DALHOUSIE UNIVERSITY

VAWQuum: dV/dQ Analysis Software

For user-friendly differential voltage battery analysis

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Please send comments/bugs/suggestions to Jeff Dahn @ Jeff.Dahn@dal.ca

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About

VAWQuum is software meant to be used to calculate, display, and analyze dV/dQ vs Q of a battery. Its main purpose is to compare a battery over many cycles to reference materials.

For example, the user can load in the data from a battery that is composed of graphite and LCO3. Then, he/she can load in reference data of graphite and LCO3, ideally at the same temperature and current. After this, one can compare the calculated dV/dQ (from the reference curves) to the measured dV/dQ (from the battery), and adjust the positive & negative mass & slippage to improve the fit. Once the fit is completed, the user will have a pretty good sense of how much cathode and anode mass is left and how their respective slippages.

This can be repeated for the different cycles of the battery (to examine how the slippages/masses change over cycles).

VAWQuum was created by Asher Wright (asher.wright@dal.ca) under the supervision of Jeff Dahn (Jeff.Dahn@dal.ca). It was **largely** based off of the similar software made by Hannah Dahn, also under the supervision of Jeff Dahn.

Quick Start

This quick start guide will give minimal information on how to quickly load in a couple of files. It is recommended that you first read the other sections. However, if you just need a reminder on how the program works, or if you just want to quickly test it out, this section should be appropriate. For a more in depth guide, see **Detailed Sample Run**.

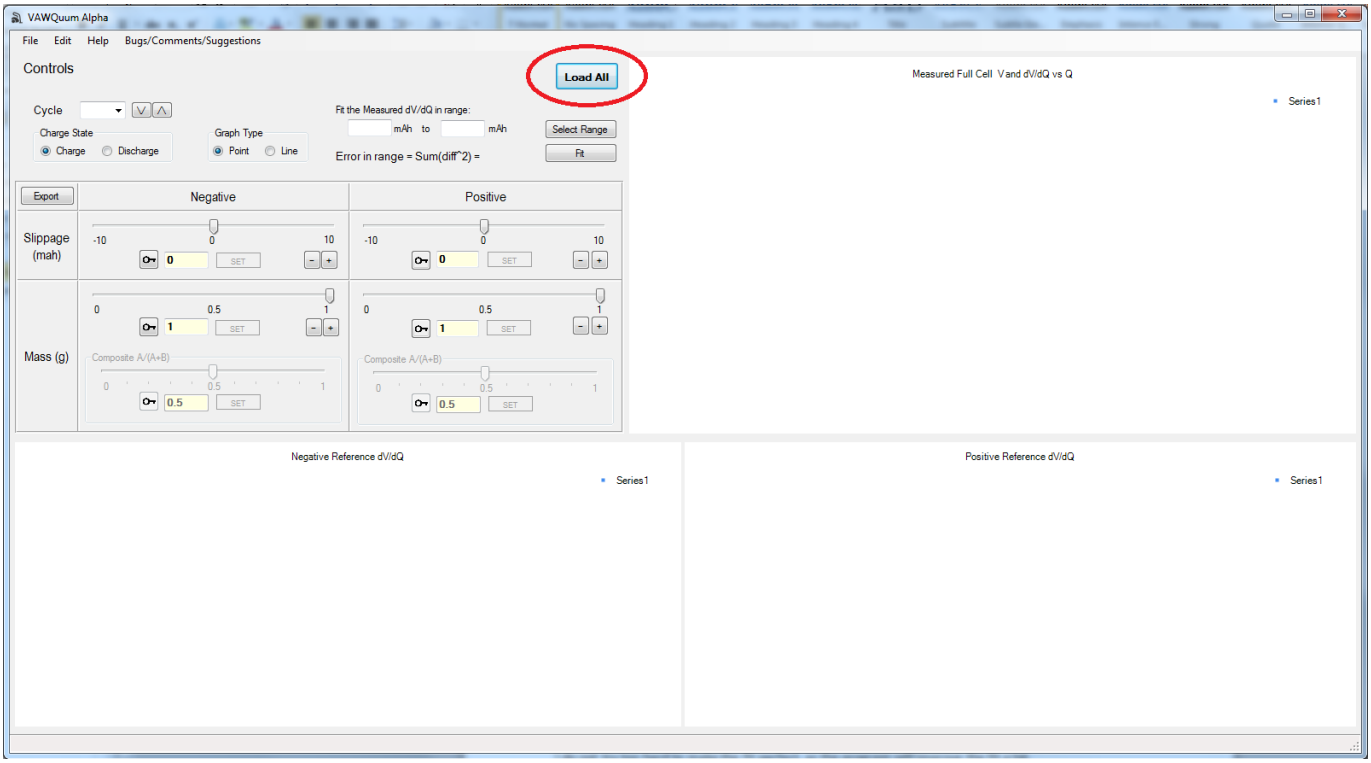
In order to use the fitting portion of this software, the program must have programmatic access to Excel (see: Giving VAWQuum Access to Excel).

Steps:

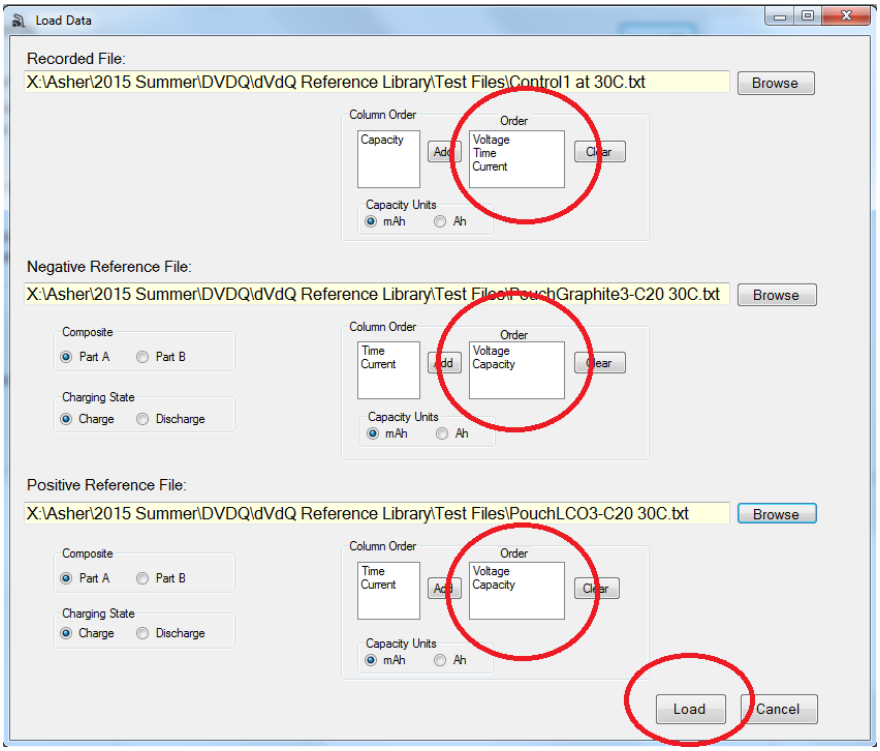
1. Loading in the negative reference, positive reference, and full cell files
2. Adjusting the parameters to improve the fit by hand
3. Selecting a range and fitting
4. Exporting the parameters.

1. Loading in the negative reference, positive reference, and full cell files

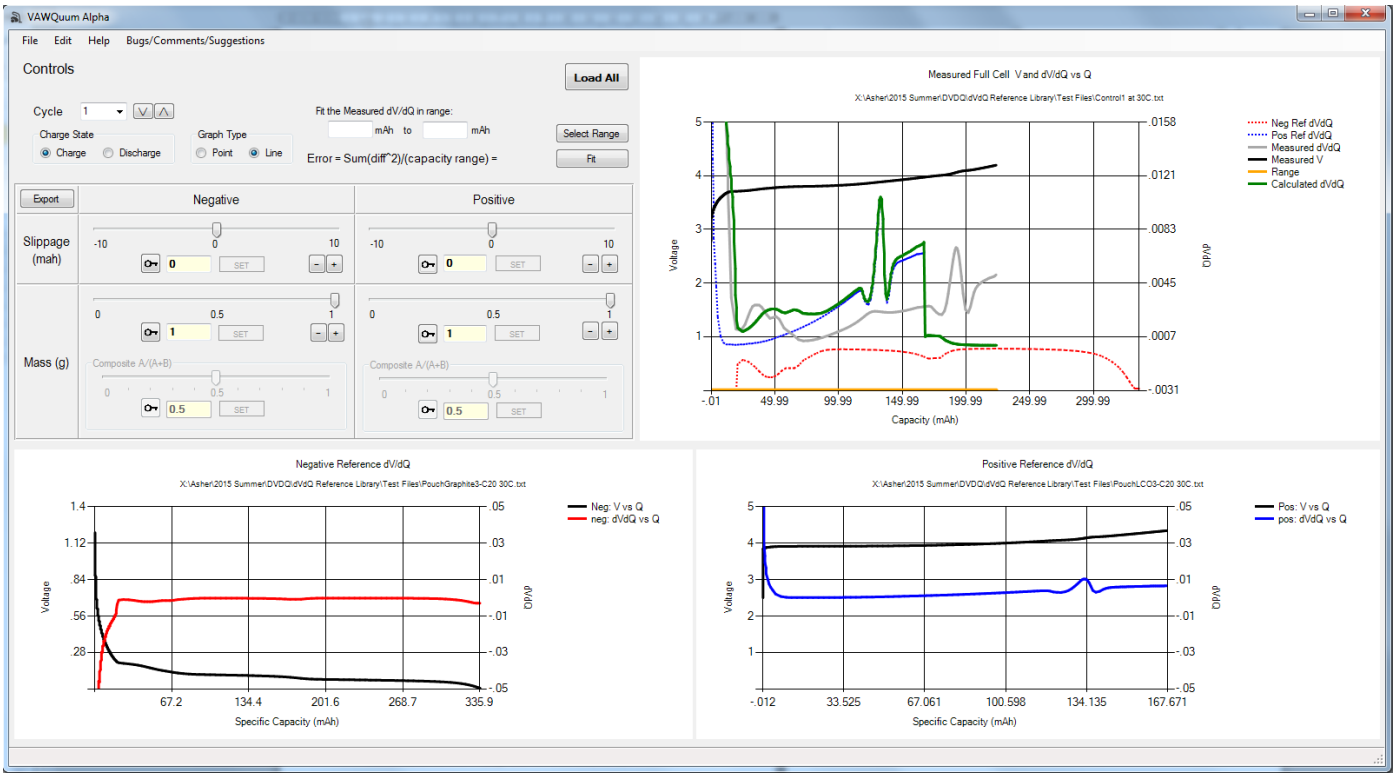
To load in all three files at once, simply click the “Load All” Button near the top of the program.



Then select the file paths, and the column order. For the picture below, the TOP file is ordered Voltage,Time,Current, so I select Voltage > Time > Current to be the order. The next two files are ordered Voltage,Capacity so I select Voltage > Capacity to be the order.



Now select “Load”, and the data will be displayed on the main program.

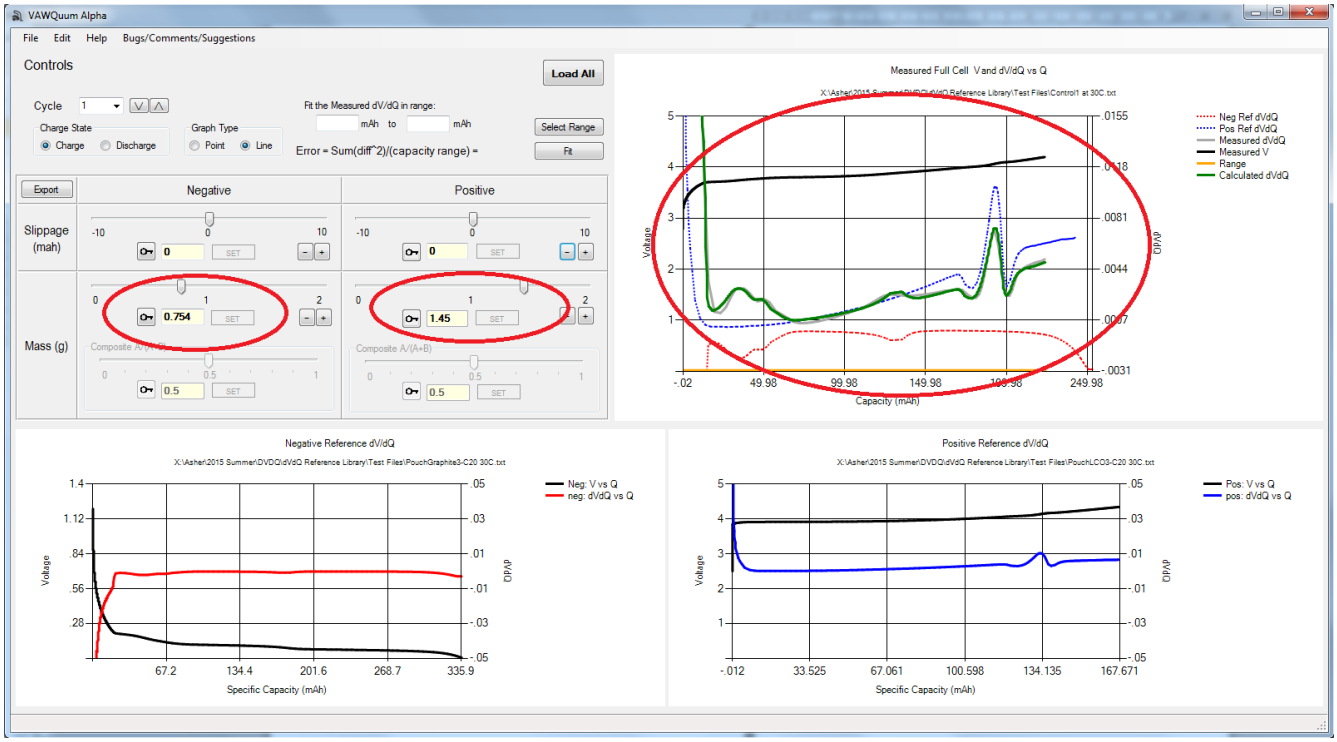


2. Adjusting the parameters to improve the fit by hand

We are trying to fit the green curve (calculated dV/dQ from the reference curves) to the gray data (dV/dQ from the full cell).

Drag the sliders for the positive and negative mass to get to a close mass to that of the cathode and anode in your cell. If you do not have any idea what the mass is, simply move the sliders until the fit improves. Alternatively, you can enter a mass into the box, and press “Set”.

If you can’t get a decent fit with only adjusting mass, drag the sliders for the positive and negative slippage to try to make the fit even better (or skip this and go to the next step). Alternatively, you can enter a slippage value into the box and press “Set”.

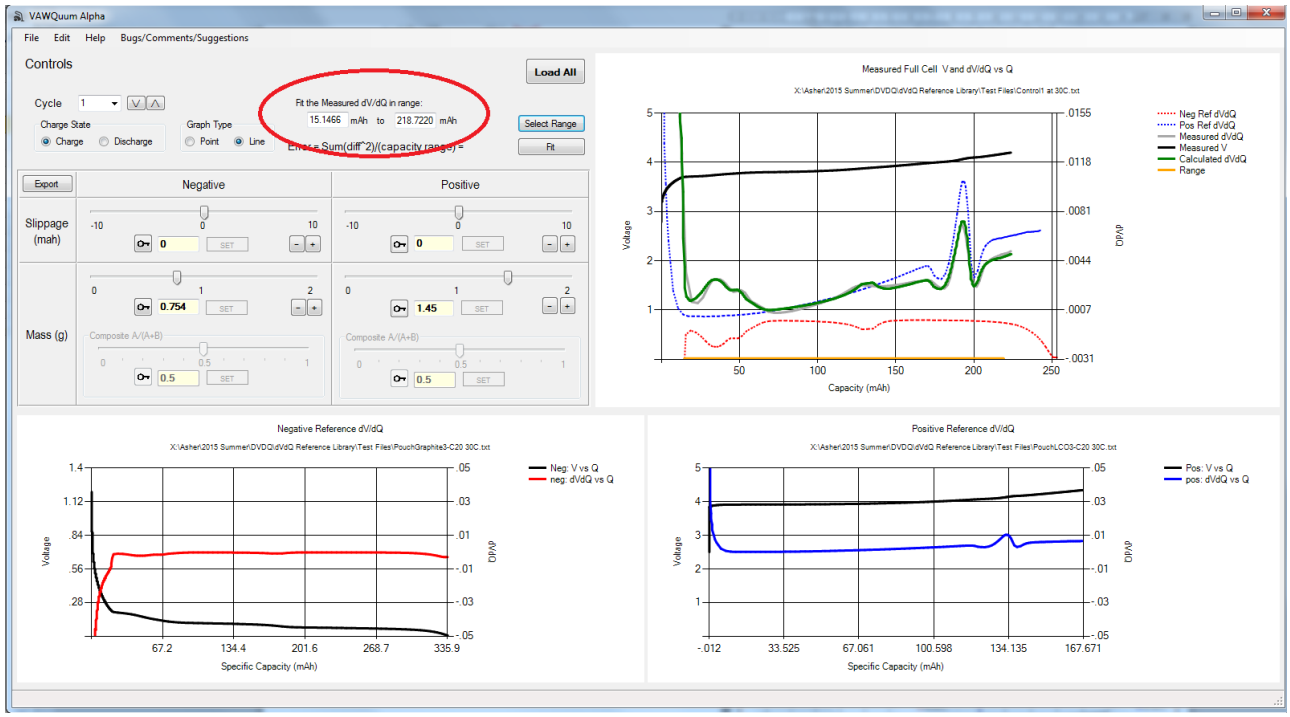


Hopefully your fit looks OK at this point. We will now go on to fit it better.

