

BattMoApp: A Web-Based application for running cell-level battery simulations

Lorena Hendrix¹, Oscar Bolzinger¹, Eibar Flores¹, and Simon Clark*¹

¹ SINTEF Industry, Norway

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Summary

BattMoApp is a web-based application built upon the command-line based battery modelling software, BattMo. It features a user-friendly graphical interface that simplifies the simulation of battery cells. The development of BattMoApp has been centered on accessibility, intuitiveness, and usability, with the aim of making it a practical and valuable tool for both educational and research purposes in the battery field. Its design allows users to simulate, obtain, analyze, and compare results within just a few minutes. While BattMoApp leverages a small yet crucial portion of BattMo's capabilities, its intuitive and explanatory design also makes it an ideal starting point for those looking to explore the more comprehensive and complex BattMo software.

Statement of need

The Battery Modelling Toolbox (BattMo) is a framework for continuum modeling of electrochemical devices. Built primarily in Matlab, it offers a pseudo X-dimensional (PXD) framework for the Doyle-Fuller-Newman model of lithium-ion battery cells. Additionally, extensions for other battery chemistries and hydrogen systems are in development. BattMo provides a flexible framework for creating fully coupled electrochemical-thermal simulations of electrochemical devices using 1D, 2D, or 3D geometries. Besides the Matlab toolbox, the framework is also being developed in Julia to leverage increased simulation speed and the non-proprietary nature of Julia.

The primary objective of BattMoApp is to unlock access to battery simulations for users without coding experience. Most researchers who can benefit from battery simulations are not familiar with any scripting language. A simple to use graphical user interface brings battery simulations to laboratory engineers and battery scientists who can use the results to inform their cell design and development activities.

BattMoApp builds upon the P2D model implemented in the Julia version of BattMo. The development of BattMoApp has focused on accessibility, intuitiveness, and usability. Users can quickly and easily obtain results using the default input parameter sets available in the application or input their own values in a straightforward manner. The results can be easily analyzed and compared using the predefined plots that can handle multiple sets of simulation results. Users can also download their results and later upload them back into the application to review. Furthermore, significant effort has been made to ensure the parameters are realistic for both computational research and lab use, making it easier for experimentalists to fulfill the necessary inputs.

Another important aspect, besides accessibility, intuitiveness, and usability, is interoperability. To ensure that the input data of the simulation is inter-operable, the selected data format adheres to the FAIR principles and the 5-star open data guidelines. The data entered by the

41 user is automatically formatted into a JSON Linked Data (LD) format which includes all
42 the semantic metadata along with the actual data. This semantic data connects the actual
43 data to the ontology documentations, EMMO and BattINFO, which contain descriptions of
44 the linked data definitions. With this, the JSON LD format eliminates any confusion about
45 definitions. If the user wishes to publish their results, they can include the JSON LD file in
46 their publication, allowing anyone seeking to replicate the results to simply upload the JSON
47 LD file into BattMoApp and obtain the anticipated results.

48 The documentation of BattMoApp includes an overview on what the application has to
49 offer and a troubleshooting section that provides insights into the relationship between input
50 parameters and results. As BattMoApp is designed to be informative and explanatory, it can
51 also be a powerful tool for educational purposes, helping students understand batteries, battery
52 modelling, and the impact of material and cell design parameters on battery cell performance.

53 Technical setup

54 The application consists of two main components: the graphical user interface (GUI), which
55 includes the frontend, a database, and the backend that provides the frontend's functionality,
56 and the application programming interface (API) that runs the BattMo software in the
57 background. These two components are isolated from each other, each running in its own
58 Docker container.

59 BattMo GUI

60 The frontend is Python-based and developed using the Streamlit framework. Streamlit was
61 chosen due to its user-friendly framework, which greatly accelerates the development process.
62 The backend, also written in Python, supports the frontend's functionality. The database that
63 supports both the frontend and backend is created using the sqlite3 Python package.

64 BattMo API

65 The API runs the Julia package BattMo. Integrating Julia, a pre-compiled language, with
66 Python, a runtime language, to form a smoothly running and stable application turned out to
67 be complex. Therefore, a Julia-based API was created and containerized within a separate
68 Docker container, isolating it from the BattMo GUI. This separation ensures that the Julia and
69 Python components do not interfere with each other. The framework used for creating the API
70 is Genie. Within the BattMo API's docker image a system image of BattMo's pre-compilation
71 is created to ensure an instantaneous API response.

72 Examples

73 The application provides a list of features:

- 74 ▪ Access to parameter sets from literature, and customization of these sets.
- 75 ▪ Download input parameter values as a BattMo formatted JSON file or as a linked data
76 formatted JSON file.
- 77 ▪ Visualization of 3D grids.
- 78 ▪ P2D model.
- 79 ▪ Quick calculations of key indicators.
- 80 ▪ Interactive plots that zoom, hover, and downloads PNGs.
- 81 ▪ Visualization of not only voltage curves but also internal states to provide further insight
82 into gradients of concentrations and potentials.

- 83 ■ Comparison of multiple simulation results.
- 84 ■ Download full results as HDF5.

