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A three-dimensional multi-physics model for a Li-ion battery

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HIGHLIGHTS

- A 3D multi-physics model for a lithium-ion battery module with three cells in series is developed.
- This model is used to predict the distributed electrical/thermal behavior of the battery.
- A physics-based pseudo-2D model is used to describe the electrochemical behavior.

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ABSTRACT

A multi-geometry and multi-physics model is developed for a Li-ion battery module which includes three cells connected in series by electrical busbars. The model can be used to predict the 3D profiles of the electrical potentials and temperature in the battery. The physics-based porous electrode (P2D) model is used to predict the electrochemical behavior of the cells, and the coupling between the P2D model and the electrical/thermal equations is simplified through a linear approximation method. This approximation is useful at rates of at least 5 C and reduces the computation time significantly. The anisotropic conductive properties for the regions where conductors are separately arrayed are discussed in detail, and the model predictions are presented and discussed.

1. Introduction

Currently, as battery packs including multiple large-format Li-ion cells are widely used in the hybrid electrical vehicles (HEV) and space craft [1,2], there is an increasing demand for computer-aided tools that enable the battery community to design and simulate batteries. These software tools are expected to have access to the latest numerical methods and algorithms and facilitate battery design by integrating battery modeling components within an open architecture. Therefore, a standardized model template which can capture most physical features of cells and batteries and be implemented within an open architecture would be ideal to meet such demands.

As the thermal and electrical behavior is quite non-uniform through the cells during the charge/discharge operations at high-current rates [3–6], multi-dimensional and multi-physics models are usually suggested for large-format batteries. In recent years, various multi-dimensional mathematical models and model order reduction approaches have been proposed to simulate effectively the distributed thermal, electrical, and electrochemical behavior within an electrode plate pair or a single cell [7–15]. However, very little work has been reported concerning the 3D multi-physics modeling for large batteries.

The huge computational load is one of the major problems that prevents the single-cell-level models from being extended to the multi-cell-level, especially for those cell models including the full-order physics-based electrochemical sub-models [16–18]. In the most recent work of our research group, a very efficient model simplification method, the linear approximation method [19], was developed based on a two-dimensional electrode plate pair domain; the linear model developed with this method can be used to simulate the charge/discharge operations using only a few seconds of computation time; and the thermal/electrical results from the linear model agree well with the results from the full-distribution model which requires about 1000 times more computation time than the linear approximation method. Another issue in developing this 3D battery model is the difficulty in identifying the transport properties in the connecting regions between the cell electrodes and external parts. The current collectors of

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electrodes are connected to the external parts through many thin metal foils arrayed in complex patterns, and the apparent thermal/electrical conductive parameters in these connecting regions vary significantly with position. No literature report has been found so far on how to evaluate these anisotropic transport phenomena.

Our research group is currently working on the solutions for those above-mentioned problems. In the first step, our goal is to develop a three-dimensional multi-physics model template using the linear approximation approach presented in Ref. [19]. In this model template, a battery module including multiple cells is divided into different computational domains according to the transport and reactive properties and the general electric and thermal equations are specified in each domain. It is noted that we have found a way to identify the transport properties in the connecting regions between the cell electrodes and external parts based on basic geometry relations. The governing equations and inputs are standardized and users can implement this model with different commercial or non-commercial software for various simulation purposes. The details of the model development and the simulation results are presented in this paper, and extended research will be covered in our future work.

