Simulation of Lithium-ion Battery by COMSOL

No.201960 Dapartment: Mathematical Sciences

Abstract

Simulation calculation plays a key role in the studies of lithium-ion batteries due to its advantage of low cost, time saving but systematic prediction and design. In this project, properties of lithium-ion batteries, such as charging/discharging characteristics and thermal behaviors, are studied by mathematical modeling with COMSOL's Multiphysics software. We use COMSOL to simulate the 2D and 3D models of lithium-ion batteries, and get the results of particle distribution and temperature distribution after the batteries react. The battery model is further optimized by adding thermal management system to improve efficiency and to prolong service life of the battery.

Background

Lithium-ion batteries (LiB) have been widely used in our daily life. The growing energy demand and increasing safety concerns have attracted many research interests in batteries with higher energy density and safety. With a view to estimating electrical characteristics of a polymer Li-ion battery during specific charge and discharge conditions, a COMSOL Multiphysics model of 1 Cell 300mAh has been developed in our project to account for electrochemical phenomena inside the device. The cell model has been created by setting up the Li-ion battery interface, customized material properties and electrochemical reactions in the software. The electrochemical parameters required for the calculation have been determined by laboratory tests, manufacturer datasheets and literature survey.

2D Model

In order to see the chemical reactions inside the battery more clearly, we first developed a 2D lithium-ion battery model, acting as a cross-section of the 3D model as shown in Figure. 1 (geometric diagram of the cross-section shown in Figure. 2).