Note: It is not necessary to improve the fit by hand before using the Fit Button to fit it, but it is recommended, and can sometimes make a difference.

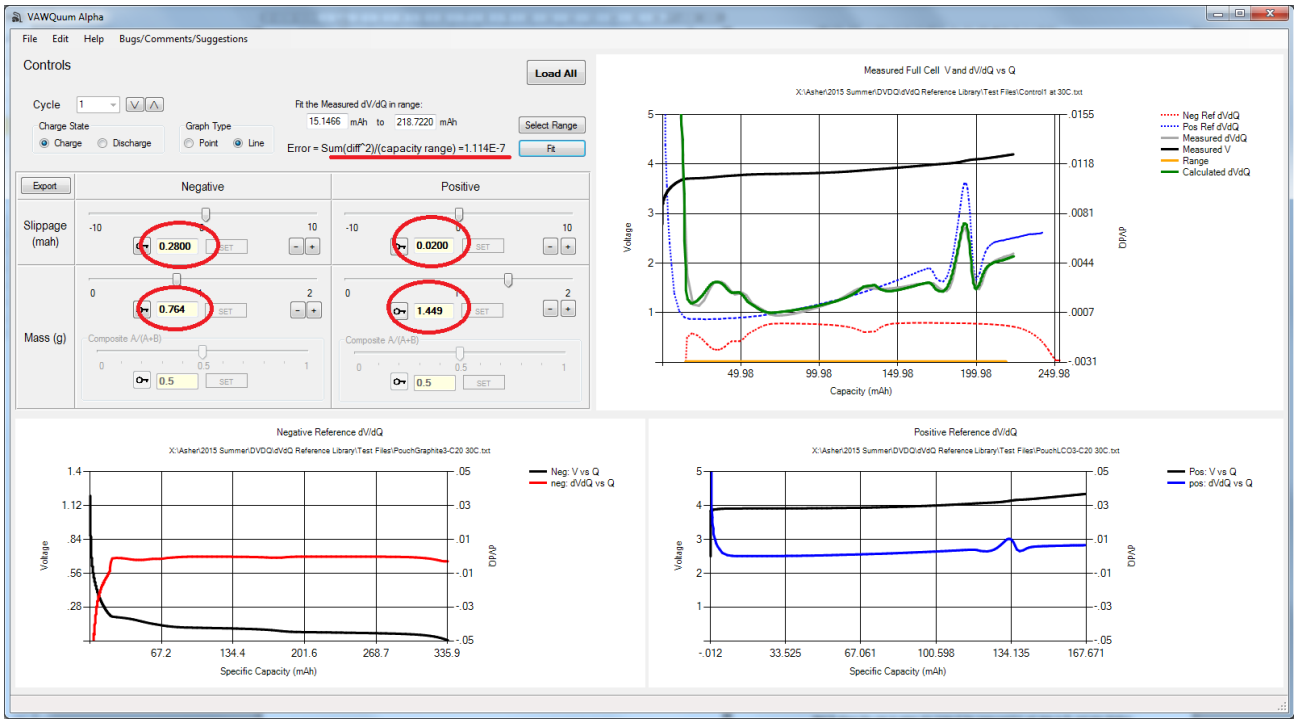
3. Selecting a range and fitting

You must now select a range to fit, either by entering the minimum and maximum capacity values to consider into the boxes, or by pressing “Select Fit”. If you do the latter, you must then click the minimum and maximum values on the full cell chart.



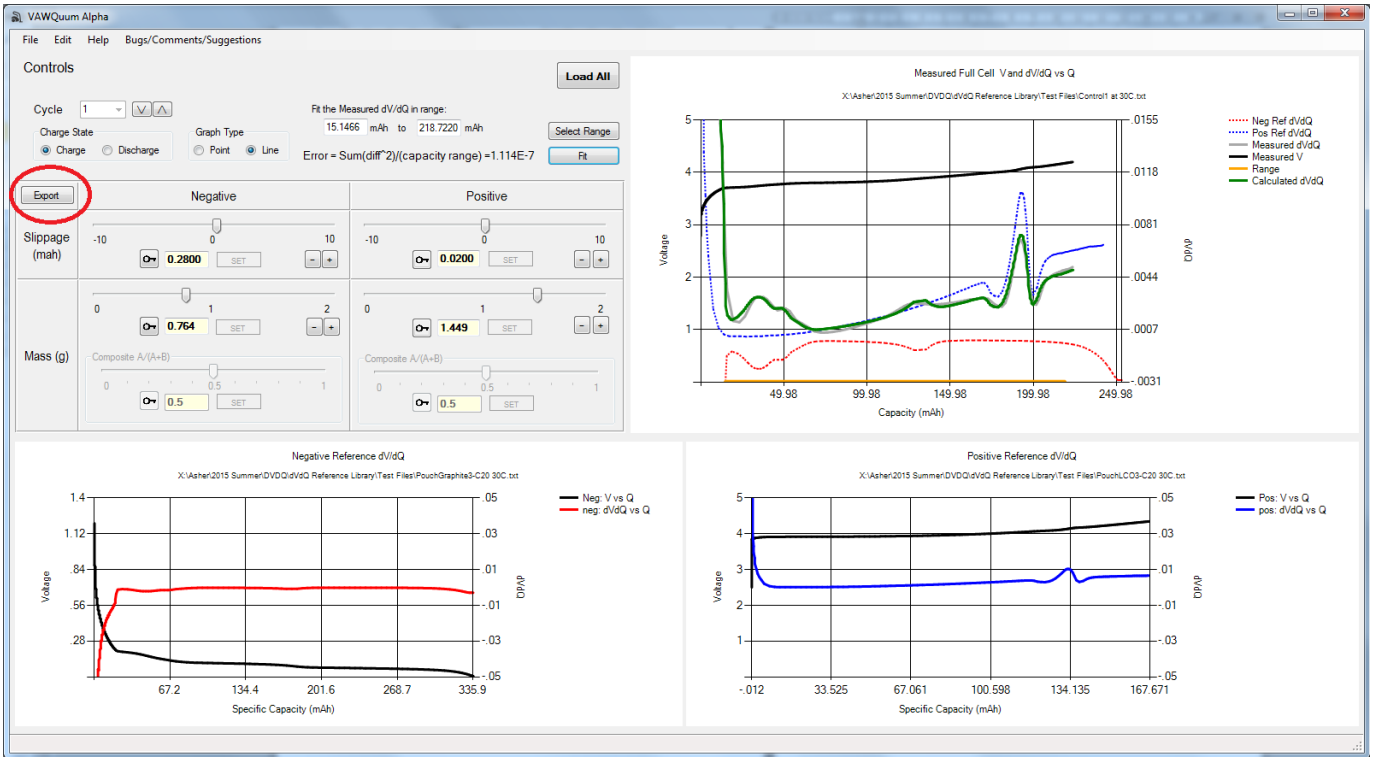
Once the range is selected, hit “Fit”. The first fit may take a while (10s), but the subsequent fits should be much faster.

The click “Fit” a few more times to make sure that the fit settles down. Sometimes it is necessary to slightly move a slider (like positive slippage) to “Refresh” the fit. The relative error of the fit will now be displayed as well as the updated parameters.



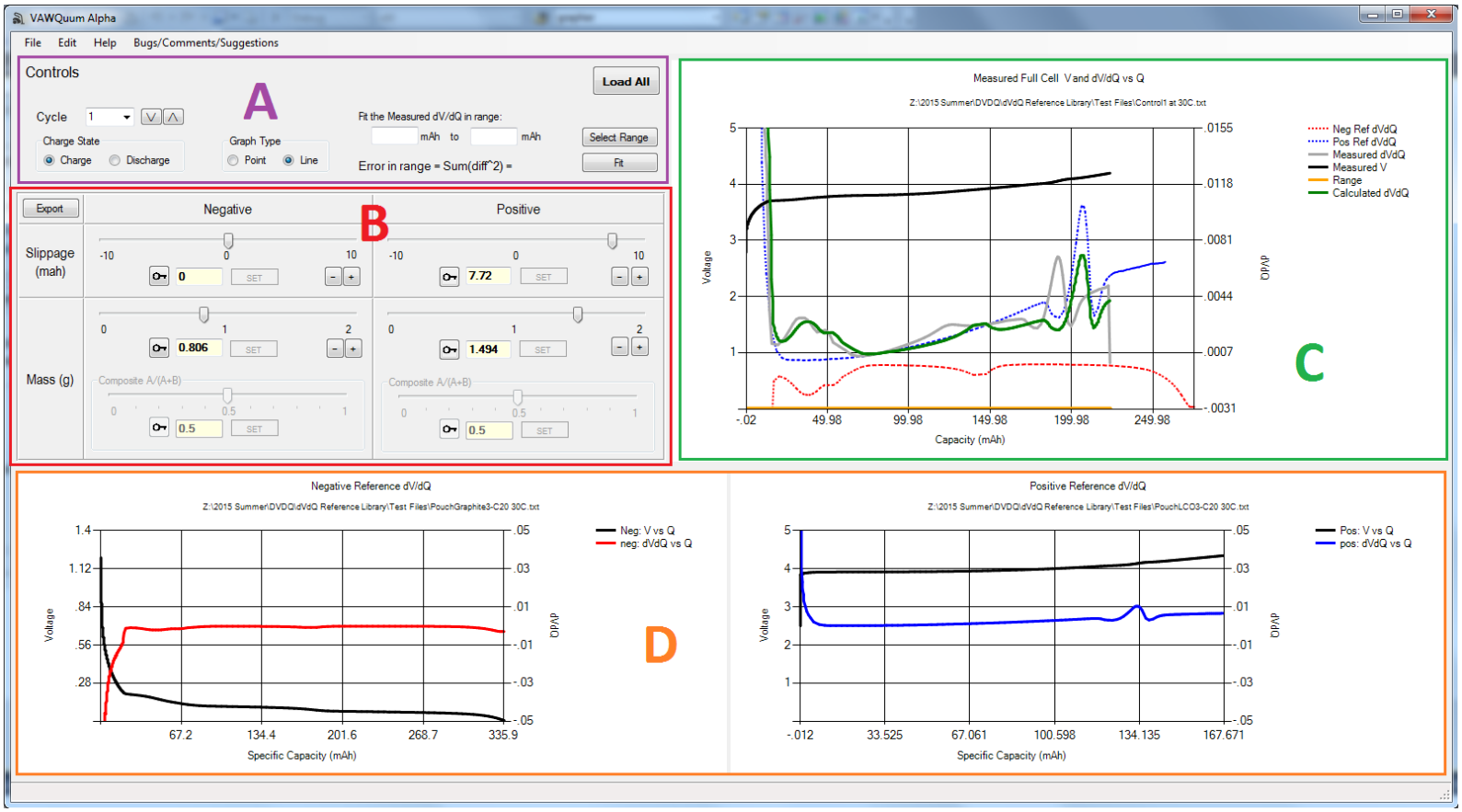
4. Exporting the parameters.

To export the parameters to a text-file, simply click the Export button near the sliders. Then select the location to which you want to export. The parameters and filenames will be exported but the data will not be. For other exporting, please see the more detailed sections of the user manual.

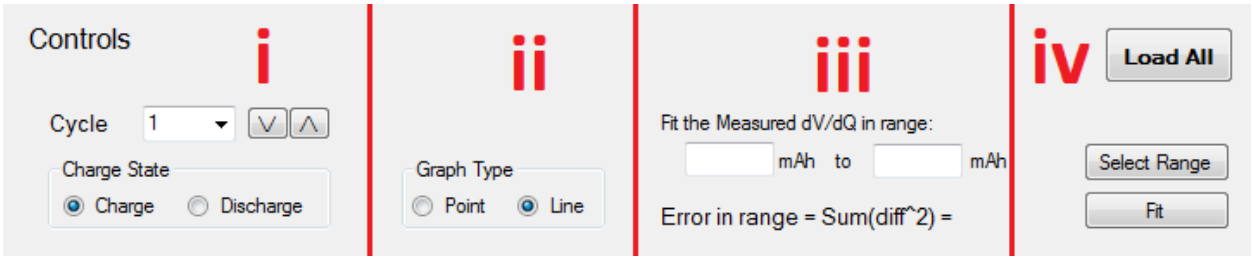


Overview

Main Window



A. Graph Control Panel



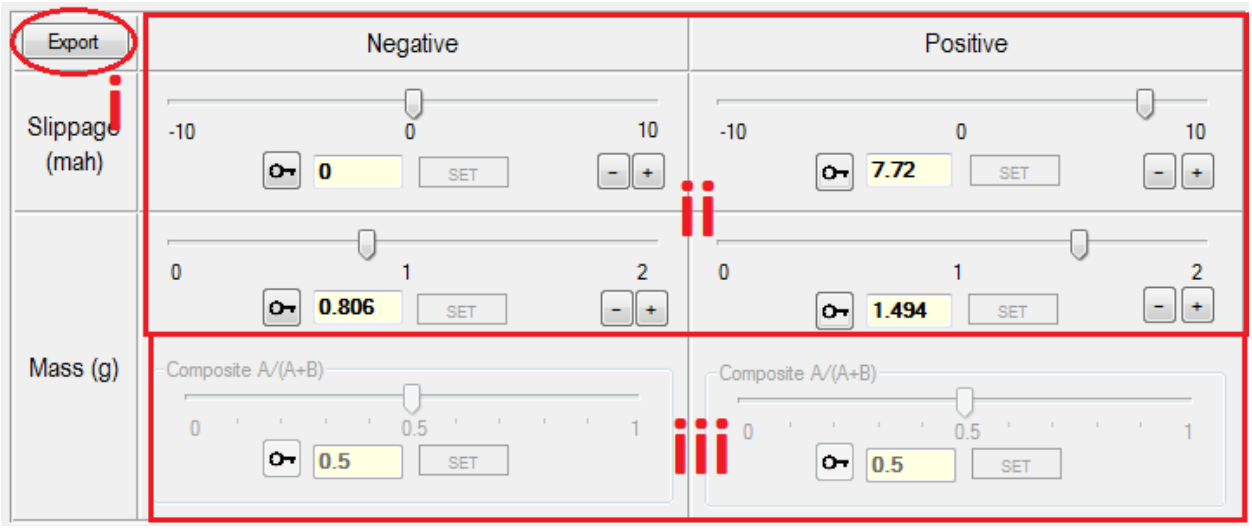
Part i of the control panel allows the user to choose the cycle to display, and whether to display the charging portion of the cycle or the discharging.

Part ii allows the user to choose between displaying point-graphs or line-graphs.

Part iii allows the user to select the range of the measured/full cell data to fit, and also displays the error in that range (after fitting).

Part iv contains the buttons, and allows the user to load data, select the range to fit (by clicking directly on the chart), and fit the data.

