

Mathematical modelling and numerical simulation of batteries



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Background

Lithium-ion batteries have become essential for energy storage in applications such as smartphones, electric vehicles, and grid systems. To enhance their performance, safety, and lifespan, accurate modelling is critical.

This work focuses on electrochemical models, which simulate the internal physical and chemical processes of the battery—such as ion transport, intercalation, and SEI (Solid electrolyte interphase) layer formation. These models provide detailed insights that are valuable for the design and optimization of cells and materials.

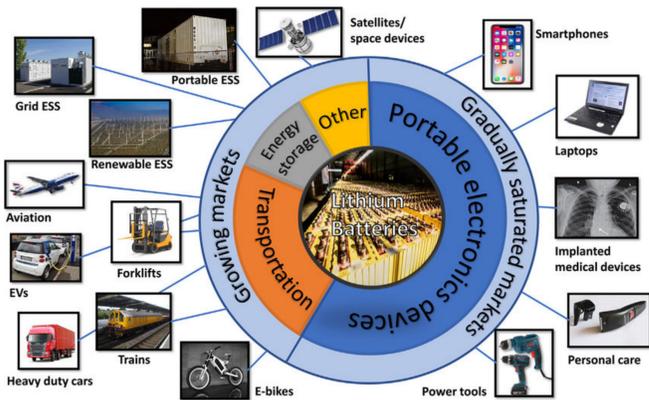


Fig. 1: Current applications of lithium-ion batteries in portable electronics, transportation, medical devices, and energy storage. Source: [1]

Pseudo 2-D Model (Doyle, Fuller, Newmann)

Schematic representation of the pseudo-2D model geometry (Doyle–Fuller–Newman), showing the spatial domains of the anode, separator, and cathode, along with key transport and electrochemical variables.

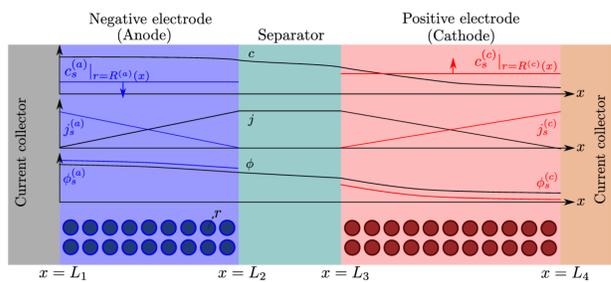


Fig. 2: A sketch of a cross section of a typical device as well as the macroscopic variables and their domains of definition. Source: [2]

Model Equations

The lithium-ion battery model [2] describes transport and electrochemical phenomena across different regions of the cell: the anode, separator, and cathode.

The equations account for:

- **Mass and charge conservation** in both solid and electrolyte phases.
- **Lithium-ion diffusion** in the electrolyte and inside solid particles.
- **Charge transport** driven by electric potential and concentration gradients.
- **Electrochemical reactions** at the electrode–electrolyte interfaces (Butler–Volmer kinetics).

The model includes:

- Diffusion equation for lithium in solid particles.
- Ionic transport and current equations in the electrolyte.
- Charge conservation in the solid phase.
- Boundary and initial conditions for realistic operation.

This coupled system enables the simulation of battery dynamics under various charging and discharging conditions.

Example: Electrolyte Mass Conservation

$$\epsilon_v \frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left(D_{\text{eff}} B_{11} \frac{\partial c}{\partial x} - \frac{t_0^+(j)}{F} \right) + \frac{S}{F}$$

This equation (see the QR code above for the full set of model equations) models the **lithium-ion concentration dynamics** in the electrolyte, accounting for:

- Diffusion of ions.
- Electric field effects via migration.
- Reaction sources/sinks at electrode interfaces (term S).



Simulation Results

• **COMSOL Multiphysics 6.3:** We implemented a standard Lithium ion cell model using the **Battery Module**, which solves the governing electrochemical equations in a multiphysics environment <https://www.comsol.com/model/1d-isothermal-lithium-ion-battery-686>.

• **Dandeliion Model:** A specialized solver designed for electrochemical simulations, providing an alternative approach to battery simulation. More details about this model can be found at <https://www.dandeliion.com/>.

