Polymath tutorial on non-linear regression (Example 10-3)

The following table shows the raw data for performing nonlinear regression using Polymath (refer Table E10-3.1, Elements of chemical reaction engineering, 5th edition)

PE	РЕА	Рн	Rate
1	1	1	1.04
1	1	3	3.13
1	1	5	5.21
3	1	3	3.82
5	1	3	4.19
0.5	1	3	2.391
0.5	0.5	5	3.867
0.5	3	3	2.199
0.5	5	1	0.75

Determine the model parameters for each of the rate law equation given below

a)
$$-r'_{E} = \frac{k P_{E} P_{H}}{1 + K_{EA} P_{EA} + K_{E} P_{E}}$$

b)
$$-r'_{E} = \frac{k P_{E} P_{H}}{1 + K_{E} P_{E}}$$

c)
$$-r'_{E} = \frac{k P_{E} P_{H}}{(1 + K_{E} P_{E})^{2}}$$

d)
$$-r'_{E} = k P_{E}^{a} P_{H}^{b}$$

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

When you open Polymath, following window would appear

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Step 2: 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:

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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

Enter the column name as PE and click Ok

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Similarly, rename C02 to PEA, C03 to PH and C04 to Rate

Step 4: To input the data for PE, select the first cell (row 01, column PE) and enter the first data. Similarly, enter the remaining data of PE in subsequent rows. Repeat this procedure to input the data for PEA, PH and Rate. 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 Spreadsheet should look like this:

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02	1	1	3	3.13				
03	1	1	5	5.21				Linear & Polynomial Multiple linear Nonlinear
04	3	1	3	3.82				fly
05	5	1	3	4.19				
06	0.5	1	3	2.391				
07	0.5	0.5	5	3.867				
08	0.5	3	3	2.199				e.g. y = 2*x^A+B
09	0.5	5	1	0.75				Model Parameters Initial Guess:
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Part (a)

Step 5: Now, you need to input the model form you wish your equation to match. In this case, there are 4 equations for rate law. We will first do the nonlinear regression for the part (a) and then repeat the same for part (b) to (d).

For part (a), the rate expression is given by

Rate=k*PE*PH/(1+KEA*PEA+KE*PE)

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, you need to provide initial guesses for the parameters in your model, in this case, k, KEA, and KE. (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

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03	1	1	5	5.21					Linear & Polynomial Multiple linear Nonlinear
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05	5	1	3	4.19					
06	0.5	1	3	2.391					RATE=k*PE*PH/(1+KEA*PEA+KE*PE)
07	0.5	0.5	5	3.867					
08	0.5	3	3	2.199				_	e.g. y = 2*x^A+B
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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.

Step 6: Click on the pink arrow \blacktriangle to have Polymath perform the regression. If you selected "Report" you will see a screen like this that details the statistical results (such as R², Variance etc.) from the regression analysis.

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4	3	3	1	3.82	3.9253	-0.1053004
5	5	3	1	4.19	4.150869	0.0391314
6	0.5	3	1	2.391	2.33749	0.0535101
7	0.5	5	0.5	3.867	3.935052	-0.0680519
8	0.5	3	3	2.199	2.247839	-0.0488395
9	0.5	1	5	0.75	0.7216039	0.0283961
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From the above report

$$k = 3.348$$

 $K_{EA} = 3.348$
 $K_E = 3.348$

Part (b)

Step 7: Go back to step 5 and enter the RATE equation as

RATE=k*PE*PH/(1+KE*PE)

with

Initial Guess: k= 1, KE= 1

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Step 8: Click on the pink arrow to have Polymath perform the regression

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From the above report,

$$k = 3.187$$

 $K_E = 2.1$

Part (c)

Step 9: Go back to step 7 and enter the RATE equation as

RATE=k*PE*PH/(1+KE*PE)

with



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02	1	1	5	5.21				Linear & Polynomial Multiple linear Nonlinear
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05	5	1	3	4.19				
06	0.5	1	3	2.391				RATE=K"PE"PH/(I+KE"PE) 2
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Step 10: Click on the pink arrow to have Polymath perform the regression

