

# Instructions for Using “General Spreadsheet Length id.xlsx” and for Fitting Conductance and Voltage data using Origin Software®

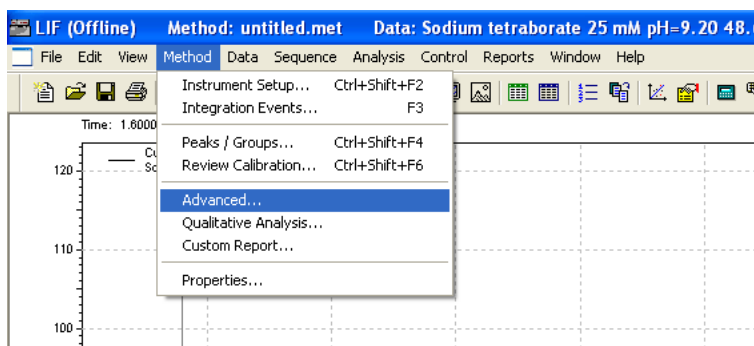
## Introductory Notes about “General Spreadsheet Length id.xlsx”

The spreadsheet is designed to be suitable for capillaries of any length and internal dimensions for which the lengths of the cooled and un-cooled regions are known. It contains three worksheets: “Raw Data”, “Average” and “Collated”. There is space for the input of 20 averaged voltages and currents in “Collated” Cells A8:B27. If high electrical conductivity buffers are used or capillaries with large internal diameters, it will not be possible to collect data for higher voltages, so that several rows in the spreadsheet may become redundant. It is suggested that the worksheet be saved by another name and surplus rows removed. These instructions are written for use with Beckmann CE instruments but can be easily adapted for use with other instruments.

### 1. Input of data for “Raw Data” (using a Beckmann CE instrument)

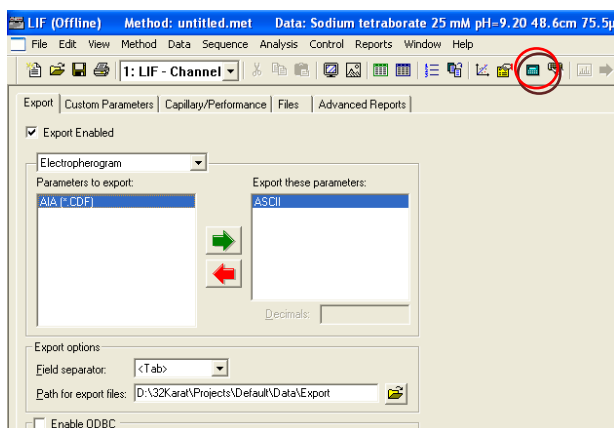
1.1 Open the 32 Karat software and locate the data file.

1.2 Click on the Methods pull down menu and select Advanced Methods



1.3 Click on the Export Tab and place a √ in the box “Export enabled”

1.4 Click on ASCII and the green arrow.



- 1.5 Click on the yellow folder to the right of “path for export files” and specify where you would like your ASCII file to be saved
- 1.6 Click on the “Analyze” icon (shown in the red circle).
- 1.7 Open the program Excel and use it to open the ASCII file. For the file type, it is necessary to select “All files”. The file name will be the same as your original data file but will have the extension “.dat.asc”
- 1.8 If you get a message “The file you are trying to open, “File name” is in a different format than specified by the file extension.....Do you want to open the file now?”, Click Yes
- 1.9 The file will open with file information followed by the raw data, starting with the electropherogram followed by the voltage in multiples of  $10^{-2}$  V and the current in multiples of  $10^{-11}$  A.
- 1.10 For the purpose of determining the electric field strength or temperature the electropherogram data is not needed and should be removed. Take note of the number of data points that were collected. There will be a 0 at the start of the voltage data and at the start of the current data. Select and cut the current data and make a new column next to the voltage data and paste them there.
- 1.11 Copy and paste the two columns (voltage and current) into the “Raw Data” worksheet of General Spreadsheet Length id.xlsx.
- 1.12 Save your ASCII data file as an excel file. This will make it easier to open in the future.
2. **Processing the Raw Data.** The raw data contains voltages and currents for when the voltage was ramping and for when the voltage was stable. Assuming that the duration of each voltage was for one minute and the ramp time was 10 s, there are 50s of data collected at each constant voltage giving rise to 200 data points if the collection rate is 4 Hz.
  - 2.1.1 Copy and paste 200 data points from the two columns (voltage and current) for which the voltage has stabilized (a multiple of  $\sim 1$  kV) into the “Average” worksheet of General Spreadsheet Length id.xlsx.
  - 2.1.2 Select cells A202:B202. The short cut for this repetitive task is Ctrl G. After selecting A202:B202 once, this command is remembered in the future. These cells average the data and convert the voltage to kV and the current to  $\mu$ A. **Different multipliers** may be involved if collecting data from alternative CE instruments.
  - 2.1.3 Copy the cells A202:B202
  - 2.1.4 Type Ctrl G again and select A1:B200 in preparation for the next 200 data.

