

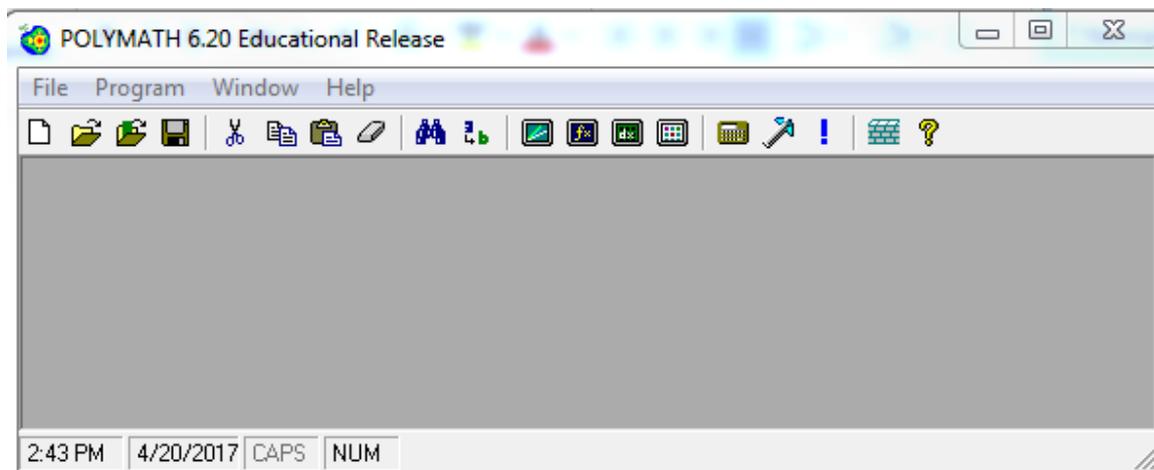
## Polymath Tutorial for estimating the Yield Coefficients and Rate-law parameters (Example 9-4)

### a) Estimating Yield Coefficients

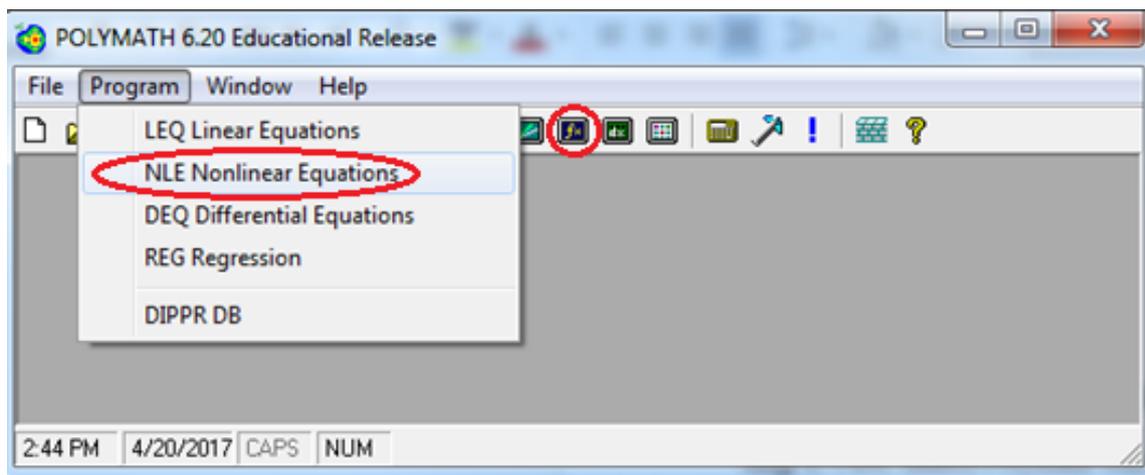
To estimate yield coefficients, we will use Polymath nonlinear equation solver.

