

# Lithium-Ion Battery Multi-Physics Simulations Using LS-DYNA<sup>®</sup>

Jie Deng<sup>1</sup>, Chulheung Bae<sup>1</sup>, Theodore Miller<sup>1</sup>, Min Zhu<sup>1</sup>, Pierre L'Eplattenier<sup>2</sup>,  
Inaki Caldichoury<sup>2</sup>

<sup>1</sup>Ford Motor Company, Research and Innovation Center, Dearborn, Michigan 48124

<sup>2</sup>Livermore Software Technology LLC, Livermore, California 94551

## Abstract

*The market share of electrified vehicles grows rapidly in recent years. One of the top priorities in the electrified vehicle design is to improve the robustness of lithium-ion battery system during a crash. Various abuse tolerance tests have been developed to evaluate the performance and robustness of lithium-ion batteries. These tests can be resource intensive, and in some cases, provide limited information on the failure mechanisms of batteries. As such, computational modeling becomes an important tool to evaluate the battery under different abuse scenarios. Here we present a multi-physics battery model that can predict coupled mechanical, thermal, electrical and electrochemical responses of automobile lithium-ion batteries under abusive conditions. In this model, the electrochemical behavior of batteries is described by a spatially distributed equivalent circuit model, where polarization and damping effects are captured by a resistance-capacitance network. During simulations, the mechanical solver predicts the onset of short circuit, and then the coupled thermal, electrical and electrochemical solver captures the evolution of temperature, voltage and current distribution after short circuit initiation. In order to make the proposed model applicable to module or pack level simulations, various element formulations and strategies have been developed to improve computational efficiency without sacrificing much accuracy. Details of model set up, parameters evaluation, and case studies that demonstrate the model capabilities will be presented. Experimental validation of model prediction and the future development of this framework will also be discussed.*

Battery robustness is a key design factor for electrified vehicles. Both abuse tests and numerical simulations have been applied to evaluate the responses of batteries under extreme conditions [1]. Since conducting abuse tests on large-format batteries can be resource intensive, computational modeling as a tool to examine battery performance has gained interest in the automotive industry. Nevertheless, due to complex internal structures of batteries, there are three main challenges in battery multi-physics modeling [2]. First, a battery model should couple different physical processes (such as mechanical, thermal and electrochemical) that may occur simultaneously during an abuse event. Second, simulations should be able to extend from component level to pack level, which is several orders of magnitude different in length scale. Third, material properties of battery components need to be measured and modeled accurately, which is not straightforward since they usually depend on various factors such as strain rate and temperature. To address these challenges, Ford and LST-LLC collaborated to develop new keywords and solver capabilities for battery simulations in LS-DYNA. In this paper, we briefly introduce the progress in model development and solver capabilities.

The battery model in LS-DYNA currently can capture coupled mechanical, electrical, electrochemical and thermal responses of batteries during abuse testing [3]. In particular, the momentum, charge and energy balance equations are solved to get the mechanical, electrical and thermal responses of batteries, respectively. The electrochemical behaviors of batteries are described by the Randles circuit model [4] that is computationally efficient (required by large-scale simulations). A Randles circuit contains an open-circuit voltage, an internal resistance and a resistance-capacitance pair for polarization and damping effects. During short-circuit, the Randles circuits in the shorted area are replaced by short-circuit resistances to allow large current flow. The coupling strategy of these solvers can be found in Ref. [1].

The model is implemented in LS-DYNA in three different formats (i.e., solid model, t-shell model and macro model) in order to cover simulations in different length scales. In a solid model, each individual component is represented by one layer of solid elements. It contains the most detailed information of battery components but is computationally intensive and only suitable for cell level simulations. The t-shell model [5] utilizes composite t-shell elements to represent the cell bulk, which has computational advantages in mechanical solver. In impact simulations where the mechanical solver dominates the entire simulation time, using t-shell model can save simulation time by one order of magnitude compared to the solid model [5]. The macro model [6] assumes that the cell properties are homogeneous and uses standard solid elements to represent a cell. It is efficient in all solvers and therefore applicable for module and pack level simulations. It is demonstrated that with appropriate material properties, a macro model can achieve similar results as a solid model using much less computational time [6].

An accurate material model is essential in a battery multi-physics modeling to enhance its predictive capability. Most of material models for battery components or cell bulk are elastic-plastic models (isotropic or anisotropic), crushable foam models and granular material models [7]. These material constitutive models are available in the LS-DYNA material library, and some of them includes the effects of strain rate and/or temperature. The mechanical properties of a separator may depend on orientation, strain rate and temperature in which the current available material models within the solver library does not address these effects. In that case, new constitutive material models need to be developed to capture these effects and coded to be used as a “User Subroutine” in LS-DYNA.

In summary, LS-DYNA can be used to simulate a multi-physics behavior in Lithium-ion batteries subjected to impact or abuse at the cell, module and pack levels.

### Acknowledgements

Ford authors acknowledge the support of the Vehicle Technologies Office, Office of Energy Efficiency and Renewable Energy, U.S. Department of Energy under DOE Agreement DE-EE0007288.

### References

- [1] J. Deng, C. Bae, J. Marcicki, A. Masias, T. Miller, *Nature Energy*. 3, 261-266, 2018.
- [2] J. Deng, C. Bae, A. Denlinger, T. Miller, *Joule*, 2020, DOI: <https://doi.org/10.1016/j.joule.2020.01.013>
- [3] J. Marcicki, M. Zhu, A. Bartlett, et al., *J. Electrochem. Soc.*, 164, A6440-A6448, 2017.
- [4] P. L'Eplattenier, I. Caldichoury, J. Marcicki, et al., *LS-DYNA conference proceedings*, 2016.
- [5] J. Deng, C. Bae, T. Miller, P. L'Eplattenier, S. Bateau-Meyer, *J. Electrochem. Soc.* 165, A3067-A3076, 2018.
- [6] J. Deng, C. Bae, T. Miller, P. L'Eplattenier, I. Caldichoury, *J. Electrochem. Soc.* 166, A3119-A3121, 2019.
- [7] J. Zhu, T. Wierzbicki, W. Li, *J. Power Sources* 378, 153-168, 2018.