Mathematical modelling for Lithium-ion batteries

Investigating the level of complexity needed for a P2D model and looking at the significance of conductivity values

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Abstract

The project aims to develop an optimal Python code for **simulating lithium ion concentration profiles inside a cathode**. Additionally, it discusses the **importance of conductivity values** in achieving accurate concentration profiles.

During the project, it was discovered that processes within the electrolyte could be overlooked without introducing significant errors. It was also found that conductivity values have a substantial impact on the final total concentration. This underscores the **importance of pursuing further research on modeling the single crystal particle** considering a range of conductivity values for different planes.

Motivation

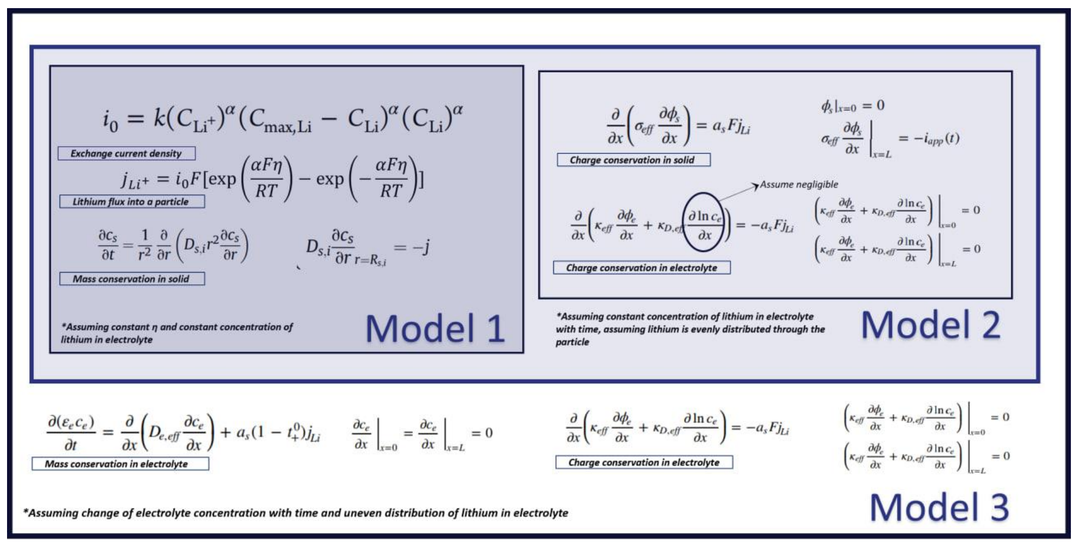
- The efficient and accurate modeling method for charge/discharge processes is of great importance as it can reduce the number of experiments required to enhance existing battery materials and introduce new ones.

Methods

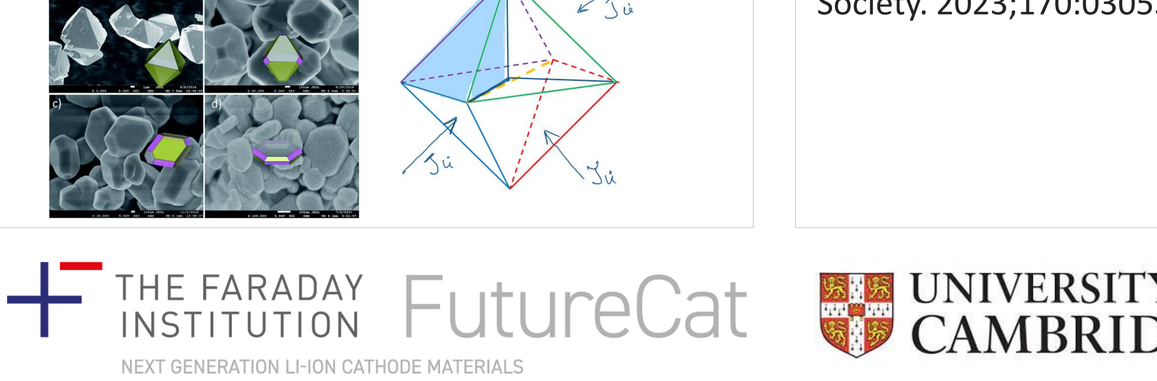
- The code was developed in Python. Finite Difference Methods were used to simulate both PDEs and ODEs. Parameters for the calculations were taken from the literature, as per reference 1. The system was approached as a pseudo-two-dimensional (P2D) model[1].

Section 1: How complicated should we make things?

- Models of different levels of complexity were created. **Model 1** was assuming no change in overpotential and concentration of electrolyte. **Model 2** was updating overpotential value at each step and included ODEs for electric potential inside the solid and electrolyte. **Model 3**[2] included a PDE describing change in electrolyte concentration with time.