**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>

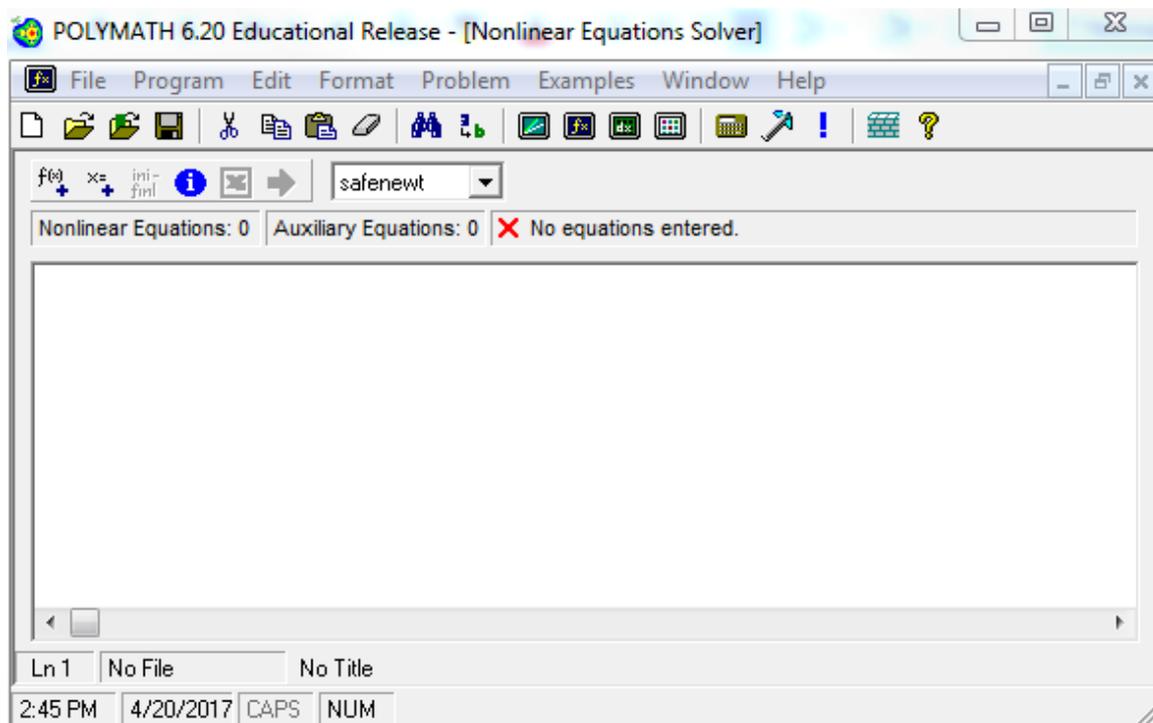
When you open Polymath, following window would appear



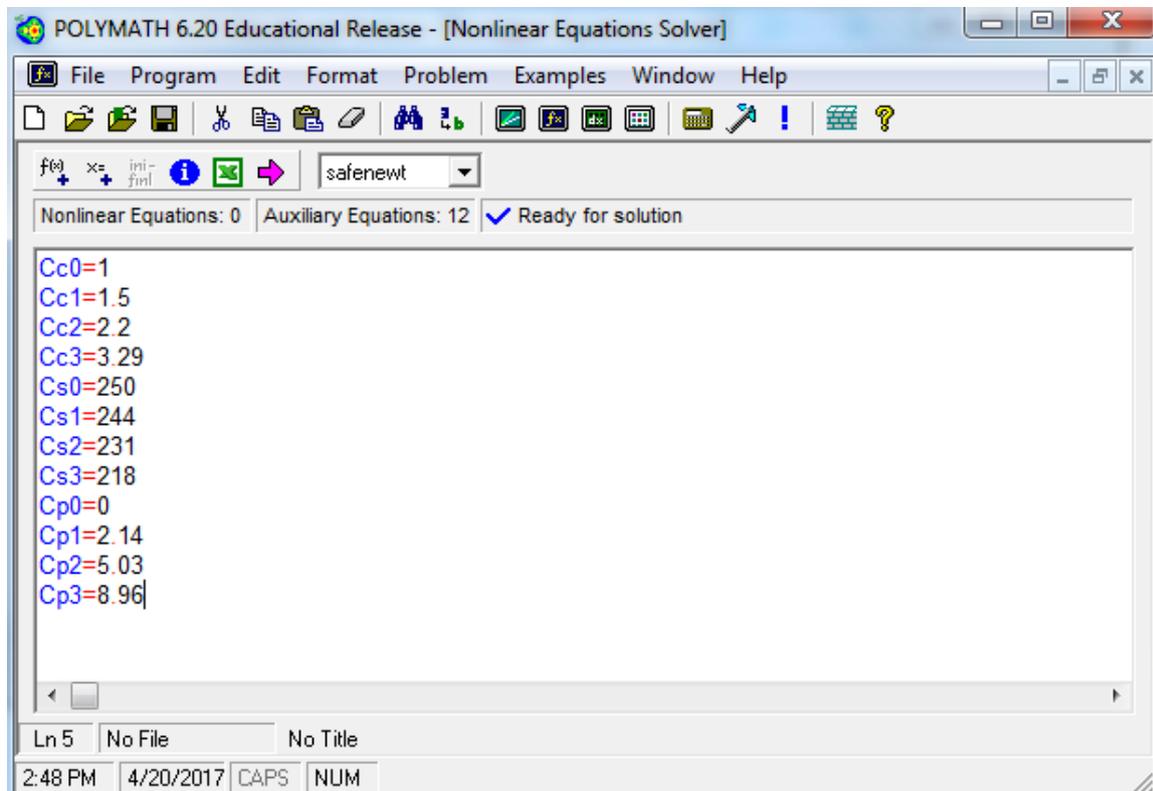
**Step 2:** Click on the “Program” tab present on the toolbar. This will bring up a list of options from which you need to select. In this case we need to find slope of line which can be done using nonlinear equations solver. Select "NLE Nonlinear Equations". The shortcut button “ $fx$ ” for nonlinear equation solver is also present on the menu bar (  ) as shown by red circle in below screenshot