B. Parameter Control Panel



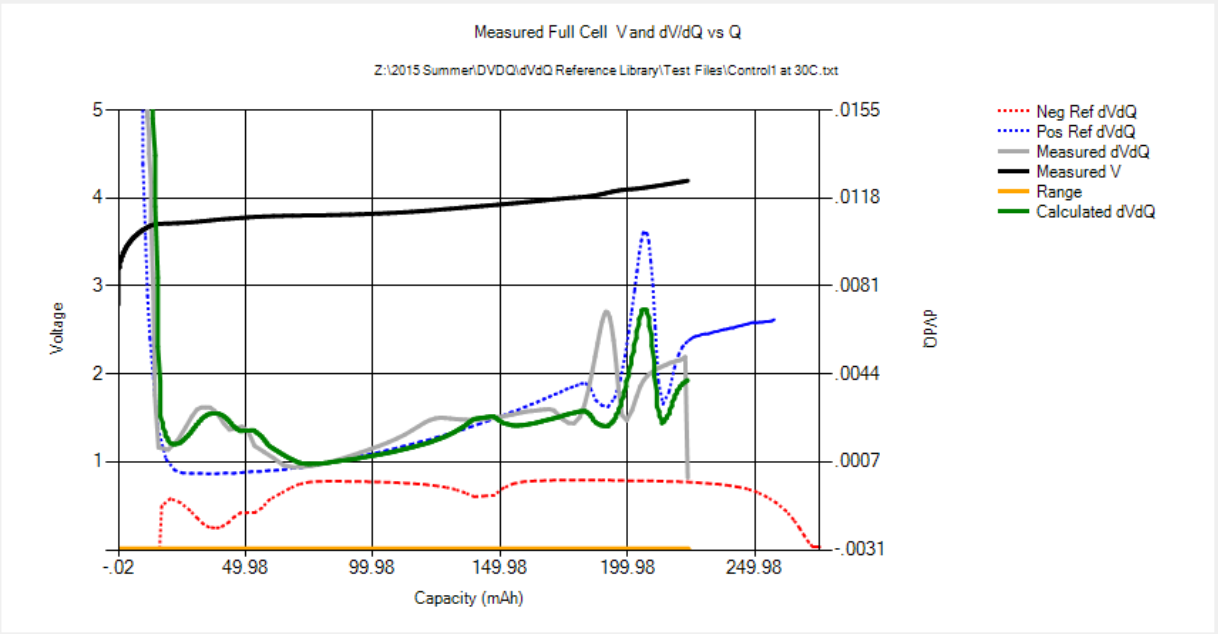
This control panel is what allows the user to adjust the parameters (or view the parameters found by the fitting).
The Export button (**Part i**) allows the user to export the current parameters (with the loaded file names) to a text file.
Part ii of the control panel is where the typical parameters are displayed (mass and slippage for cathode and anode).
Part iii of the control panel is only enabled once there is a composite electrode loaded in. It then allows the user to select the fraction of Part A in the electrode.

In Parts ii and iii, the user can either adjust the parameters by moving the slider, or by entering the value in the textbox, and then hitting Enter or the “Set” Button. The lock button can be seen below:

It allows the user to “lock” the parameter. This means that when the fit is calculated, it will not adjust this parameter.

The Plus and Minus buttons allow the user to increase/decrease the range of the slider bar. It will be automatically changed upon hitting the “Set” Button.

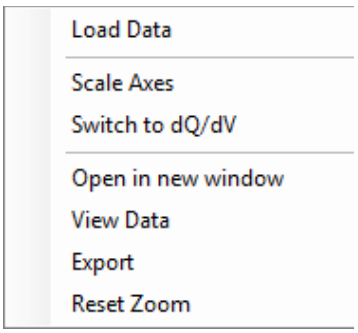
C. Measured/Full Cell Graph



This chart displays all of the data listed in the legend, namely:

1) The negative reference (anode) dV/dQ vs Q
2) The positive reference (cathode) dV/dQ vs Q
3) The measured/full cell dV/dQ vs Q
4) The measured/full cell Voltage vs Q
5) The range of data we are fitting (can be changed, see A: Graph Control Panel)
6) The calculated dV/dQ vs Q (found with the anode dV/dQ, cathode dV/dQ, and parameters)

After right-clicking on the chart area, the following menu appears:

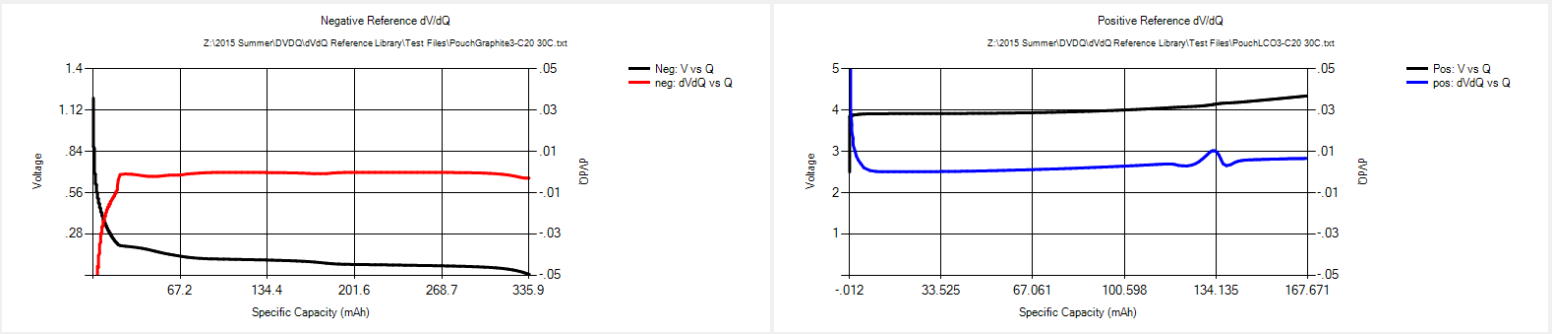


1. Load Data
   Allows the user to load in measured/full cell data (starts load form)
2. Scale Axes

This allows the user to set the minima and maxima for the axes of the measured/full cell chart. This is an alternative to selecting the zoom amount by clicking on the chart and drawing the zoom rectangle.

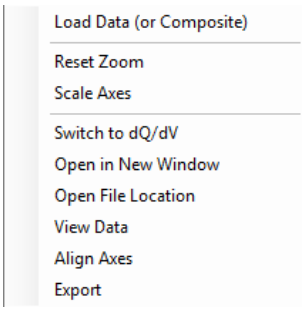
3. Switch to dQ/dV
   Switches from dV/dQ vs Q to dQ/dV vs V. This can be clicked again to switch back.
4. Open in new window
   This opens the graph in a new **Chart Window**, in which the user can select series to display/export/examine.
5. View Data
   This displays the data contained by the chart in a temporary text file (not recommended for actual exporting). It is useful for quickly looking at data.
6. Export
   This displays an **Export Window** that allows the user to quickly export the chart however they want.
7. Reset Zoom
   This resets the zoom of the chart to the zoom when it was loaded into the program. Useful if the user zooms into a detail, and then wants to zoom out.

D. Negative and Positive Reference Graphs



These charts display the negative and positive reference curves (both V vs Q and dV/dQ vs Q). They can also be composite electrodes, in which case they display this information for both components.

After right-clicking either of these chart-areas, the following menu appears:

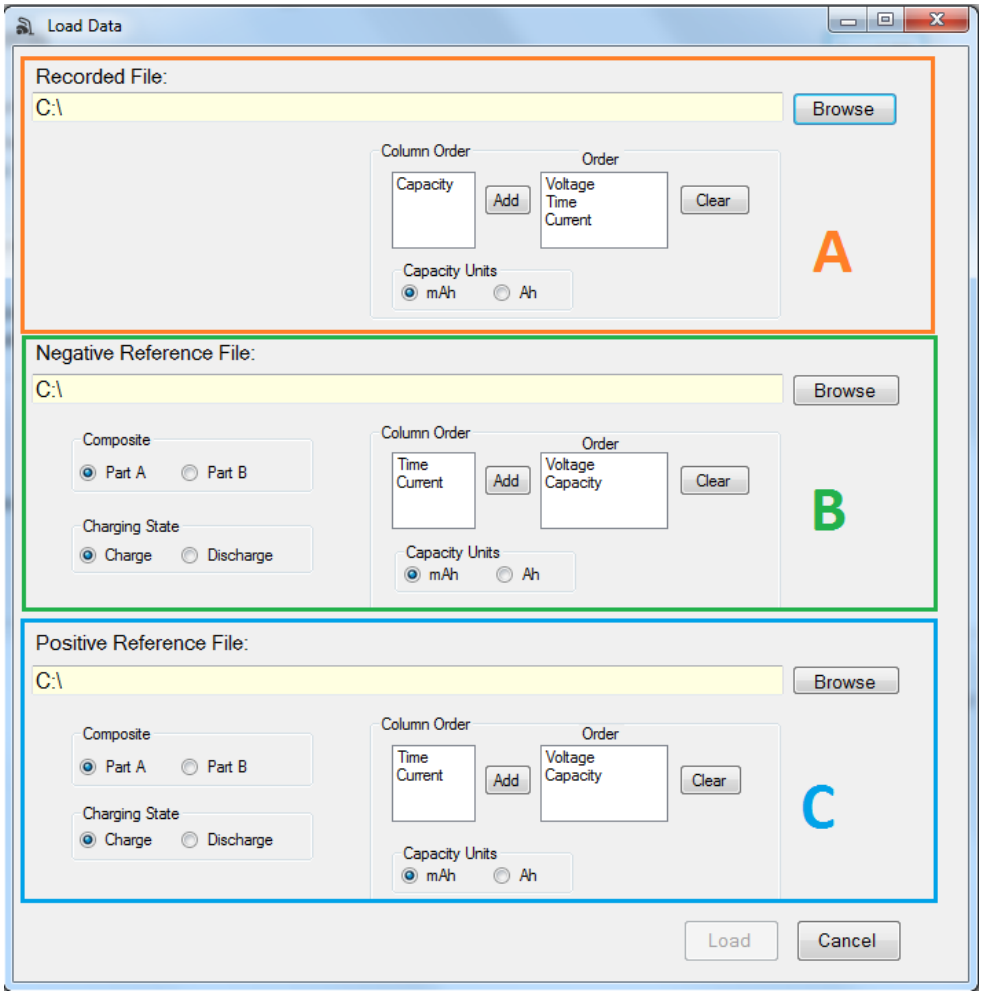


Many of these options are identical to the ones in “C. Measured/Full Cell Graph”, and so only the differences will be explained.

1. Load Data
   This allows the user to load in negative/positive reference data, and potentially composite data.
2. Open File Location
   This opens the location (in Windows) of the reference file that has been loaded in).
3. Align Axes
   Sometimes the two y axes of the chart do not match up. This can be fixed by selecting this option.

Load Window

There are three states to the Load Window. The first (shown below) is when you have clicked the “Load All” Button. It allows you to load all three files at once. The other states appear if you have right-clicked on a chart and selected “Load Data”. In this case, only the corresponding file to your chart will be enabled to load.



A. Measured/Full Cell Data

This is where you can load in your full cell data. The only things to fill out are:

1. The file location (click Browse)
2. The order of the columns in your text file (which can be separated by commas or by tabs). Example: If the file is formatted as: *Voltage,Current,Time* Then Select *Clear*, and then click *Voltage* and then *Add*, *Current* and then *Add*, *Time* and then *Add*. This will display the names in the same order as the file (which is necessary).
3. The units of the capacity in the file (if the file contains capacity information).

B. Negative Reference Cell Data

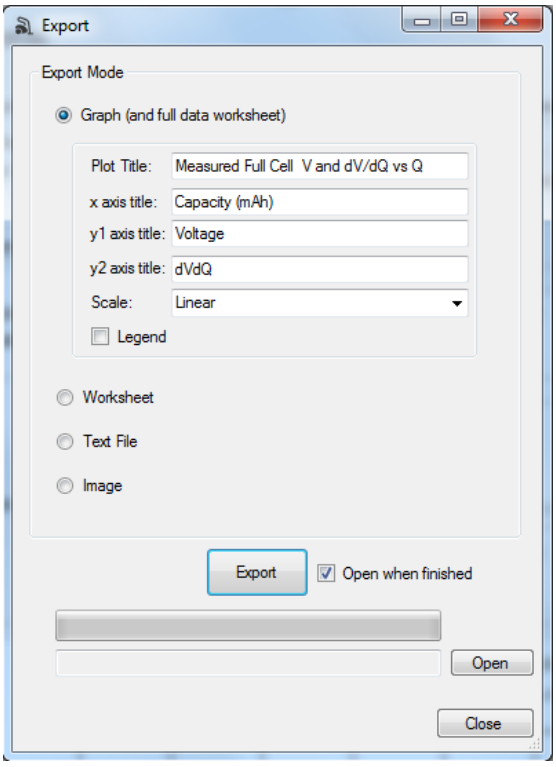
This is where you load in your negative cell reference data. The format is mostly the same as the measured, with a few minor differences. These are:

1. Charging state (i.e. if your reference cell is charging or discharging).
2. Composite (select Part B if this is the second file you are loading in for the electrode and you want it to be a composite electrode).
3. It defaults to the column order being *Voltage,Capacity*. This can be changed (just as before).

C. Positive Reference Cell Data

This is nearly identical to the negative reference cell loading in. It also defaults to the column order being *Voltage,Capacity*.

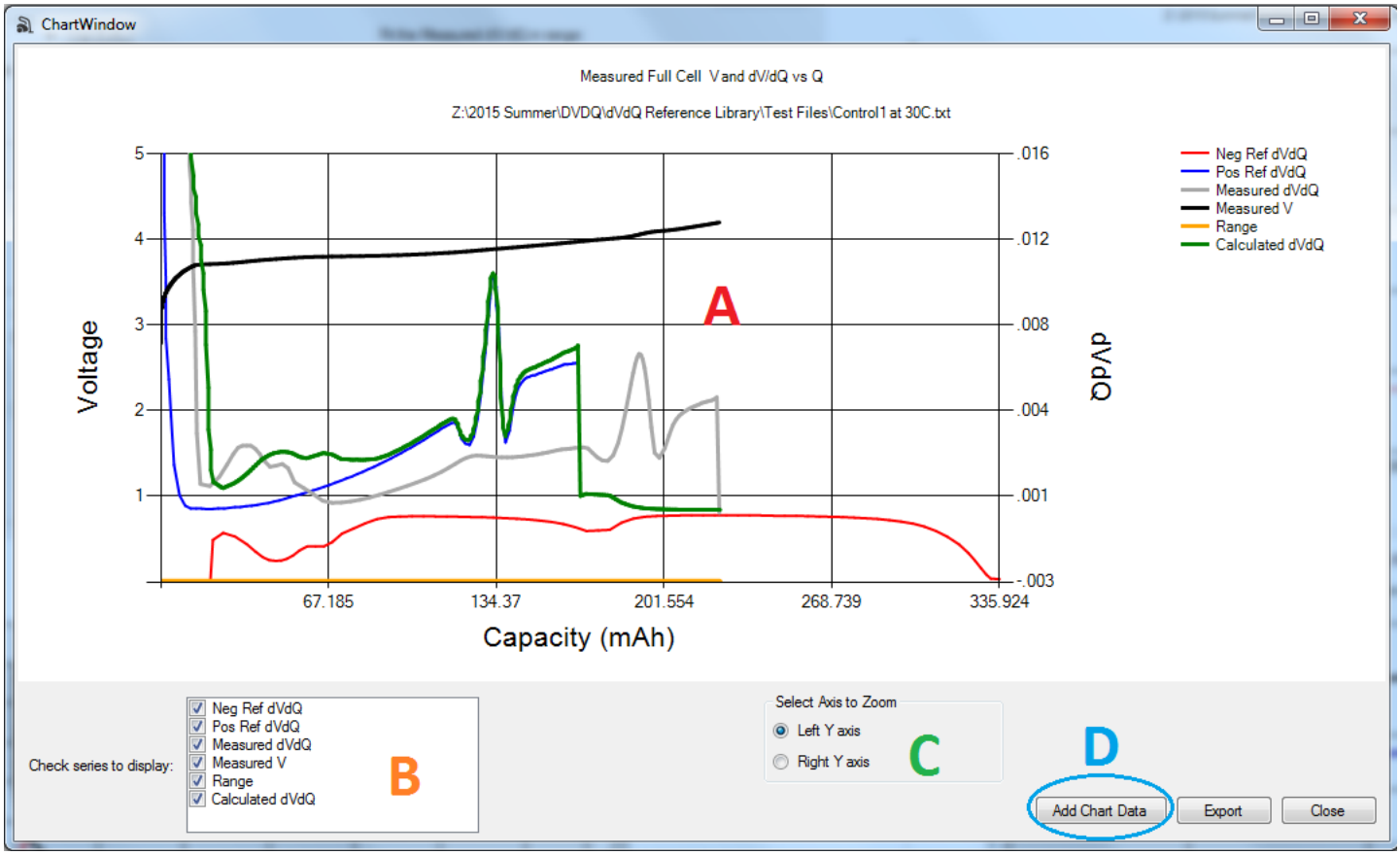
Export Window



This window allows the user to export the data they have. It will appear when the user either selects “Export” from the **Chart Window**, or if the user right-clicks on a chart and selects “Export”. There are 4 different ways to export the data:

1. Graph (and full data worksheet)
   Exports the graph to Grapher 7.0. Does not work if Grapher 7.0 is not installed.
2. Worksheet
   Exports the data to an Excel worksheet. Does not work if Excel is not installed
3. Text File
   Exports the data to a text-file
4. Image
   Exports the data as an image (not recommended)

Chart Window



The **Chart Window** displays any chart, and can be used to examine specific series, or compare data from multiple charts (See D. Add Chart Data Button). It has a few key sections:

A. Chart Area
   This is where the data is displayed. It can be zoomed in (and reset zoomed) just like the other charts in the program.
B. Series to Display
   This is where the user can choose which data to display (and subsequently export).
C. Axis to Zoom
   This allows the user to select between the two Y Axes to decide which one to zoom in on when the user draws a rectangular zoom box (while the other remains constant).