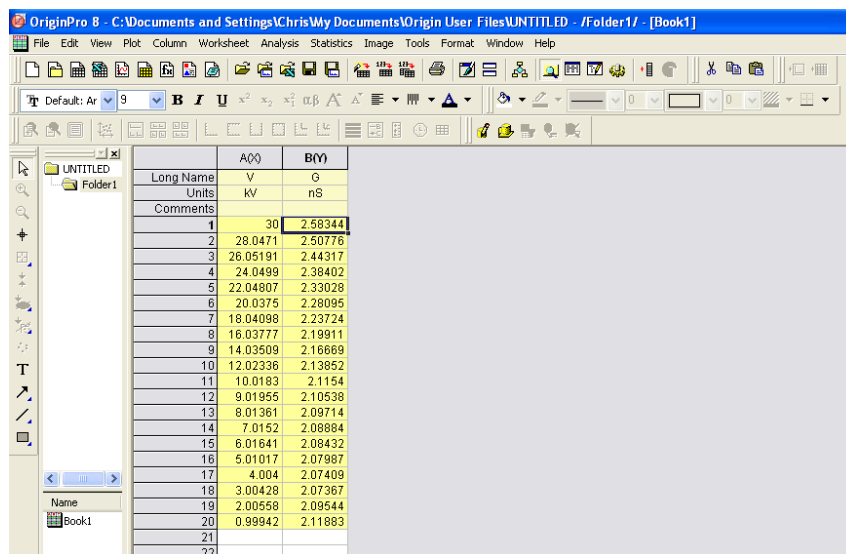
2.1.5 Paste the copied cells from step 1.2.3 into the first two columns of the worksheet “Collated Data”


2.1.6 Repeat steps 1.2.1 to 1.2.5 until you have averaged and collated all the raw data.

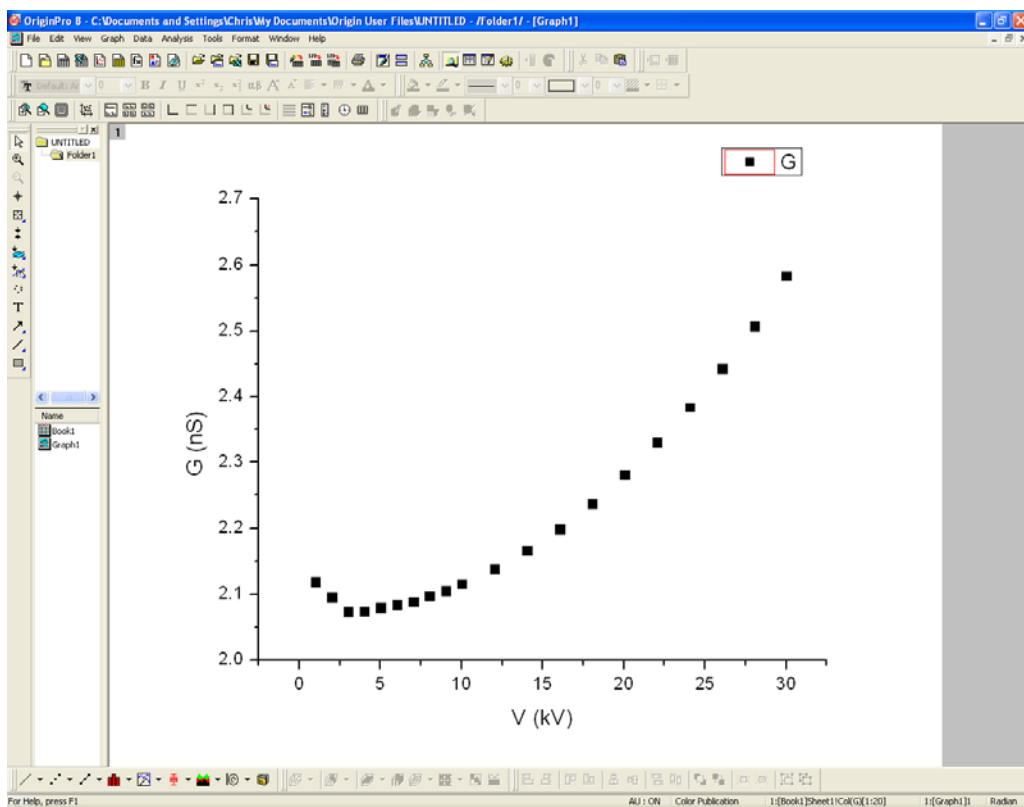
### 3. Fitting the Conductance vs Voltage data using Origin® software