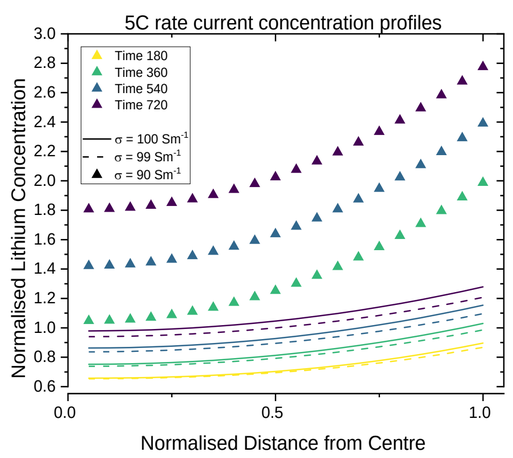


Comparing concentration profiles simulated by all three models at 25%, 50%, 75% and 100% SOC

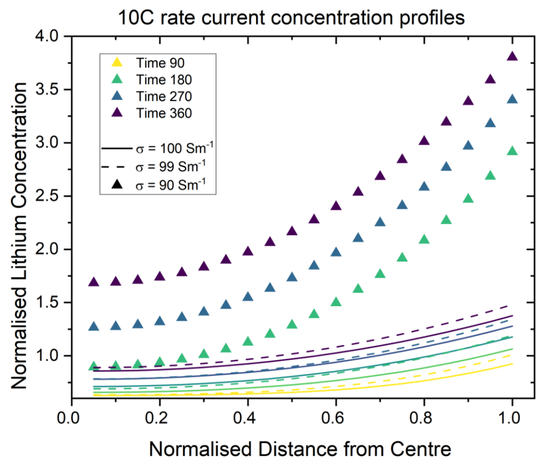


Section 2. Conductivity: a parameter that shouldn't be ignored

- In the majority of papers on modeling, the conductivity parameter is consistently set to 100Sm^{-1}. However, **the conductivity depends on the plane at which lithium ions penetrate the cathode material.** Upon closer examination of how this parameter influences the system, it's evident that it cannot remain constant in all scenarios: **even the slightest change of 1% leads to a large alteration in overall concentration (5%).**



Decrease in σ value (%)	Increase in concentration(%)
1%	5%
10%	107%



Decrease in σ value (%)	Increase in concentration(%)
1%	5%
10%	132%

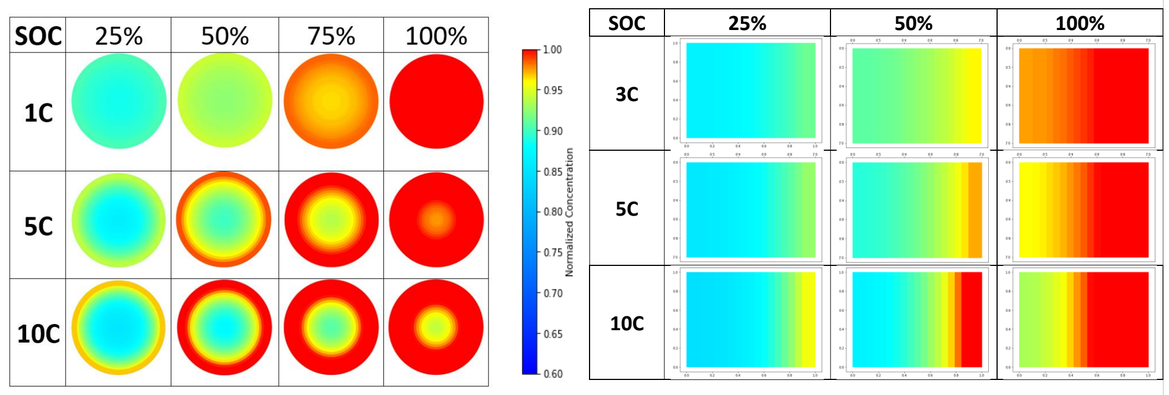
Conclusions

1. Developed three computational models of varying complexity for predicting concentration profiles and revealed that **assuming electrolyte concentration constant does not lead to significant errors.**

	25% SOC	50% SOC	75% SOC	100% SOC
1C rate	0.01	0.02	0.03	0.04
2C rate	0.01	0.02	0.03	0.04
3C rate	0.01	0.03	0.04	0.05
4C rate	0.02	0.04	0.05	0.06
5C rate	0.01	0.03	0.04	0.05
10C rate	0.01	0.02	0.04	0.05

Relative Deviation between model 2 and model 3

2. Revealed that **concentration profiles at identical SOC vary significantly with different C-rates.**



3. Conductivity sensitivity analysis reveals **minor alterations significantly impact total concentration value** at identical applied currents.

Impact / Next steps

In many cases, it has been found that modeling the processes inside the electrolyte isn't necessary. Based on this discovery, **adjustments to the model are being made to fit pyramids of any shape**. Once this is achieved, models for other polyhedron shapes can be created. This would allow us to account for different conductivity values depending on the plane and to **recommend optimal particle shape.**

References

1. Li C, Cui N, Wang C, Zhang C. Reduced-order electrochemical model for lithium-ion battery with domain decomposition and polynomial approximation methods. Energy. 2021;221:119662.

2. Jané E, Medeiros R, Varas F, Higuera M. A Time-adaptive order reduction technique for the Doyle-Fuller-Newman electrochemical model of lithium-ion batteries. Journal of The Electrochemical Society. 2023;170:030539.

Intern bio

Anastasia is a Chemistry with Molecular Physics student at Imperial College London aspiring to pursue a PhD in Computational Chemistry field. Outside of her studies, she is involved in outreach events hosted by Imperial College London helping high school students, especially those from underrepresented backgrounds, to understand the beauty of science. She hopes to encourage more students to explore and embrace STEM fields for their academic and professional journeys.

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