85 The following figures display screenshots of the application's 'Simulation' and 'Results' pages.
86 On the 'Simulation' page, users can define input parameters, visualize their cell geometry,
87 and initiate a simulation. The 'Results' page then allows for the visualization of simulation
88 outcomes using predefined plots. In Figure 2, the results of two simulations are visualized to
89 show an example. The two simulations were conducted using the default parameter sets from
90 Chen et al., with the electrode coating thicknesses varied to illustrate a comparison of results.
91 Both pages also present key indicators of the battery cell, such as capacities, cell energy, and
92 round-trip efficiency.

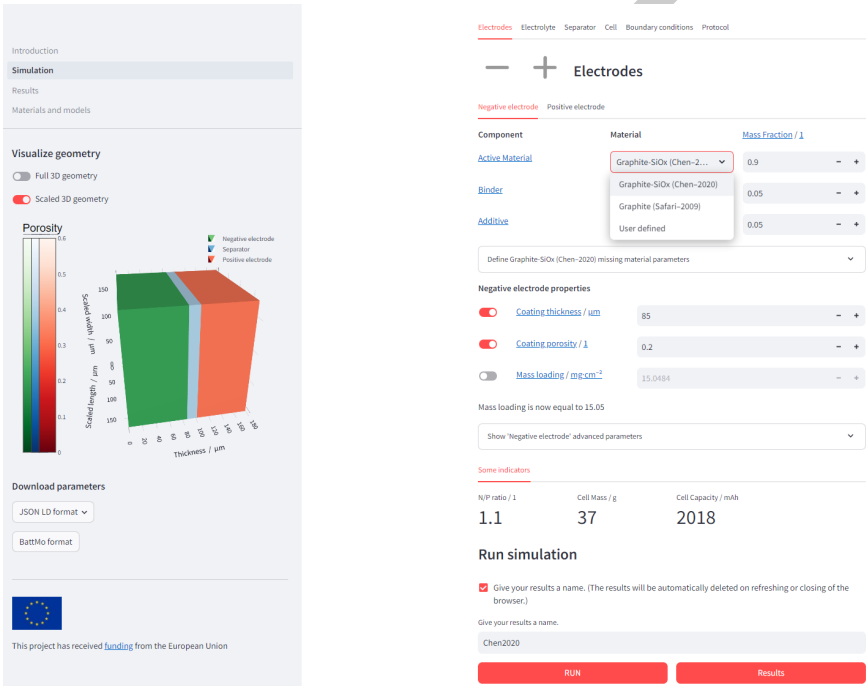


Figure 1: A screenshot of the Simulation page of BattMoApp.

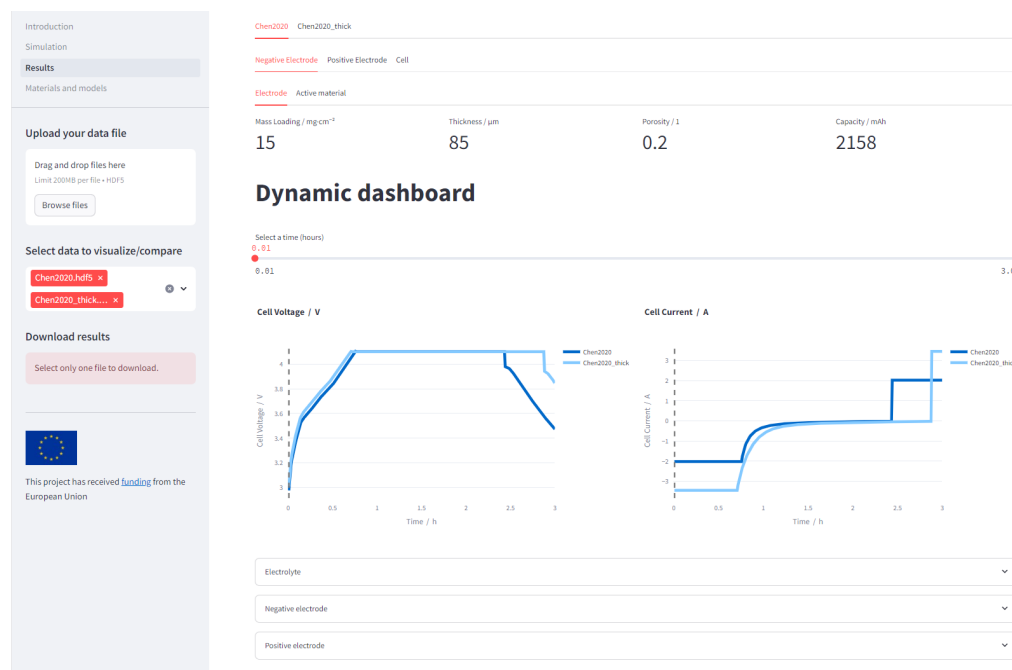


Figure 2: A screenshot of the Results page of BattMoApp.

Future work

While BattMoApp has reached a mature state and offers a valuable platform for P2D simulations, there are still countless possibilities for further development. Its evolution will continue in parallel with BattMo.jl, allowing for the future integration of additional simulation models and features like parameterization. BattMoApp will continue seeking feedback from its target audience to enhance usability and practicality. Additionally, more effort will be dedicated to improving the performance BattMo GUI to improve user interactivity.

Installation and contribution

BattMoApp can easily be used online at the following address: app.batterymodel.com. Furthermore, it can be locally installed using Docker. The Docker images and a detailed instruction on how to install BattMoApp locally can be found in the Github repository.

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References