

Battery Software Available for Licensing

<u>A Two-Dimensional Thermal-Electrochemical Model</u> <u>for Prismatic Lithium-Ion Cells</u>

A team of NREL scientists developed this cost-reducing software model that incorporates material parameters, electrochemical characteristics, and thermal design aspects to provide a customized, physics-based estimate on the remaining capacity or useful life of prismatic lithium ion batteries. This model in C++ can provide real-time updates of electrochemical states when interfaced with a battery, can predict the voltage under specified conditions and initial states, and has been used to demonstrate a 50% reduction to charge times of lithium-ion cells and a 10% reduction to the size of a PHEV battery pack.

<u>Lithium-Ion Batteries: Predictive Computer Models</u> for Lithium-Ion Battery Performance under Standard and Potentially Abusive Conditions

Scientists at NREL have developed four advanced computer models to predict thermal, electrical, and electrochemical battery performance to enable developers to optimize battery designs for improved life, overall performance, cost, and safety. These models are faster and more accurate than currently available models and can stimulate three-dimensional regions of temperature, cell behavior under internal short circuits, and interactions between cells within a battery pack. These models include: the Electrochemical Lithium-Ion Battery Performance Model, the Multi-Scale, Multi-Dimensional Lithium-Ion Battery Performance Model for Lithium-Ion Batteries, and the Electrical Thermal Network Model for Multi-Cell Lithium-Ion Batteries.

Battery Life Predictive Model

This novel software model developed by NREL scientists analyzes the performance of batteries over a lifetime of use in real world environmental and loading scenarios. Developed in the commercial platform MATLAB, the Battery Life Predictive Model utilizes an extensive database of previous experiments and a series of empirical models to simulate lifetime performance requirements, to minimize the size and cost of a battery, and to produce accurate estimates of battery life, increases in battery resistance, and the reduction in capacity over a given number of cycles.

A Material Model for Simultaneous Coupling of Mechanical and Electrochemical Phenomena

This model developed by NREL researchers enables simultaneous coupling of the material's mechanical loading to electrical, electrochemical, and thermal response through the use of numerical

solvers compatible with the commercial software platforms of ANSYS, CCM+, Comsol, or LS-DYNA. This model promotes good computational efficiency, enables end users to study physical processes with large time constants, and captures the two-way interactions of the different physical phenomena in battery systems.

MSMD/GH-MSMD Baseline Suite

This computer software is composed of executables to run multiscale, multi-dimension (MSMD) and GH-MSMD multi-scale multiphysics framework battery model simulations and includes baseline options of particle domain models (PDM), electrode domain models (EDM), and cell-domain models (CDM). This model in C++ greatly reduces computational costs, resolves the impacts of design and application characteristics, and solves the details of kinetic, transport, and geometric attributes of electrode particulates including morphology, size distribution, and mixture composition of active materials.

A Representative Sandwich Model to Simulate the Mechanical-Electrical-Thermal Response of a Pouch format Lithium-Ion Cell Subjected to Mechanical Crush

Built in the commercial platform of LS-DYNA, this simulation tool developed by NREL researchers evaluates the propensity of a given short-circuit event based on given test conditions and specific test articles. This model accounts for heat dissipation versus accumulation during the same time frame and utilizes separate criteria for the mechanical, electrical, and thermal failure of individual layers to quickly and efficiently estimate each criterion's time for failure and the sequence of follow-on reactions that result in thermal runaway.

Contact Information

For more information or for licensing opportunities, please contact Doreen Molk, Licensing Coordinator, National Renewable Energy Laboratory, at (303) 275-3014 or *Doreen.Molk@nrel.gov*.

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