3.1 Copy the fitting file named “ConductancevsVoltage.fdf” into your fitting files into the location:  
Origin User Files\fitfunc\ConductancevsVoltage.fdf

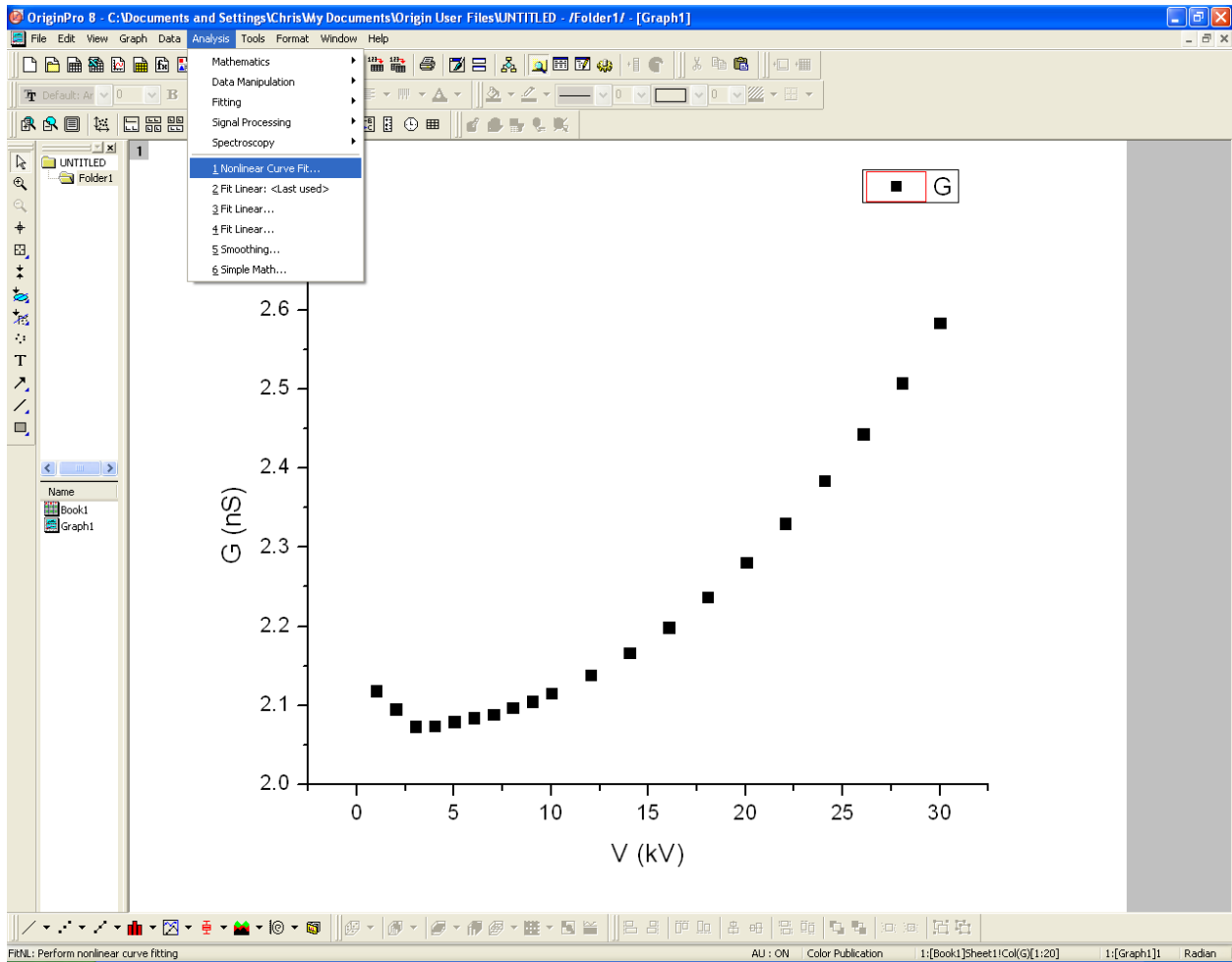
3.2 Input the values of the total voltage ,V (Column A), and experimental conductance,  $G_{\text{exp}}$  (Column D), into a new Origin worksheet.



