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Three dimensional thermal-, electrical-, and electrochemical-coupled model for cylindrical wound large format lithium-ion batteries

Kyu-Jin Lee [a,b], Kandler Smith [a], Ahmad Pesaran [a], Gi-Heon Kim [a,*]

[a] National Renewable Energy Laboratory, 15013 Denver West Parkway, Golden, CO, USA
[b] Department of Mechanical Engineering, Myongji University, 116 Myongji-ro Cheoin-gu, Yongin-si, Gyeonggi-do, South Korea

HIGHLIGHTS

- The wound potential-pair continuum (WPPC) model is developed.
- It serves a cell-domain model of the Multi-Scale Multi-Domain (MSMD) framework.
- It resolves temperature and current collector phase potential variation in cell composites.
- It is coupled with submodels solving lithium diffusion dynamics and kinetics.
- Electrical/electrochemical/thermal coupled behavior of 20 Ah cylindrical cells was investigated.

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ABSTRACT

A numerical model for cylindrical wound lithium-ion cells, which resolves thermal, electrical and electrochemical coupled physics, is presented in this paper. Using the Multi-Scale Multi-Domain (MSMD) model framework, the wound potential-pair continuum (WPPC) model is developed as a cell domain submodel to solve heat and electron transfer across the length scale of cell dimension. By defining the cell composite as a wound continuum, the WPPC model can evaluate layer-to-layer differences in electrical potential along current collectors, and electric current in the winding direction to investigate the effects of thermal and electrical configurations of a cell design, such as number and location of tabs, on performance and life of a cylindrical cell. In this study, 20-Ah large-format cylindrical cell simulations are conducted using the WPPC model with the number of electrical tabs as a control parameter to investigate how macroscopic design for electrical current transport affects microscopic electrochemical processes and apparent electrical and thermal output.

1. Introduction

To meet the system demands of high-energy and high-power energy storage in electric vehicle applications, lithium-ion cells with increased size and capacity have the advantage of reducing the number of interconnectors and control circuits when integrated in a battery pack. Although the technology of small lithium-ion batteries (LIBs) for consumer-electronic devices has made significant progress regarding performance, cost, life, and safety in the past 20 years, the scale-up of batteries is still challenging because of unexpected size effects. As cell size increases, spatial non-uniformity of temperature and current collector electrical potential in a cell excessively grows and significantly influences electrical, thermal, electrochemical, and mechanical response of a LIB system. Thus, without knowledge of the interplays among interdisciplinary multi-physics occurring across varied length scales in LIB systems, it is difficult to design long-lasting, high-performing, large-format LIB cells retaining the quality of small capacity LIB systems. Cylindrical cell formats, widely adopted by the consumer electronics battery market because of their low production cost and well-established manufacturing process, face difficulties in scaling-up capacity. One well known issue is poor thermal characteristics, such as decreased surface-to-volume ratio and increased radial dimension of cells. The adverse impacts of non-optimized electrical pathway design on cell performance and degradation become significant in such a scenario. In a typical large-format cylindrical cell with discrete electrical tabs, electrical pathways carrying current along continuous wound metal foil are longer, causing excessive non-uniformity in kinetics and transport.

* Corresponding author. Tel.: +1 303 275 4437; fax: +1 303 275 4415.
E-mail addresses: gi-heon.kim@nrel.gov, kgheon@gmail.com (G.-H. Kim).

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To avoid unexpected loss of cell performance in large-format designs, it is important to know how thermal and electrical design of large-scale cylindrical cells affects cell physics. The build-and-break design process, typically used by the battery manufacturing industry, is costly, extremely time-consuming for large-format cells, and provides only limited information. In contrast, numerical models which resolve the interactions between long-range transport and short-range physics can help to shorten design processes and optimize batteries. Since Newman and his team [1] suggested a numerical model for a LIB resolving lithium diffusion dynamics and charge transfer kinetics in porous electrodes, various mathematical approaches [2,3] have been used to understand physics in LIB systems and predict their electrical response. However, it is challenging to extend these approaches to simulate large capacity system responses. Most numerical models for wound cells suggest various simplification strategies to achieve effective solutions [4–14]. Previous studies on heat conduction in spirally-wound geometry assumed uniform kinetics throughout the cell volume, with volumetric heat generation evaluated from experimental data [4–7] or from a lumped cell model [8–10]. Heat conduction in cylindrical cells has been studied in various simplified geometry models: lumped thermal mass [4], 1-D radial direction [7,8], 2-D spiral geometry [5,6,11], 1-D radial spiral modeling with the domain reduced from a 2-D spiral model through the coordinate-transform technique [12], 2-D concentric rings [9], and 3-D concentric rings [10]. On the other hand, several studies only solved electrical current along wound metal current collectors assuming uniform kinetics over a cell volume without temperature calculation [13,14]. To date, there has not been a numerical study solving a thermal-, electrical-, and electrochemical-coupled system in a 3-dimensional cell domain resolving spirally-wound geometry.