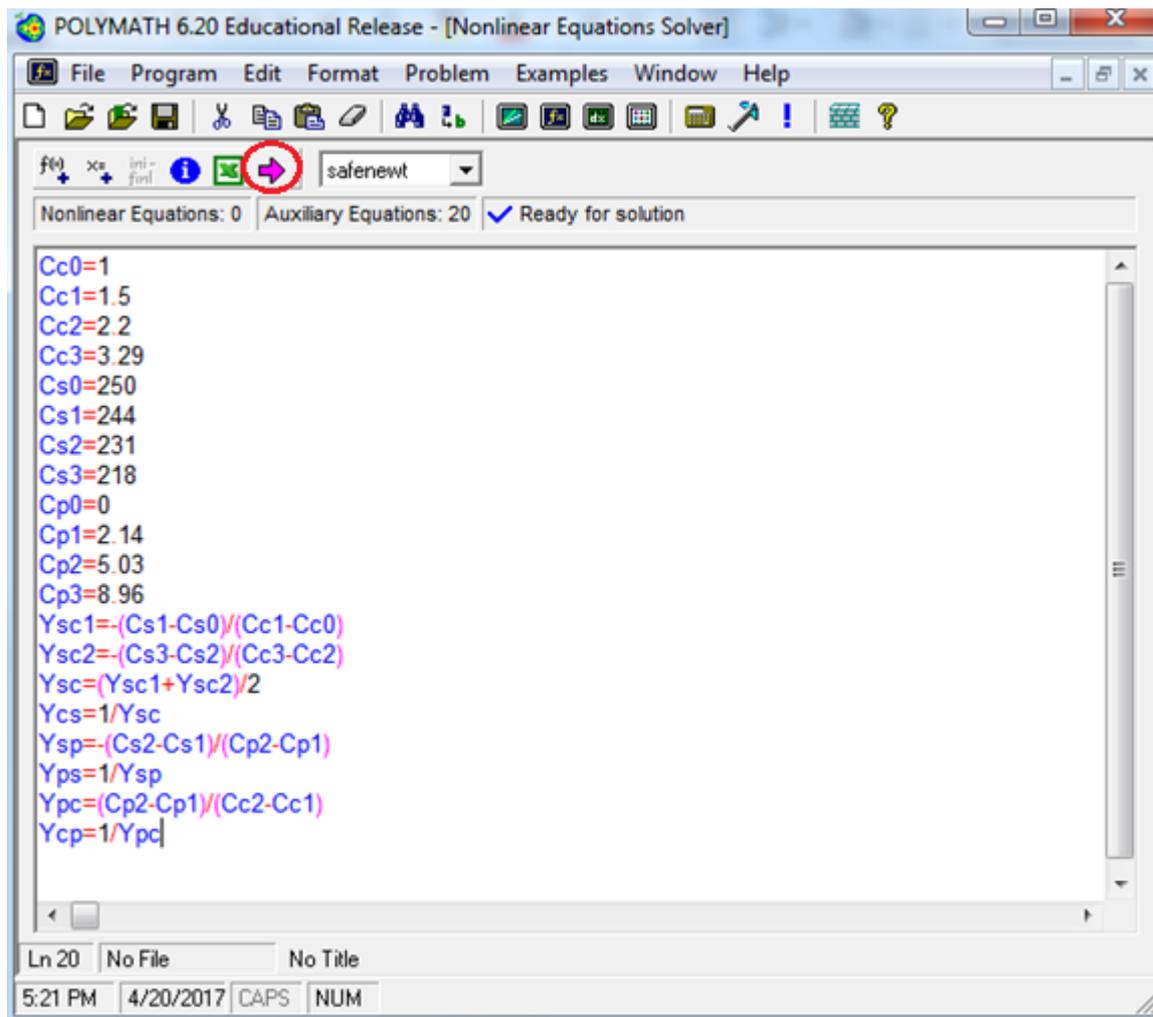
This will open up another window, which looks like this.