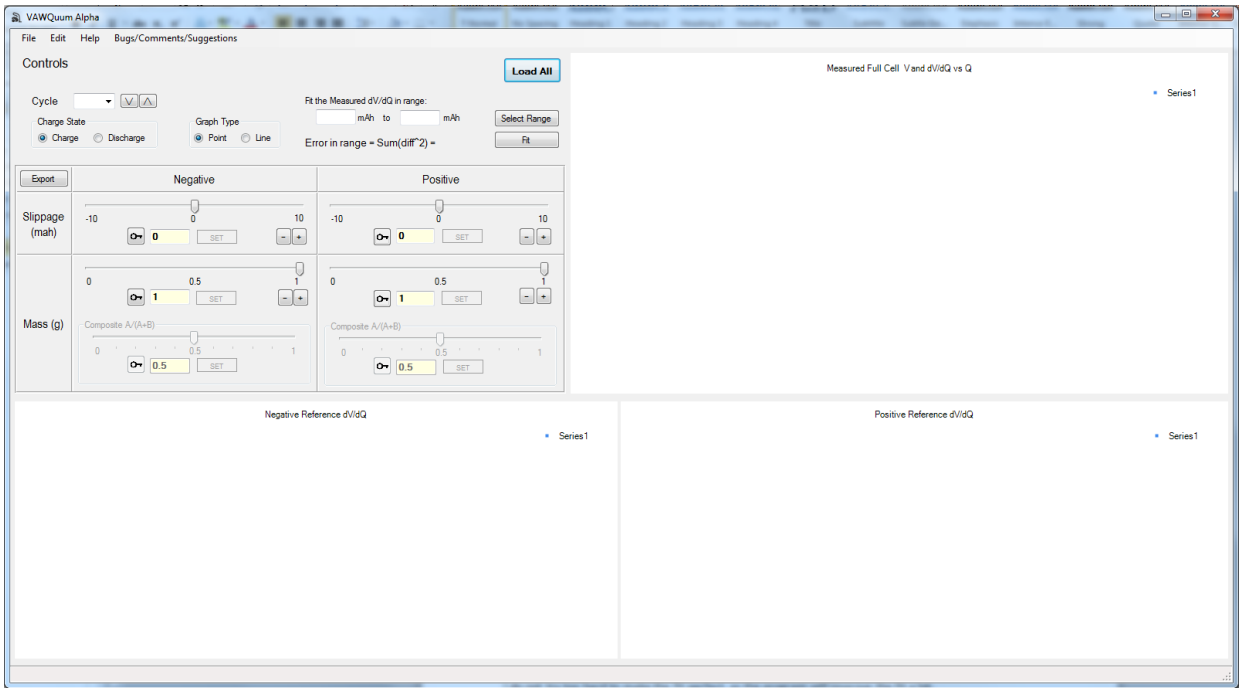
D. Add Chart Data Button

This button allows the user to add another chart's data to the current Chart Window. For example, the user could right-click on the negative reference chart, and select "Open in new window". Once this Chart Window is open, the user can select "Add Chart Data", and then click on the positive reference chart. Now, the negative and positive reference data is on the same chart! It can then be exported/examined together.

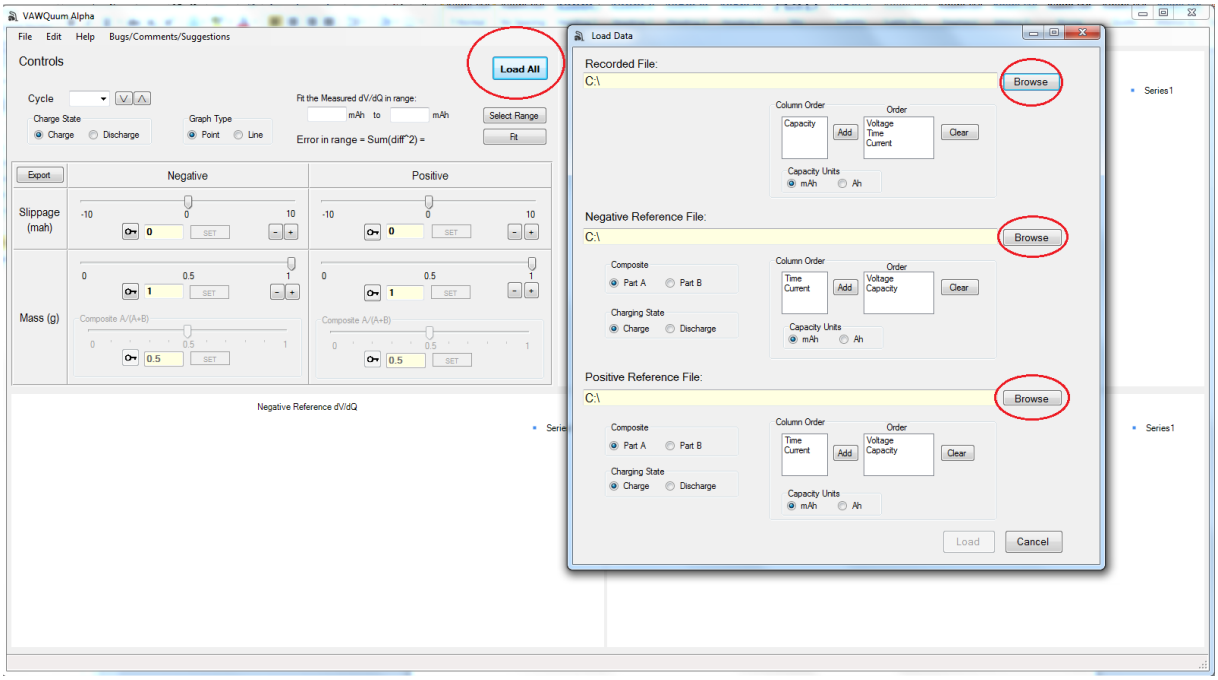
Detailed Sample Run

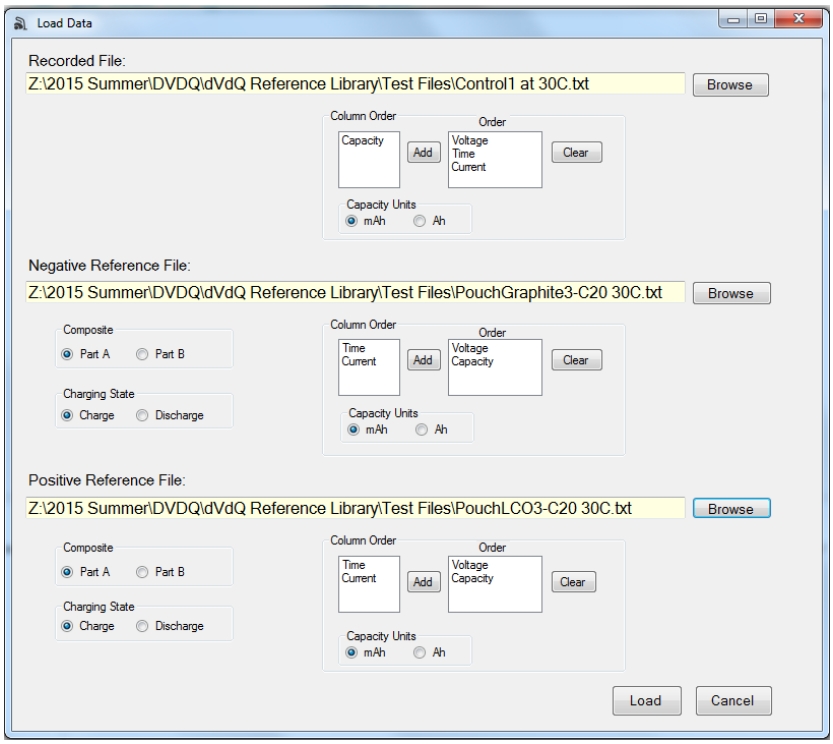
In order to use the fitting portion of this software, the program must have programmatic access to Excel (see: Giving VAWQuum Access to Excel).

First, I will load up the program.

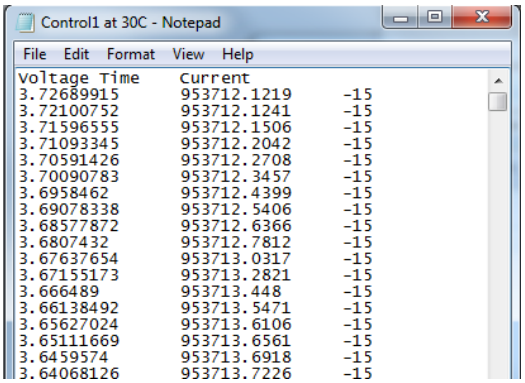


Next, I will choose "Load All" (since I know the three files I want to load). After this, I will select the three files to load. {See **What Files to Load**}.

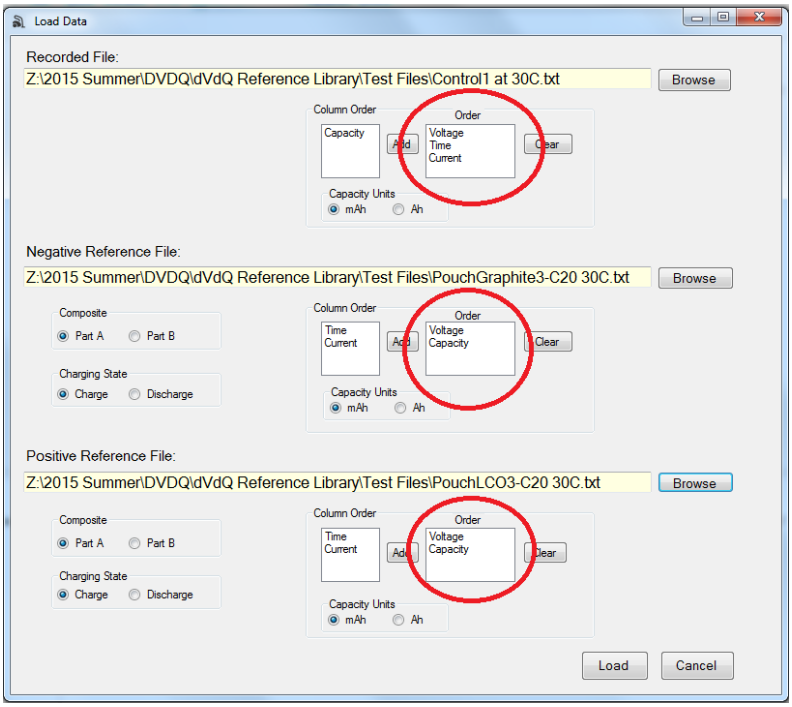




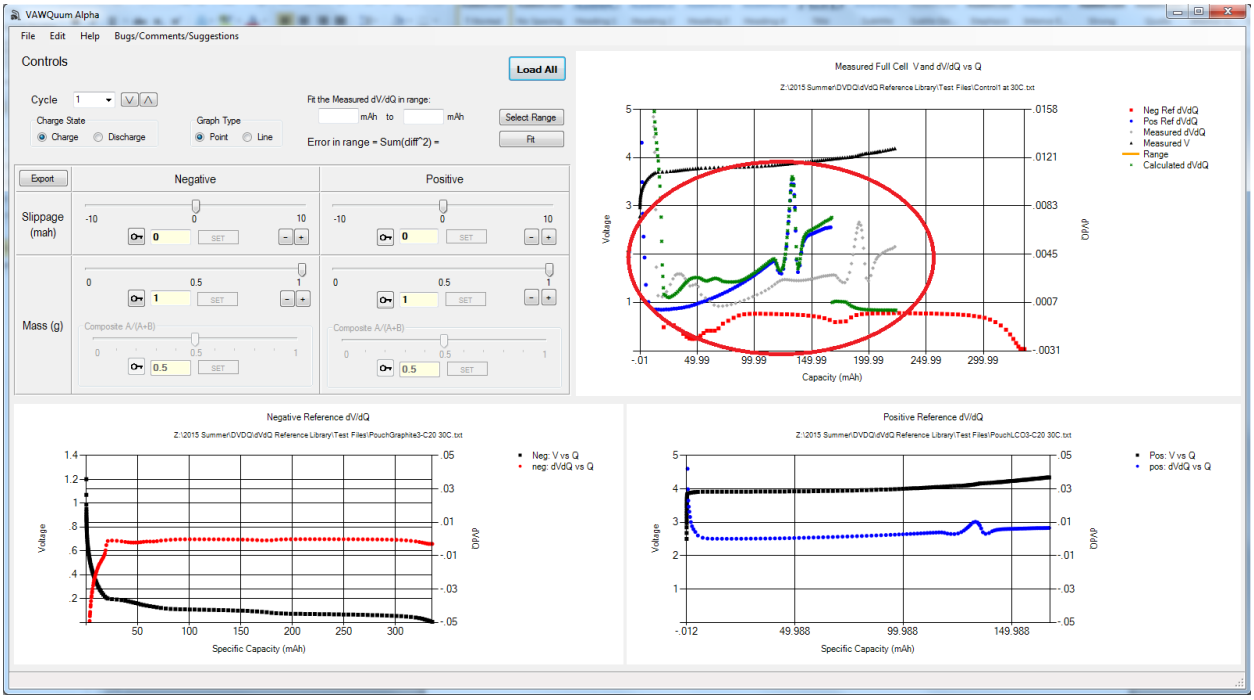
I have forgotten the order of my full-cell file, so I open it in a text-editor and look at the file.



