New Lithium-Ion Battery Performance Prediction Tool Combining Experimental State-of-the-Art Technology and Kinetic Thermal Modeling

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Predicting a battery's response to thermal, electrical and mechanical abuse is a key factor to successful product development. Advanced thermal modeling can predict a battery's response to these abuse scenarios as well as what conditions will lead to a hazardous response from the battery. Efforts at TIAX continue development of cheaper, faster, more reliable and more flexible approaches to ensuring safety in lithium-ion batteries by integrating accurate thermal modeling software in combination with selected experimental verification and thermal hazard screening methods.

To advance safety and performance modeling, TIAX combines detailed understanding of the individual chemical reactions within a lithium-ion battery with a microkinetic approach that builds on a set of specific chemical reactions within a finite element method. The finite element method takes input from "real" battery chemistry, known from the lithium-ion battery community's library of measurement data, and tracks the resulting conditions through an array of hundreds of thousands of defined battery elements. For lithium-ion batteries, we specifically model the individual exothermal events associated with reactions between electrolyte, cathode and anode during charge/discharge or decomposition scenarios. By tracking heat flow and diffusion of individual reaction species, and by iterating calculations through the array of defined elements, temperature and chemical species can be mapped at various points in the battery as a function of time. These results can then be related to real temperature and pressure conditions that define a battery's safety performance.

The TIAX thermal model has incorporated more detailed battery chemistry into the modeling equations predicting heat generation and flow and performed specific experiments to guide and evaluate modeling accuracy. Recent results demonstrate the effect of materials changes and the effectiveness of external cooling. In this paper, we illustrate the use of these models for two critical functions: (1) to screen safety related properties of new materials being considered in battery development, and (2) to evaluate the effectiveness of undesired, yet required, non-energy producing additions to lithium-ion battery systems.

Figure 1 shows TIAX modeling results on a temperature profile of a lithium-ion 18650 cell placed into an oven at 4 different temperatures (120 - 160 °C). These conditions are similar to the "Hot Box" test required by UL testing procedure. TIAX modeling shows that internal cell reactions contribute to temperature overshoot at 150 and 160 °C. Additional modeling results combined with experimental validation will be given at this presentation. Also addressed will be how this information can be used to better understand materials properties and their role in determining lithium-ion battery safety.

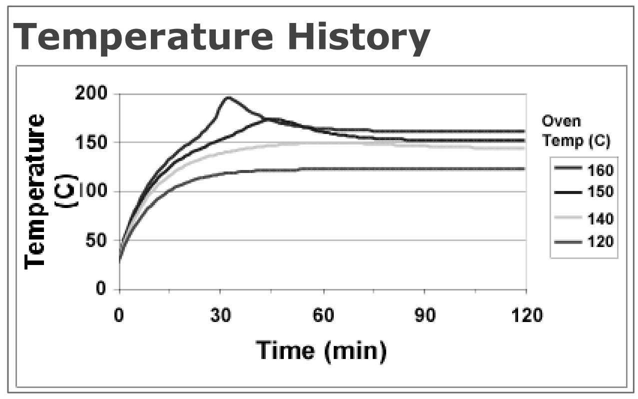

Figure 1. TIAX modeling of the temperature response by an 18650 Li-ion cells under elevated temperature conditions from 120 – 160 °C.