**Step 3:** Enter the values of Cc, Cs, and Cp at different times as shown below

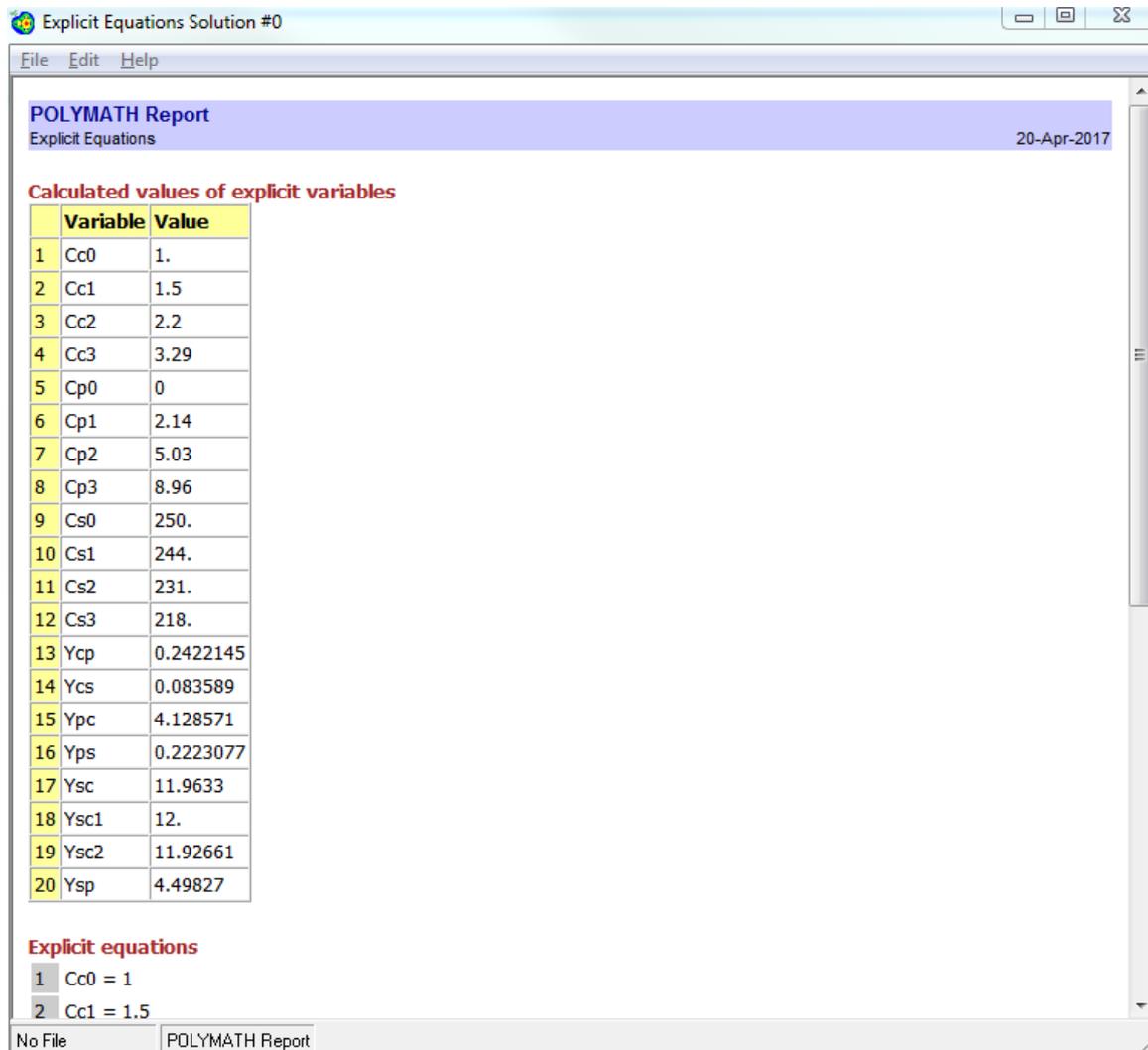


**Step 4:** Next, enter all the equations for yield coefficients as per given in the textbook



Now you have entered all your data and equations in the Polymath.