3.3 Select the data in columns A and B and select the  scatter plot icon (bottom left hand corner) to plot.



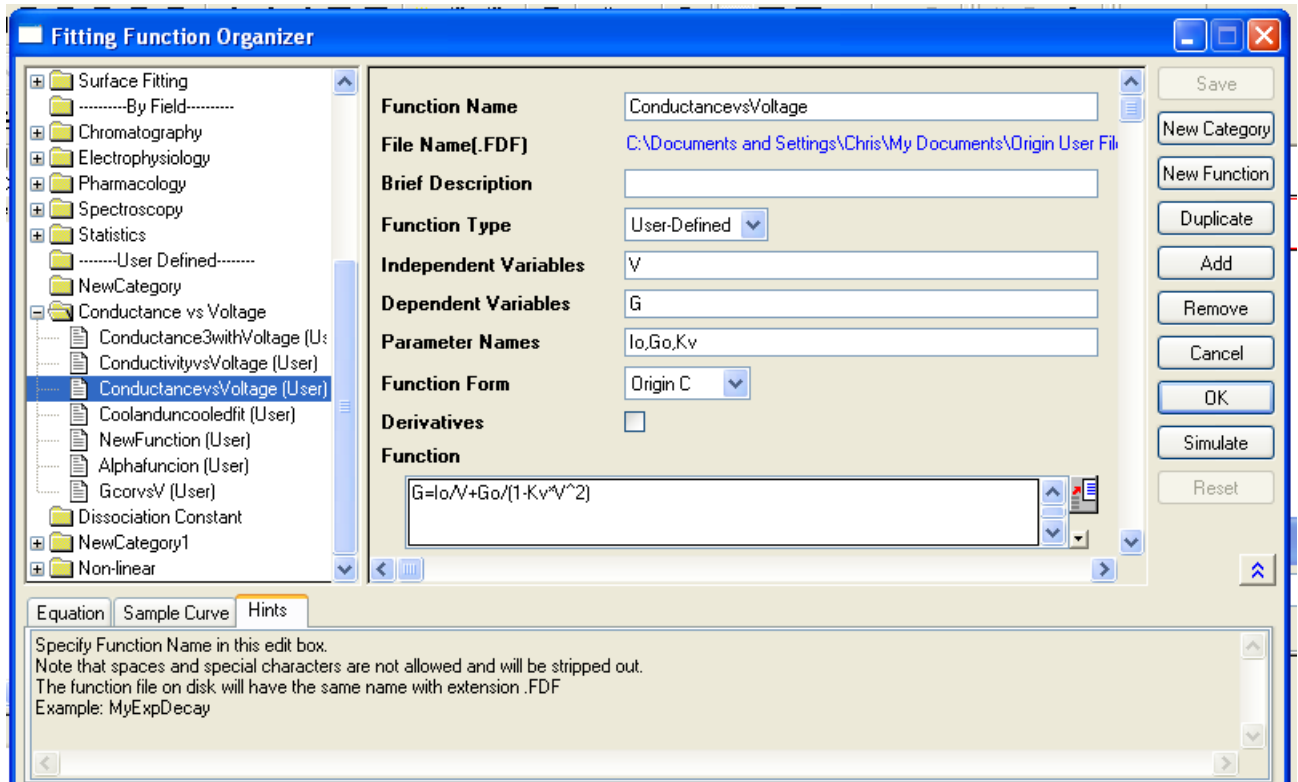
3.4 Click the scroll down Analysis menu and select the non-linear curve fit tool.