In our previous study by Kim et al. [15], we introduced the Multi-Scale Multi-Domain (MSMD) model framework, able to investigate the interplay among various length scale physics in lithium-ion batteries by decoupling submodel geometries. In the MSMD framework, electric potential variation along current collectors and heat transfer are solved in a computational domain representing the battery cell length-scale, coupled with lithium diffusion dynamics and charge transfer kinetics in smaller length-scale subdomains. In this paper, we introduce development of the wound potential-pair continuum (WPPC) model, a cell domain submodel of the MSMD framework, and apply the model to investigate electrical, thermal and electrochemical behaviors of large-format cylindrical wound cells.

2. Model description

The computational model geometries of the MSMD framework are separated into a particle domain, an electrode domain and a cell domain. Model geometries in each domain are completely decoupled and the solution variables are solved for corresponding length-scale physics while coupled through inter-domain communication between the adjacent hierarchical model domains. The solution variables in each domain and the inter-domain coupling quantities are summarized in Fig. 1. The MSMD model framework solves lithium diffusion inside solid electrode particles and charge transfer kinetics in the particle domain. Charge balance in solid matrices and the liquid phase, as well as species transport across the electrode pair are solved in the electrode domain. In the cell domain, electrical current flow in metal current collector sheets and heat flow over a cell composite volume are calculated in consideration of macroscopic cell geometries and boundary conditions. Thanks to its modularized hierarchical architecture, the MSMD framework allows flexible choice of submodels in each modeling domain. In this study, the submodel chosen for the particle domain model is a one-

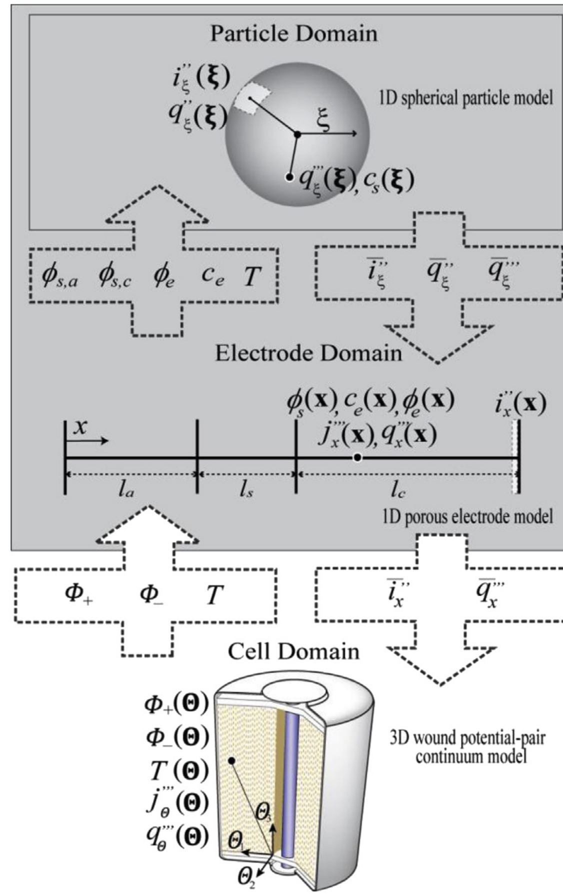

Fig. 1. The MSMD model framework: summary of submodel choice, solution variables in each submodel domain, and coupling variables.

dimensional spherical particle model, and the submodel chosen for the electrode domain is a one-dimensional porous electrode model as presented in Fig. 1. The governing equations of the particle domain and the electrode domain are summarized in Table 1. A model-reduction scheme, the state variable model (SVM), which calculates the governing equations as a quasi-linear system, is adopted to enhance computational speed [16]. Detailed information regarding the submodels and the MSMD framework is found in Kim et al. [15].

2.1. Wound cell geometry

Cylindrical lithium-ion cells typically have a pair of long, wide continuous current collectors wound as shown in Fig. 2. As electrical current generated from charge transfer kinetics across the pair of electrode layers is delivered through external circuitry, electric current convergence causing large potential change occurs near the electrical tabs. Where a cell has extended foils functioning as continuous tabs in Fig. 2(a), electric current mainly flows in the axial direction of the jelly roll, wound with negligible difference of electrical potential in the azimuthal direction. For continuous tabbed cells, it is reasonable to represent an arbitrary finite volume of jelly roll with a single pair of electric potentials to define a single potential-pair continuum (SPPC). On the other hand, in the cell represented in Fig. 2(b), which has discrete and localized electrical terminals, electric current flows in the azimuthal direction, resulting in significant change of electrical potential in the azimuthal direction. This means that electrical potentials in an