**Step 5:** Click the pink arrow  to run the file. You should get a report window that looks like this. In the report, you can find the value of all the yield coefficients along with the equations which you entered



The screenshot shows a window titled "Explicit Equations Solution #0" with a menu bar (File, Edit, Help). The main content is a "POLYMATH Report" for "Explicit Equations" dated "20-Apr-2017".

**Calculated values of explicit variables**

	Variable	Value
1	Cc0	1.
2	Cc1	1.5
3	Cc2	2.2
4	Cc3	3.29
5	Cp0	0
6	Cp1	2.14
7	Cp2	5.03
8	Cp3	8.96
9	Cs0	250.
10	Cs1	244.
11	Cs2	231.
12	Cs3	218.
13	Ycp	0.2422145
14	Ycs	0.083589
15	Ypc	4.128571
16	Yps	0.2223077
17	Ysc	11.9633
18	Ysc1	12.
19	Ysc2	11.92661
20	Ysp	4.49827

**Explicit equations**

- Cc0 = 1
- Cc1 = 1.5

The status bar at the bottom shows "No File" and "POLYMATH Report".

From the above report,

$$Y_{s/c} = 11.96 \text{ g/g}, Y_{c/s} = 0.084 \text{ g/g}$$

$$Y_{s/p} = 4.5 \text{ g/g}, Y_{p/s} = 0.22 \text{ g/g}$$

$$Y_{p/c} = 4.13 \text{ g/g}, Y_{c/p} = 0.242 \text{ g/g}$$

For more step-by-step tutorial on Polymath Nonlinear equation Solver, refer to tutorial [http://umich.edu/~elements/5e/software/Non\\_linear\\_equation\\_tutorial.pdf](http://umich.edu/~elements/5e/software/Non_linear_equation_tutorial.pdf)

## b) Determination of Rate- law parameters

The rate law equation is given by

$$\frac{C_c C_s}{r_g} = \frac{K_s}{\mu_{max}} + \frac{C_s}{\mu_{max}}$$

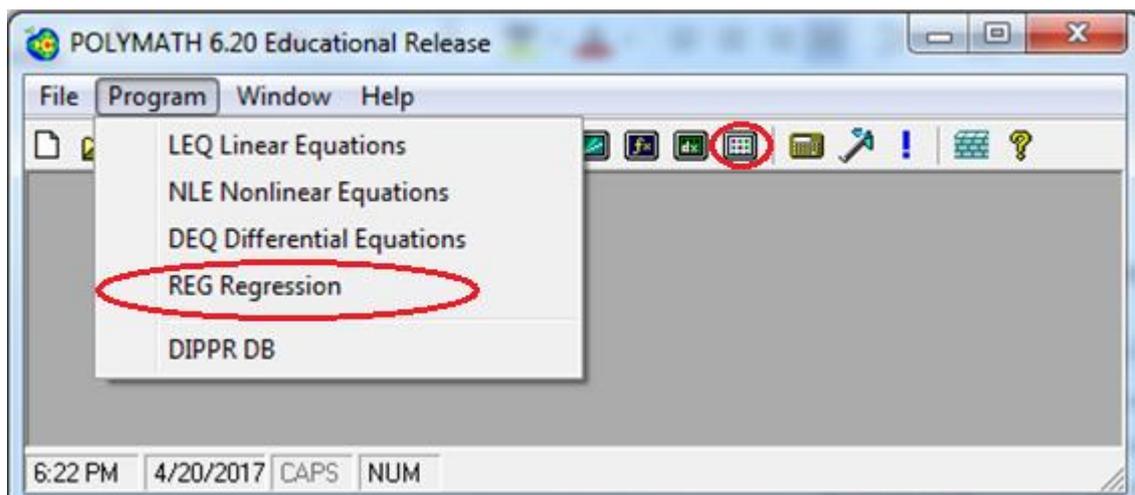
Where,  $K_s$  and  $\mu_{max}$  are model parameters