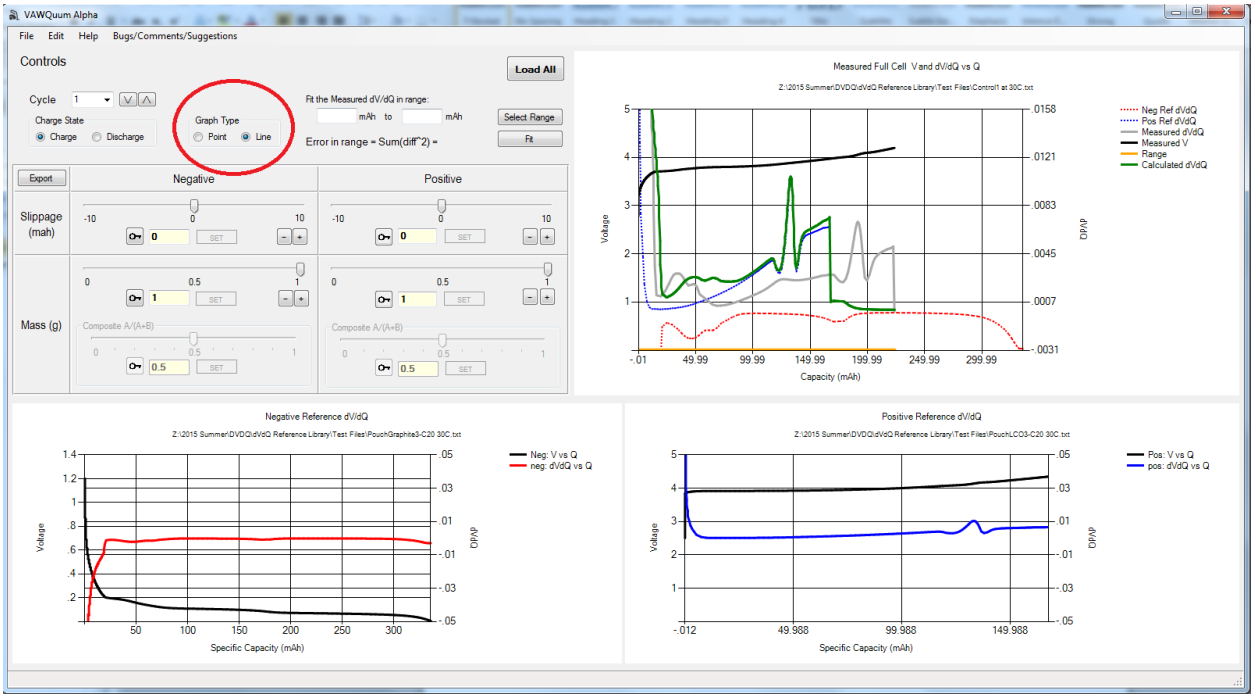
It appears to be Voltage-Time-Current, so my column order selection (see below) is correct. I also know that my reference files are Voltage-Capacity, so my column order selection is also correct for them.



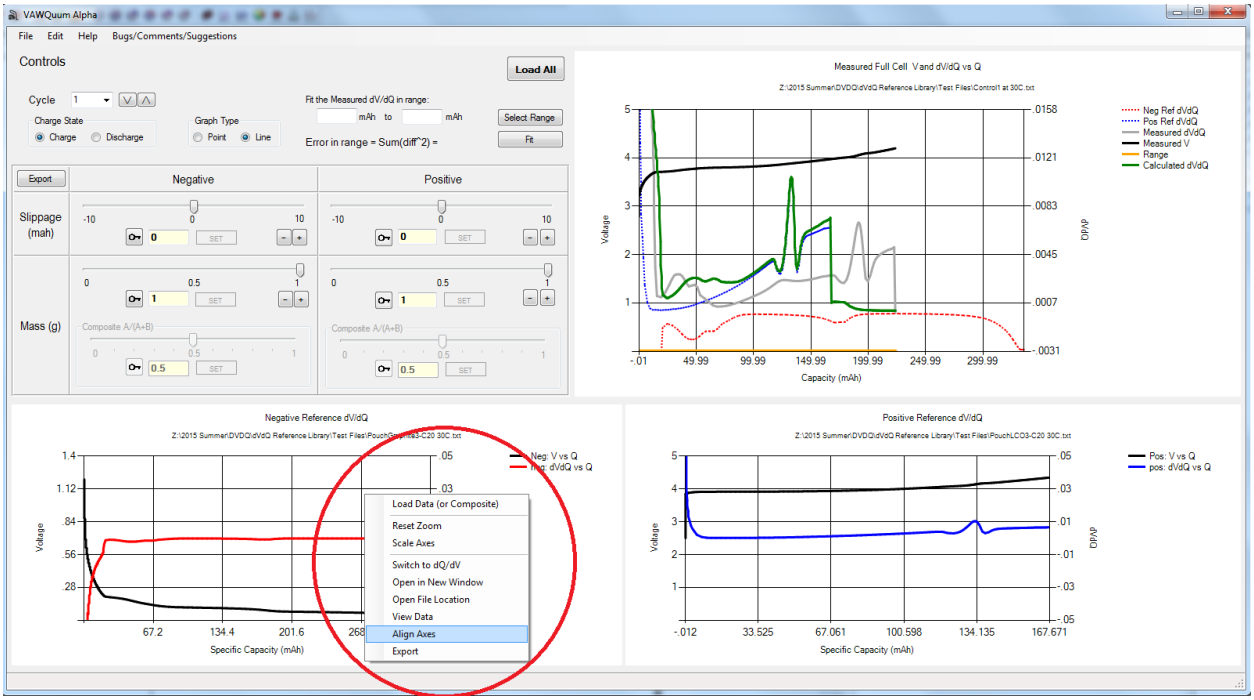
Now I can press “Load”. My data shows up, and I know that I want to fit the calculated dV/dQ vs Q to the measured/full-cell dV/dQ vs Q. This shows up on the full cell chart as trying to fit GREEN to GREY.



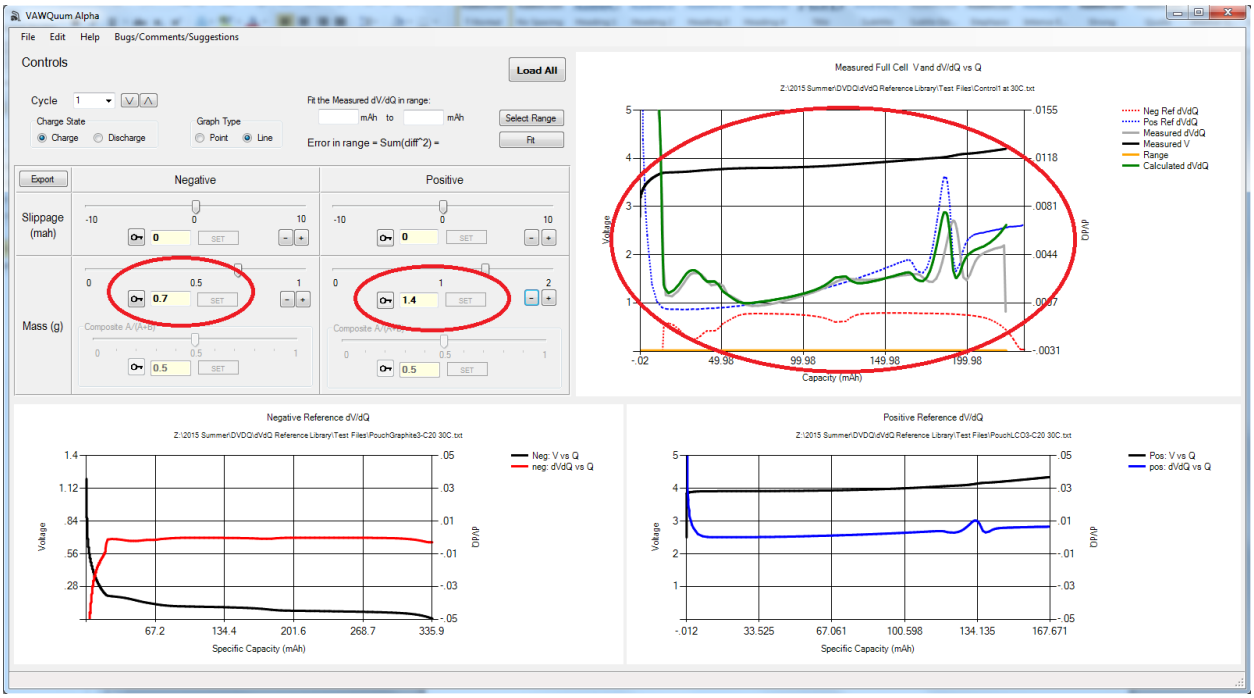
I prefer line-graphs to point-graphs, so I select Line in Graph Type:



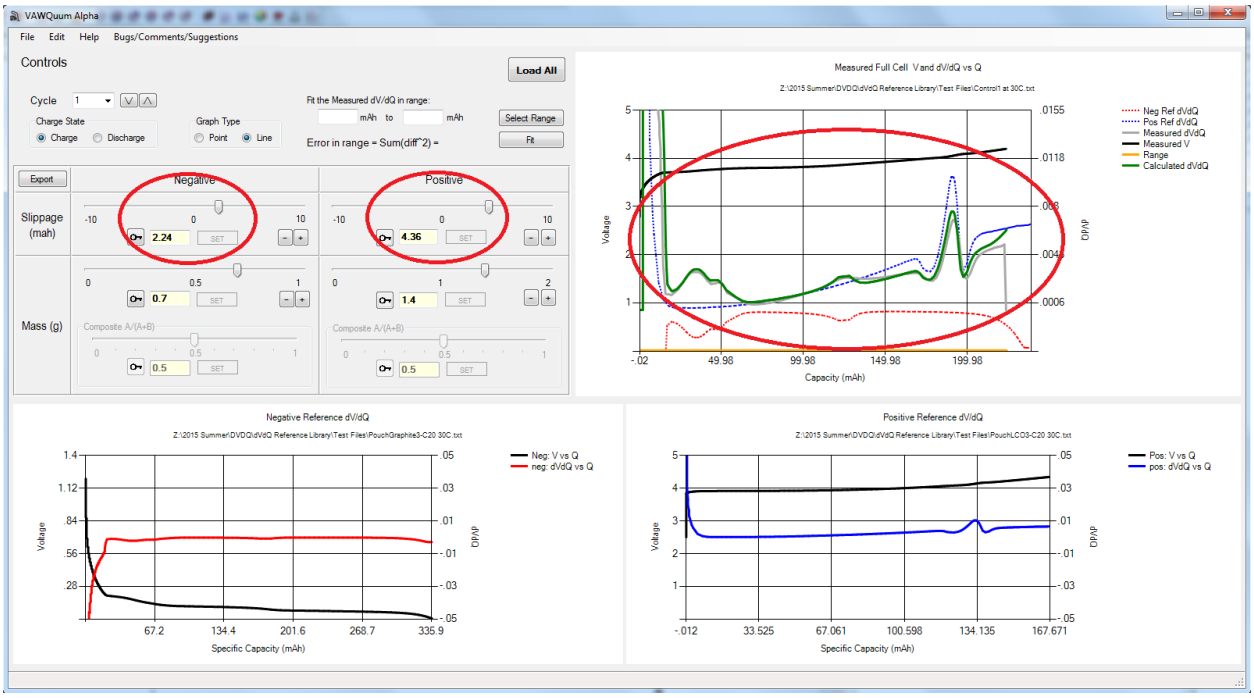
I also notice that the negative reference chart has conflicting axes. I can fix this by right clicking and selecting “Align Axes”.



I now input the negative/positive electrode masses that I think my cell has (roughly), and the fit improves significantly.

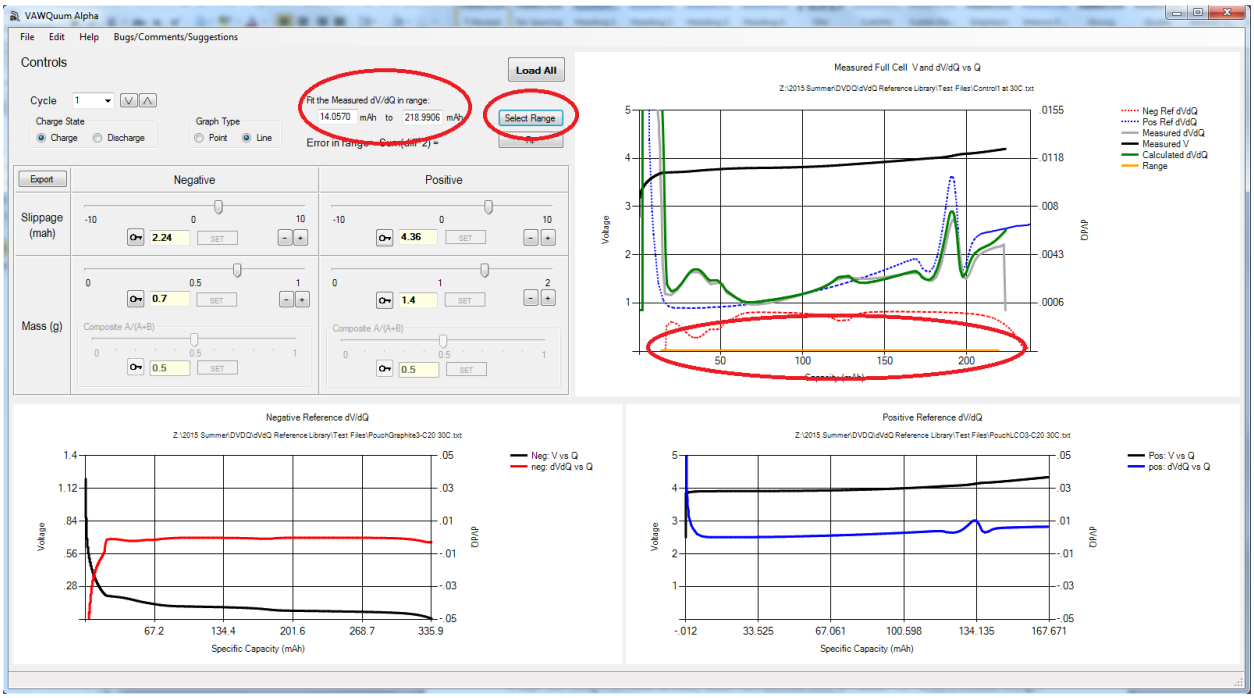


It is still not excellent, so I then try to adjust the slippages to match my curve somewhat.



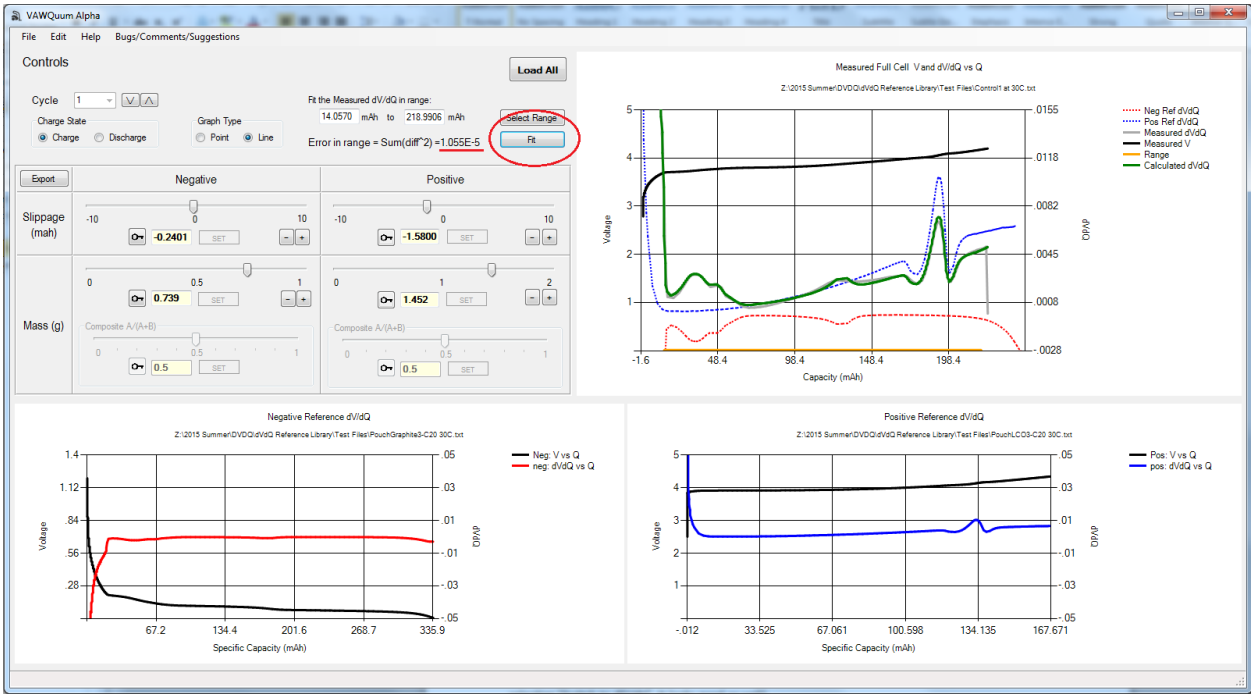
I like the fit, but I do not thing my slippage parameters reflect real life (this is only cycle 1). However, I do not try to improve it any further, as the program will improve the fit significantly.

