How can we increase the robustness of optimisation-based diagnostic tools for battery life & performance?

Mathematical and Electrochemical approach to Battery Modelling

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Abstract

A battery's lifetime, power and capacity are all functions of the degradation mechanisms that act from the end of manufacturing to the decommissioning of the battery.

These degradation mechanisms can be categorized into 3 main modes: the loss of lithium inventory (LLI), the loss of active anode material (LAM NE) and the loss of active cathode material (LAM PE) (1).

The current working model maps experimentally measured OCV to lithiation fractions. The aim is to increase its robustness by developing its ability to handle different types of data including faster cycles (higher C – Rate). This would involve a consideration of the now considerable internal resistance and overpotential.

This approach will outline the approach used, the results, as well as a study of different optimisation solvers and constraint set ups that could possibly supplement the implementation of this correction.

Motivation

Identifying the degradation mode from measurable OCV is a non – destructive diagnostic tool that can quantify and give better understanding of the underlying degradation mechanisms. (2).

There is an assumed link between measured OCV and the underlying degradation mode (2). If a robust link is established between OCV and degradation modes, real time recommendations can be made to extend and improve battery life and user – experience.

By including handling for higher C – Rate data, the toolbox will be more accurate when implemented in consumer used lithium – ion batteries, as many practical applications of batteries involve fast cycles such as supercharging EV packs.

Generating a model that is robust enough to successfully be implemented in commercial batteries is tough but worthwhile and helpful to the industry as it expands and continuously develops.

Methods

Good battery modelling software must be able to accurately and repeatedly predict battery degradation in the operational setting and commercial use of the battery.

This includes handling higher C – Rates by:

1. Devise an iR correction mechanism.
2. Implement this in the software. This includes changing the optimiser's objective function, creating new frameworks to compute and store the iR data, and altering the model that is passed to the optimizer.
3. Robustness is achieved by running the tool on different data sets and evaluating the results in line with scientific expectations and theory.

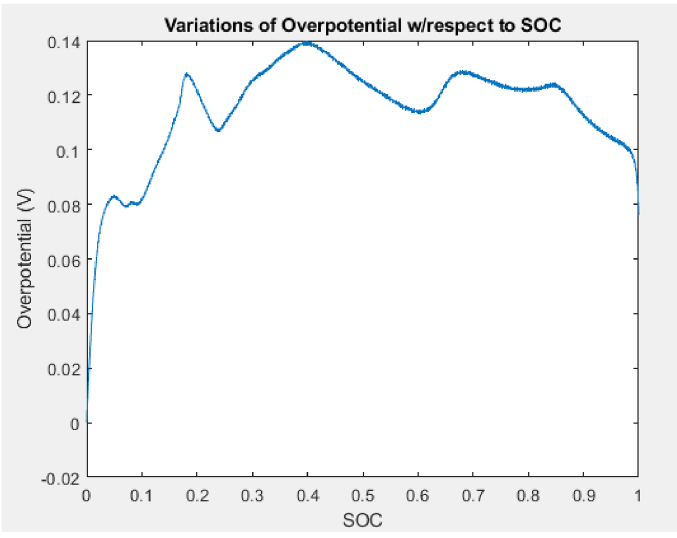
This is coupled by iterating through different optimisation solvers.

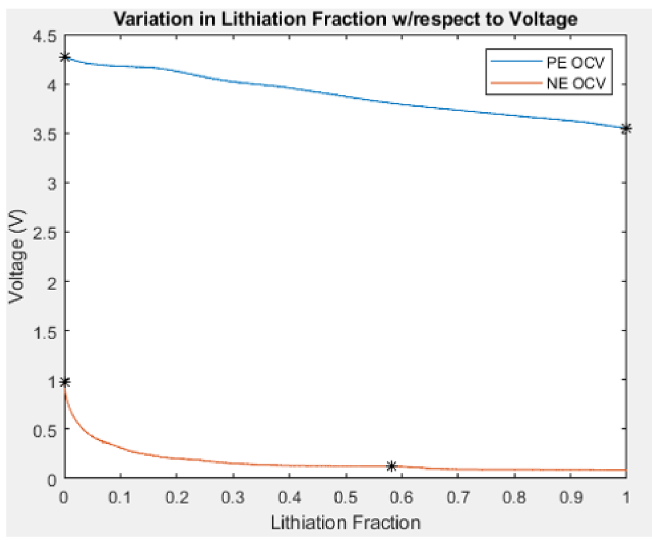
Results 1 – Confirming Optimisation algorithm