The data for  $\frac{C_c C_s}{r_g}$  and  $C_s$  are given below

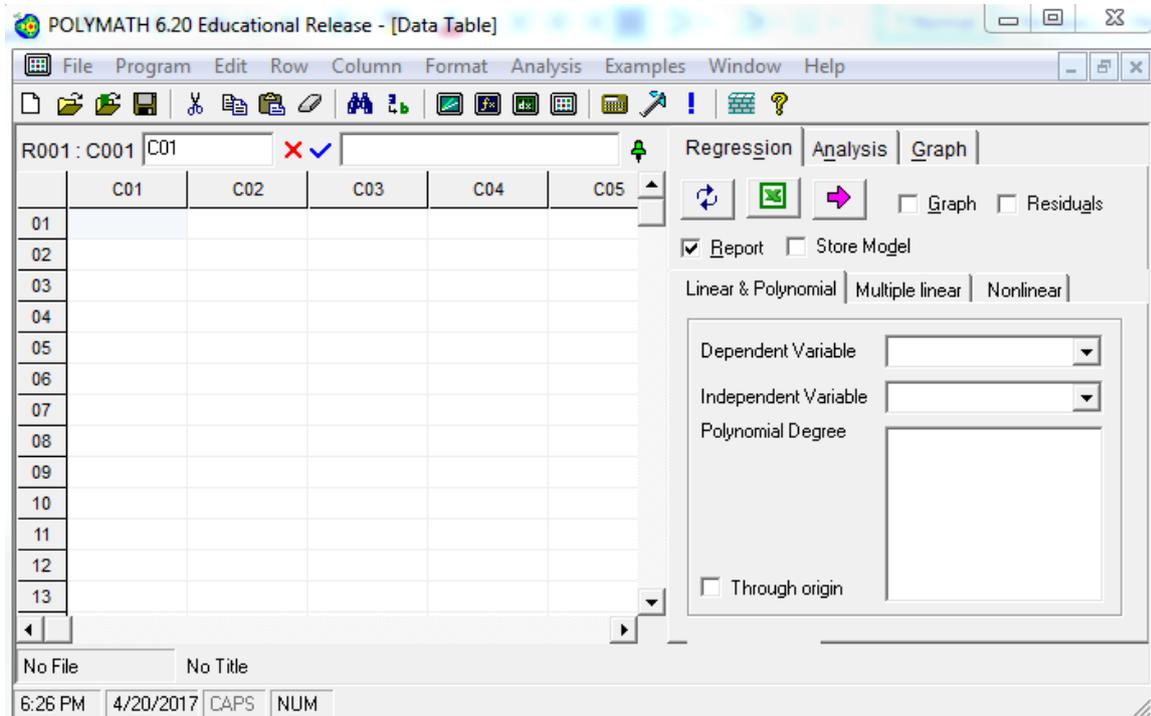
$t$	0	1	2	3
$C_c C_s / r_g$	625	610	567.8	558.1
$C_s$	250	244	231	218

We will use Polymath nonlinear regression solver to determine the model parameters

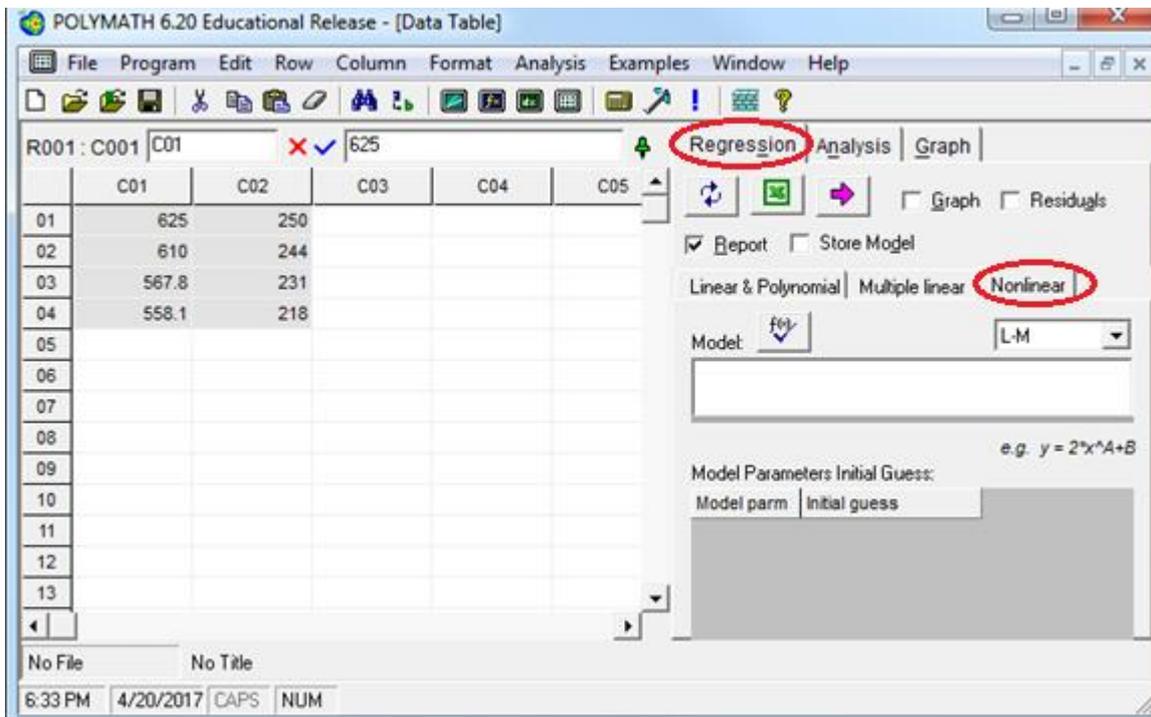
**Step 1:** Open Polymath and click on the “Program” tab present on the toolbar. Select "REG Regression". The shortcut button for nonlinear regression solver is also present on the menu bar as shown by red circle in below screenshot