I select the range I want to fit by hitting “Select Range”, and then clicking the minimum x value I want to fit, followed by the maximum x value I want to fit. It shows up as an orange line on my graph.



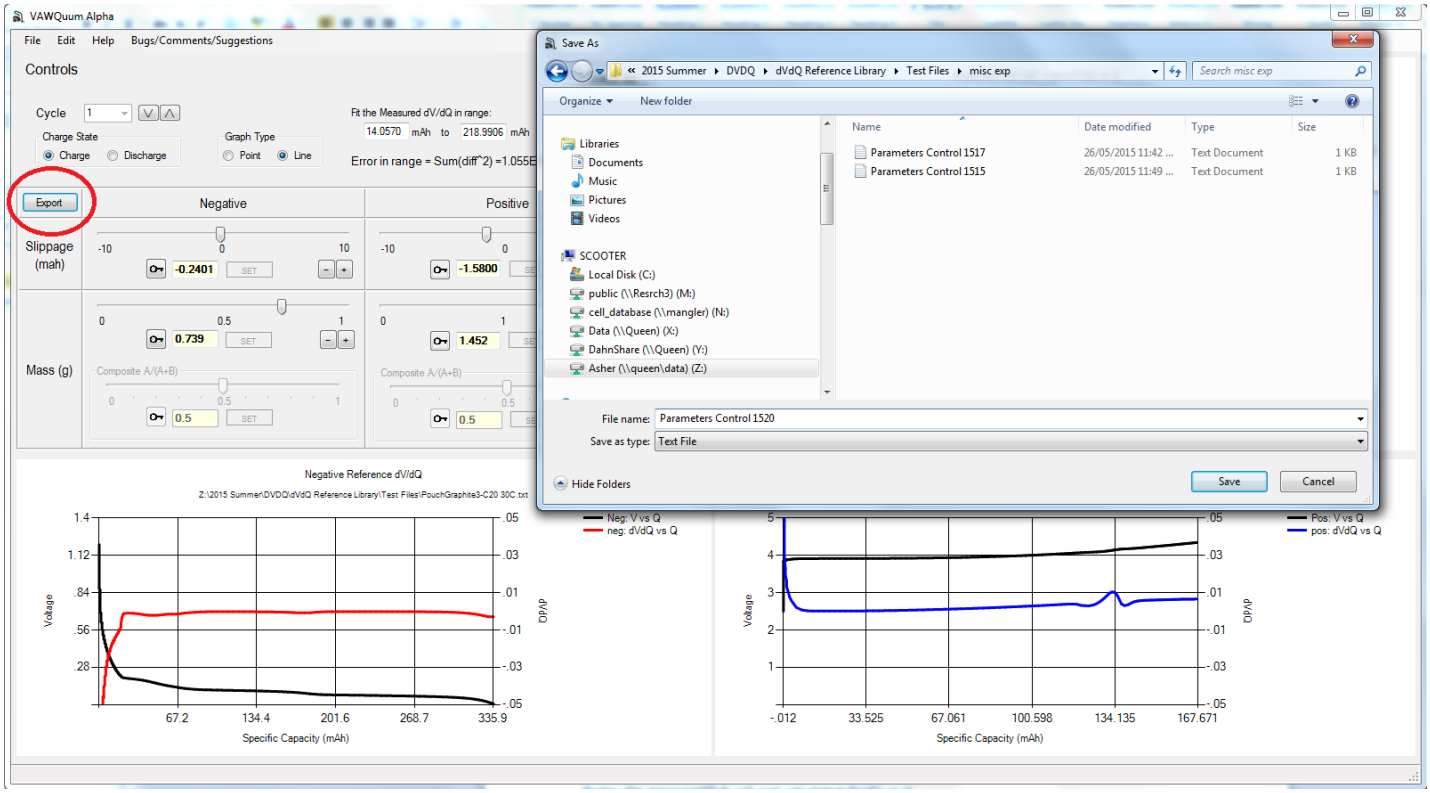
It says I am fitting from ~14 to ~219, which I am satisfied with, so I select “Fit”. Once it finishes fitting, I press it a few more times, just to make sure the fit is consistent. I may have to move one of the sliders

slightly to “refresh” the fit, and make it “snap” into place. It also displays an Error with my fit (depends on amount of points), and is only useful for comparing one fit of Data X to another fit of Data X.

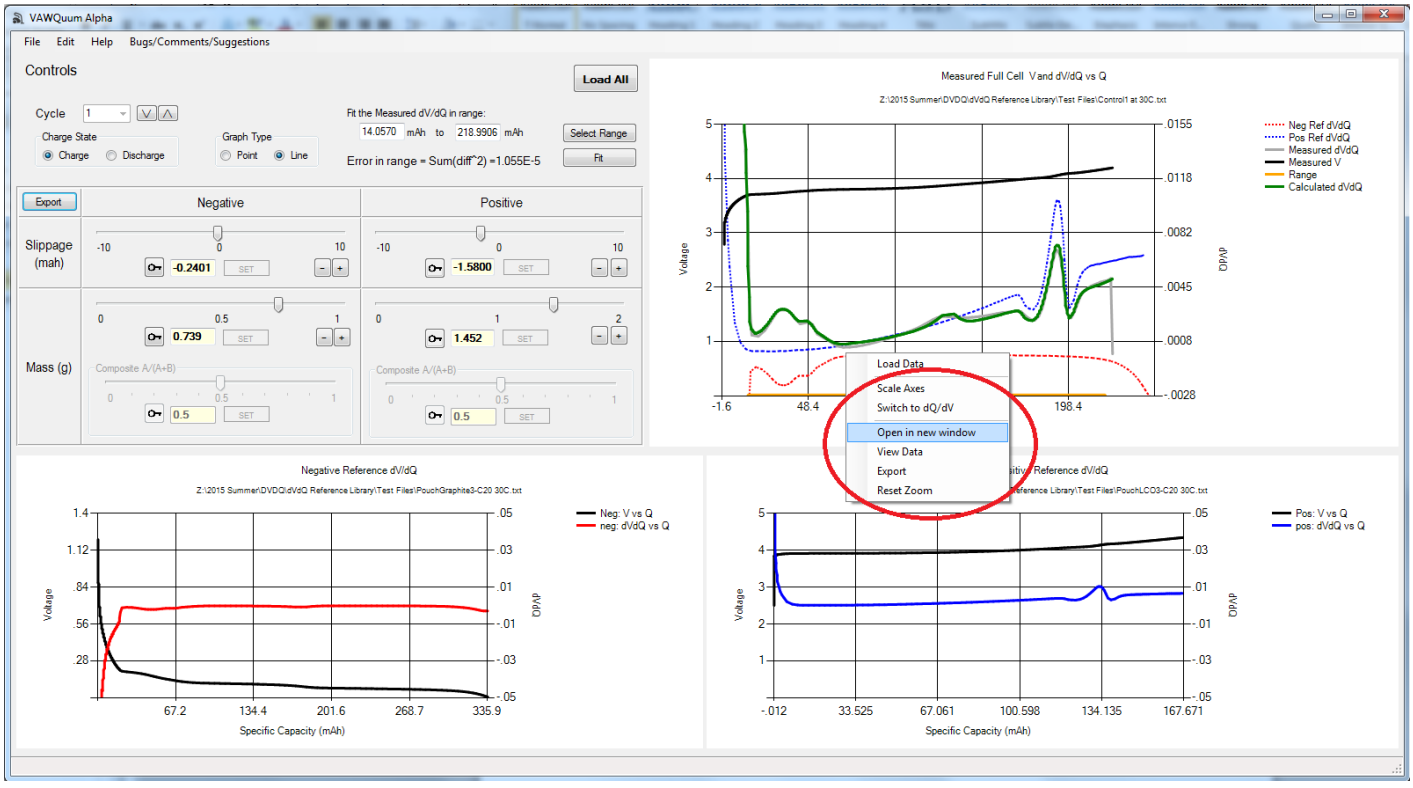


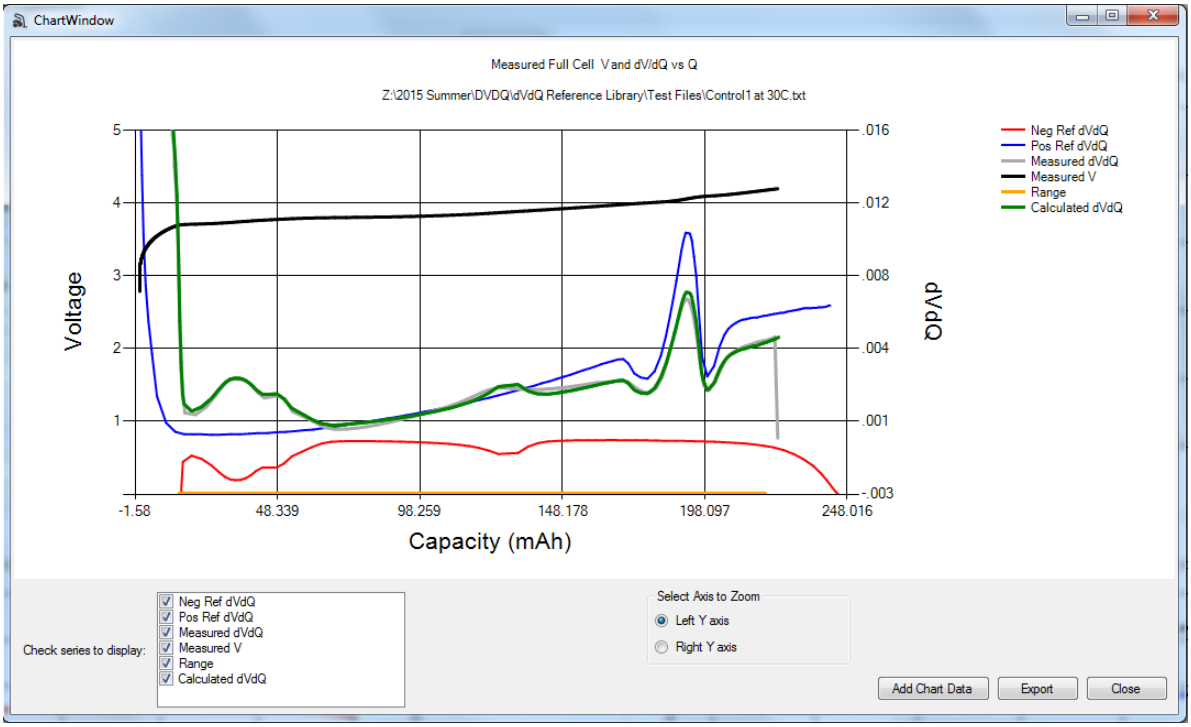
The fit of dV/dQ vs Q looks great, but I also decide to check dQ/dV vs V by right-clicking on the chart and selecting “Switch to dQ/dV”. I have to zoom in a bit (by clicking and drawing a rectangle and clicking again), but I can see that It looks good as well! [Image added after bug fixes]

I press “Switch to dQ/dV” again to switch back. I am fully satisfied with the fit, and I want to save the values of the parameters (the [positive, negative] [mass, slippage]). So I click the “Export” button, and choose where to save the text file.

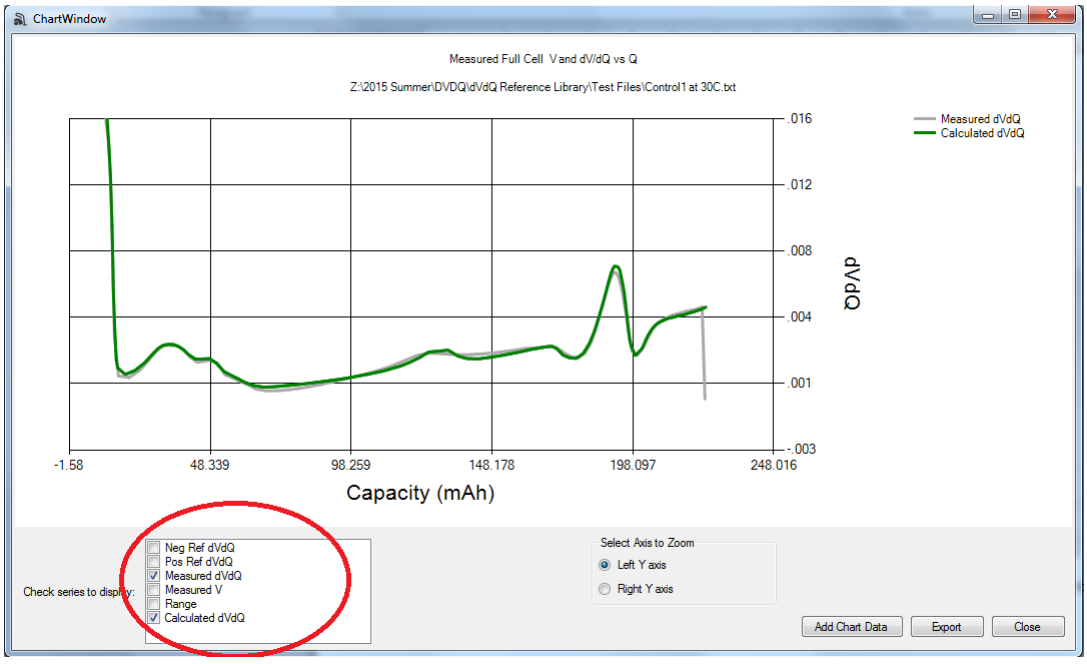


I also want to save a graph of the fit, but I don't want all of the series that are currently present on the full-cell chart. Thus, I right-click, and select "Open in new window".

