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Mathematical model for a spirally-wound lithium-ion cell

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HIGHLIGHTS

- A mathematical model for the thermal behavior of a wound cylindrical Li-ion cell was developed.
- The new numerical method significantly saves computation time and memory allocation.
- The coordinate transform and variable extrusion algorithms were validated.

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ABSTRACT

A new computational method is proposed that can be used to reduce the numerical difficulties in modeling the electrical and thermal behavior of a spirally wound Li-ion cell. By analyzing the winding locus of the electrodes, some important geometric relationships of the spiral surfaces are identified, and algorithms for coordinate transform and variable extrusion between 2-D and 3-D domains are derived. Our method reduces the computation time and memory requirements needed to simulate the cell performance. The accuracy of our method was validated by model-to-model comparisons.

1. Introduction

Today, most of the safety issues for Li-ion cells and batteries are related to the electrical and thermal properties of the composite electrodes. [1–4] Therefore, mathematical models that deal with the charge balance and heat transfer in cells have become important tools for cell design. However, the implementation of these models is significantly affected by the cell geometry and electrode configurations. There are basically two types of electrode structures in Li-ion cells, the laminated or pouch structure and the wound structure. For the laminated electrode structure, all the electrodes are flat and arrayed in parallel, and the transfer of charge and energy goes along the orthogonal directions in the Cartesian coordinate system. Therefore, building and meshing the computational domains for laminated electrodes can be done easily in commercial CAD software. For the wound electrode structure, however, the electrodes are put through a complicated winding locus, and the electrical potentials of the solid phases are non-continuous along the normal direction of the winding surface due to the insulating separator layer. Therefore, electrical insulation zones with full winding details must be included in the model domains for wound electrodes, and the meshing of these domains becomes extremely difficult if the electrodes have many winding turns.

Due to the numerical difficulties discussed above, most 3-D physical models have been developed for cells with laminated electrodes [5–9], and modeling for the wound-structure electrodes have been rarely reported. Gomadam et al. [10] developed a 2-D thermal model for a cylindrical jell-roll based on the spiral geometry relations, but the charge balances in the current collector foils, which are supposed to be the most difficult parts for the wound electrode models, were neglected. Santhanagopalan et al. [11] and Ye et al. [12] also developed physics-based models for the wound cells, but their models are limited to 2-D. In a recent paper by Lee et al. [13], a multi-scale multi-dimensional (MSMD) model for wound cells was reported; however, their approach involves two mesh groups in which the size for geometry units are no larger than twice the electrode pair

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thickness, and thus requires a large number of mesh elements which would make the model computationally expensive.

In this work, a new modeling approach different from all the above-mentioned ones is developed. The charge balance and heat transfer in a jelly-roll are solved separately in different computational domains, and coupled through a coordinate transform and variable extrusion algorithm derived from analytical geometry relationships. The mesh requirement for the 3-D domain is significantly lowered by using these geometric algorithms.

2. Mathematical approach

2.1. Basic geometric relations

Our model was developed from an assumption that all the cell sandwich layers (current collectors, coatings, and the separator) in the jelly-roll of a18650-type cylindrical cell are of uniform thicknesses and are wound through an Archimedean spiral locus which can be described by the following polar coordinate equation:

$$r = r_0 + \frac{D}{2\pi}\theta \tag{1}$$

where r is the radius coordinate, θ is the angular coordinate, r_0 is the initial radius of the spiral at $\theta = 0$, and D is the separation distance. The geometry details for a spiral surface are presented in Fig. 1, where the surface is wound spirally around the z axis and the cross section on the x–y plane is an Archimedean spiral curve described by Equation (1). The Archimedean spiral has the property that any ray from the origin intersects successive turnings of the spiral in points with a constant separation distance D, and the difference in the polar angle between two intersecting points, $\Delta\theta$, is 2π. In Fig. 1, ξ is the tangential arc length along the spiral curve and differentiation of ξ can be expressed as follow:

$$d\xi = \sqrt{r^2 + \left(\frac{dr}{d\theta}\right)^2} d\theta = \sqrt{\left(r_0 + \frac{D}{2\pi}\theta\right)^2 + \left(\frac{D}{2\pi}\right)^2} d\theta \tag{2}$$