This will open up a spreadsheet which looks like this:

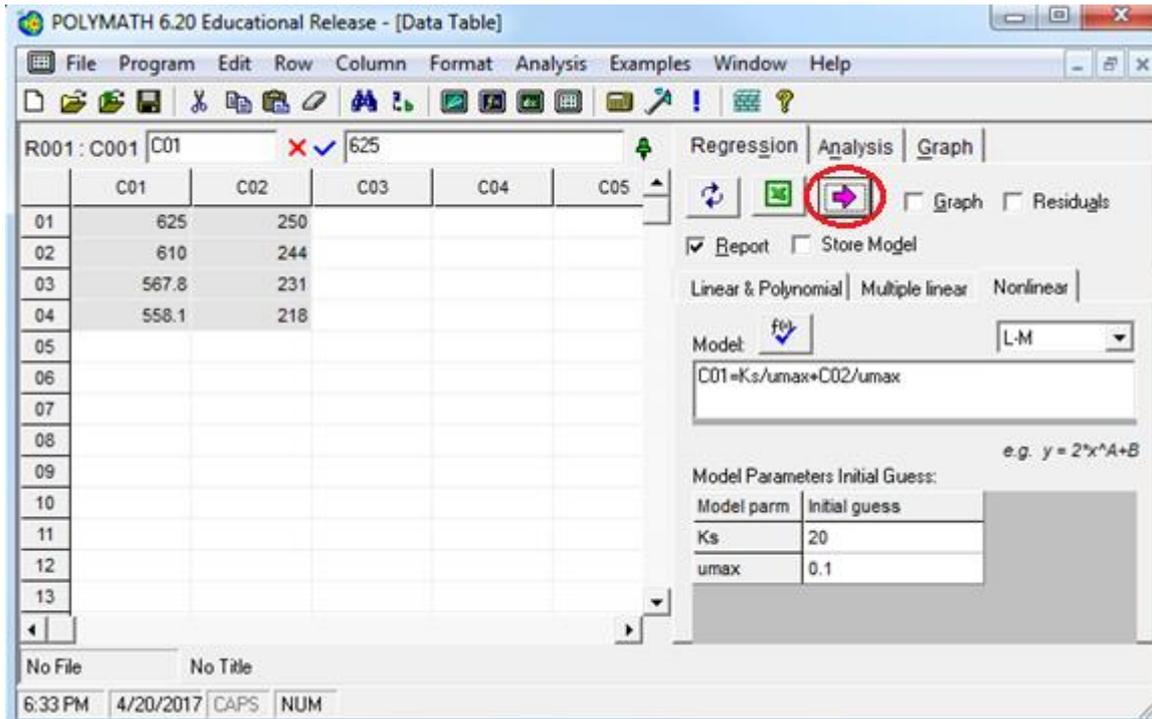


**Step 2:** Now enter the data for  $C_c C_s / r_g$  and  $C_s$  in Column C01 and C02 respectively as shown below. For nonlinear regression, click on the Regression tab on the right side of the window, and select the "Nonlinear" regression tab under the "Report" and "Store Model" check boxes.