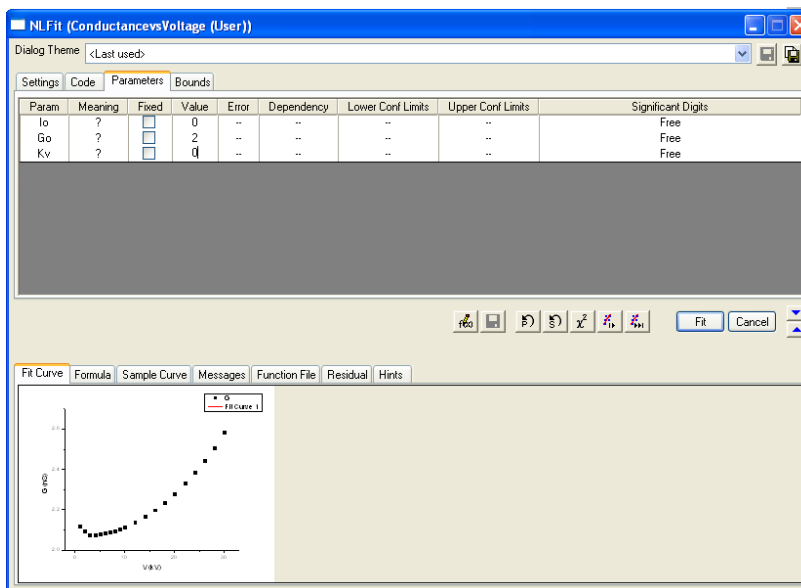
3.5 Select the category pull down menu and select (User) New Category and create Conductance vs Voltage

3.6 In the "Function" menu select "New".

3.7 The code for the fitting function is inputted using the  $f(x)$  icon. After filling in the boxes hit "OK".  
(In future select the Category: Conductance vs Voltage and Function: Conductance vs Voltage)

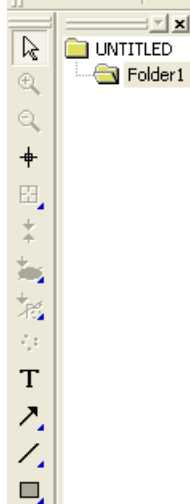
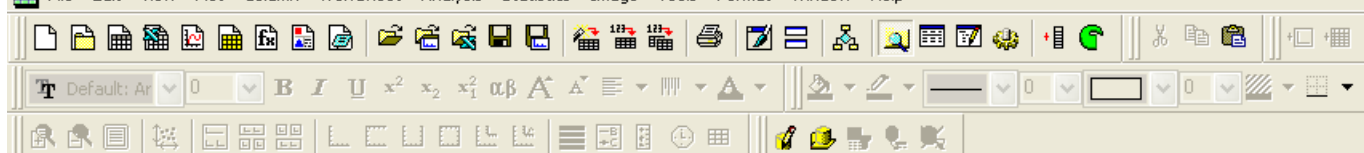


3.8 Select the Parameters button and input values for Io, Go and Kv. Input values of 0 for Io and Kv and use the minimum value of G as your estimate of Go in this case approximately 2.



Now click on the fit button.

The following screen should appear.



&lt; &gt;

Name

Book1  
Graph1  
Table1

## 1 NL Fit (Conductance vs Voltage (User)) (28/07/2010 12:06:09)

## Notes

## Input Data

## Parameters

	Value	Standard Error
Io	0.05119	0.00759
Go	2.06283	0.00273
Kv	2.27049E-4	2.14485E-6

Iterations Performed = 5

Total Iterations in Session = 5

Fit converged - tolerance criterion satisfied.