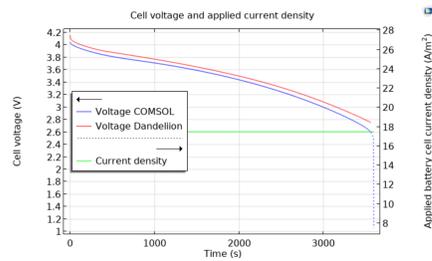


Fig. 1: Voltage and applied battery cell current density (I/A) until final simulation time (3562 s for the Dandeliion curve and 3594.4 s for the COMSOL curve).

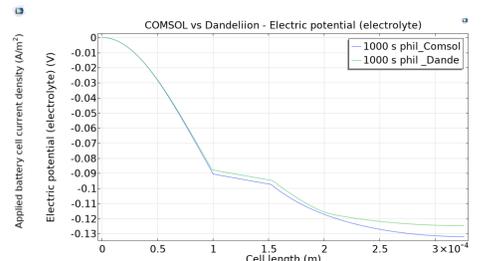


Fig. 2: Electric potential in the electrolyte measured with a reference Lithium electrode at t = 1000 s.

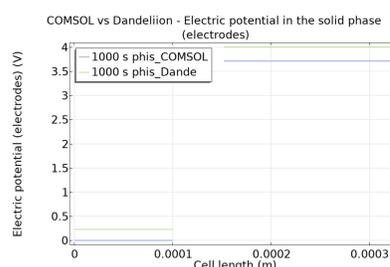


Fig. 3: Electric potential in the solid phase of the electrodes at t = 1000 s.

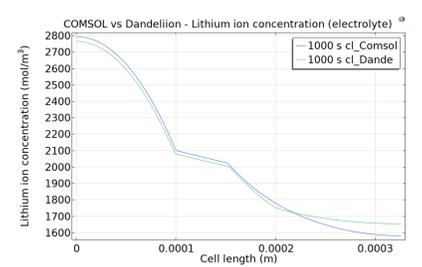


Fig. 4: Lithium-ion concentration in the electrolyte at t = 1000 s. Comparison between COMSOL and Dandeliion.

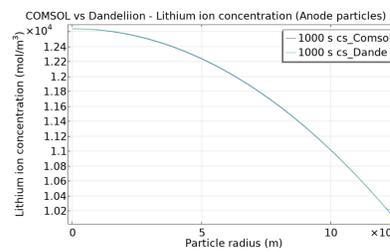


Fig. 5: Lithium concentration in the solid particle at the middle of the anode at t = 1000 s.

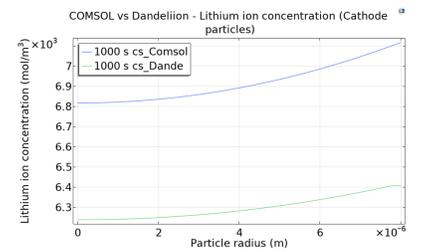


Fig. 6: Lithium concentration in the solid particle at the middle of the cathode at t = 1000 s.

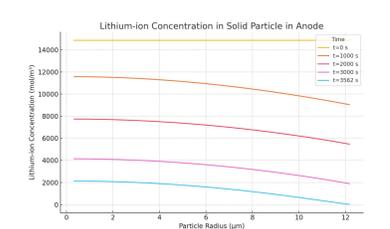


Fig. 7: Lithium concentration in the solid particle at the interface of the anode with the separator at different times. Solution of the solver Dandeliion.

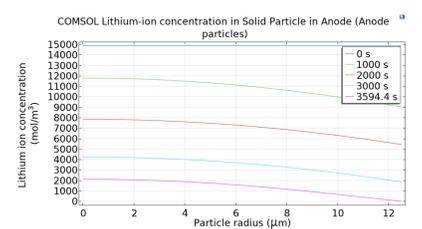


Fig. 8: Lithium concentration in the solid particle at the interface of the anode with the separator at different times. Solution of the solver COMSOL.

Conclusions

- We studied a lithium-ion battery model using the pseudo-2D Doyle–Fuller–Newman framework [3], incorporating transport and electrochemical dynamics. Simulations with COMSOL and Dandeliion showed good agreement in cell voltage, electric potential and concentration behavior.
- Results confirm the model's reliability and its utility for analyzing battery behavior and exploring design improvements.
- Future work includes modelling novel battery concepts where both positive (e.g., Li⁺) and negative ions can intercalate into the electrodes.

Acknowledgements and References

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References

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