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A distributed thermal model for a Li-ion electrode plate pair

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HIGHLIGHTS

- A distributed thermal model for a lithium-ion electrode plate pair is developed.
- This model has multiple dimensions and multiple length scales.
- The model was developed by coupling the heat equation with a P2D electrochemical model.
- Reduced order model was also produced to significantly reduce the simulation time.

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ABSTRACT

This paper presents a distributed thermal model for a lithium-ion electrode plate pair used to predict the distributed electrical and thermal behavior of the electrode pair including tabs. Our model was developed by coupling the heat equation with a pseudo two dimensional (P2D) physics-based electrochemical model. The local heat generation rate is predicted by the P2D model at every node point in the 2D electrode pair. To reduce significantly the computation load of the model, a linear approximation method is introduced to decouple the electrochemical model from the heat equation with a very slight loss in accuracy.

1. Introduction

Currently, large-format Li-ion cells are widely used in the hybrid electrical vehicles (HEV), and these cells are often operated at very harsh electrical and thermal conditions such as the high and fast-changing current rates or extreme ambient temperatures. Under such conditions, the thermal and electrical behavior will be quite non-uniform through the cell volume [1–4]. Multi-scale and multi-dimensional (MSMD) modeling approaches have been proposed to simulate the distributed thermal, electrical, and chemical behavior of large format Li-ion cells [5–7]. The length scales of computational sub-domains in an MSMD model have typically three different levels: the microscopic, mesoscopic, and macroscopic [7,8]. Modeling in the microscopic scale generally focuses on the molecular-level quantum behavior, modeling in the mesoscopic scale specifically deals with the electrochemical processes and transport phenomena in the electrode coatings and the active material particles, and modeling in the macroscopic scale mainly describes the non-uniformity of the electric potential along the current collectors in electrode composites and the temperature throughout the cell volume [7,8]. In the fields of engineering and industry, models with mesoscopic-to-macroscopic length scales are more preferable for application; and among these models, the electrochemical-thermal (ECT) coupled models [1] are commonly used for the thermal management design and thermal runaway analysis.

Unfortunately, the physics-based MSMD models require a significant amount of computation time. The widely accepted physics-based model for Li-ion cells, Newman's pseudo-2D (P2D) porous electrode model [9–11], involves a large non-linear DAE system in the mesoscopic scale. Although various model order reduction techniques have been suggested to simplify the Newman's P2D model and reduce the computation time for a MSMD model [12–17], the reduced order models (ROM) still have disadvantages in terms of the accuracy for high current rates simulation. For example, the SVM model, which was derived by Smith et al. [12,13] and employed in the MSMD model by G-H Kim et al. [7] show poor agreement with the full-order model in the voltage response when the current rate exceeds 5C. Therefore, the goal of

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good time-efficiency in simulation as well as sufficient accuracy in predictions is a great challenge for researchers in the MSMD modeling for the Li-ion cells.

In this work, we present our full physics-based (P2D) MSMD model and an associated ROM for a Li-ion electrode pair with planar electrode. We derived our ROM by segregating the mesoscopic and the macroscopic sub-domains, that is, we decoupled the Newman's P2D model from the charge balance in the current collectors and the energy balance in the cell volume. Significant improvements in the simulation speed were achieved through our model order reduction approach. To ensure that our ROM also maintains sufficient accuracy in predictions, extensive model-to-model validations were made between the ROM and the full-order full-distribution model.

2. Mathematical model

In this part of work, the model developments and simulation case studies are based on one single electrode plate pair; and in the future, the model will be extended to cell stacks that include multiple electrode pairs.

2.1. The modeling scales and sub-domains

The planar electrode plate pair of the Li-ion cell can be divided into several computational sub-domains in terms of length scales (see Fig. 1). As shown in Fig. 1, the thickness of electrode pair (the x dimension) and the radius of particles (the r dimension) are much smaller than the length and width of the electrode pair (the X and Y dimensions). Therefore, in our model, the macroscopic sub-domains include the electroactive part of the electrode plate pair (the cell sub-domain) and the two electrode tabs; the mesoscopic sub-domains include the porous electrode coatings and separator (the porous electrode sub-domain), and the active material particles (the particle-sub-domain). According to a dimensional analysis, the temperature and the electrical potential of each current collector can be considered to be distributed only in the two macroscopic (X and Y) dimensions; the mass and charge transport in the electrolyte and the solid phase in the porous electrode sub-domain follow the mesoscopic (x) dimension; the mass balance in the particle sub-domain is described by another mesoscopic dimension, the r dimension. Table 1 summarizes the dependent variables to be solved in the different sub-domains.