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80	0.5 3	2.199	2.16095	/ 0.0380	43	
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From the above report,

$$k = 2.009$$

 $K_E = 0.3617$

Part (d)

Step 11: Go back to step 9 and enter the RATE equation as

with

Initial Guess: k= 1, a=1, b=1

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Step 12: Click on the pink arrow to have Polymath perform the regression

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k		:	1.	0	.8940237	0.2505474		
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Ge Sa Ma In Ite	nera ample odel dep v eratio	al e siz vars vars ons	2e 9 3 3 4 2 6					
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Ge Sa Ma In Ite So	odel odel dep v eratio urce PE	al e siz vars vars ons e da PH	22 9 3 3 4 2 6 ta po RATE 1.04	ints and RATE ca 0.894023	calculate	ed data points RATE 1763		
Ge Sa Ma In Ite So 1 2	nera ample odel dep v eration PE 1 1	al e siz vars vars ons e da PH 1 3	 2 3 2 6 ta po RATE 1.04 3.13	ints and RATE ca 0.894023 2.869717	calculate b Delta 7 0.1459 0.2602	ed data points RATE 1763 1829		
Ge Sa M In Ite So 1 2 3	nera ample odel dep v eratio PE 1 1	al e siz vars vars ons e da PH 1 3	2 9 3 3 4 2 6 1.04 3.13 5.21	ints and RATE ca 0.894023 2.869717 4.935641	calculate b Delta 7 0.1459 0.2602 0.2743	ed data points RATE 1763 1829 1591		
6e Sa M In Ite So 1 2 3 4	nera ample odel dep v eratio PE 1 1 1 3 3	al e siz vars vars ons e da PH 1 3 3	2 3 2 6 ta po RATE 1.04 3.13 5.21 3.82	ints and RATE ca 0.894023 2.869717 4.935641 3.811947	calculate k Delta 7 0.1459 0.2602 0.2743 0.0080	ed data points RATE 1763 1829 1591		
6e Sa M In Ite So 1 2 3 4 5	nera ample odel dep veration 1 1 1 3 5 5	al e siz vars vars ons e da PH 1 1 3 3 5 3 3	2 3 2 6 ta po RATE 1.04 3.13 5.21 3.82 4.19	ints and RATE ca 0.894023 2.869717 4.935641 3.811947 4.349924	Calculate Delta 0.1459 0.2602 0.2743 0.0080 -0.159	ed data points RATE 1763 1829 1591 1529 9245		
Ge Sa M In Ite So 1 2 3 4 5 6	nerational dep variable dep var	al e siz vars vars ons e da e da 11 1 3 3 3 3 3 3	re 9 3 2 6 6 ta po RATE 1.04 3.13 5.21 3.82 4.19 2.391	ints and RATE ca 0.894023 2.869717 4.935641 3.811947 4.349924 2.399057	Calculate Delta 0.1459 0.2602 0.2743 0.0080 -0.159 -0.008	ed data points RATE 1763 1829 1591 1529 9245 0569		
Ge Si M In Ite So 3 4 5 6 7	nera ample odel 1 dep v eration PE 1 1 1 3 5 5 5 0.5 5	al vars vars ons e da 1 1 3 3 3 3 3 5 5	1 2 2 6 1.04 3.13 5.21 3.82 4.19 2.391 3.867	ints and RATE ca 0.894023 2.869717 4.935641 3.811947 4.349924 2.399057 4.12615	Calculate Delta 0.1459 0.2602 0.2743 0.0080 -0.159 -0.008 -0.259	ed data points RATE 1763 1829 1591 1529 9245 0569 15		
Ge Sa M In Ite So 3 4 5 6 7 8	nera ample odel dep v dep v eratio 1 1 3 5 0.5 0.5 0.5	al e siz vars vars ons e da PH 1 1 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	Image: Point of the second s	ints and RATE ca 0.894023 2.869717 4.935641 3.811947 4.349924 2.399057 4.12615 2.399057	Calculate Delta 0.1459 0.2602 0.2743 0.0080 -0.159 -0.008 -0.259 -0.200	ed data points RATE 1763 1829 1591 1529 1529 1559 1559 1559 1559		

From the above report,

k = 0.894
a = 0.258
b = 1.062