2. Mathematical model

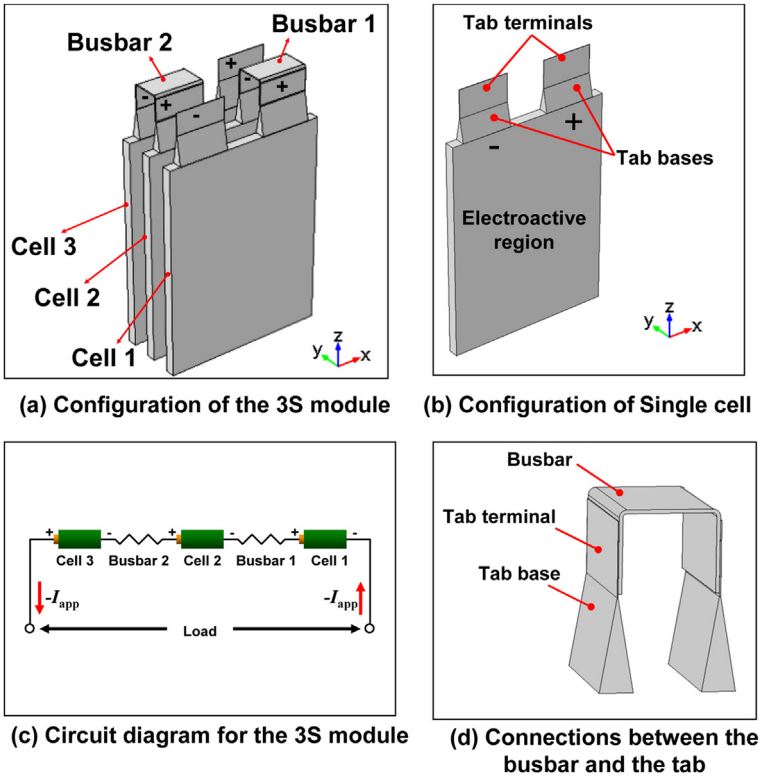
2.1. Configuration of battery module

The battery module presented in this paper includes three Li-ion pouch cells connected in series (3S module) through two electric busbars. The geometry and electrical circuit diagram for this 3S module are presented in Fig. 1. Each single pouch cell forming this module is divided into different parts in terms of electrical and thermal conducting properties. In the electroactive region of each cell, current and electrochemical heat sources are included and the conductive current flows only in the two planar directions (in the x–z plane) along the current collector foils; the thermal conductivity in the transversal direction (the y direction) is much smaller than in the planar directions because the y direction heat flux goes through the less-conductive separator layers. The lower parts of the electrode tabs are labeled as the tab bases, where the current collector conductor foils extend separately from the current collector in the electroactive regions of the cells to the tab terminals. The upper parts of electrode tabs, which are labeled as the tab terminals, have isotropic properties and are connected to the electric busbars or serve as the inlet/outlet for the applied current. The dimensions for the cells are shown in Fig. 2, the thickness of each cell (d_{Cell}) is 9 mm, the distance between two adjacent cells (Δ_{Cell}) in the module is 27 mm, the thickness for the positive and negative electrode tab terminals (d_{Tab}) are respectively 0.375 mm and 0.24 mm, and the thickness of the busbar (d_{BB}) is 1 mm.

2.2. Definitions of reference and modified electric potentials

In this model, four reference electric potentials, V_0, V_1, V_2, andV_3, are defined at different locations as shown in Fig. 3; where V_0 is set to zero, while $V_1(t)$, $V_2(t)$, and $V_3(t)$ are state variables which change only with time.

In this model, two modified electric potentials, Φ_{L} and Φ_{R}, are defined throughout the module domains (as shown in Table 1). The modified potentials are expressed as the difference between the actual potential (Φ_+, Φ_-, or Φ) and the reference potential in each conductive domain. Details for the definitions of modified potential in different domains are presented in Table 1, where Φ_+ and Φ_- are the actual potentials of the positive and negative electrode current collectors and tabs, and Φ is the actual potential of the busbars. According to the definitions, the modified potentials are zero at locations chosen for the reference potentials, and these constraints are used as imposed limiting conditions to obtain solutions for the electrical equations.



(a) Configuration of the 3S module (b) Configuration of Single cell

(c) Circuit diagram for the 3S module (d) Connections between the busbar and the tab

Fig. 1. Configuration and circuit diagram for the 3S battery module.