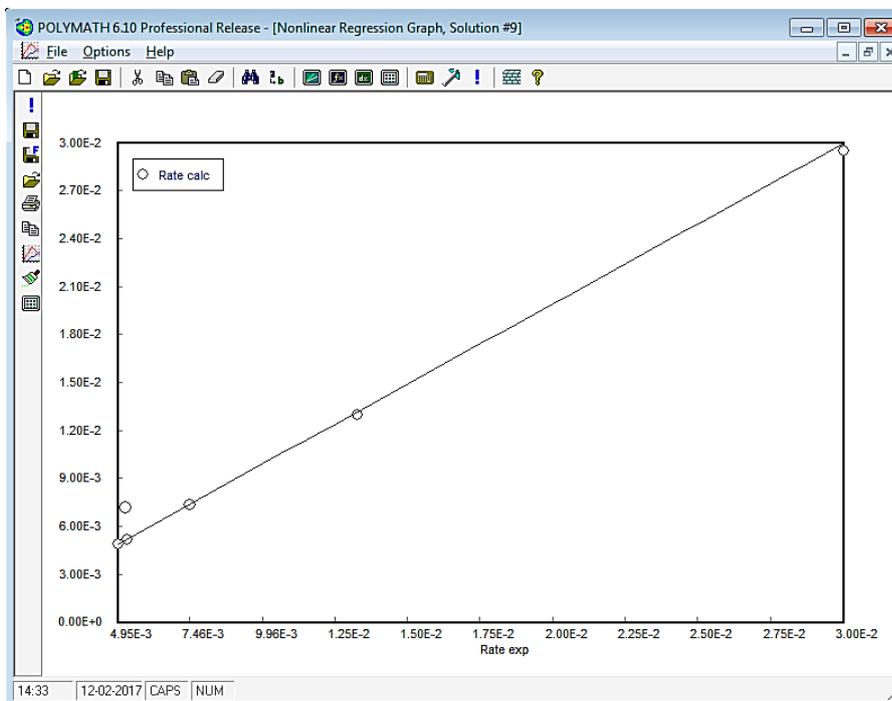
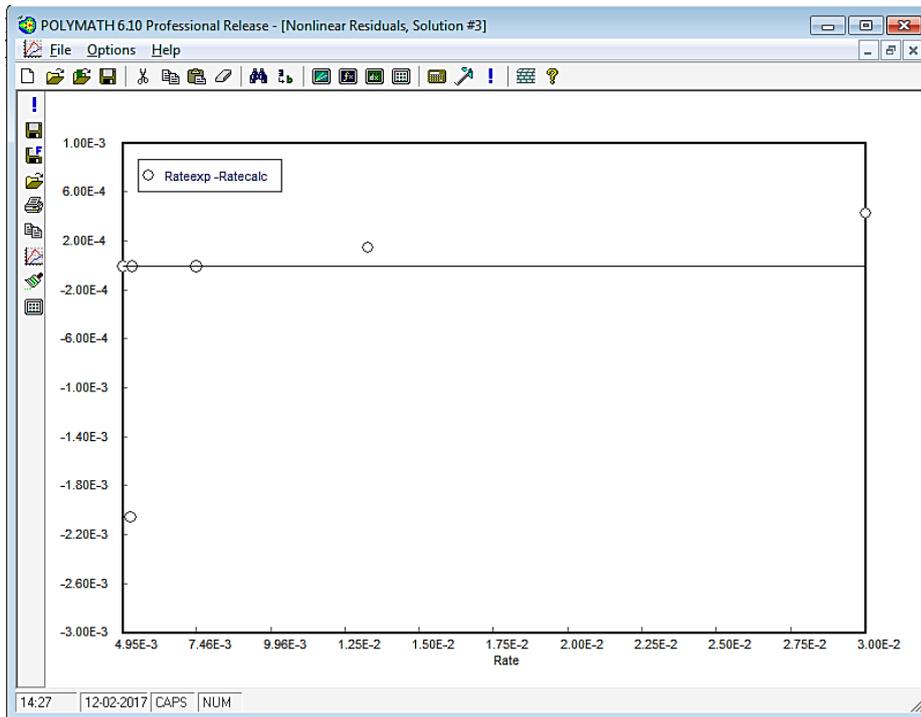


Now select what you want polymath to output by checking the boxes on the right side of the window. The options are Graph, Residuals, Report, and Store Model. Click on the pink arrow  to have Polymath perform the regression.

