

fuelcell: A Python package and graphical user interface for electrochemical data analysis

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Overview

fuelcell is a Python package designed to standardize and streamline the analysis of electrochemical data. This package includes modules for data processing and data visualization, as well as a graphical user interface (GUI) for interactive use.

Introduction

As the demand for sustainable, carbon-free electricity increases globally, development of electrochemical energy conversion devices is increasing rapidly. These devices include fuel cells, flow batteries, and water electrolysis cells. A wide range of diagnostic experiments is used to assess the performance, durability, and efficiency of electrochemical devices. ([Bard & Faulkner, 2001](#); [Newman & Thomas-Alyea, 2004](#)). Among the most commonly used techniques are chronopotentiometry (CP), chronoamperometry (CA), cyclic voltammetry (CV), linear sweep voltammetry (LSV), and electrochemical impedance spectroscopy (EIS) experiments. ([Bard & Faulkner, 2001](#); [L. Wang, 2003](#); [Newman & Thomas-Alyea, 2004](#); [Orazem & Tribollet, 2008](#)). Although these experimental protocols have been well-established in the field of electrochemistry, the protocols for analyzing electrochemical data have not been clearly standardized. Standardizing electrochemical data analysis will also aid in applying machine learning frameworks to extract valuable information from electrochemical data sets.

Statement of need

A single electrochemical experiment can generate on the order of ten thousand data points, and several individual experiments are frequently used to assess a single cell. Electrochemical experiments also generate large quantities of raw data, which require extensive preprocessing before the data can be used to assess the performance of an electrochemical device completely. Processing and analyzing the data from a single experiment using conventional methods often is a bottleneck and time consuming. Manually processing this data also introduces unnecessary human error into the results, resulting in increased variation both between individual researchers and between research groups within the electrochemical field ([Agbo & Danilovic, 2019](#)). Therefore, an application that efficiently processes electrochemical data will standardize and expedite the analysis of data generated from electrochemical experiments.

Functionality

`fuelcell` includes modules for both data processing and visualization to enable a smooth, efficient workflow from raw data to publication-ready figures. These modules can be imported and used programmatically as a standard Python package, and `fuelcell` also includes a standalone GUI that allows users with little or no programming experience to utilize these modules. `fuelcell` also serves as a platform that can be expanded to facilitate new and more advanced techniques as the needs of the electrochemical community evolve.

`fuelcell.datums`

Every experiment requires a unique protocol to process the raw experimental data, so the `datums` module contains experiment-specific functions to read and process data for each experiment. Currently, functions to process CV, CP, CA, LSV, and EIS data are included in `fuelcell`, and new protocols can be added to the project by opening an issue on GitHub. The complexity of these processing protocols varies depending on the experiment, and the specific data processing steps carried out for each experiment are detailed in the documentation. The `datums` module also includes functions to determine the Tafel slope and exchange current density from LSV data as well as to extract the high-frequency resistance (HFR) value from EIS data (Agbo & Danilovic, 2019; Orazem & Tribollet, 2008).

`fuelcell.visuals`

The `visuals` module includes functions to generate visualizations, which are commonly used in the electrochemical community. `fuelcell` currently includes functions to generate polarization curves, cyclic voltammograms, linear sweep voltammograms, and Nyquist plots (Figure 1). This module is built around the `matplotlib` library, which allows for highly customizable visualizations. The `visuals` module is designed to integrate both seamlessly with the `datums` module and to function as an independent module that can be incorporated into an existing workflow.