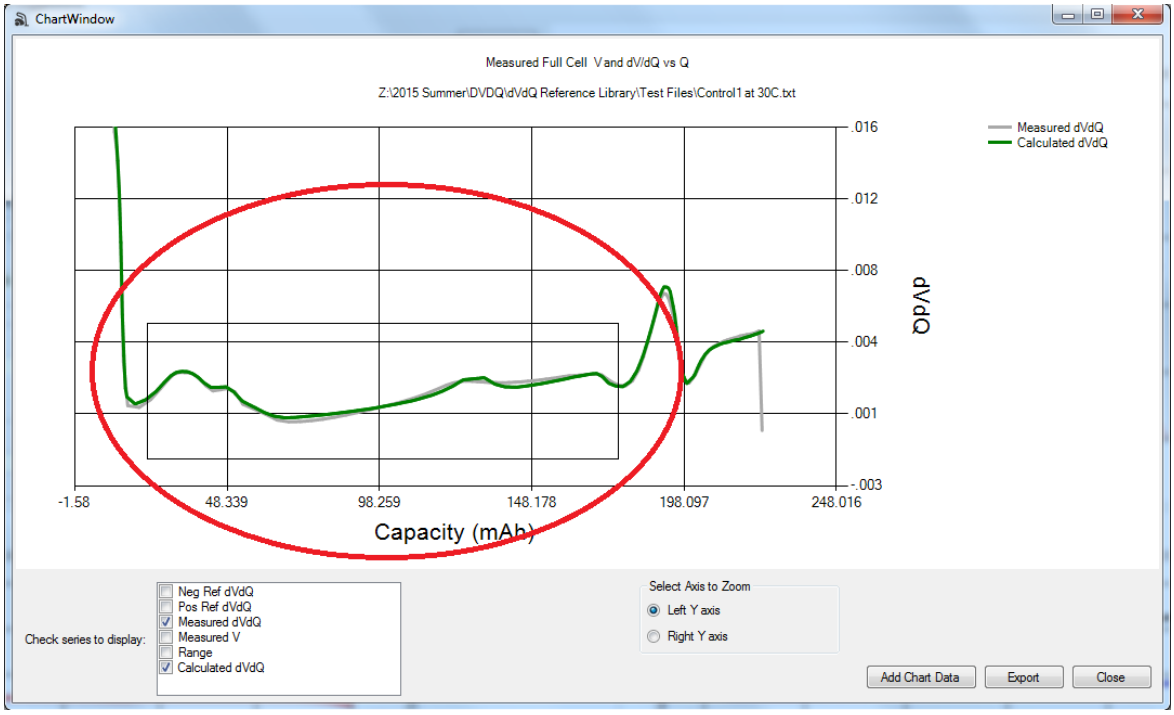




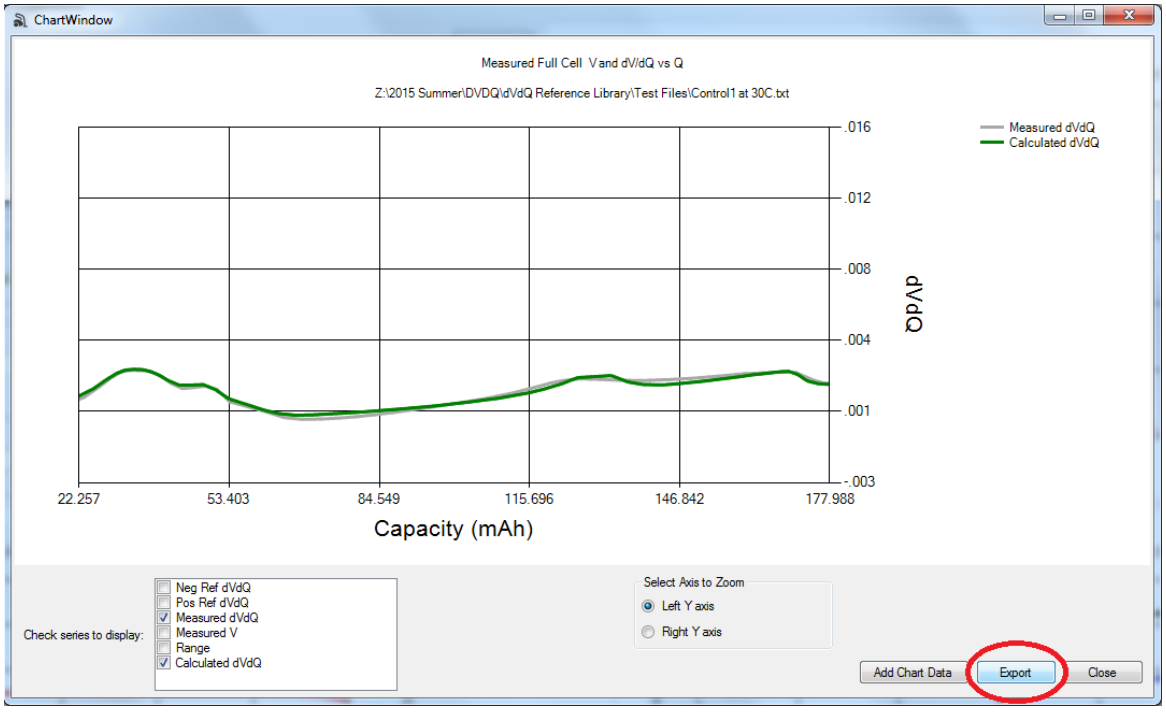
Now that this window is open, I can choose which series I want to display. I decide that I only want to display the measured/full-cell and calculated dV/dQ vs Q.



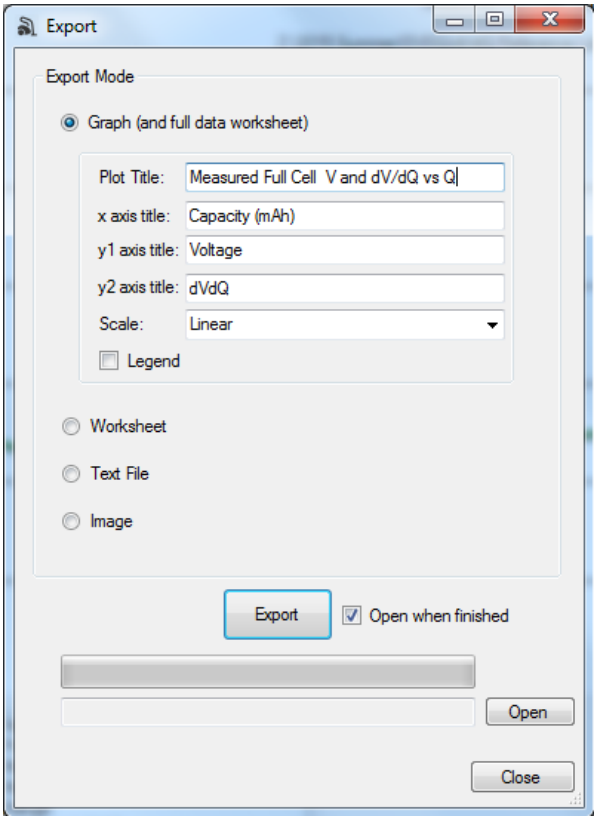
I want to zoom in on a specific region, so I click on the graph to start a zoom-rectangle, and then click again when I am finished.



I like the graph I have, and I want to export it to Grapher. So I click “Export”.



I choose the titles that I want, and choose Grapher, and then hit “Export”.



Once the Export is complete, I have everything I want. [Image put in after bugs fixed]

File Loading Guide

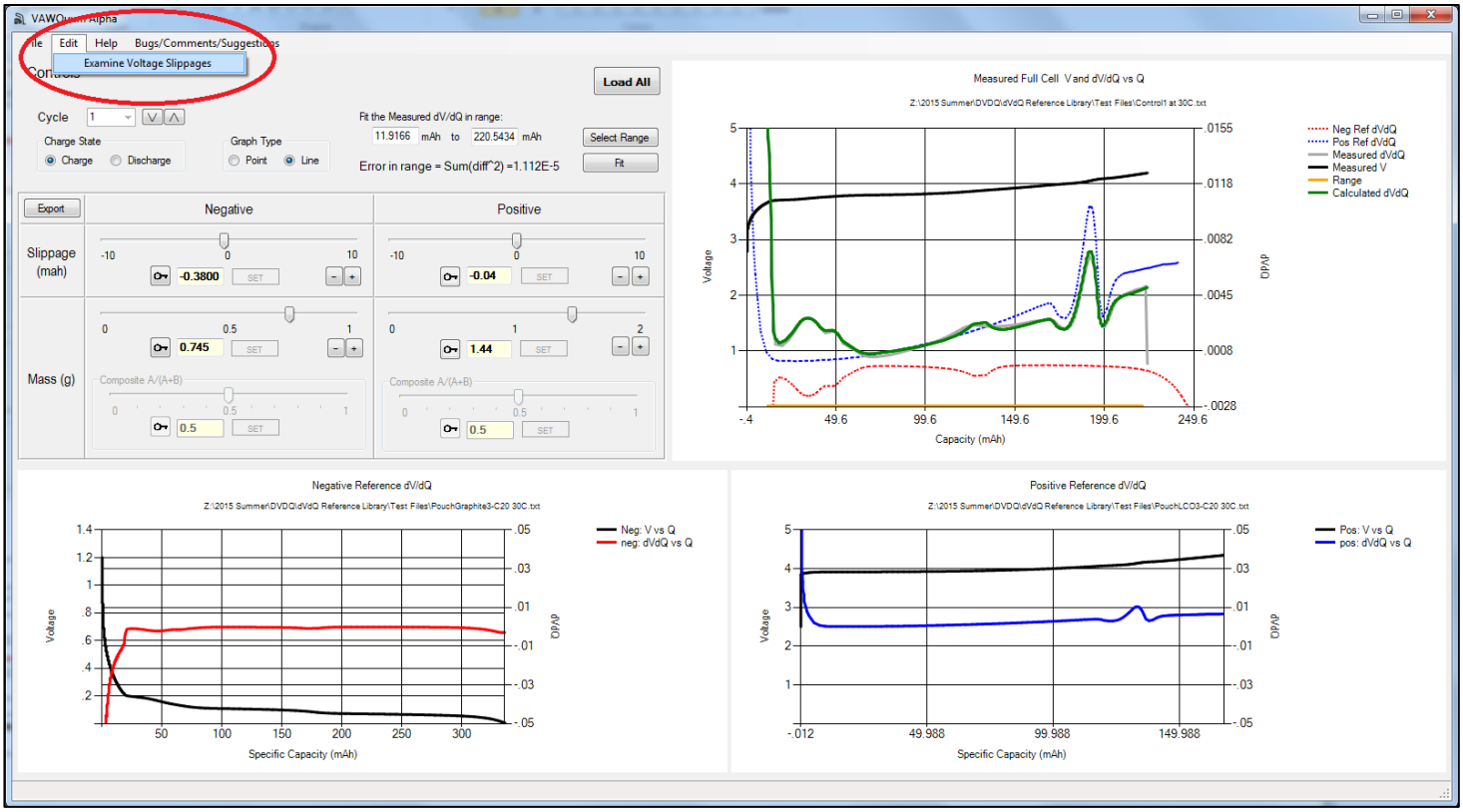
This software takes regular text files that are either tab-delimited or comma-delimited. The files are allowed to have a header (e.g. Voltage,Current,Time), but cannot have more columns than the data (e.g. C:/uselessFileName,Voltage,Current,Time). Basically, the header must match the data.

Since we want to know the dV/dQ of the cell, we need to know the voltage and the capacity. There are two ways that the program does this. Either it reads the voltage and the capacity directly, or it reads the voltage, the current, and the time, and it calculates the capacity. That being said, the files being load MUST either contain {Voltage, Capacity} OR {Voltage, Time, Current}. Cycling information tends to be more accurate when {Voltage, Time, Current} is loaded in (as it is easier to tell exactly when it is charging/discharging, and one does not need to worry as much about noisy voltage).

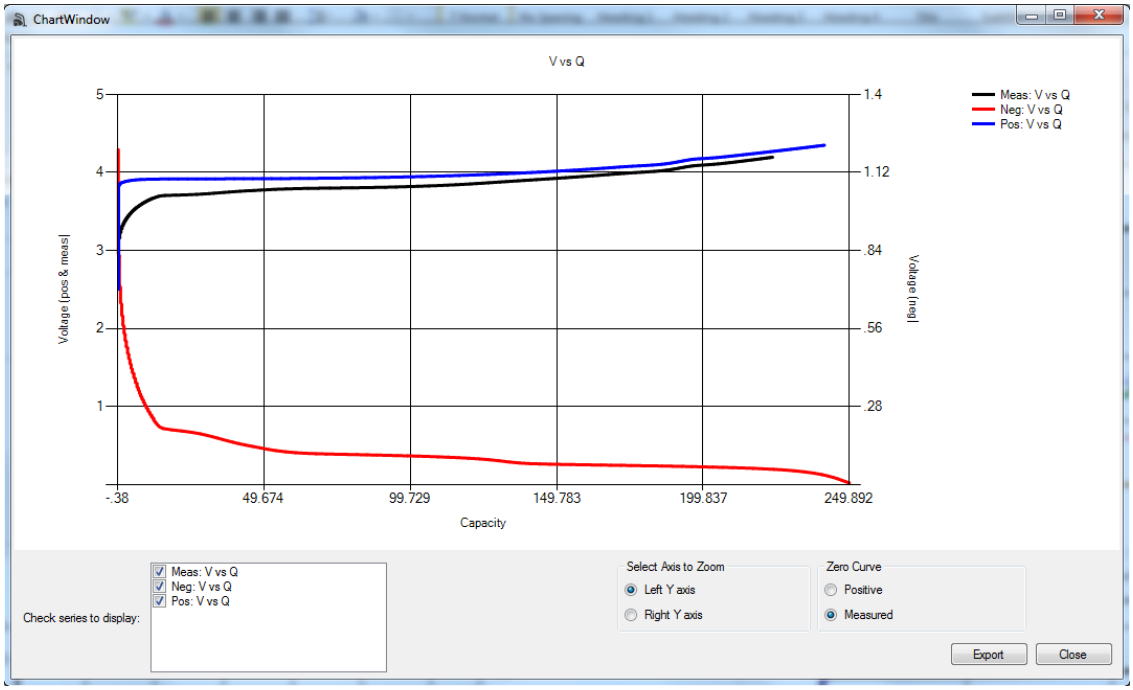
Please contact either Asher Wright (Asher.wright@dal.ca) or Jeff Dahn (Jeff.Dahn@dal.ca) if you would like sample files to test/examine.

Slippage Analysis Feature

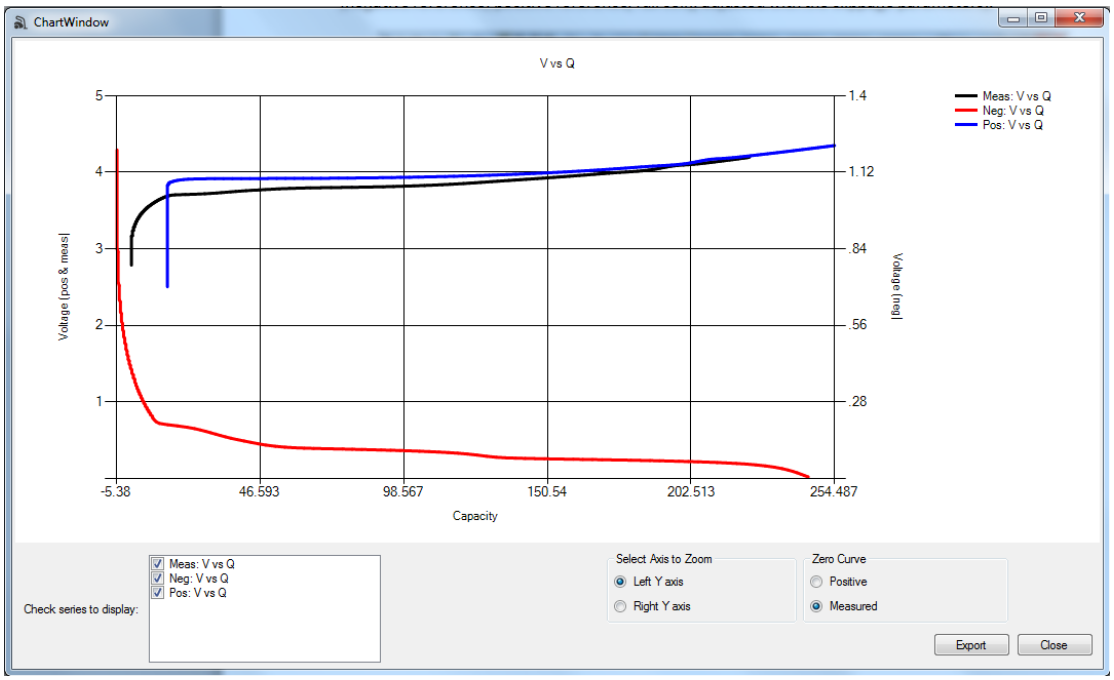
One feature that was added to add to the overall utility of the program is the Slippage Analysis feature. This feature can be accessed (after loading in the appropriate data) by right-clicking on Edit, and selecting “Examine Voltage Slippages”.



This takes the user to a modified Chart Window that displays the three measured voltage curves (negative reference, positive reference, full cell), adjusted with the slippage parameters).



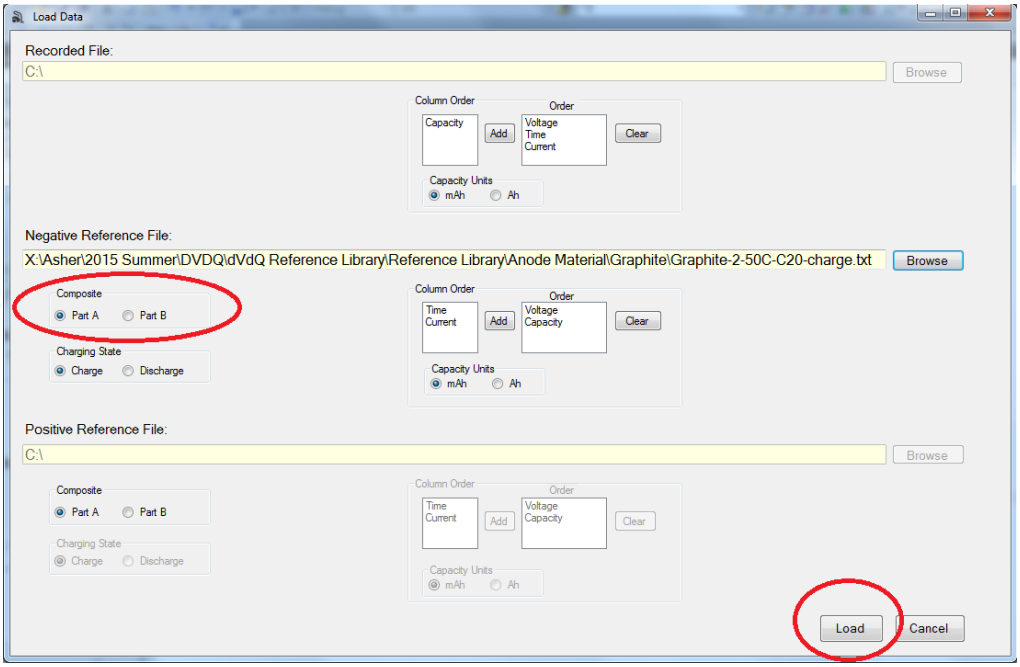
In the above example, the slippage values are low (the cell is on its first cycle), so each curve appears to start at the same point. However, when the slippage values are increased, the graph can look very different (see below). This chart can be used to examine the slippage of the full cell.