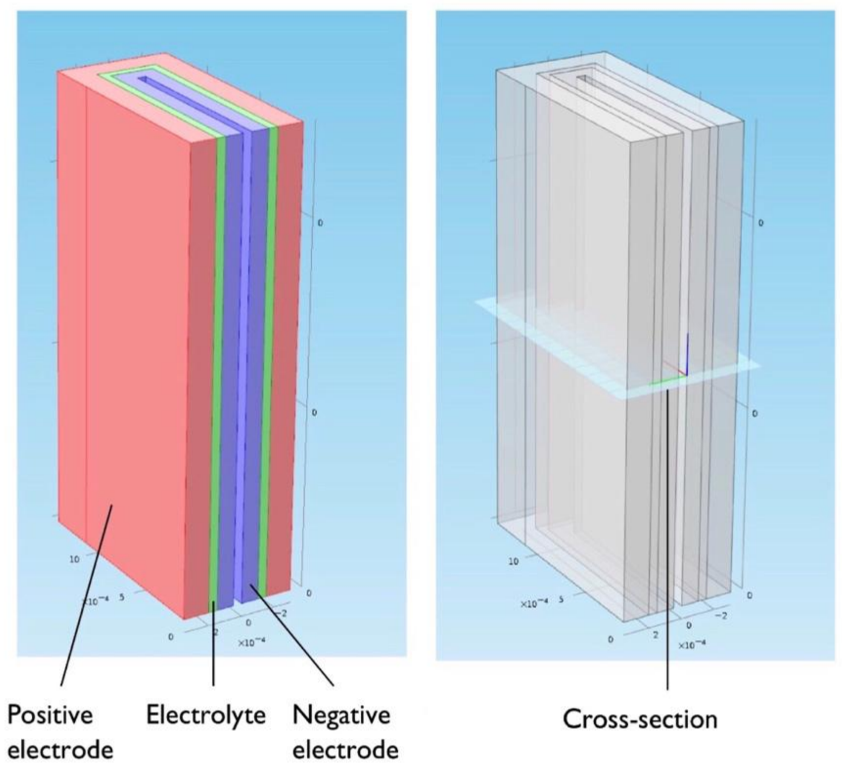

Figure1 The geometric model of Lithium-ion battery

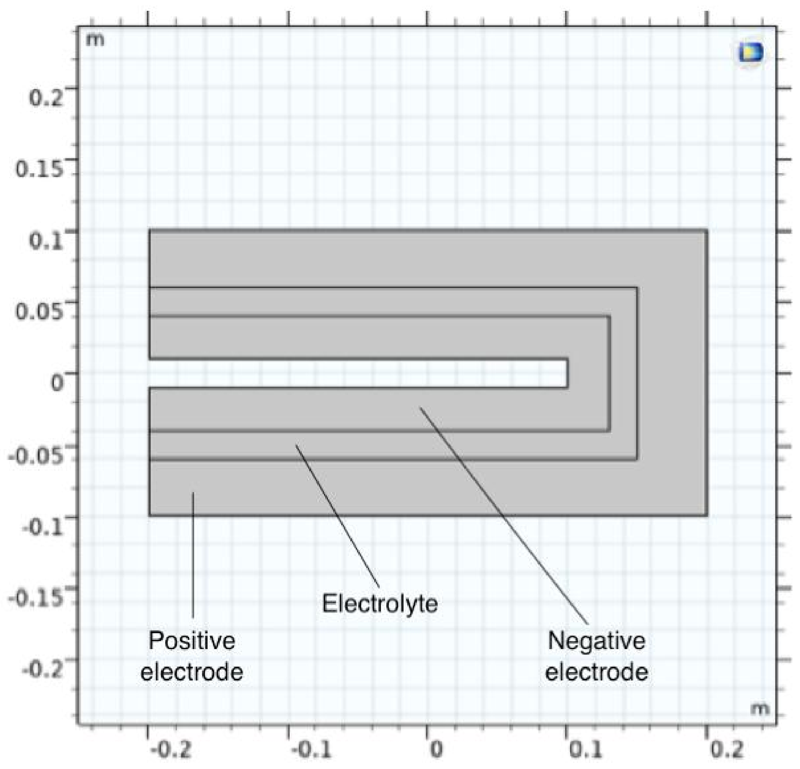

Figure 2 Geometric model of cross-section

The steps of developing a COMSOL model to study the charge-discharge characteristics and thermal behavior of lithium-ion batteries are as follows.

First, 2D model, coupling electrochemical and heat transfer modules by using COMSOL Multiphysics, is developed. Then Multilayer cells consisting repeating units of positive electrode, separator, and negative electrode are developed (Figure.2). And electrochemical and thermal parameters are obtained by fitting model to experimental data using least square method. Finally, principles of mass transfer, heat transfer, charge transfer, and electrochemical kinetics are used to develop model.

