The Battery Modelling Toolbox (BattMo)

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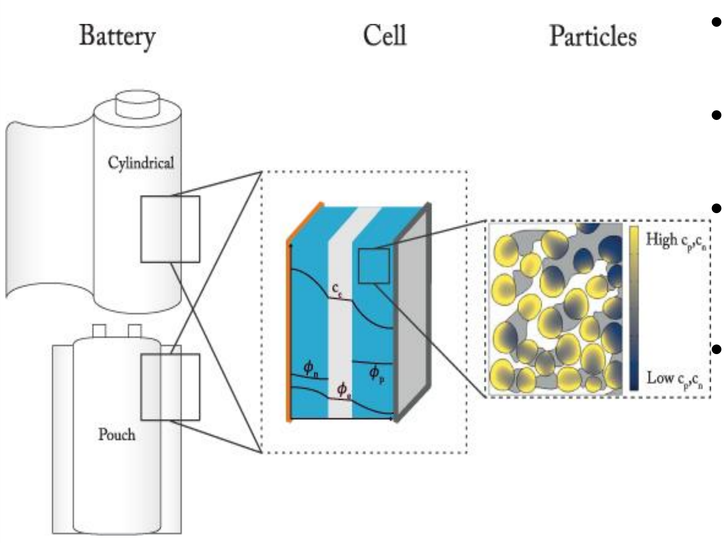
What is BattMo?

- BattMo [1] is an opensource framework for performing continuum-scale simulations of electrochemical devices.
- Can be run in MATLAB [2] and Julia [3], or (partly) as a web GUI [4].
- Primarily developed for modelling Li-ion battery cells, it is based on the pseudo-X-dimensional (PXD) framework of Doyle-Fuller-Newman model.
- Has been applied to other battery chemistries and hydrogen systems.

The Doyle–Fuller–Newman (DFN) model



- Established physics-based model for Li-ion batteries.
- Cell is divided into three regions.
- Electrodes are modelled as spherical particles of active material.
- The continuity equations for charge, mass and heat yield the concentration, electric potential and temperature.

Sketch of the battery components at different scales [5].

Inputs to a general PXD model in BattMo

Cell geometry
- Coin cell
- Prismatic cell or pouch cell
- Cylindrical cell
- Arbitrary shapes in 1D, 2D and 3D

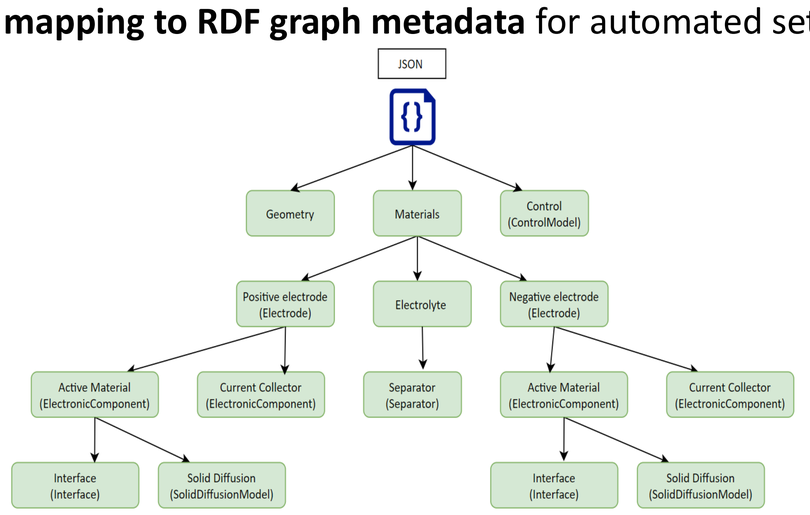
Electrode
- Thickness
- Porosity
- Active particle radius
- OCVs
- Li diffusivity
- ...

Electrolyte and separator
- Separator width and thickness
- Porosity
- Ionic conductivity
- Ionic diffusivity
- ...

PXD models require lots of parameters, but given geometry and half-cell OCVs we can calibrate critical parameters against experiment. This is done in two stages: first against low C under equilibrium assumption, then at high C.

Workflow in BattMo

The code is structured using a **hierarchical holistic perspective**. This enables (i) **plug-and-play encapsulation** of component models and (ii) **direct mapping to RDF graph metadata** for automated setup and post-processing.



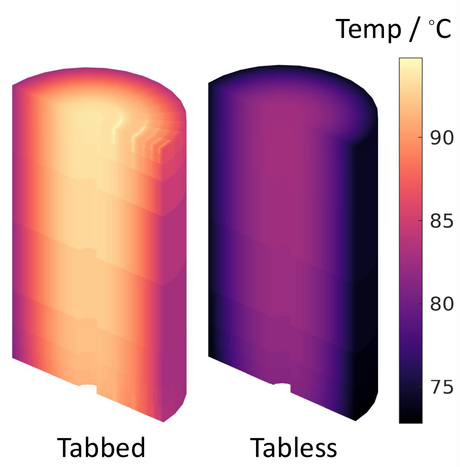
- Control module allows to set the protocol of the simulation, such as CCCV or CC or CV.
- Battery geometry module can be used to build your own 1D, 2D or 3D cells.