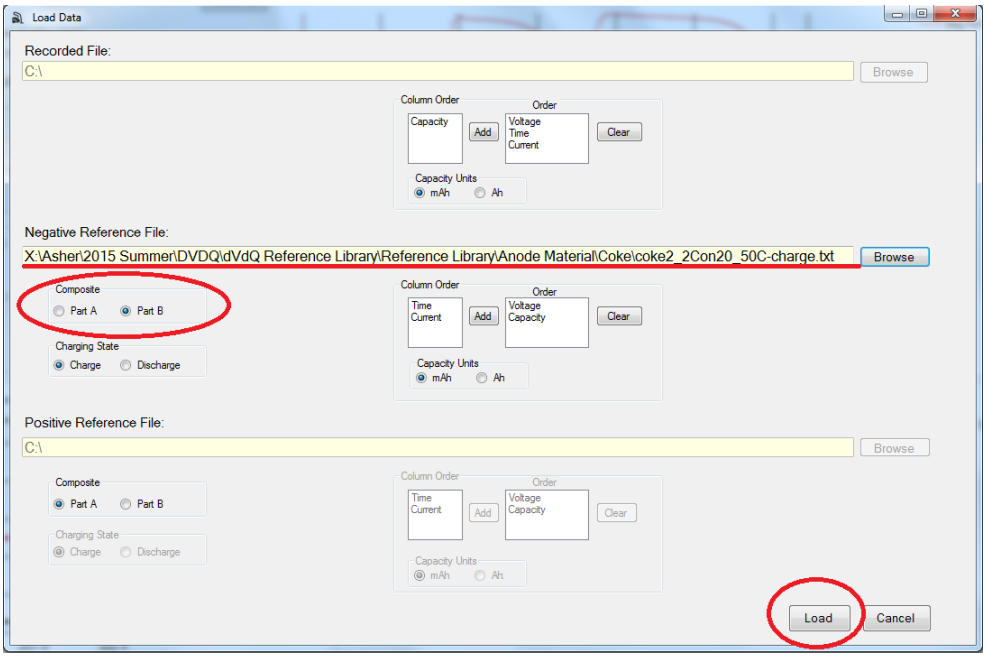
Composite Electrode

This software can also be used to fit cells with composite electrodes (cathode/anode electrodes composed of two materials).

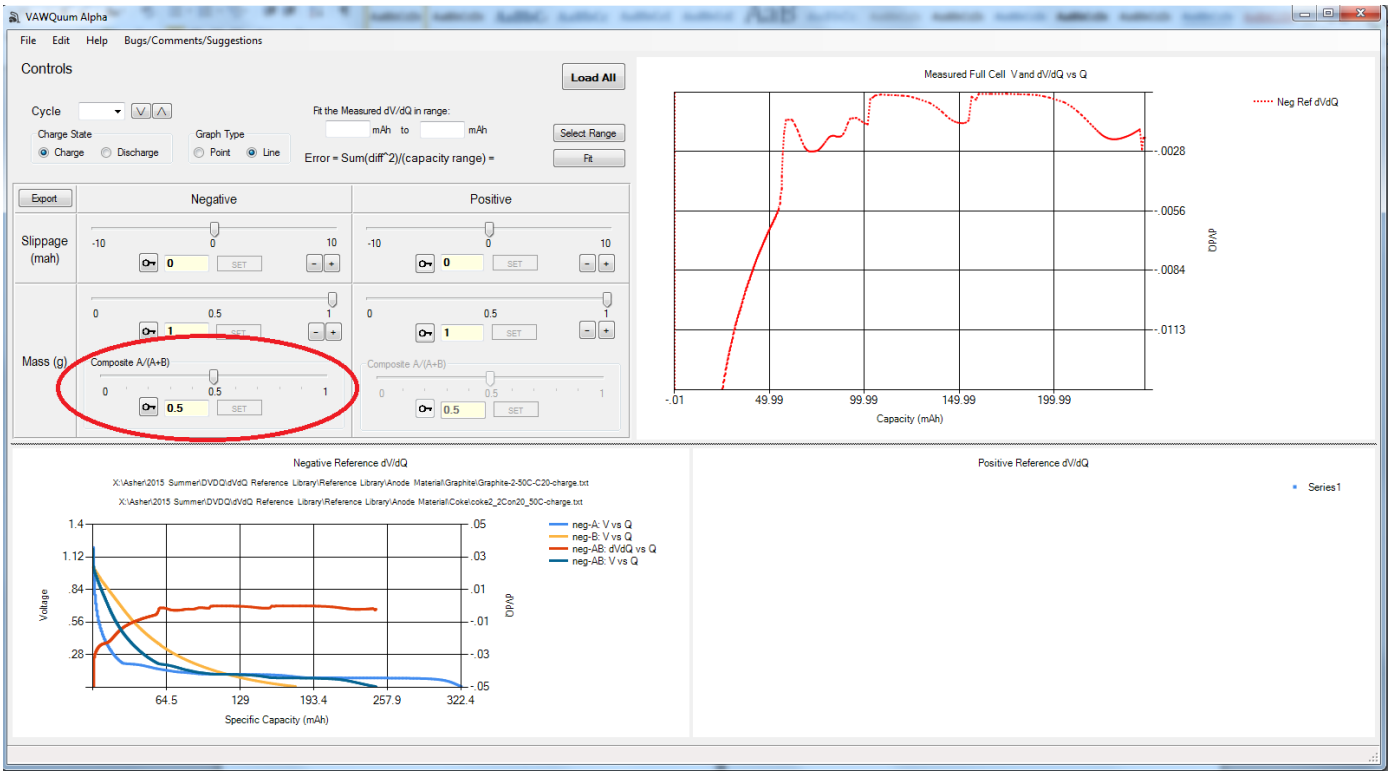
First, load in the first component of your electrode (here we do this with the anode), just as you normally would.



Next, right-click on the same chart and click “Load File” again. This time, select the second component. The first file’s path will be originally written in this box, but you can overwrite this (it will not remove the file from the program). Now, however, **make sure you check the “Part B” radio-button.**



After clicking “Load”, the two components should be shown on the same chart (whichever electrode you are loading). Additionally, the slider for Composite will be enabled for the electrode. This allows you to change the fraction of Part A that is in the electrode, and see how this changes the dV/dQ vs Q.



Moving this slider to 1.0 will mean it is completely Part A (and should be the same as if you only loaded in the Part A file). Moving it to 0 will mean it is completely Part B (and should be the same as if you only loaded in the part B file).

Note that moving the slider too quickly can result in the slider being in a location that is not representative of the actual fraction value. To set specific values (accurately), please use the box and press "Set".

From here on, you can use the program just as you would normally. The only difference is the fraction of Part A in the electrode. This parameter **must** be adjusted by hand, **and is not fitted by the program.**

Fitting Method

This program uses Microsoft Excel and the Solver Add-in to fit the data. The program writes all of the data to excel, and then writes the formulas to find the calculated dV/dQ in the appropriate Excel cells. After this, it writes a Macro that tells Excel to use Solver to minimize the error between the calculated dV/dQ and the measured dV/dQ by changing the four parameters (positive mass, positive slippage, negative mass, negative slippage). This Macro is then run, and the final parameters are read off of the Excel worksheet. This is why it is necessary for the user to enable the Trust Setting in Excel (see **Giving VAWQuum Access to Excel**).

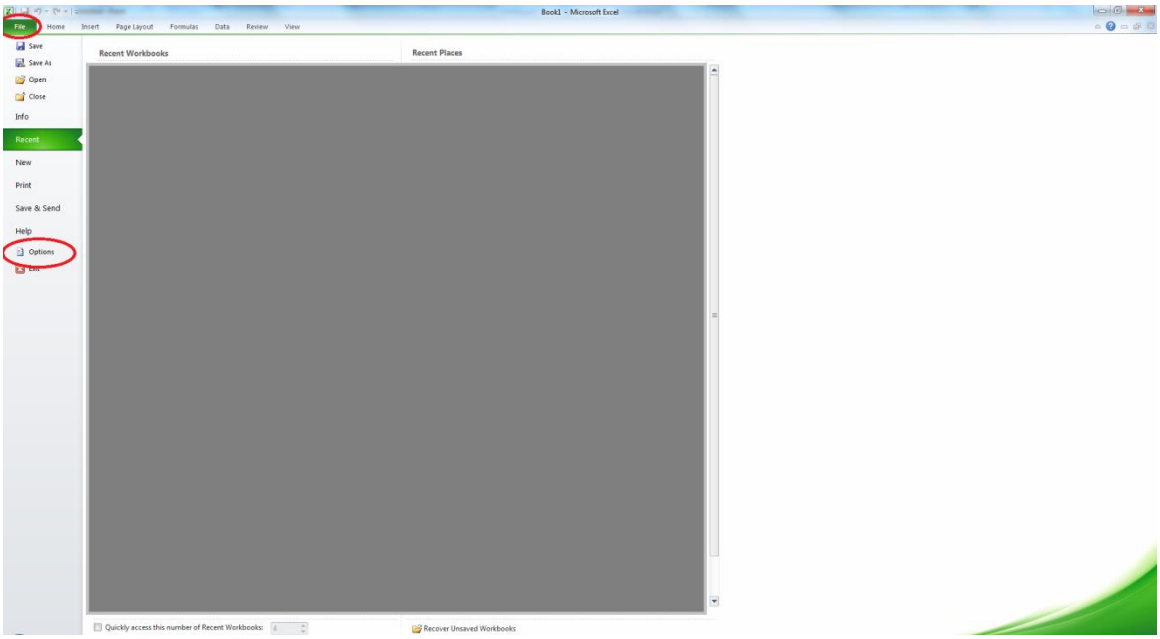
This method of fitting was chosen because it is already optimized, and much faster than any similar algorithm I could write myself.

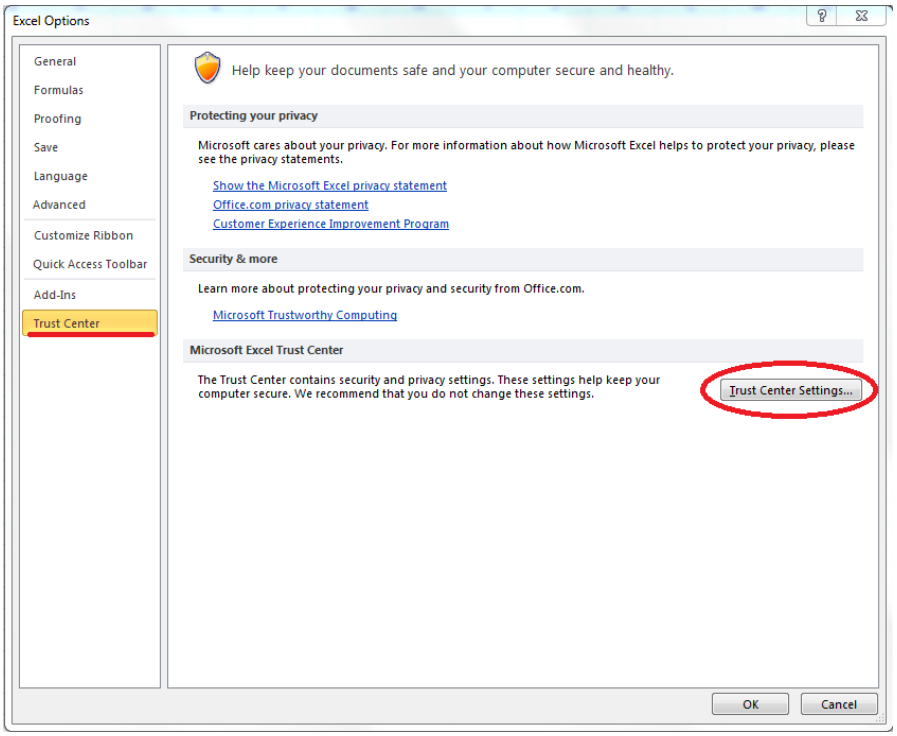
Giving VAWQuum Access to Excel

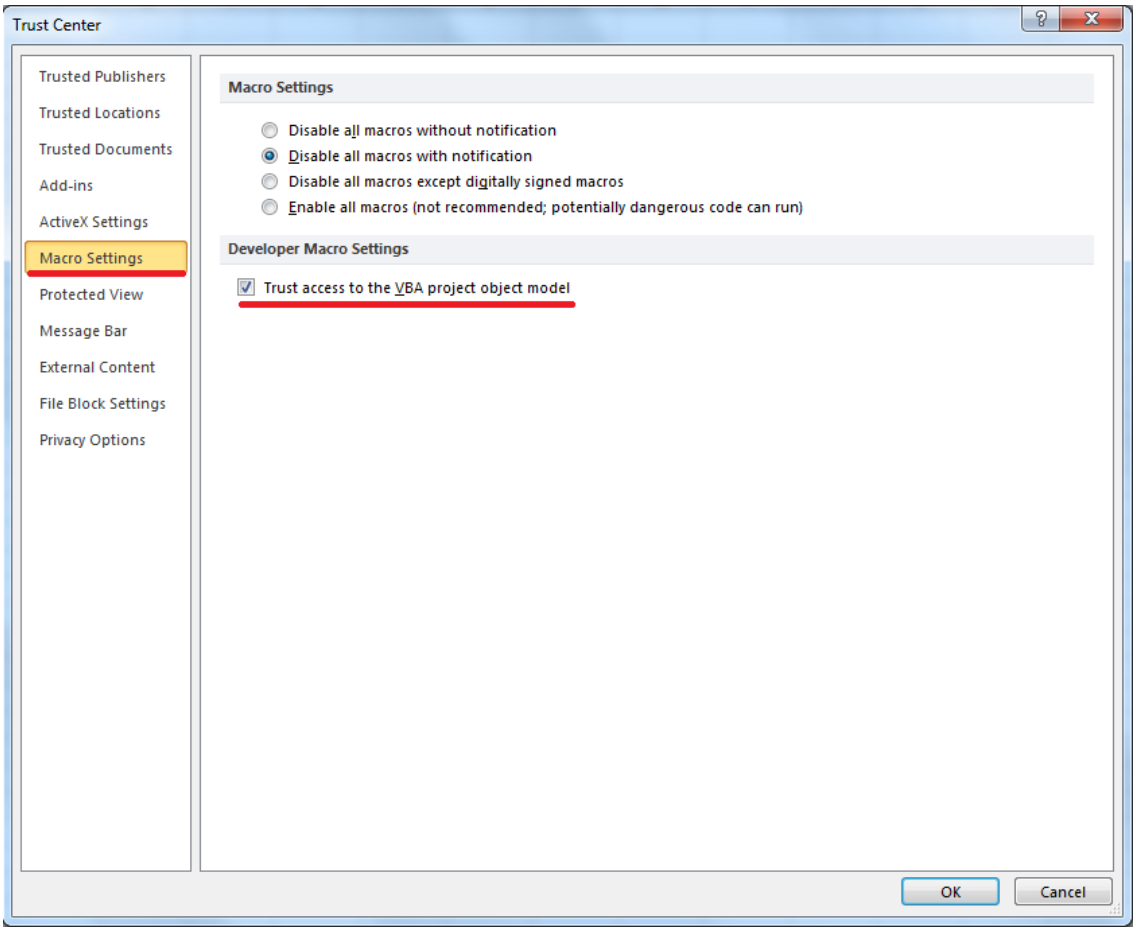
This program is powered partially by Excel, and as such, needs to use it to run fully (see **Fitting Method**). Thus, it is necessary to enable access to Excel. To do this, go to:

Excel>File>Options>Trust Center>Trust Center Settings>Macro Settings> Trust Access to the VBA Project Model

This can be seen below:







Sometimes, when you first enable this, it is automatically disabled after the first use of the program. Simply re-enable it and the program should be able to operate correctly.