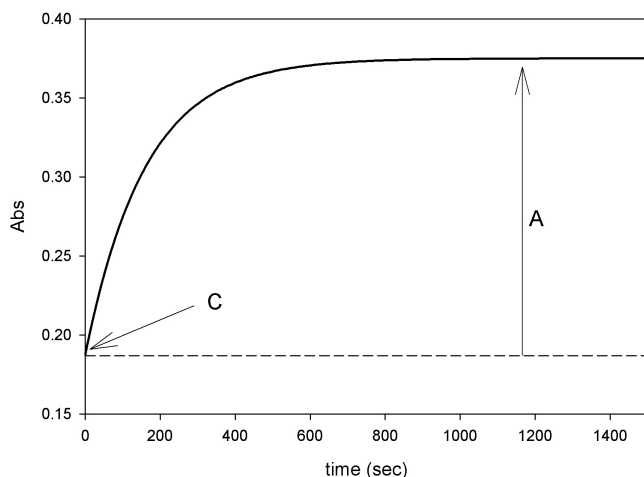Using "Solver" in Excel for non-linear curve fitting

Create a spreadsheet similar to the one pictured below. Import your kinetics data into columns A and B. Column A should be the time values and B the absorbance values.

	A	B	C	D	E	F	G
1	0	0.17376	0.18743	0.00018687		A	0.187596
2	5	0.1821	0.19321	0.000123432		k	0.006259
3	10	0.19035	0.198812	7.16025E-05		C	0.18743
4	15	0.19761	0.204241	4.39712E-05		X^2	0.001225
5	20	0.20554	0.209503	1.57057E-05			
6	25	0.21286	0.214603	3.03767E-06			
7	30	0.21881	0.219546	5.41118E-07			
8	35	0.22485	0.224336	2.6416E-07			
9	40	0.23062	0.228979	2.69331E-06			

For an exponential rise to a maximum value the equation is

$$Abs = C + A(1 - e^{-kt})$$

Where A is the amplitude of the curve, c is the offset from zero and k is the rate constant. A and c are easily estimated from inspection of the data, see the figure below. The rate constant can be estimated as $1/t_{1/2}$ ($t_{1/2}$ = half-life).

Column C is the predicted curve based upon the guess values of A, C and k. The following formula should be entered into cell C1: =$G$3+$G$1*(1-EXP(-$G$2*A1)) and copied into all of column C. Column D is the square of the difference between the real data (column B) and the predicted data (column C), called chi squared(χ^2). The following formula should be entered into cell D1: =(B1-C1)^2 and copied into all of column D. Cell G4 is the sum of the chi squares values, $\sum_i \chi_i^2$. If the predicted curve is very close to the experimental curve then the value for $\sum_i \chi_i^2$ will be small. The best fit

curve is then expected to have the minimum value of $\sum_i \chi_i^2$. We can use the "Solver"

add-in in Excel to find the values of A, C and k that result in the minimum value for $\sum_i \chi_i^2$ (cell G4)

Procedure to Fit the Data

1. Under the "Tools" menu select "Solver".* A new pop-up window will appear.
2. In the box labeled "Set Target Cell" type in $G$4.
3. Below this select "Equal To" the "min" function since we are trying to minimize the value in cell G4.
4. In the box labeled " By Changing Cells" type $G$1:$G$3 . This allows the solver to vary the values for A, C and k to minimize the sum of chi squared.
5. Now click on "Solve". The program will alter your initial values to fit the data.
6. A new pop-up will appear asking if you want to keep the new values or revert to your original values. Select "keep solver solution" and click the "OK" button.
7. The best fit values for A, C and k will now be in cells G1:G3. To be sure the values make sense, plot the columns B and C vs. column A. The two curves should match very closely. If they do not, then you need to make better guesses for A, C, and k to start with. Enter new guess values and repeat the procedure.

* If you do not see this as an option the add-in needs to be installed. To do this select "Add-Ins" under the "Tools" menu and check the solver add-in. Note: You may need the Excel installation disk to add this feature.