Battery modelling and the Goldilocks zone

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oorja

With the global shift towards electrification as a primary energy storage solution, there is an escalating need to better understand the behaviour of batteries. As battery technologies advance, incorporating several rare-earth elements and achieving higher energy densities, safety considerations become paramount.

Therefore, understanding the behaviour and performance of batteries under different operating conditions is critical to the large-scale adoption of batteries. Predictive modelling that can accurately forecast safety, performance, and lifetime is therefore indispensable.

The traditional approach to this type of analysis involves physics-based modelling, which, while powerful, presents considerable challenges. Batteries are complexly designed devices consisting of multiple materials layered together. Their functionality depends on an intricate interplay of various phenomena — electrochemistry, heat transfer, and fluid dynamics, to name a few — that control the transport of ions and electrons and the production of heat within the battery.

To effectively model these phenomena within the overall structure of an electrochemical cell, accurate design, transport, and degradation parameters are required to get physically relevant results from a physics-based model.

A key challenge during digital battery twinning is identifying the “Goldilocks zone” for parameters. For predictions to be dependable, the entire set of parameters must be precisely calibrated over the battery's lifecycle. However, obtaining and validating the correct set of parameters is not easy. Inaccuracies in parameter estimation can lead to significant errors in model predictions, reducing the reliability of safety assessments and performance predictions.

This complexity underlines the need for sophisticated tools capable of offering robust multi-parameter optimization, like -the hybrid software solution, oorja, which extracts essential information from HPPC (hybrid pulse power characterization) data to simulate real-world battery behaviour under various operating conditions.

Approach

At oorja, engineers have pioneered a hybrid approach that combines data and physics-based models to perform multi-parameter optimization with limited data sets to provide detailed information on transport and degradation parameters for Lithium-ion (Li-ion) cells.

Multi-parameter optimization techniques for estimating parameters using HPPC data involve adjusting the model parameters until a satisfactory fit is achieved between the model and the experimental data. The objective function for optimization is defined by the sum of the squares of the errors between the predicted and experimental values. The error is split into two parts.

- At the beginning of the step change in the pulse (e_{step}).
- During the pulse (e_{pulse}).

During the step change in the pulse, the loss function is computed using the following formula:

$$e_{\text{step}} = \sum [\ V_{\text{model}}(t_i) - V_{\text{exp}}(t_i)\ ]^2,$$

where t_i corresponds to the first of the pulses at which the step change in the current occurs, and during the pulse, the loss function is given by:

$$e_{\text{pulse}} = \sum [\ V_{\text{model}}(t_i) - V_{\text{exp}}(t_i)\ ]^2,$$

where t_i is the time duration of the pulse. Thereafter the total loss function is computed as the weighted sum of the e_{step} and e_{pulse}:

$$e_{\text{total}} = (e_{\text{step}} \cdot w_{\text{step}} + e_{\text{pulse}} \cdot w_{\text{pulse}}),$$

where w_{step} and w_{pulse} are the respective weights.

Among all the electrochemical parameters associated with the Single Particle Model (SPM), a set of five parameters (namely the internal resistance of the cell, the Li-ion diffusion coefficients of positive and negative electrodes, and the reaction rate constant of the positive and negative electrodes) are found to be sensitive to operating conditions, especially when considerable temperature fluctuations occur. Optimization algorithms adjust these parameters to minimize the differences between model predictions and experimental data. After optimizing the set parameters and obtaining the prediction fit, users can adjust these parameters to improve the prediction fit further based on their informed judgment.

Results

In HPPC tests, the battery is subjected to a sequence of charge and discharge pulses of different magnitude and duration in different states of charge (SoC). Its voltage response is observed and recorded.

Using the technique described previously, parameter optimization simulations were performed on experimentally obtained HPPC data sets of cylindrical 21700 commercial cells (LGM50) with a nominal capacity of 3Ah at temperatures 0°C, 25°C, and 40°C. Conditioning was carried out for 40 minutes. The resulting parameter values at various temperatures are shown in Table 1.

The prediction voltage responses obtained from the simulations and the percentage error plots are shown in Fig.1. ((a)-(c)) and ((d)-(f)), respectively, at different temperatures. The prediction responses obtained from the simulations correspond well with the experimental data, as seen in Fig.1. The error is limited to 7% in most of the test except in some cases in the middle and final part of the test where the error spikes above 7%.

Table 1 clearly shows the sensitivity of the model parameters to the varying operating conditions, particularly temperature. As the temperature increases cell resistance decreases, while the reaction rate constants of the positive and negative electrodes increase. Due to strong interactions with other factors, the solid-state diffusion coefficients of the positive and negative electrodes show no correlation with the temperature.

Discussion

The cell's internal resistance and reaction rate constants (of the anode and the cathode) are expected to decrease and increase with temperature, respectively. These relevant trends are captured through our simulations. In general, the diffusion coefficient for both positive and negative electrodes is expected to decrease with temperature, which was not observed in our simulations, thus requiring further investigation. In addition, larger deviations are

About oorja

Headquartered in Bangalore in India, oorja aims to empower automotive companies to design better batteries. Through a first of its kind cutting-edge technology that combines the best of Machine Learning and Physics, oorja enables automotive OEMs to make informed decisions to optimize battery packs by reducing time to market and costs.

