ABSTRACT

In this paper, we demonstrate the AutoLion™ suite: a collection of battery simulation tools for electric drive vehicle (EDV) Li-ion cell and pack development. At the heart of each simulation tool is a thermally coupled battery (TCB) model that simultaneously computes electrochemical and thermal effects of large format cell and pack operation. As we will demonstrate through illustrative examples, TCB modeling is critically important for properly simulating EDV Li-ion cells and packs under conditions of interest to the automotive industry (cold-start, rapid charge, safety simulations, etc.). Furthermore, we highlight a one-of-a-kind degradation model that simultaneously predicts cell performance and degradation over the life cycle of the battery.

INTRODUCTION

Significance

Lithium-ion batteries are very sensitive to temperature and heat generation during operation. Battery systems in electric vehicles are required to withstand extreme operating conditions, including high rates of charge/discharge, very high/low ambient temperatures, and must be able to maintain integrity in the event of a vehicle crash. Battery systems that function under these strict criteria are notoriously difficult and expensive to design, produce, and test, particularly for safety testing in which cells and packs are irreversibly destroyed. Executing the battery development cycle in a virtual environment saves valuable resources that would otherwise be used to optimize the system through experimental practice. It is for this reason that advanced computer modeling for large-format cells and full EV battery packs provides an invaluable tool to the automotive industry.

The nature of large-format cells and packs makes the modeling and simulation of these systems an extremely difficult task. The model must be powerful, robust, and take into account the wide variety of conditions to which the battery system is subjected. This requires advanced algorithms that are electrochemically and thermally coupled (ECT) to take into account thermal behavior during operation, and how it influences system safety and performance. TCB architecture is a key feature of any accurate, reliable model because of the extremely complex, non-linear interaction between the electrochemical and thermal behavior that must be captured during simulation. Equally significant to the TCB approach is a high quality database from which material properties can be drawn, including both electrolyte and active materials properties, over wide-ranging conditions such as temperature, state of charge (SOC), and electrolyte concentration. These algorithms, combined with a high quality materials database, must be executable in three dimensions, allowing for the design and simulation of these systems in a complete virtual environment.

The work described here outlines a proprietary modeling approach (the TCB model), and the subsequent commercial implementation of this model, AutoLion™. Incorporating such modeling software into a battery product development cycle can drastically reduce the amount of time, effort, and capital that would normally go into the development of EV/HEV powertrains. The entire process can be carried out in a virtual environment, reducing time and money spent fabricating test rigs, developing cooling strategies, and the costly mistakes made during the process. In addition, insights into the behavior of the cell/pack are made available that would otherwise be unobtainable with standard empirical analysis.
Current Technology
Li-ion battery modeling traces its roots to the early nineties, when the first 1D electrochemical model was developed using a macro-homogeneous, isothermal model approach [3]. Current modeling technology is largely based on this approach [1-2], with various modifications to accurately capture temperature evolution within the cell during operation.

Contemporary approaches to li-ion battery modeling often use a combination of both electrochemical and thermal models in an iterative process to obtain temperature values during cell operation. When electrochemical effects are used to determine temperature, but these values are not fed back into the electrochemical model, it is referred to as one-way coupling [4]. Subsequently, when the temperature values are fed back into the electrochemical model, this is called two-way coupling [4]. One-way coupled models can be useful in a narrow window of operating conditions and in a limited range of applications. However, for cases where Li-ion batteries exhibit strong temperature dependence, rapid internal heat generation, or near instantaneous transient behavior (e.g. cold-start from < −20°C, high charge/discharge rates, and safety events such as internal shorting), a TCB modeling approach is necessary.

MODEL DESCRIPTION
The TCB model described in this work is based on a multi-scale, physics-based approach that simultaneously calculates both electrochemical and thermal effects of li-ion battery operation. Early models using this approach were developed by CY Wang and co-workers, using what is now called “computational battery dynamics” to fully capture electrochemical and thermal behavior ranging from the microscopic material level to the macroscopic pack level [5].

The model can be summarized by five governing equations that determine the electrochemical and thermal response of a li-ion battery, which are tabulated in Table I. Equations (1) and (2) represent the conservation of charge in the solid phase and the electrolyte phase, respectively. Equation (3) gives the Li⁺ species conservation in the electrolyte phase, while equation (4) represents the Li diffusion in the active material particles.

The evolution of temperature within the cell over time is governed by the conservation of energy (5), where the heat source term includes entropic, reaction, and joule heating components. The electrochemical-thermal (ECT) coupling of these equations is reflected in the transport properties of equations (1) through (4) being properly described as strong functions of temperature, local electrolyte concentration, SOC, etc., which enables a truly accurate simulation of highly non-linear battery dynamics over wide-ranging conditions.