Individual JSON files that capture the parameters of the specific battery modules.

Example: 3D geometry effects

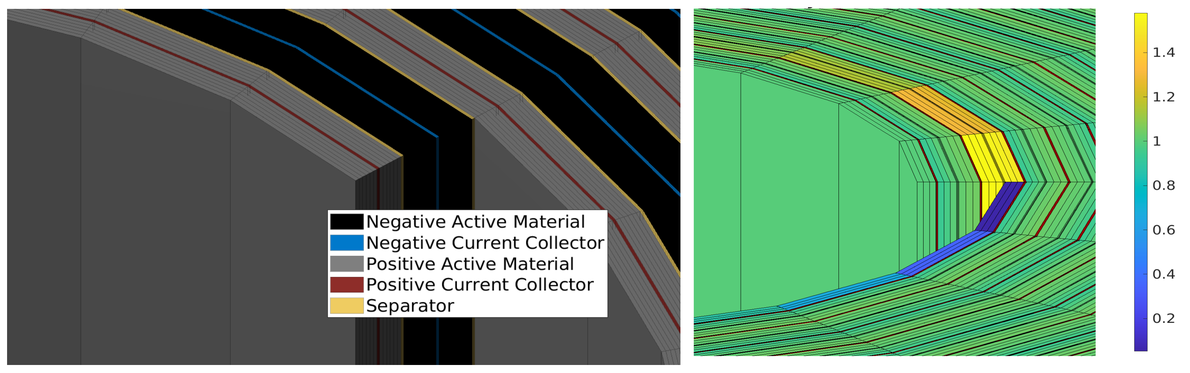
Tab effects in 4680 cylindrical cells

Tabless cell designs have been proposed to improve heat management and enable high-rate operation. Simulated discharge at 2C and 100 W/m^2 external cooling indicates that **the tabless design stays ca. 10°C cooler than the design with tabs** (right). **Tabs can also lead to preferential (de)lithiation** in the electrodes and in-homogeneous lithium distribution. This is difficult to reveal in experiments, but not in simulation.



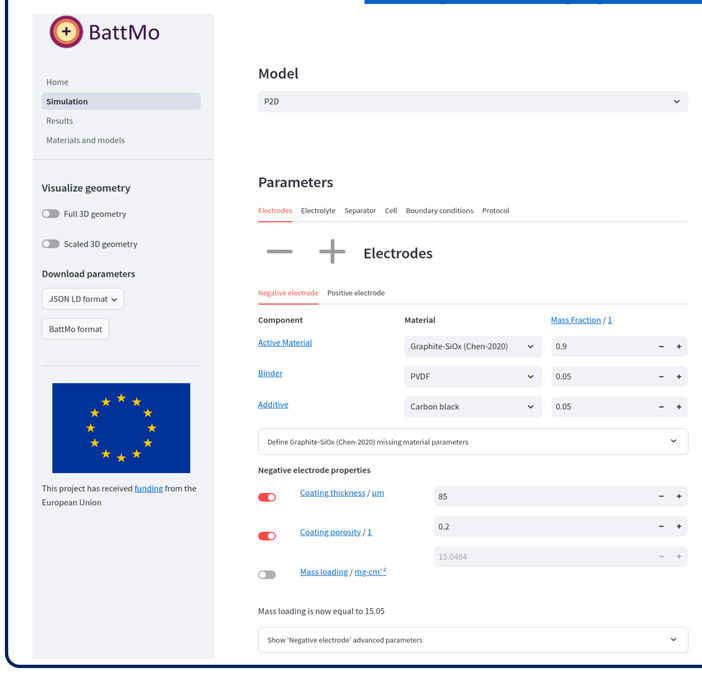
Winding effects in jelly-rolls

Inner-most and outer-most layers of jelly rolls often contain some section of electrode that is coated with active material but lacks a counterpart. **At the interface where this layer wraps back around on itself, there may exist strong local gradients in lithium and electrolyte concentration (left).**



Grid resolution and battery components for the 4680 simulations (left).
Strong electrolyte concentration gradients in the inner-most layer (right).

BattMo GUI: http://app.batterymodel.com



This project has received funding from the European Union

- Offers intuitive interface to run P2D simulations in real-time with the Julia backend.
- Access a comprehensive default parameter list for a range of materials: NMC, LFP, SiGr, etc, or provide yourself.
- Allows testing P2D model parameters effortlessly.
- Provides interactive visualization tools for simulation results.
- In progress! Lacking features of the MATLAB version.

Outlook

- Support interoperability via ontologies with other frameworks.
- Port more features of BattMo in MATLAB to Julia.
- Model integration in cell research and engineering workflows.
- Develop and couple degradation mechanisms (Li plating, mechanics).

References

[1] www.batterymodel.com
[2] https://github.com/BattMoTeam/BattMo
[3] https://github.com/BattMoTeam/BattMo.jl
[4] http://app.batterymodel.com
[5] F Brosa Planella et al 2022 Prog. Energy 4 042003. https://doi.org/10.1088/2516-1083/ac7d31.

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www.h2020hydra.eu
www.digibattproject.eu
www.batmaxproject.eu