A functional relationship between the arc length ξ and the polar angle θ can be derived by integrating Equation (2):

$$\begin{aligned}\xi(\theta) &= \int_0^\theta \sqrt{r^2 + \left(\frac{dr}{d\theta}\right)^2} ds = \int_0^\theta \sqrt{\left(r_0 + \frac{D}{2\pi}s\right)^2 + \left(\frac{D}{2\pi}\right)^2} ds \\ &= \frac{1}{2}\left(\frac{2\pi}{D}\right)\left[\left(r_0 + \frac{D}{2\pi}\theta\right)\sqrt{\left(r_0 + \frac{D}{2\pi}\theta\right)^2 + \left(\frac{D}{2\pi}\right)^2} \right. \\ &\quad \left. - r_0\sqrt{r_0^2 + \left(\frac{D}{2\pi}\right)^2}\right] \\ &\quad + \frac{1}{2}\left(\frac{D}{2\pi}\right)\ln\left[\frac{\left(r_0 + \frac{D}{2\pi}\theta\right) + \sqrt{\left(r_0 + \frac{D}{2\pi}\theta\right)^2 + \left(\frac{D}{2\pi}\right)^2}}{r_0 + \sqrt{r_0^2 + \left(\frac{D}{2\pi}\right)^2}}\right]\end{aligned} \tag{3}$$

Equation (3) sows that ξ is a unique function of θ; therefore, at a fixed z, any variable defined on the spiral surface can be expressed as a function of the polar angle θ. Due to the small thicknesses of the Li-ion cell electrodes, it can be found that $(r_0 + (D/2\pi)\theta)^2$ is at least three orders larger than $(D/2\pi)^2$ for all θ, and Equation (3) can be approximated as:

$$\begin{aligned}\xi &= \int_0^\theta \sqrt{\left(r_0 + \frac{D}{2\pi}s\right)^2 + \left(\frac{D}{2\pi}\right)^2} ds \approx \int_0^\theta \left(r_0 + \frac{D}{2\pi}s\right) ds \\ &= r_0\theta + \frac{D}{4\pi}\theta^2\end{aligned} \tag{4}$$

therefore, an approximate functional relationship between θ and ξ can be derived from Equation (4):

$$\theta(\xi) \approx \frac{-r_0 + \sqrt{r_0^2 + \frac{D\xi}{\pi}}}{\frac{D}{2\pi}} \tag{5}$$

As shown in Equation (5), at a fixed z, any variable defined in the spiral surface can also be expressed as a function of the arc length ξ.

According to references [5–9], the current collector foils can be regarded as surfaces due to the small thickness, and the electrical potential of a current collector distributes only in the two tangential directions of the surface (ξ and z directions). Therefore, the charge balance equations on the current collector surfaces are:

$$\sigma_j \frac{\partial^2 \Phi_j}{\partial \xi^2} + \sigma_j \frac{\partial^2 \Phi_j}{\partial z^2} + i_{v,j} = 0 \quad (j = +, -) \tag{6}$$

where Φ_j is the electric potential of the current collector of electrode j, σ_j is the electric conductivity for the current collector of electrode j, and $i_{v,j}$ is the volumetric current source in the current collector of electrode j. It can be found that Φ_j solved from Equation (6) is a function of ξ and z; therefore at a fixed z, Φ_j can be expressed as a function of the polar angle θ.

As discussed later in our work, certain electrical and thermal variables need to be evaluated along the spiral surface and extruded into the 3-D Cartesian coordinate system. The extrusion of variables can be performed through a coordinate transform algorithm. As shown in Fig. 1, $\psi'(\theta)$ is a variable defined on the spiral surface at a fixed z, and (x,y) is a specific Cartesian coordinate point which has the same z coordinate as $\psi'(\theta)$. Point (x,y) could be located either on or outside the spiral surface. The first step for variable extrusion is to project point (x,y) to the spiral surface along a specific direction defined by a ray from the origin and passing (x,y), the elevation angle θ_E (where $0 \le \theta_E < 2\pi$) for the projecting direction can be calculated as follow:

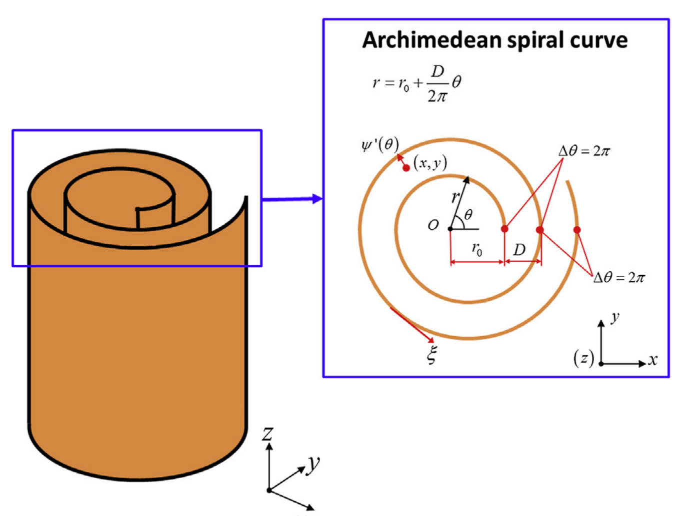

Fig. 1. Schematic for a surface wound through an Archimedean spiral locus.