

Improving efficiency of a numerical solver for microscopic Li-ion battery simulation including SEI degradation

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With the ongoing electrification of the transport sector as well as the shift of the energy sector to renewable energies, Lithium-ion batteries have gained significant attention as electrical power sources and storage devices, in particular due to their high energy density. To further optimize cell design and cell life time, it is crucial to understand and minimize degradation processes inside the battery. The overall designing process can be supported by developing suitable mathematical models and solvers.

In this talk we focus on a numerical solver for a microscopic electrochemical model for Lithium-ion batteries [1] including a model for the Solid Electrolyte Interphase (SEI) [2], one of the major degradation processes leading to capacity fade of the battery. In the isothermal setting of the original model [1] we solve for two quantities, the lithium ion concentration c and the electro-(chemical) potential ϕ . This results in a coupled system of parabolic and elliptic PDEs of the form

$$(1) \quad \begin{pmatrix} \partial_t c \\ 0 \end{pmatrix} = \begin{pmatrix} G^c(c, \phi) \\ G^\phi(c, \phi) \end{pmatrix}.$$

Introducing the SEI model, the Butler Volmer reaction kinetics at the anode interface are mostly replaced by an expression describing the total current density i_{tot} flowing across the interface, which can no longer be directly eliminated, as it is given by an implicit nonlinear equation. The SEI layer itself is not spatially resolved, but the local thickness of the layer is stored in corresponding variables L . Adding the set of nonlinear algebraic constraints for the total current density and a set of ODEs capturing the SEI layer growth, we obtain a system

$$(2) \quad \begin{pmatrix} \partial_t c \\ 0 \\ 0 \\ \partial_t L \end{pmatrix} = \begin{pmatrix} G^c(c, \phi, i_{\text{tot}}, L) \\ G^\phi(c, \phi, i_{\text{tot}}) \\ G^{i_{\text{tot}}}(c, \phi, i_{\text{tot}}, L) \\ G^L(\phi, i_{\text{tot}}, L) \end{pmatrix},$$

containing additional types of equations and physical processes compared to (1). Using a fully implicit monolithic solver, we notice a significant performance degradation comparing simulations with and without SEI.

Thus, we propose an alternative solver combining operator splitting and preconditioning of the resulting linear systems in order to separate the newly introduced equations step by step. The obtained linear systems exhibit a similar structure compared to the ones of the basic battery model. First numerical results suggest that the new solver can improve the performance for SEI simulations, yielding performance results in line with the ones observed for non SEI simulations.

REFERENCES

- [1] A. Latz and J. Zausch, Thermodynamic consistent transport theory of Li-ion batteries, *Journal of Power Sources* **196** (2011), 3296–3302.
- [2] T. Schmitt, *Degradation Models and Simulation Tools for Lithium and Zinc Batteries*, PhD Thesis, Ulm University, 2019.