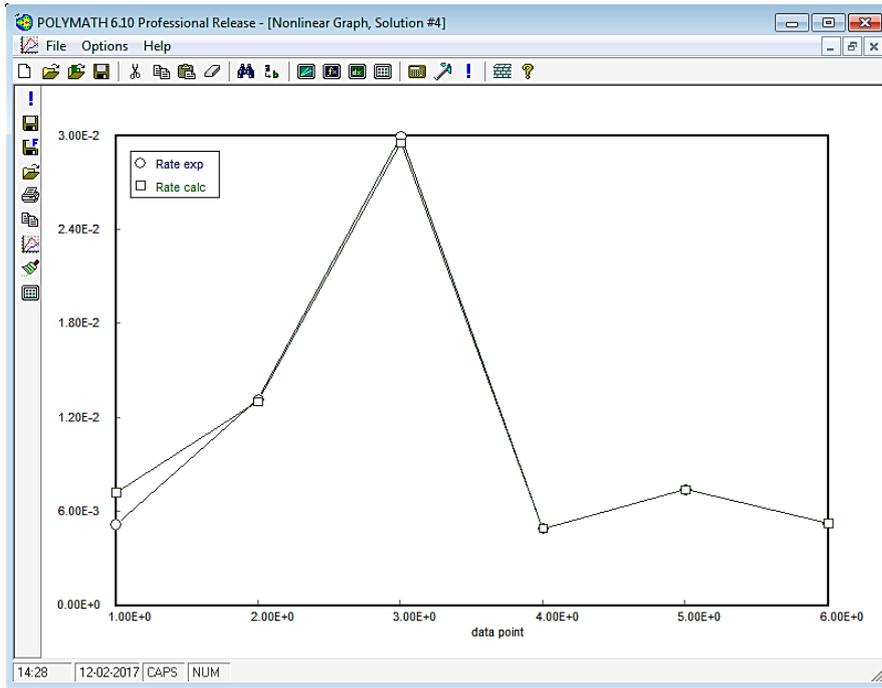
If you selected "Report" you will see a screen like this that details the results from the regression analysis.



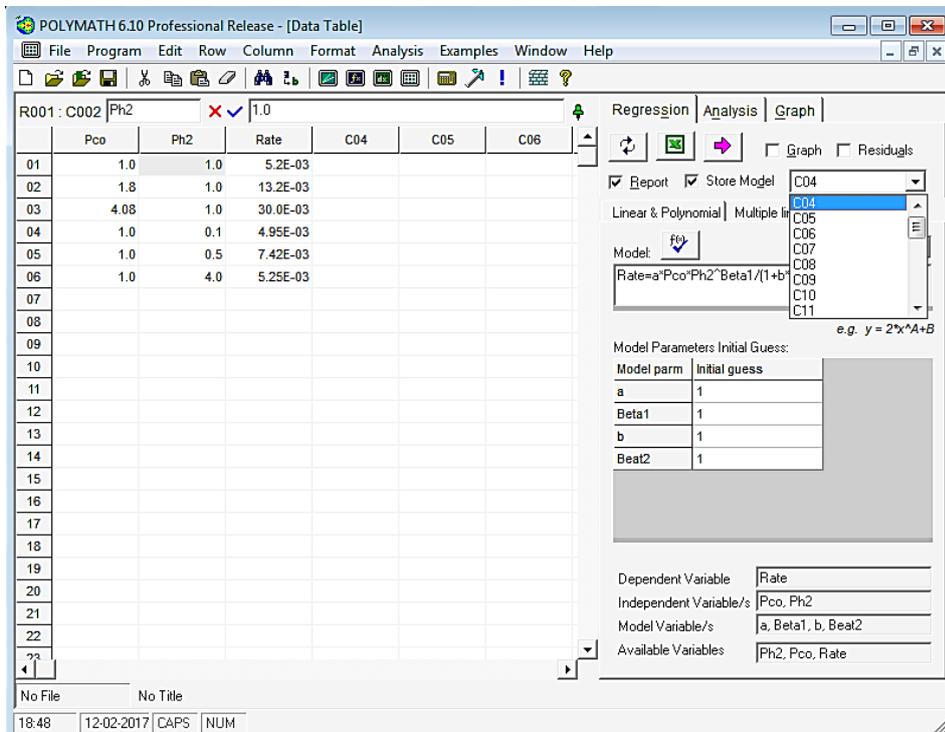
If you selected residuals, then you will get two plots: one with difference of experimental and model values plotted against experimental value and another as an X-Y graph between experimental and model values



