dV/dQ Analysis Tool Documentation

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**System Requirements:**

1. Computer must be running Windows, macOS, or Linux (there is a different version of the software available for each operating system)

2. Computer must have Anaconda installed

**To run the application:**

1. Navigate to the downloaded application folder in your file explorer

2. Double click on the file entitled “run\_dVdQAnalysis\_win.bat” if you are on PC, and “run\_dVdQAnalysis” if you are on Mac or Linux.

3. You should see a command line window appear on your screen. If it is your first time running the application, it may take some time to install he required packages. Eventually, your default browser (works best when Chrome or Safari is default), with the application running as a webpage. Despite the app being a web tool (ie: it is run using a browser), it is not dependant on an internet connection as it is being run locally on your computer.

**To load a file:**

1. Click the expander entitled “Load files here”.

2. You can drag files or select them from a directory on your computer by pressing “Brows files”. If your intentions with the app are simply to plot V vs. Q for the various cycles in your file, all you need is to load the cycler data file. If your intentions are to perform dV/dQ analysis, you must also load two reference files. When you are finished loading files, press the “ - “ icon at the top right of the expander to close the file selection window.

**Selecting a file path (Windows and Linux only):**

If the user navigated to the path selection expander, and uses the tool to select a file path, then every file that is outputted by the software will be saved to this directory. If no path is selected, the directory in which the application file is save will be the default directory.

**Performing dV/dQ analysis:**

This program gives users the option of either performing dV/dQ analysis on an individual cycle from the imported file, or fitting a calculated dV/dQ curve to a range of cycles. The user can navigate between these two options by selecting it in the left sidebar under the header “Fit over range of cycles or individual cycle?”

**Individual Cycle:**

After loading the file and selecting “Individual”, the measured and calculated dV/dQ curves from the first cycle will be automatically plotted. The constants that are used to compute the calculated curve can be found int he expander in the left sidebar entitled “Adjust active mass and slippages”. The user can manually adjust the values using the number inputs. The user can also select the cycle they wish to analyze using the slider located in the left sidebar.

*Selecting C-Rate:*

The user can change the C-Rate which will in turn change the cycles that are available to select using the slider (they depend on the C-Rate selected), however for dV/dQ analysis only C-Rates of C/20 or slower are available.

Fitting the cycle:

*Automatic fit:*

To automatically fit a calculated curve to the individual cycle, the user can do so with either a brute force fit, least squares fit (which is less likely to produce an accurate result, but is typically computationally less intensive), or a combination of the two where the brute force fit serves as the initial guess to the least squares fit. All of these fits are performed using the three buttons located above the plot. Whenever a fit is performed, the actives masses and slippages in the left sidebar are adjusted to the results of the automatic fits, and the user can then further adjust them manually even after an automatic fit has been performed.

*Adjusting the brute force fit:*

To adjust the grid over which the brute force fit algorithm operates, whether it be to adjust the range or the precision, navigate to the “Adjust brute force fit parameters” expander in the left sidebar.

*Fitting over a range:*

To fit the curve specifically over a capacity range, navigate tot he “Fit over specified range” expander to select the capacity range. If the user selects the “Fit over specified range” checkbox, a grey transparent window will appear on the plot to indicate the range over which the fits will occur.

*Locking parameters:*

To lock a parameter (meaning it will not change during an automatic fit), navigate to the expander located about the plot entitled “Locking fit parameters”.

*Smoothing data:*

The measured data is smoothed by default, however this can be adjusted (either to turn it off or adjust the smoothing) using the “Smoothing measured data” expander.

**Range of Cycles:**

When “Range of cycles” is selected, the user can still select different cycles to have their dV/dQ curves plotted, however the calculated curve is no longer plotted because the focus of this functionality is not on individual cycles, but on a range of them.

The controls are largely the same as with the individual cycle section with some key differences.

*Fit over specified range:*

The “Fit over specified range” expander is now devoted to selecting the range of cycles to fit, and the capacity range to fit over for each cycle. The slider in the expander is used to select cycles, and when the user selects the “Adjust Range Fit Bounds?” checkbox, the available controls change.

After pressing the checkbox, the user can select either the first cycle or the last cycle in the range to input their respective capacity ranges. When “First Cycle” is chosen, the first cycle will be plotted and the user will be given the opportunity to decide on the capacity range that should be used to fit this first cycle. The same can be done for the last cycle, and what the algorithm does is linearly interpolate values between the two capacity ranges such that the fit window changes as each cycle within the range is fitted. This will result in a fit window moving with the features the user wishes to include in the fit as features move with cycle number.

The parameters and shift loss that resulted from each fit within the range will be outputted to a .txt file located in the selected file path (or the application directory by default). The user can input the name of this file using the text field, and they can decide on a header for the file, which will be the first line of the file, using the other text field.

*Plot parameters vs. cycle number:*

If the user navigates to the “Plot parameters vs. cycle number” expander, they can select the checkbox which plots all four parameters vs. cycle number after the range fit has completed.

*Plot intermediate fits:*

The “Plot intermediate fits” expander enables the user to plot intermediate fits from the range fit. If the “Display intermediate fits” checkbox is selected, every *n* fits is plotted after the range fit has completed where *n* is the number that is inputted using the expander. If “Export intermediate fits” is selected, these plots are outputted to the selected file path (or the application directory by default).