

Open Architecture Software (OAS) for modeling multi-physics phenomenon of Li-Ion Batteries

S. Pannala, S. Allu, W.R. Elwasif, S. Simunovic, and J. A. Turner

Oak Ridge National Laboratory
One Bethel Valley Road, Oak Ridge, TN-37831

In this paper, we will present a flexible, robust, and computationally scalable open-architecture framework that integrates multi-physics and multi-scale battery models. The physics phenomena of interest include charge and thermal transport, electrochemical reactions, and mechanical stresses. They operate and interact across the porous 3D structure of the electrodes (cathodes and anodes), the solid or liquid electrolyte system and the other battery components. The underlying lower-length processes are accounted for through closure equations and sub-models that are based on resolved quantities. The schematic of this framework is given in Fig. 1.

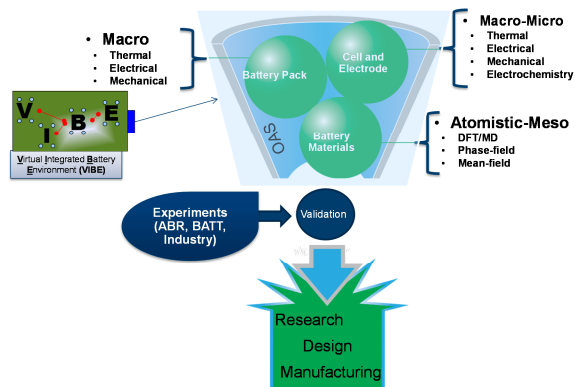


Figure 1: Schematic of the OAS modeling framework and interactions with other tasks within the CAEBAT program and external activities.

This framework will enable seamless integration of the following physical phenomena that are necessary for development of realistic and predictive battery performance and safety models. This open architecture software (OAS) framework as part of DOE CAEBAT (Computer Aided Engineering for Batteries) is derived from Integrated Plasma Simulator (IPS) [1]. The framework is designed with a lightweight Python backplane and is highly modular in structure. This would support integration of multiple modeling approaches and by design allows for switching between different components to accelerate design of batteries. The framework provides services for the component execution coordination, resource management, data management, and inter-component communication.

We will present results for two different simulation cases. The first modeling study shows the variation of internal temperature distribution in a cylindrical cell (with current collectors resolved) on the electrochemistry model (NTG (Newman, Tiedemann and Gu model) [2] vs. Pseudo-2D model) for various discharge rates as well as different coarse-grain mappings between the electrochemistry, electrical and thermal transport. We use AMPERES (Advanced MultiPhysics for Electrical and Renewable Energy Storage) components for both thermal and electrical transport. Fig. 2a shows the geometry and the finite element mesh used to resolve the geometry of the cylindrical cell and the current collectors. The top hierarchy model has 168 (56 each for the cell-sandwich and positive and negative current collectors) zones in 4 quadrants. The zones describe different current collector

and cell sandwich regions. The simulation uses 56 concurrent Dualfoil simulations for different cell-sandwich zones. Typical results are shown in Fig. 2b. The maximum temperature occurs at the cell core as expected.

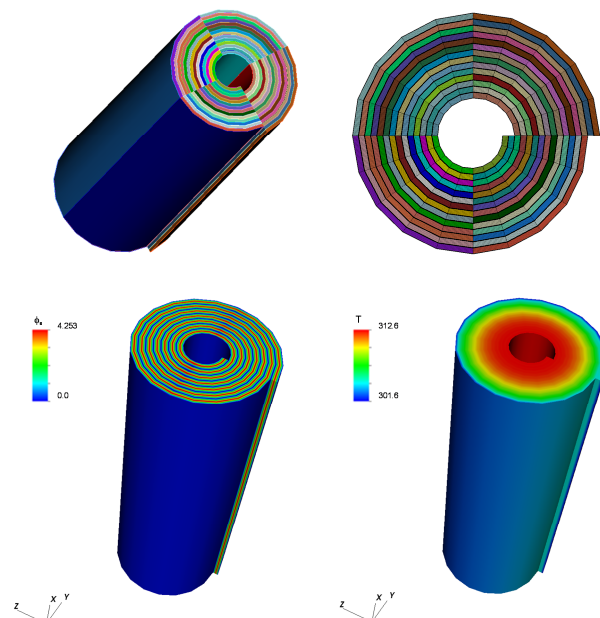


Figure 2: Geometry, mesh, electric potential, and temperature of the simulated cylindrical cell.

In the second study, a battery module is simulated with transient current, thermal and electrochemical transport in a three-dimensional stack as shown in Figure 3. Results for this scenario with AMPERES component for the electrical and thermal transport and Dualfoil component for electrochemical transport will also be presented.

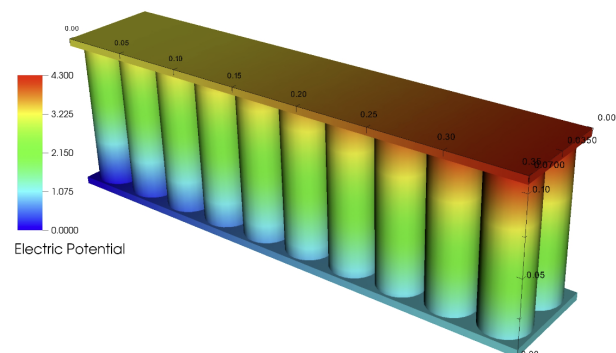


Figure 3: Electrical Solution profiles (preliminary) of simulation results for a Battery Module.

Acknowledgement

Research sponsored by the U.S. Department of Energy, Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Vehicle Technologies, as part of the Energy Storage Program, under Contract No. De-AC05-00OR22725 with UT-Battelle, LLC.

References:

1. Elwasif, W.R. and Bernholdt, D.E. et al., "The design and implementation of the SWIM Integrated Plasma Simulator", Parallel, Distributed and Network-Based Processing (PDP), IEEE, 419-427, 2010.
2. Kim, U.S. et. al., "Modeling the Dependence of the Discharge Behavior of a Lithium-Ion Battery on the Environmental Temperature", Journal of the Electrochemical Society, 158, A611, 2011.