Optimization parameters	Initial values	Optimized parameter values obtained at		
		0°C	25°C	40°C
Internal resistance (mΩ)	2	1.91	1.65	1.46
Positive electrode diffusion coefficient (m^2/s)	3×10^{-15}	3.0251×10^{-15}	2.9586×10^{-15}	3.0006×10^{-15}
Negative electrode diffusion coefficient (m^2/s)	2×10^{-14}	1.9547×10^{-14}	2.0781×10^{-14}	2.0551×10^{-14}
Positive electrode reaction rate constant ($mol^{1.5}/m^{5.5}$)	2×10^{-6}	2.3384×10^{-6}	2.8279×10^{-6}	2.9302×10^{-6}
Negative electrode reaction rate constant ($mol^{1.5}/m^{5.5}$)	4×10^{-7}	6.1249×10^{-7}	7.8374×10^{-7}	8.1862×10^{-7}

Table 1: Optimization parameters obtained at various temperatures.

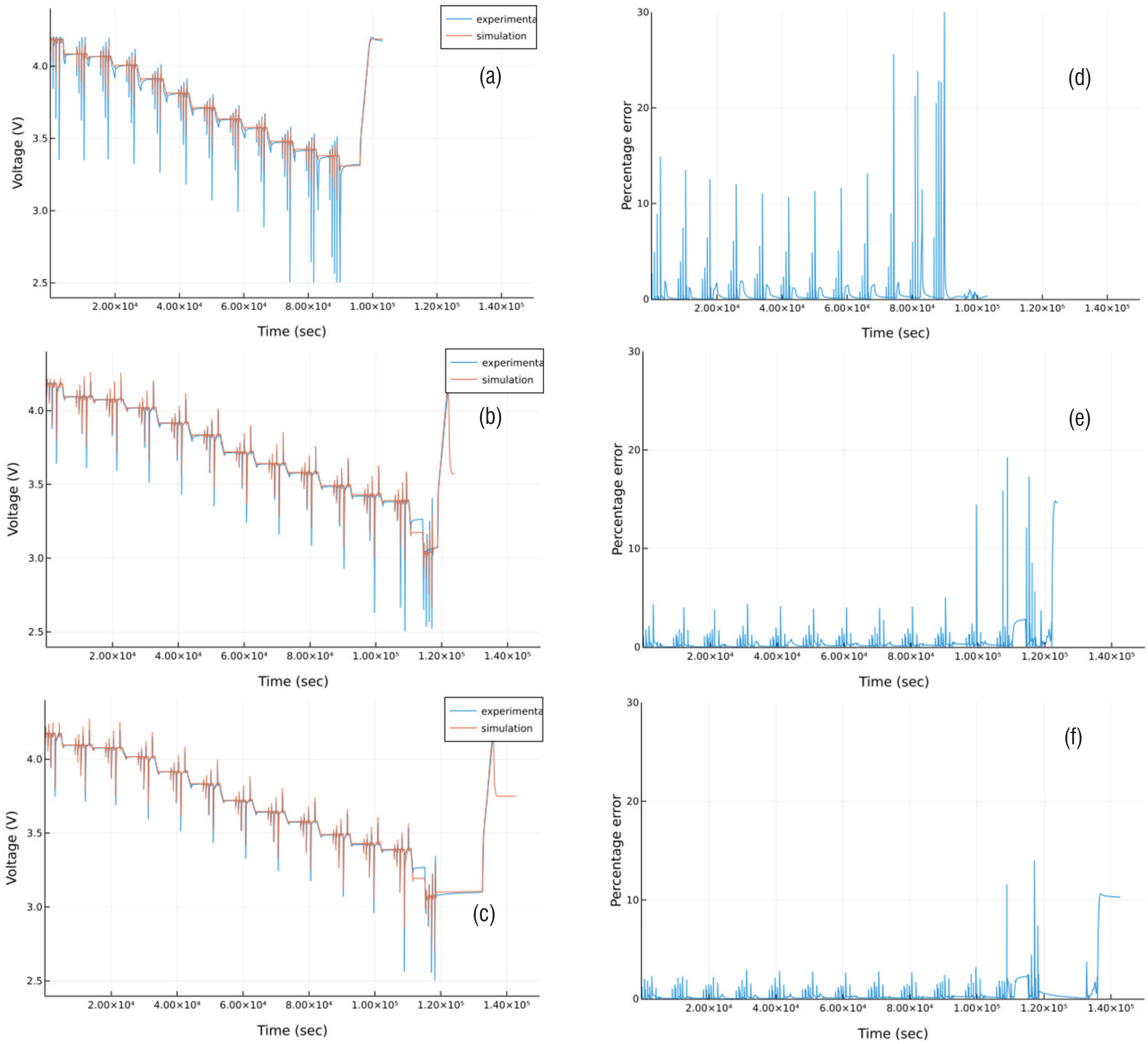

Fig. 1. Comparison of responses obtained from simulation and experiment for the HPPC data set at 0°C, 25°C, and 40°C are shown in (a)-(c). The error plots, showing the error between the experimental data and model prediction, are shown in (d)-(f).

observed in the voltages mounted to the lower SoC. This is due to the low sensitivity of the SoC to open circuit voltage (OCV). During regularization, higher weights can be used at low SoC to improve the quality of the fit.

Conclusion

This work shows the successful identification of the Goldilocks Zone for electrochemical parameters using the HPPC data. The optimization parameters show good physical trends with respect to temperature sensitivity. Furthermore, the comparison of voltage responses between predicted and experiment data shows a good match.

The accuracy of the parameters is also sensitive to the load on the different parts of the HPPC pulses. Further improvements can be made by adjusting of the individual error terms.

In the present method oorja regularizes the parameters obtained on different SoCs to obtain a set of parameters representing the cell for the SoC range. The weight of the regularization can be controlled to make the parameters dependent on the SoC. This will improve the adaptation to different states of charge. Moreover, in the current exercise, the cell design parameters are taken from the literature, and the accuracy of fit can be further improved by using design parameters obtained from the cell measurements.

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