Three dimensional thermal, electrical and electrochemical modeling of Li-ion batteries

Sergiy Kalnaus, Srikanth Allu, Sreekanth Pannala, Wael Elwasif, Srdjan Simunovic, and John A. Turner

Computational Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN-37831

Accurate predictions of performance and thermal behavior are essential for development of lithium-ion batteries and their integration into automotive drivetrains. Such predictions are based on solutions of mathematical problems representing several physical processes responsible for the overall cell behavior. Integration of electrochemical models with electrical and thermal models is essential for accurate description of cell performance. Development of computational software capable of integration of available models into one suite of tools with capability of accurate cell modeling will accelerate the design process as well as enable better in-use thermal management of Li-ion cells.

The CAEBAT (Computer Aided Engineering for Batteries) [1] program involves collaboration among several National Laboratories and industrial partners aiming at development of such software. Within this effort we have developed the computational framework which combines physics-based models developed by the research community with latest advanced numerical methods and algorithms. The CAEBAT Open Architecture Software (OAS) framework has a modular structure with each component representing physics-based model (Fig.1.). The control of the components, as well as processing of input and output data, occurs by the component adapters. The state adapters update the battery state based on the output from the components. The battery state file serves as data collection describing the state of the system at each time step, thus passing the information to each component. This system constitutes the Virtual Integrated Battery Environment (VIBE).

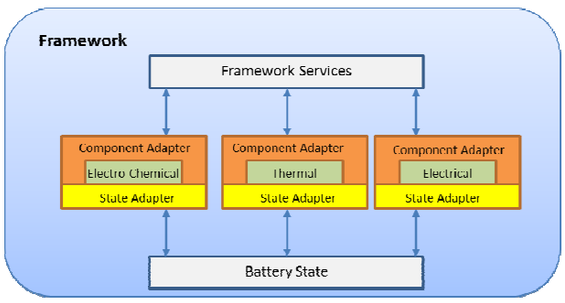

Fig. 1. Schematic of the Virtual Integrated Battery Environment

At the present stage capabilities include coupled electrochemical thermal and electrical models integrated within VIBE. Electrochemical models include the pseudo-2D model based on the porous electrode theory and concentrated solution behavior for electrolyte as well as the model based on linear approximation of cell polarization functions. The solutions of potential provided by electrochemical model are updated by solutions from electrical model which solves the equations for the continuity of current resolving the current collectors. These solutions are used in computation of heat sources. The heat sources are used as input for thermal modeling. Solution of both electrical and thermal 3D transport models is performed by ORNL developed AMPERES (Advanced Multi-Physics for Electrical and Renewable Energy Storage) code [2].

We demonstrate the capabilities of the framework by performing case study simulations of different cell geometries (Fig. 2.). Selection of the models as well as their influence on the solution is discussed. Optimization of cell parameters with the goal of temperature minimization is performed. Finally the simulations are validated by experimental thermal measurements at different applied current densities.

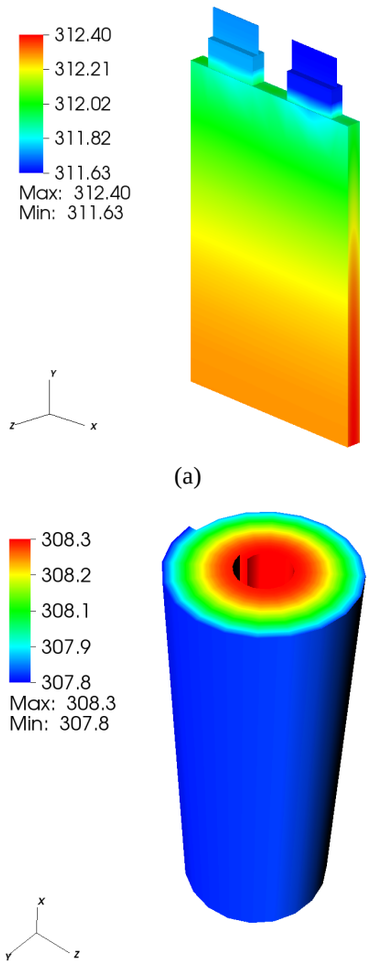

Fig.2. Temperature distribution (in K) in a) 16.4 Ah/m^2 pouch cell at the end of 5C discharge; b) 14 Ah/m^2 rolled cylindrical cell at the end of 2C discharge.

Acknowledgment: This work at Oak Ridge National Laboratory (ORNL) was supported by the Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Vehicle Technologies of the U.S. Department of Energy. ORNL is managed by UT Battelle, LLC, for the U.S. Department of Energy under contract DE-AC05-00OR22725.

References

[1] Turner, J., Pannala, S., Mukherjee, P., Allu, S., Elwasif, W., Simunovic, S., Bernholdt, D., 2012 DOE Hydrogen and Vehicle Technologies Program Annual Merit Review Report, Project ID ES121: Open Architecture Software for CAEBAT.

[2] Pannala, S., Mukherjee, P. P., Allu, S., J. Nanda, Martha, S. K., Dudney, N. J. and Turner, J. A., "A micro-mesoscopic model for Li-Ion intercalation batteries," *219th ECS meeting* (2011).