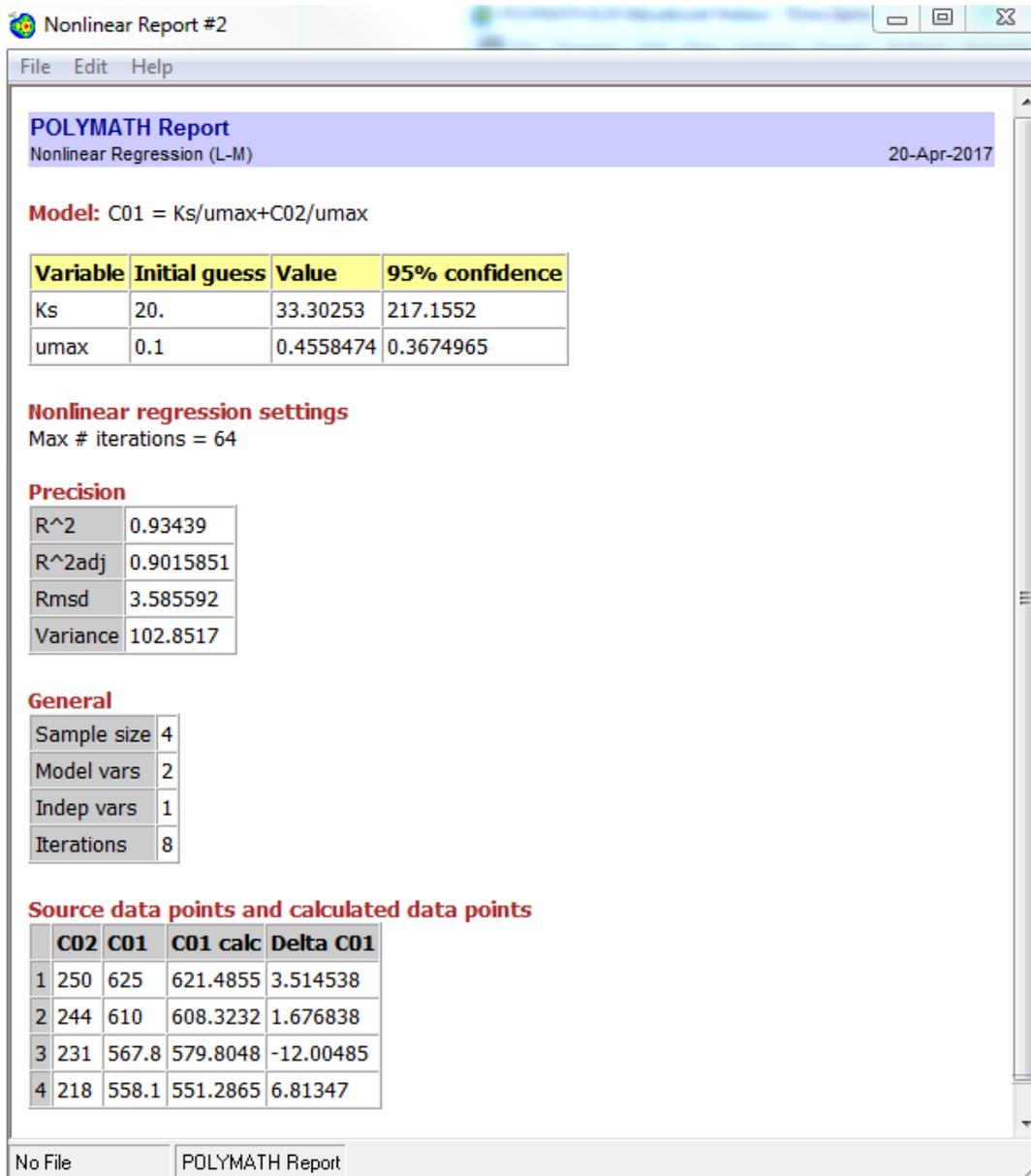
**Step 3:** Now, you need to input the model form you wish your equation to match. In this case, the form is  $C01 = K_s / u_{max} + C02 / u_{max}$ , where  $C01$  represents  $C_c C_s / r_g$  and  $C02$  represents  $C_s$ . To input the model, place the cursor in the rectangular box below “Model:” and type the equation as shown in the below screen shot.

Next, you also need to provide initial guesses for the parameters in your model, in this case,  $K_s$  and  $u_{max}$ . Let’s put 20 and 0.1 as initial guess for  $K_s$  and  $u_{max}$  respectively. 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.

**Step 4:** If you selected "Report" you will see a screen like this that details the results from the regression analysis.



From the above report,  $R^2 = 0.93$  which shows model fits well to the data.

The model parameters are

$$K_s = 33.3$$

$$\mu_{max} = 0.46$$

For more step-by-step tutorial on Polymath Nonlinear regression Solver, refer to nonlinear regression tutorial at <http://umich.edu/~elements/5e/software/polymath.html>