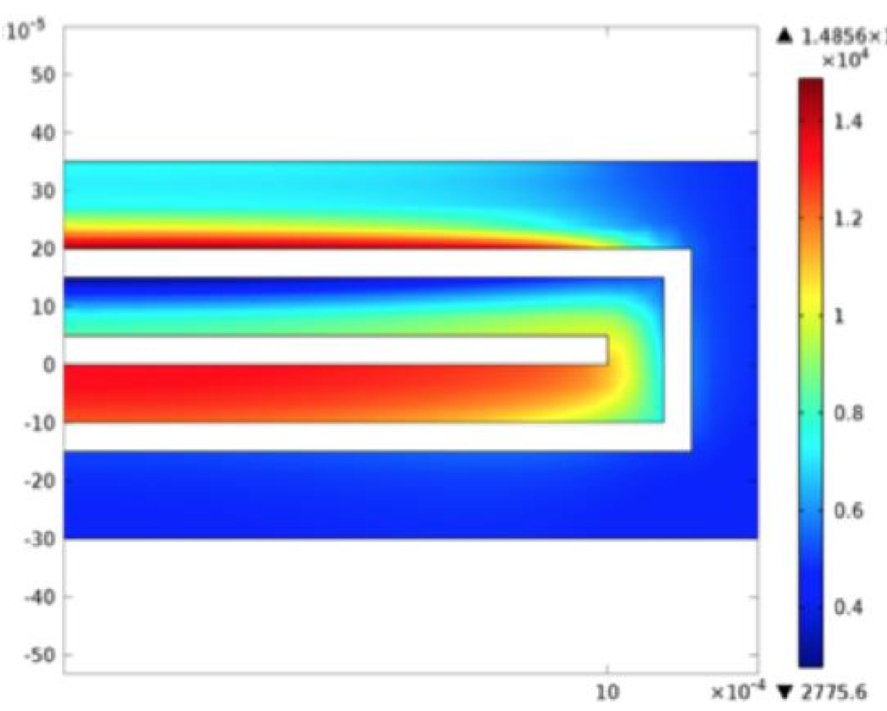

Figure 3 Surface: Insertion particle concentration

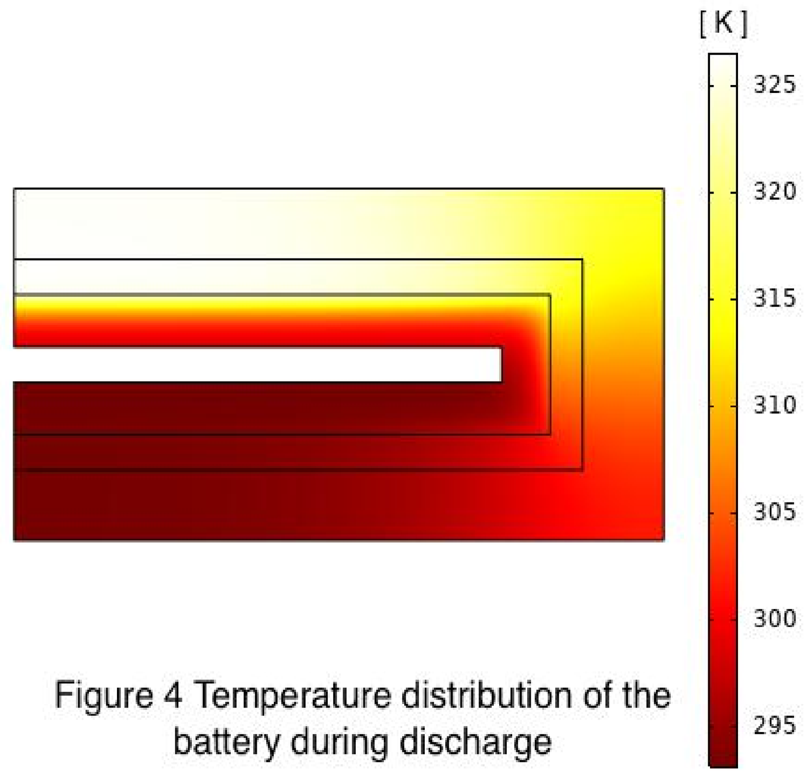

Figure 4 Temperature distribution of the battery during discharge

Figure 3 shows the lithium-ion concentration distribution in the cross-section. During the discharge, as lithium is dissolved on the negative lithium metal electrode, the concentration in the positive electrode increases.

Figure 4 shows the thermal distribution of the battery during discharge, which is dissipated to the surrounding space by convective radiation. It can be observed that the temperature of the positive electrode is higher and the heat distribution of the battery is uneven during discharge.

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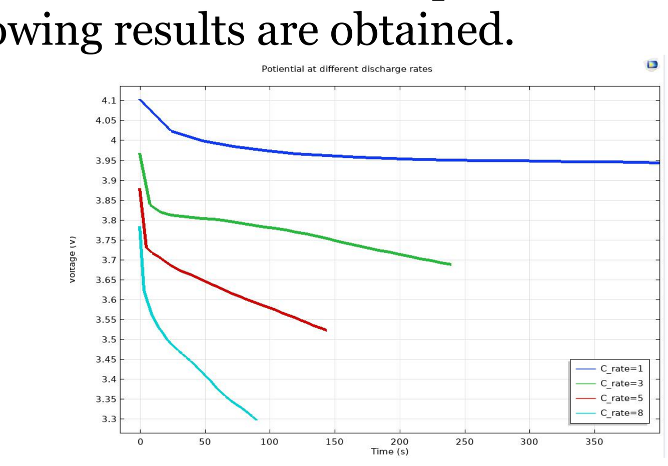
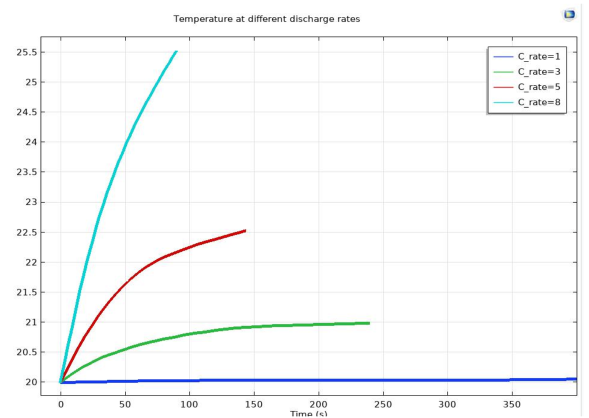
3D Model