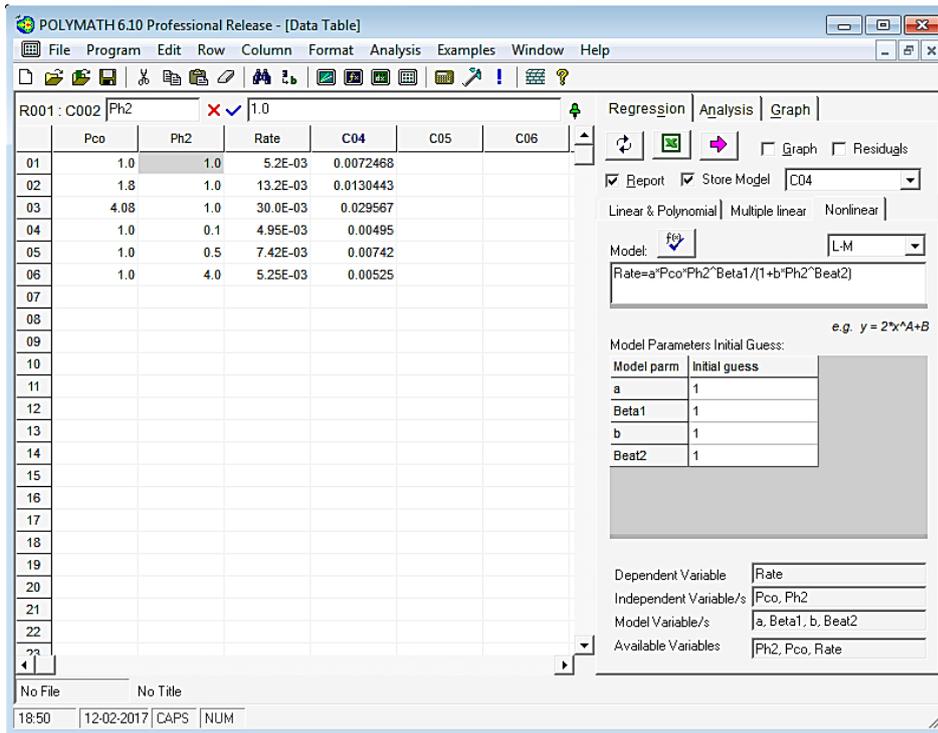
If you selected Graph, then a graph of the experimental and calculated data sets are graphed together for comparison.



If you checked the box "Store Model", your model value will be stored in the selected column. To select the column no, click on the dropdown menu present on the right side of Store Model box and select the column name where you want to store the model values. In this case, we have chosen C04



Now click on the Pink arrow to run the program. You will see that model value is stored in the column C04.



You can also export your polymath output to excel by clicking on the excel button . For this, you need to have excel workbook open prior to selecting this option. The excel spreadsheet would look like this after polymath export the data.

