VoltCycle: Cyclic Voltammetry Data Visualization and Analysis

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An interactive data visualization and analytics tool for determining electrochemical reversibility from automated batch cyclic voltammetry

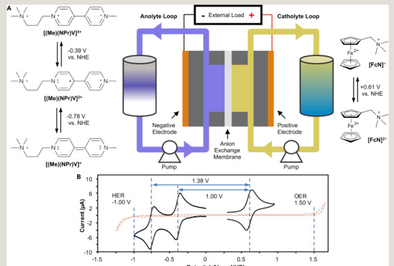
MOTIVATION

Introduction:

Cyclic Voltammetry (CV) is an electrochemical technique utilized to measure the the current that develops in a cell under excess voltage. This method enables the classification of materials to determine if they are optimal for use in batteries. Currently, with the mass production of data, CV analysis is a time consuming procedure, where each raw file has to be analyzed individually. The purpose of this project is to develop a tool for high throughput analysis, that is able to draw relevant information from multiple data files with relatively minimized user input.

Objectives:

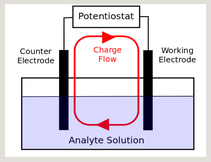
1. Data Mining and Cleaning
   - Read raw data files from Gamry
   - Parse required data for analysis
2. Data Visualization
   - Create an interface for visualization
     - based on user inputs
3. Classification
   - Collect pertinent information
   - Classify reversibility of the material
4. Machine Learning

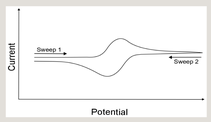


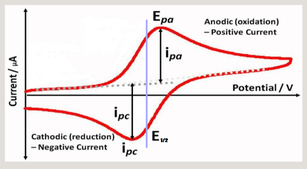
BACKGROUND

Fundamentals:

Voltammetry is an experimental method in which an analytic solution is exposed to two electrodes. When the voltage is manipulated on one of the electrodes, current flow is observed and the voltage required for electron transfer is determined. In cyclic voltammetry, the potential is swept in one direction and then reversed till the starting value is reached. This range delivers the potential window. Such experiments give thermodynamic and kinetic information on electron transfer for different analytes.







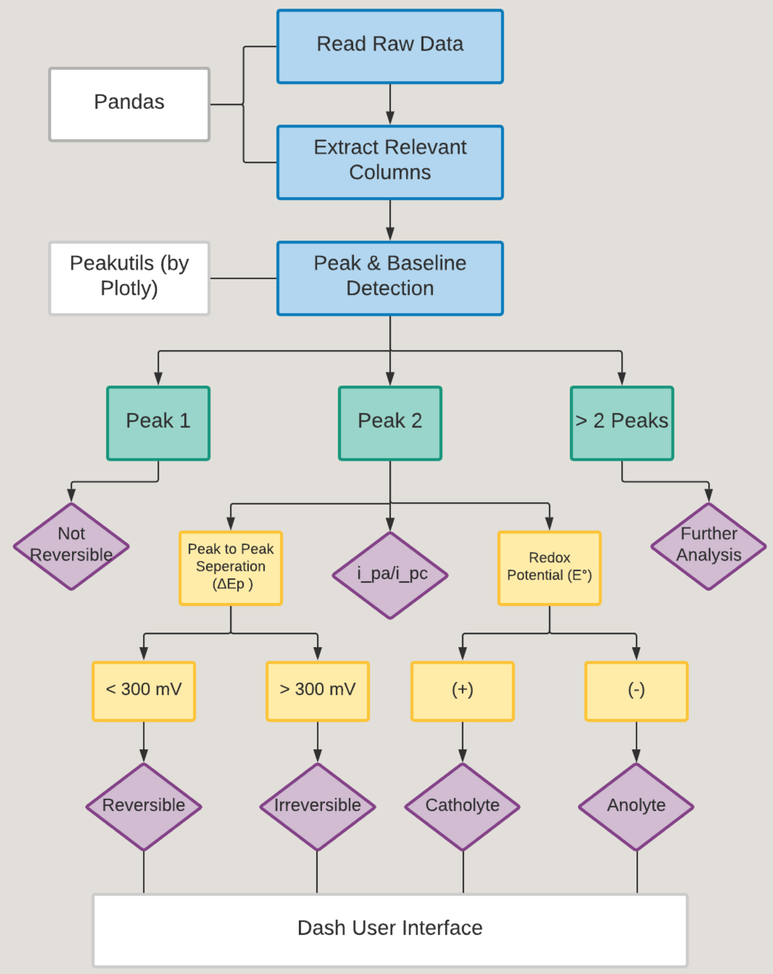
Notable values to determine reversibility:

- Peak potentials (E_{pa}, E_{pc})
- Peak-to-peak separation (ΔE_p)
- Peak Currents (Adjusted baselines, I_{pa}, I_{pc})
- Peak Current Ratio (I_{pa}/I_{pc})

Important factors to consider:

- For completely reversible electron transfer, the peak potentials will not change with different scan rates
- Ideal peak separation at 25°C is 59mV for one electron wave CV (reversible)
- Peak:current ratio should be approximately 1
- Both anolytes and catholytes are necessary for a functioning battery
  - Positive standard reduction potential ($E_{1/2}$) - catholyte (vise versa)

WORKFLOW



User Interface:

- Dash (by Plotly)
- Visualize and analyze multiple datasets simultaneously with ease

Limitations:

- Negative peaks proved to be a challenge
  - Used a function to split the negative values and take their absolute value
- Detecting 1 or greater than 2 peaks - further user-based analysis required
- Classifyinging multiple experimental cycles from the same file - current focus

RESULTS

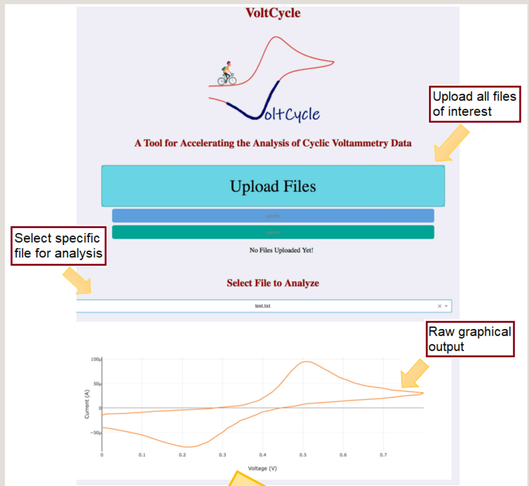
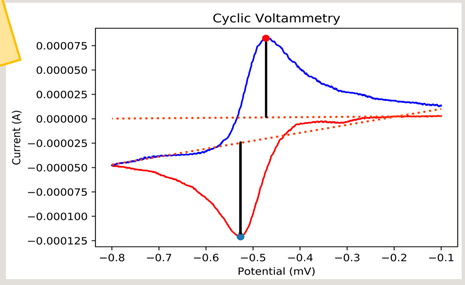


Figure representing the Dash interface consisting of the logo and introduction, the file upload and selection portals and the raw data plot.



Graphical output on github package and Dash showing the predominant peaks, baselines and peak current (I_{pa}, I_{pc}) values.

CONCLUSION & FUTURE WORKS

Conclusion:

The final package includes a Dash interface based on a single wrapper function that outputs a graphical image with the relevant parameters calculated and labeled. It also results in a dictionary consisting of important values and the final classification.

Future Direction:

- Process more complex CV raw files
  - Perform analyses for files with more than two peaks

  Output materials classification comparison table for all input files
- Machine learning
  - Once enough data has been classified, develop design features for materials that are good candidates for this application

Acknowledgements

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All packages used and generated are open source, and documentation can be found on github at https://github.com/sabiharustam/voltcycle

References

[1] https://sop4cv.com/index.html
[2]http://urrjaa.blogspot.com/2013/08/cyclic-voltammetry-urrjaa-p0110-2013.html