Large lithium-ion batteries are widely employed in electric vehicles and for stationary energy storage applications. In the (stacked) pouch battery cell design, all current exits the cell on the cell "tabs", and as the cell size and power increases, the voltage gradients in the highly conductive metal foil current collectors may come into play, resulting in a non-uniform current distribution and electrode utilization in the cell.

We build this 3D model to study the current distribution and electrode utilization in a large format lithium-ion pouch cell, and how it depends on the cell current. And the following results are obtained.





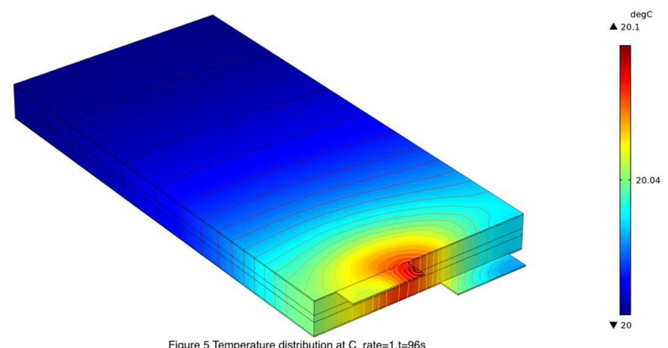


Figure 5 Temperature distribution at C_rate=1,t=96s

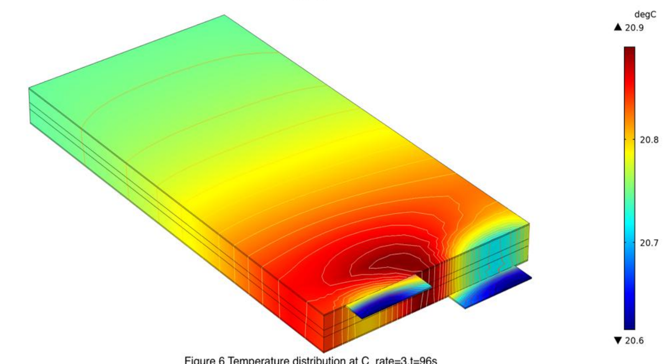


Figure 6 Temperature distribution at C_rate=3,t=96s

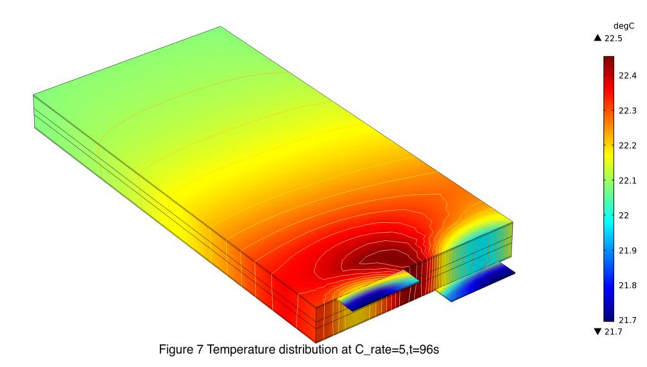


Figure 7 Temperature distribution at C_rate=5,t=96s

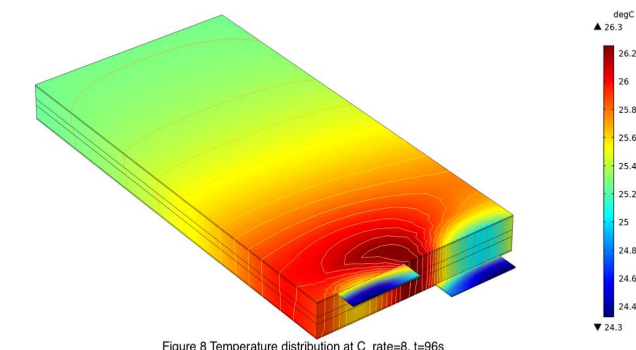


Figure 8 Temperature distribution at C_rate=8,t=96s

These are the simulation results of the temperature distribution 96s after the battery begins to work at different rates. It is shown that the higher the rate, the higher the maximum temperature. The elevated temperature shows that heat diffuses from the battery tab into the inner part of the cell. And the highest temperature is located close to the tab, so this area is more prone to aging and degradation. Therefore, it is also necessary to control the temperature in the battery.