The model itself is critical to accurate simulations, but is ineffective without high quality materials properties corresponding to the given conditions. In this work, the TCB model is accompanied by a materials database that has been developed by testing over 100,000 coin cells. The resulting database consists of data for anode and cathode active materials and electrolytes, including NCM, LCO, LTO, LFP, and graphite, among others. All relevant properties are characterized over wide-ranging temperatures, states of charge, electrolyte concentrations, etc., in order to yield accurate simulations under the extreme conditions demanded by the auto industry.

### Table 1. Conservation Equations

<table>
<thead>
<tr>
<th>Equation</th>
<th>Description</th>
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<tbody>
<tr>
<td>(1)</td>
<td>( \nabla \cdot (\sigma \text{eff} \nabla \phi_s) = j^{\text{Li}} )</td>
</tr>
<tr>
<td>(2)</td>
<td>( \nabla \cdot (k \text{eff} \nabla \phi_e) + \nabla \cdot (k_p \text{eff} \nabla \ln c_e) = -j^{\text{Li}} )</td>
</tr>
<tr>
<td>(3)</td>
<td>( \frac{\partial (c_e c_o)}{\partial t} = \nabla \cdot (D_e \text{eff} \nabla c_e) + \frac{1 - t^{\text{Li}}}{T} j^{\text{Li}} )</td>
</tr>
<tr>
<td>(4)</td>
<td>( \frac{\partial c_o}{\partial t} = \frac{D_o}{\tau^2} \frac{\partial^2 c_o}{\partial r^2} )</td>
</tr>
<tr>
<td>(5)</td>
<td>( \frac{\partial (\rho c_o T)}{\partial t} = \nabla \cdot (k \nabla T) + q_r + q_j )</td>
</tr>
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</table>

\( q_j = \sigma \text{eff} \nabla \phi_s \nabla \phi_e + k \text{eff} \nabla \phi_s \nabla \phi_e + k \text{eff} \nabla \ln c_e \nabla \phi_e \)

CASE STUDIES
Model Validation
The TCB model has been validated against empirical data from HEV pulse testing profiles [6], and extensive validation is currently ongoing. Sample cell validation in Figure 1 shows cell operation at 1C discharge at temperatures of −20,
−10, 0, 25, and 45°C. As shown in the figure, the experimental data and simulation results have strong agreement. The distinct “dip”, seen at the beginning of discharge in the −20°C curve in Figure 1 is caused by complex electrochemical-thermal interaction as the battery discharges, clearly showing the temperature sensitivity of cell performance. The strong agreement between the experimental and simulation data demonstrates the robustness and accuracy of the model, particularly at low temperatures with highly complex, non-linear ECT phenomena. As was previously stated, experimental validation for the model is ongoing, and includes large-scale, multi-dimensional validation for cells and packs.

**AutoLion-3D™: Battery Pack Model**

The model is capable of rendering cell and pack simulations in 3D, while simultaneously outputting electrochemical and thermal results. In this case, a 1C discharge was modeled for an air cooled, 2.8kWh Li-ion battery pack. The air cooling system for the pack used a flow rate of .36kg/s and an inlet temperature of 20°C. The initial cell temperature was set to 50°C to simulate a pack cooling in a high temperature environment.

Figure 2 shows pack temperature (max, min, and average) (°C) and pack voltage (V), respectively. Figure 3 is a 3D rendering of the pack with the temperature contours shown at t=3000 sec. Figures 2 and 3 were generated simultaneously, giving thermal and electrochemical output with just one simulation, and was performed on an 8-CPU desktop in ~15 minutes (simulation of ~ 58 minutes).

**AutoLion-3D™: Cell Model**

The model has been developed for simulating all types of large-format cells typically used in the automotive industry, including both cylindrical and prismatic rolled electrode designs (RED) (i.e. “jelly rolls”) and stacked electrode designs (SED). Several case studies have been performed to highlight the AutoLion-3D™ cell model.

The first case is a 2.3 Ah 18650 cell simulation at 6C discharge. The active materials are graphite for the anode, and LCO for the cathode. Figure 4a shows a simple thermal distribution of the cell at t=200 seconds. Figure 4b shows the same cell unwound, and displays the local current density across the electrode.

The second case is a 3Ah prismatic RED “jelly roll”. This cell was designed using AutoLion™’s GUI feature and
simulated at 6C discharge. Figures 5a and 5b show current density and SOC respectively, in the unrolled electrode at t=100 seconds. A key strength of the model is the ability to simultaneously output both thermal and electrochemical results, as shown in this example. In addition, the model is useful in predicting local values across the system, as opposed to average values. In this case, the local current density and SOC is rendered, allowing the user to identify the detailed relationship between SOC, current density, and cell temperature. This insight is unavailable through strictly empirical testing, and is unique to TCB modeling technology.

