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Mathematical Modeling as a Tool for Understanding Lithium-Ion Batteries in Electric Vehicles

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Abstract

For a battery manufacturer, modeling and simulations can improve the design of cells and modules by identifying limitations in a design. The influence of different geometries, electrode materials, pore distribution, electrolyte composition and other fundamental parameters can be studied. This results in the intuition for a system that is required for making vital improvements. For vehicle manufacturers who incorporate batteries in their vehicles, modeling allows them to simulate performance at relevant operating conditions or at relevant failure modes. For both a battery manufacturer and a vehicle manufacturer, mathematical modeling enhances the understanding of the interaction between the processes within the cell, which ultimately saves time and cost.

A 2-D electrochemical model has been developed in COMSOL Multiphysics to simulate the discharge of a cylindrical cell. The model simulates the heat production when the battery cell is discharged or short circuited by predicting the battery voltage, current and temperature as a function of time. The model takes into account activation of the electrochemical reactions, mass transport of species in the electrolyte and in the solid phase of the electrodes, heat generation within the cell, heat conduction and convection. The benefits of modeling and simulations are discussed with examples from different types of modeling such as: performance modeling, failure mode modeling, internal short-circuit modeling and lifetime modeling.

Keywords: lithium battery, modeling, simulation, thermal management, short circuit

1 Introduction

Mathematical modeling and simulations of batteries can be used in combination with testing to enhance the understanding of battery processes on a micro scale and its impact on system level performance. Modeling can also be used to determine effects of material properties, design and operating conditions as well as narrow down the range of experimental trials needed to determine performance of prototypes.

Mathematical models describing the performance of lithium-ion battery cells were first published in the beginning of the 1990s by Professor Newman’s group at the University of California [1]-[2]. They were based on well-proven electrochemical and thermodynamic concepts. Performance models have since then been used to predict the cell voltage during different operating conditions. The advantage of the performance models is that they can be used to find out and analyze the processes that are responsible for the limitations in the performance of the battery [3]. The models can also be used to evaluate how the energy and power density are changed when the design of the electrode is varied [1] and how the electrode materials are utilized in the cell design.

Mathematical modeling has also been used to study thermal management in batteries [4]-[9]. These models often take into account heat generation inside the battery due to Joule heating, heat transfer by means of conduction and heat transfer from the surface of the cells by convection and radiation. One of the advantages of using a thermal model is that the temperature inside the cell can be estimated from the measurement at the surface of the cell.

In the models, the processes within the battery are described by equations and material properties. The values of the properties are obtained through carefully designed experiments, often based on theoretical models [10].

As an example of how models of battery cells and packs can be used, we will present a model of a cylindrical lithium-ion cell. We will show how modeling can be used to enhance the understanding of lithium-ion batteries in electric vehicles.

2 Theory

A 2-D electrochemical model has been implemented in COMSOL Multiphysics to simulate a discharge of a cylindrical cell. The model simulates the heat production when the battery cell is discharged or short circuited by predicting the battery voltage, current and temperature as a function of time. The electrochemical model includes the following processes:

- Electronic current conduction
- Ionic charge transport
- Mass transport in the electrolyte
- Material transport of lithium within the electrodes
- Butler-Volmer electrode kinetics
- Heat generation due to Joule heating
- Heat transfer inside the battery cell by means of conduction
- Heat transfer from the surface of the cell to its surrounding by means of convection

The geometry of the cell is described by Figure 1 and the cell chemistry is given in Table 1.

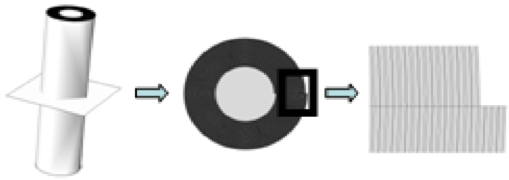

Figure 1: Geometry of the cylindrical cell.

Table 1: Cell chemistry

Positive electrode	$LiMn_2O_4$
Electrolyte	1:1 EC:DEC $LiPF_6$
Separator	Celgard 2325
Negative electrode	Li_xC_6

3 Results

The voltage of the cell described during a discharge is shown in Figure 2. Heat is produced inside the cell during the discharge which causes the temperature to rise. The temperature profile inside the cell is not uniform. This causes the electrode material closest to the core of the cell to exhibit a higher temperature compared to the material at the outer surface, as seen in Figure 3. The temperature difference will be larger at higher discharge currents, e.g., up to 10º C difference has been observed for a cylindrical $LiFePO_4$/graphite lithium-ion battery during a charge/discharge with a current of 6C [6]. The difference between the maximum and minimum temperature will also increase with more revolutions of the spiral.