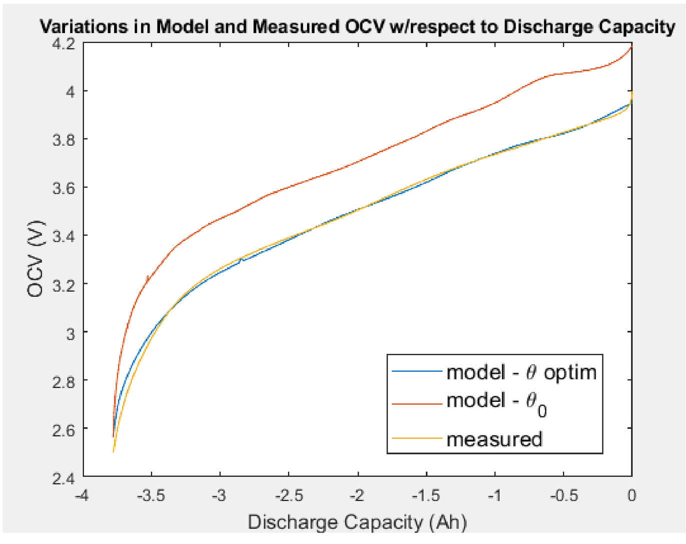
Sample	Optimisation Solver	RMSE	R2	Cathode Capacity (Ah)	Anode Capacity (Ah)
1	Fmincon (FMC)	0.0212	0.9959	6.1062	4.3532
1	Genetic Algorithm (GA)	0.0212	0.9959	6.1062	4.3532
1	Global Search (GS)	0.0212	0.9959	6.1068	4.3532
1	Simulated Annealing (SA)	0.0212	0.9959	6.1065	4.3532
2	SA	0.0205	0.9961	5.9900	4.2368
2	FMC	0.0205	0.9961	5.9974	4.2368
2	GA	0.0205	0.9961	5.9975	4.2368
2	GS	0.0205	0.9961	5.9974	4.2368

- Fmincon, the Genetic Algorithm, Global Search and the Simulated Annealing algorithm all output the same stochiometric parameters with the same error and accuracy across the same sample.
- Confirms optimized set up of fmincon and generates an appropriate degree of accuracy.

Results 2 – Higher C – Rate Correction







- The left most figure is a graphical representation of the greater iR (overpotential) correction map as a function of SOC that was applied to all fast cycles such that $V_{model} = V_{PE} - V_{NE} - (k * iR)$.
- The figure in the middle is the result of a forced minimum separation between anode lithiation fractions which was introduced as a constraint. This reflects an appropriate optimisation as the anode lithiation fractions and the difference between anode and cathode half cell utilization are in line with informed expectation.
- The figure on the right is a representation of the close tracking the model has after the correction is implemented. to the measured voltage with a Root Mean Square Error of 18.8 mV and an R2 of 0.996. The correction mechanism works and has a high accuracy.

Conclusions

- The performance of optimisation-based models is closely related to the mathematical algorithm and the set up used. The constraints, solvers and initial guess in Fmincon algorithm was evaluated based on the computing time and accuracy of outputs. The framework was set-up by editing its configurable property – value pairs, including the constraint tolerance, trust – region algorithms and in-built checks using the gradient and Hessian.
- The Genetic Algorithm were improved by editing creation, mutation and simulation functions. The Simulated Annealing algorithm was also configured by implementing hybrid options and running fmincon in parallel. These 2 algorithms are useful for benchmarking and for use when the sample space of possible solutions increases in size.
- Implementing the iR correction for higher C – Rate mandated a rework of the toolbox. New classes and workflows had to be created and introduced. Results are promising but more work is required to achieve robustness.
- For the motivation behind this project to come to fruition, the toolbox must be able to handle real time data coming from consumer usage of batteries. These conditions are different from lab testing. As such, the toolbox needs to be prepared to handle higher C – Rate data, akin to supercharging EVs and mobile/computer batteries. As batteries become more convenient, faster charging is often used. So, a diagnostic tool should handle this.

Impact / Next steps

- This project showed the complexity of optimisation based diagnostic modelling tools.
- Successfully adding functionality to handle higher C – Rate data increases the robustness of the toolbox as it can be applied to different datasets and the potential to cover a wide range of user cases.
- This approach must be expanded to handle partial data and non-constant current cycles.
- Robustness is key. Once a model is extensively validated on various datasets, it can then be deployed as an online and onboard battery management software function. This is the ceiling of this approach. Having accurate real time diagnostic tools is the worthwhile objective.

References

(1) C. Birkl, R. Matthew, E. McTurk, P. Bruce and D. Howey, "Degradation Diagnostics of Lithium Ion Cells," *Journal of Power Sources*, vol. 1, pp. 373-386, 2016.

(2) R. Prosser, J. Chen, Offer and G. J. et. Al, "Lithium-ion battery degradation: What you need to know," *PCCP - Royal Society of Chemistry*, no. 14, pp. 1 - 23, 2021.

Intern Bio

I am currently studying Mechanical Engineering at University College London. Interested in mathematical modelling, data analysis and innovations in green technology. The intersection between mathematics and technical scientific knowledge is an area of great passion to me as it can bring about true innovation and change.

As part of my engineering project, I am undertaking a research project in Lean Premixed Combustors for Hydrogen enriched fuels, in a bid to reduce emissions and increase efficiency in current adopted energy generation infrastructure.

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