A major advantage to using a TCB modeling approach is the ability to accurately simulate safety events in battery systems such as internal shorts, external shorts (e.g. nail penetration), or mechanical failure of the battery casing. The third case presented in this section demonstrates the capabilities of the TCB model by simulating a partial nail penetration in a 10Ah NCM/graphite prismatic cell. As seen in Figure 6, at just 0.5 seconds the local temperatures dangerously approach 400°C, which could easily trigger thermal runaway and catastrophic failure of the cell. This can be inferred from the virtual simulation using AutoLion-3DTM, without using any experimental resources. The contours in Figures 6b and 6c highlight the local electronic phase potential of the individual current collectors within the partially-penetrated SED cell. The vectors further highlight the substantial current flowing from the unpenetrated layers of the SED cell to the penetrated layers, generating massive amounts heat and leading to dangerously high temperatures.

**Figure 4. 2.3AH 18650 cell undergoing 6C discharge. (a) Temperature distribution. (b) Current density distribution**

**Figure 5. 3Ah unrolled prismatic RED cell undergoing 6C discharge. (a) Current density A/m². (b) SOC**

**Figure 6. Partial nail penetration of a 10 Ah NCM/graphite cell**

**AutoLion-1DTM: Cell Model**

EC Power has developed a one-dimensional software program using the TCB model to facilitate rapid simulations and high volume research. AutoLion-1DTM utilizes the same TCB model and materials database, but allows for rapid simulations by considering only the cell thickness during calculation. In addition, the program includes a proprietary degradation model that simultaneously predicts cell performance and cycle life.
The degradation model in AutoLion-1D is based on commonly understood degradation mechanisms for Li-ion batteries. Two primary mechanisms of degradation are Li deposition on the anode and interfacial film growth (e.g., solid-electrolyte interphase (SEI) layer on the anode and film growth on cathode oxides). These mechanisms lead to reduced power and capacity of the cell, thus reducing the effective cycle life of the system. The AutoLion-1D performance model includes our proprietary rate equations for surface film growth on the anode and cathode, incorporating the effects of surface film formation on species diffusion and ionic conduction into the performance model.

The following case study shows the validation of the degradation model for an 18650 NCM-graphite cell. Figure 7 shows data for 5 cycle numbers 0 to 5000 at 1000 cycle intervals at 1C discharge. Figure 8 shows the same curves at 10C discharge rate. The model predictions are in very good agreement with the experimental data. In this case, the simulations shown in Figures 7 and 8 took only \( \sim \) 15 seconds per cycle to compute on a standard laptop or desktop computer.

A second case study further supports the capability of the model by simulating a cold start scenario. Just as in Figure 1, a substantial dip and recovery in voltage of the cell is captured by AutoLion-1D™ in Figure 9. The system in this case is an NCM/graphite cell with an initial SOC of 1 at an ambient temperature of \(-20^\circ C\). The initial immediate drop-off in voltage is due to cold conditions, but the quick recovery of voltage is due to rapid temperature increase in the cell which leads to enhanced performance. This phenomenon, where voltage actually increases with discharge, can only be captured with proper ECT coupling.

**AutoLion-ST™: Software in the Loop**

AutoLion-ST™ is the implementation of the TCB model in a software-in-the-loop model block. The model facilitates the study and development of adaptive control using software-in-the-loop tools under extreme conditions pertinent to the auto industry (e.g., \(-30^\circ C<T<80^\circ C\)). Figure 10 shows Li-ion battery simulation via AutoLion-ST™ for pulse-heating scheme under cold-temperature startup. The discharge current pulse amplitude was increased from \( \sim 2C \) to \( \sim 4C \) after the average pack temperature was sensed to reach 5\(^\circ C\). As seen in Figure 11, the cell voltage response is directly in step with the Figure 10, which highlights AutoLion-ST's ability to deal with instantaneous changes in the load profile. Further, as the pack temperature rises with time, the voltage peaks gradually become smaller, owing to the reduced overpotentials at high temperature.
SUMMARY/CONCLUSIONS

This paper has demonstrated the advantages of using a thermally coupled battery model for automotive Li-ion battery simulations. The developed TCB model is the first commercially available model to simultaneously calculate both electrochemical and thermal effects of large format Li-ion cells and packs. Several case studies have demonstrated its capabilities, robustness, and its effectiveness in battery simulations of interest to the automotive industry. The nature of the model presented here is implemented in several different tools called AutoLion™ to enhance the product development cycle of automotive Li-ion battery systems. These tools enable 3D and 1D performance simulation, pack cooling strategies, investigation of safety events, and software-in-the-loop controls/system development.

REFERENCES


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