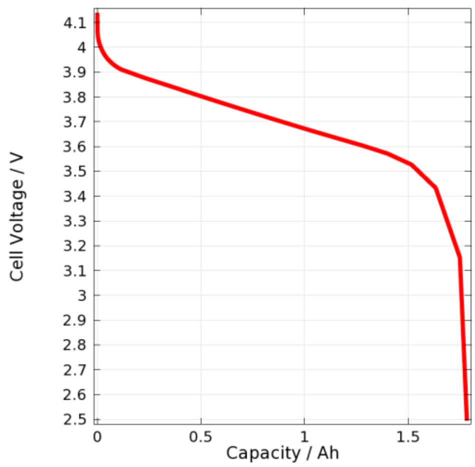

Figure 2: The cell is discharged with 2 C.

A mathematical model that describes the temperature inside a cell is a valuable tool in evaluating thermal management systems. In addition, an effective thermal management system is crucial, both for ensuring safety and a long lifetime of the cells. A detailed mathematical model could also be used to evaluate which process should be incorporated in a simplified dynamic model often used in battery management systems.

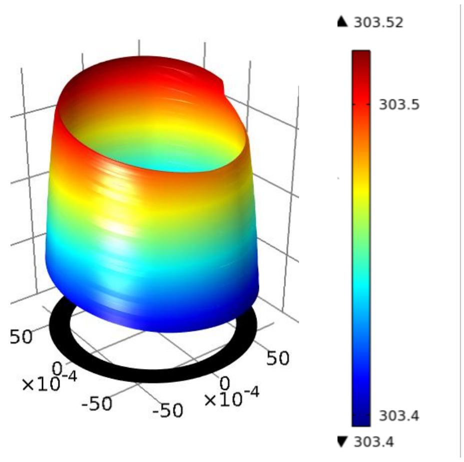

Figure 3: The temperature distribution inside the cell in Kelvin after 200 s.

As with all rechargeable battery chemistries, the lithium-ion batteries loose capacity and the internal resistance increases over time. The reactions that are responsible for this aging can be included in a performance model [11]-[14]. By combining experimental results with simulations, the lifetime can be estimated for different operating conditions. The aging models can be used to design and control the operating conditions to avoid accelerated aging.

The combination of modeling, reverse engineering and experimental testing can also be used to understand internal short circuits in cells, where hot spots may be the cause of thermal runaway [15]-[17]. One example of this is found in Figure 4, which shows the temperature profile inside a cell that is short circuited with a small metal particle.

A model of an internal short circuit will help battery manufacturers and battery users give reliable guidelines regarding temperature intervals for safe operation. It will also give valuable information for the generation of heat from the anode, cathode and electrolyte respectively, which can be used in the design of safety features such as shutdown separators [18].

4 Conclusions

Mathematical modeling can be used in combination with experimental testing and reverse engineering in evaluating the performance and safety of a battery cell and its application. Mathematical modeling enhances the understanding of the interaction between the battery processes. This knowledge will save time and cost.

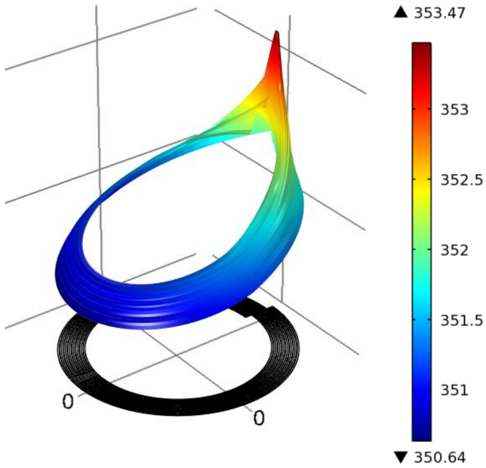

Figure 4: Temperature distribution in Kelvin during an internal short circuit. The cell is short circuited with a nickel particle

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