Thermal management system

Thermal management system is also considered to avoid battery thermal runaway during practical applications. It is a common tool to prevent the uneven temperature distribution in battery packs and modules. And in our project this is realized by designing a liquid-cooled thermal management system (TMS) in the software to enhance the battery life-time and safety when it works at 7.5C discharge rate. We could see that the temperature of the cell can be controlled by the flow of gas or liquid by adding a heat management system to the above batteries to facilitate heat dissipation and make the heat distribution more even.

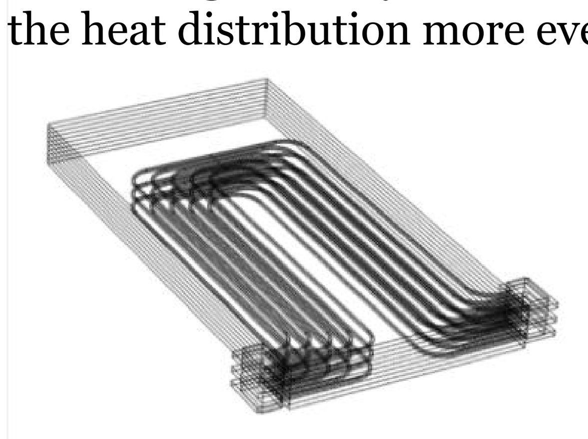


Figure 9 Perspective of Heat Dissipating Pipeline

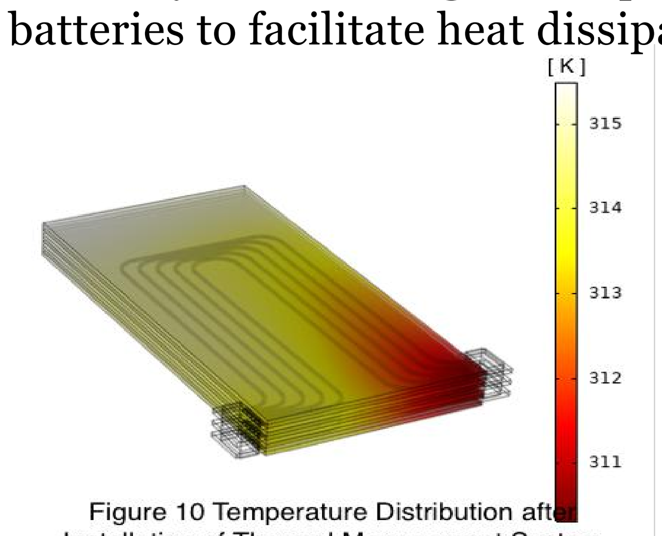


Figure 10 Temperature Distribution aft Installation of Thermal Management System

Conclusion

In general, lithium-ion battery model can be used for simulation analysis of battery cell, battery pack and battery module. It can also be developed into one-dimensional, two-dimensional or three-dimensional models for different purposes. Such models can be used to analyze the aging process of batteries and the failure mechanism of internal short circuit and simulation with experiments, the design schemes applied to various working conditions can be analyzed at relatively low cost, without being limited by the number of product designs.

Reference

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