## Statistics

	G
Number of Points	20
Degrees of Freedom	17
Reduced Chi-Sqr	4.51289E-5
Residual Sum of Squares	7.67192E-4
Adj. R-Square	0.99821
Fit Status	Succeeded(100)

Fit Status Code :

100 : Fit converged

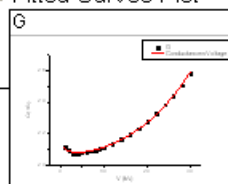
## Summary

	Io		Go		Kv		Statistics	
	Value	Error	Value	Error	Value	Error	Reduced Chi-Sqr	Adj. R-Square
G	0.05119	0.00759	2.06283	0.00273	2.27049E-4	2.14485E-6	4.51289E-5	0.99821

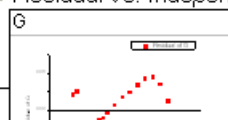
## ANOVA

		DF	Sum of Squares	Mean Square	F Value	Prob>F
	Regression	3	98.17826	32.72609	725168.47357	0
	Residual	17	7.67192E-4	4.51289E-5		
G	Uncorrected Total	20	98.17903			
	Corrected Total	19	0.47865			

## Fitted Curves Plot



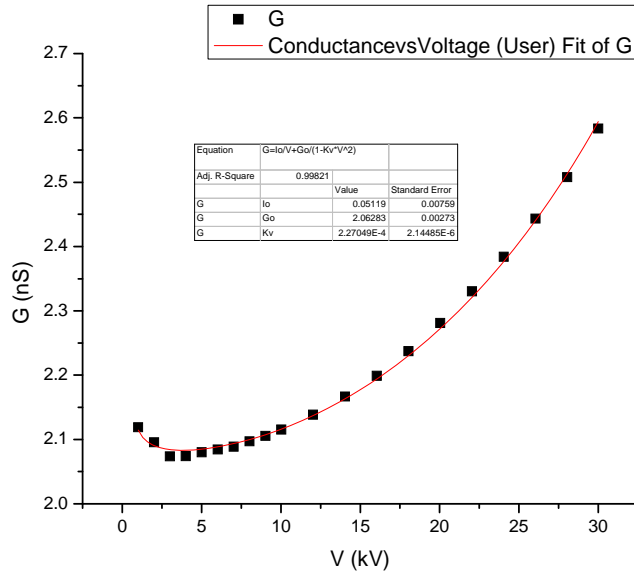
## Residual vs. Independent Plot



Sheet1 FRNL1 FitNLCurves1 /



3.9 By clicking on Graph 1 you will see your graph with the fitted curve and a table of the fitted parameters.



3.10 Input the fitted parameters from the table into the excel spreadsheet “General Spreadsheet Length id.xlsx” ie. Cells A39:C41 should contain the output from the Origin fitting table.

lo	0.05119	0.00759
Go	2.06283	0.00273
Kv	2.27049E-4	2.14485E-6

#### 4. Finding stable solutions to the conductivity, temperature, power per unit length and electric field strength in each part of the capillary.

4.1 Input the total length of the capillary (measured in cm) into cell D6. Do not add units as this value is used in calculations.

4.2 Input the length of the un-cooled part of the capillary in cell F6

4.3 Input the internal diameter, diameter of fused silica and outer diameter (measured in  $\mu\text{m}$ ) into cells K2:K4.

4.4 The thermal conductivity of water, in cell M2, is at 20°C. If you are measuring at different temperatures, consult the table of variation of conductivity of water with temperature shown below.  $\lambda$  increases by approximately 0.277% with each 1.0 °C rise in temperature.

T (°C)	10	20.0	25.0	30.0	40.0
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$\lambda \text{ (Wm}^{-1}\text{K}^{-1}\text{)}$	0.5800	0.5984	0.6070	0.6154	0.6305
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- 4.5 If you are using an alternative CE instrument to a Beckmann, input the surface heat transport coefficient for the cooled section of the capillary in cell P2. For example for an Agilent 3DCE instrument which used fan forced air with a speed of  $10 \text{ ms}^{-1}$ ,  $h_s = 566 \text{ Wm}^{-2}\text{K}^{-1}$ .
- 4.6 Now that all the data has been inputted, scroll down to cells A50:AD50 to see the result of ~1300 iterations. Convergence is indicated by  $x = 1$  for most voltages(See Column L50:L66)