2.2. The models in the macroscopic sub-domains

2.2.1. The current collector charge balance

A schematic for the planar and transverse current density distribution on the two current collectors including the tabs is presented in Fig. 2. The governing equations for the charge balance in the current collectors of the cell sub-domain are as follow:

$$\sigma_{\mathrm{cc},j}\frac{\partial^2\Phi_j}{\partial X^2}+\sigma_{\mathrm{cc},j}\frac{\partial^2\Phi_j}{\partial Y^2}+\frac{i_{N,j}}{\delta_j}=0 \quad (j=p,n) \tag{1}$$

where Φ_j is the potential in the current collector of electrode j, $\sigma_{\mathrm{cc},j}$ is the electrical conductivity of current collector, δ_j is the thickness of current collector, and $i_{N,j}$ is the normal inward current density through the coating/current-collector interfaces. In the tab sub-domains, there is no transverse current, and the charge balance equations are:

$$\sigma_{\mathrm{cc},j}\frac{\partial^2\Phi_j}{\partial X^2}+\sigma_{\mathrm{cc},j}\frac{\partial^2\Phi_j}{\partial Y^2}=0 \quad (j=p,n) \tag{2}$$

The boundary conditions (see Fig. 2) at the tops of electrode tabs are:

$$n\cdot(-\sigma_{\mathrm{cc},j}\nabla\Phi_j)=i_{\mathrm{app},j} \tag{3}$$

where n is the unit normal vector pointing out of the boundary, and $i_{\mathrm{app},j}$ is the applied outward current density based on the cross section at the top of each electrode tab.

2.2.2. The energy balance

The equation for the energy balance in the cell and tab sub-domains is:

$$\rho C_P\frac{\partial T}{\partial t}=k_{X-Y}\frac{\partial^2 T}{\partial X^2}+k_{X-Y}\frac{\partial^2 T}{\partial Y^2}+Q-Q_{\mathrm{Trans}} \tag{4}$$

where T is the temperature of the sub-domain, ρ is the density of the electrode plate pair, C_P is the specific heat capacity of the electrode plate pair, k_{X-Y} is the thermal conductivity of the

Table 1
The dependent variables in different sub-domains.

Length scale	Sub-domain	Dependent variable name	Symbol	Independent variables
Macroscopic	Cell and tabs	Temperature (K)	T	t,X,Y
		Current collector potential (V)	$\Phi_j(j=p,n)$	t,X,Y
Mesoscopic	Porous electrode	Li concentration in electrolyte (mol m^{-3})	c_e	t,x,X,Y
		Potential in solution phase (V)	ϕ_2	t,x,X,Y
		Potential in solid phase (V)	ϕ_1	t,x,X,Y
		Surface reaction rate (mol m^{-2} s^{-1})	$J_j(j=p,n)$	t,x,X,Y
	Particle	Li concentration in solid phase (mol m^{-3})	$c_{s,j}(j=p,n)$	t,r,x,X,Y

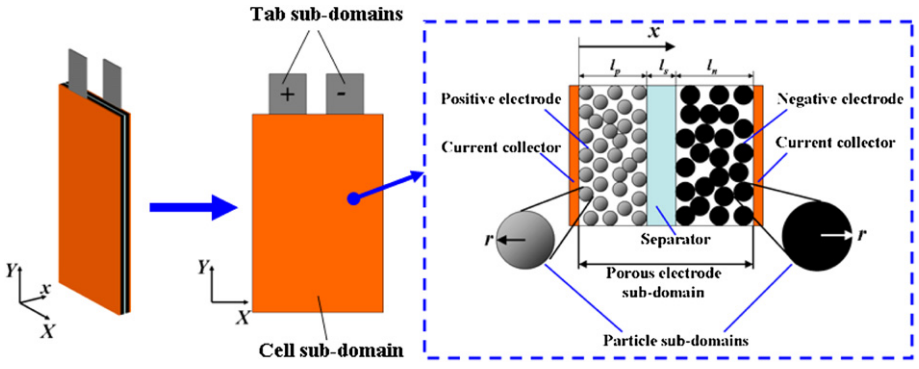

Fig. 1. The computational sub-domains in an electrode plate pair.