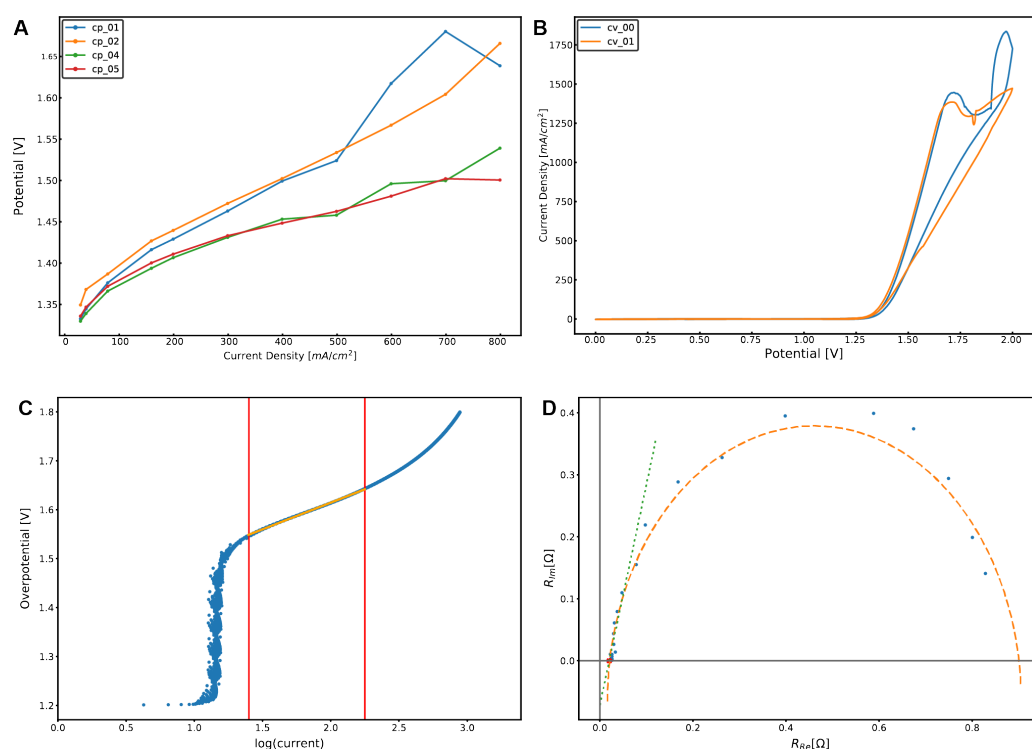


Figure 1: Examples of figures created using functions in `fuelcell.visuals`. (a) Polarization curves generated using data from CP experiments. (b) Cyclic voltammograms. (c) LSV data with the Tafel fit overlaid in yellow. (d) EIS data with the HFR value calculated using both a semicircle fit and a linear fit.

`fuelcell_gui`

The GUI is included in the standard `fuelcell` installation, but it can also be installed independently as a single executable file (Windows and MacOS) that includes all necessary dependencies. The GUI also enables users to interactively create and customize visualizations without being familiar with the ins and outs of the `matplotlib` library. This GUI has been shown to greatly reduce the time required to process electrochemical data, with researchers using the program reporting that it reduces the time required to process data from testing four cells from close to one hour to about five minutes.

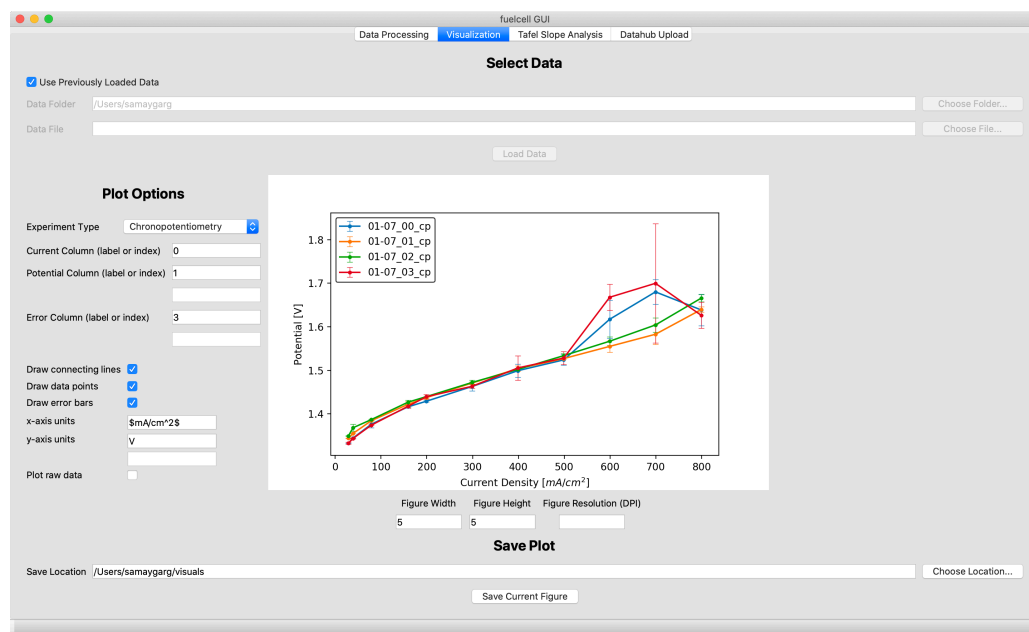


Figure 2: Data visualization tab of the GUI.

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