Impact of Tab Location on Large Format Lithium-Ion Pouch Cell Based on Fully Coupled Tree-Dimensional Electrochemical-Thermal Modeling

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ABSTRACT

This paper presents extensive three-dimensional (3D) simulations of large LiFPO$_4$ pouch cells. 3D simulations of the Li-ion battery behavior are highly nonlinear and computationally demanding. Coupling electrochemical modeling to thermal models represents an important step towards accurate simulation of the Li-ion battery. Non-uniform temperature, potential and current density through the battery induce non-uniform use of the active material and can have a negative impact on cell performance and lifetime. Different pouch cell designs, with different tab locations, have been investigated in term of performance, current density, potential and heat distributions. The model is first validated with experimental data at different current discharge rates. Afterwards, the electrochemical, thermal and electrical behaviors over each cell design under high discharge rate (4 I$_t$) are compared between configurations. It has been shown that the designs with symmetrical configurations show uniform potential and current density gradient, which minimize the ohmic heat and lead to more uniform active material utilization and temperature distributions across the cell surface.Introduction

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1. Introduction

Lithium-ion batteries have emerged as key energy storage devices, and are now the main technology for portable devices. Due to their high potential and their high energy and power densities, and also their good lifetime, they are now the preferred battery technology for Hybrid Electric Vehicles (HEVs), Battery Electric Vehicles (BEVs) and Plug-In Hybrid Electric Vehicles (PHEVs) [1–3].

Advanced research in this field enables wide use of large-format, high-capacity Li-ion pouch cells in PHEVs and EVs. This format has the advantage of reducing the number of cells in the module, increasing the capacity and reducing the size and weight at pack level. Increasing the current amplitude during the charge/discharge process subjects the large format battery to abuse situations and leads to non-uniform distributions of temperature, potential, current density and heat generation through the cell. These phenomena may reduce battery performance and lifetime [4–6], leading to thermal runaway in worst cases [7–9] and

requiring a more complex cooling strategy. Based on this observation, the main barriers to their wide use are the need for fast charging (using high current rate), and the need for BEVs to perform high acceleration (resulting in high discharge rate). Therefore, good cell design is necessary to avoid non-uniform distribution of the electrical and thermal parameters. Particle size and electrode coating thickness also have a significant impact on battery behavior. Recently, Zhao et al [10] showed that small coin cells provide much better performance and energy density than large format cells, where uneven current density is observed, leading to lower utilization of the active material. In addition, the impact of the arrangements and number of the current collecting tabs are investigated in the cases of wound design [10,11] and stacked layer design [12,13]. As a function of the number and location of tabs, the electron pathways become more or less long and thereby cause an increase or decrease of the ohmic resistance responsible for the voltage loss. In order to investigate these battery designs, electrochemical modeling techniques are more appropriate than electrical modelling because they show a clear relation between the electrochemical parameters and battery geometry. Several 1D electrochemical models are listed in the literature [14–17]. These are more suitable for describing small-format battery behavior. They also provide average values for large-format

Nomenclature

A_{tab}	Cross section of the tab (m^2)
c_1	Concentration of lithium in the active material particles (mol/m^3)
c_2	Concentration of lithium in the electrolyte (mol/m^3)
C_{dl}	Electrical double layer capacitance, (F/m^2)
c_p	Thermal capacitance (J/kg.K)
D_1	Diffusion coefficient of lithium in the solid phase (m^2/s)
D_2	Diffusion coefficient of lithium in the electrolyte (m^2/s)
$Ea_{D_{s,j}}$	Activation energy for particle diffusion [J/mol]
$Ea_{R,j}$	Activation energy for reaction[J/mol]
$f_{\pm}$	Average molar activity coefficient
F	Faraday's constant (C/mol)
h	Convective heat transfer coefficient (W/m^2K)
i_1	Electronic current density in the solid phase
i_2	Ionic current density in the liquid phase
i_N	Normal inward current density trough the electrode/CC interfaces (A/m^2)
i_{app}	Total applied current density (A)
J_0	Exchanged current density (A/m^2)
J_n	Local charge transfer current density (A/m^2)
k_0	Reaction rate constant ($m^{2.5}/mol^{0.5}$ s)
L_{PCC}	Positive current collector thickness (m)
L_P	Positive electrode thickness (m)
L_S	Separator thickness (m)
L_{NE}	Negative electrode thickness (m)
L_{NCC}	Negative current collector thickness (m)
N	Total number of single cell
r	Radius distance variable of the solid particles (m)
R	Gas constant, 8.314 (J/mol.K)
R_s	Radius of electrode particle (m)
S_a	Specific surface area (m-1)
t	Time (s)
t_+	Transferring number of Li$^+$
T	Absolute temperature (K)

Greek letters

ε_2	Electrolyte volume fraction
ε_1	Active material volume fraction
Φ_1	Solid phase potential (V)
Φ_2	liquid phase potential (V)
Φ_{cc}	Current collector potential (V)
α	Charge transfer coefficient
γ	Bruggeman tortuosity exponent
η	Local surface overpotential (V)
σ_1	Electronic conductivity of solid matrix (S/m)
σ_2	Ionic conductivity of electrolyte (S/m)
ρ	Density (kg/m^3)
λ	Thermal conductivity (W/m.K)

Subscripts, superscripts and acronyms

0	Initial value
1	Solid phase
2	Liquid phase
p	positive
n	negative
eff	Effective value
CC	Current collector
ref	Reference value
j	Indice of the electrodes
surf	surface

max	maximum
amb	ambient
rea	reaction
ohm	ohmic
act	activation
s	solid
l	liquid
PE	Positive electrode
NE	Negative electrode
SP	Separator
SOC	State of charge
DOD	Depth of discharge

batteries without taking into account the collector tabs. However, they are not sufficient to handle the issue of non-uniform thermal, electrical and electrochemical variable distributions observed in large-format cells. Recent advances in numerical simulation techniques applied to Li-ion batteries have given more attention to the development of 2D axisymmetric and 3D electrochemical-thermal modeling [10,11,18–20]. The multi-dimensional simulations are highly nonlinear and computationally demanding, and coupling electrochemical and thermal modeling represents an important step towards accurate simulation of the Li-ion battery. Most of the 2D and 3D electrochemical-thermal models are applied to the spirally wound design in order to gain insight into large-scale battery behavior and also to investigate the impact of the number of collecting tabs on battery performance. However, little work is focused on stacked layered designs and the impact of their tab positioning on performance and variable distributions. This paper presents an extensive fully coupled three-dimensional (3D) simulation of electrochemical-thermal modeling describing the behavior of large LiFPO$_4$ pouch cells. Different pouch cell designs with various tab locations have been investigated in term of performance and distribution. The model is first validated with experimental data at different discharging current rates. Afterwards, the electrochemical, thermal and electrical behaviors of each cell design under high discharge rate (4 I$_t$) are compared in order to select the best configuration. Finally, the impact of tab width on the temperature, potential and current density distributions are also investigated in depth.

2. Model Description

2.1. Model assumptions and geometry features

A 3D electrochemical-thermal modeling is developed for a high-energy LiFePO$_4$/carbon pouch cell, manufactured by European Batteries. As it is well-known, the battery is composed of several layers. Since the modeling of all layers required a lot of meshing effort and then long computational times. 1D electrochemical coupled with the thermal model applied on a single cell layer has been used in several works [21–24]. The model was validated by comparing simulation to the experimental test performed on the whole battery. Therefore a single electrode plate pair approach can be modeled to describe the pouch cell behaviors. The single electrode cell used is assumed to be a stack layered design and composed of both collectors (positive and negative) with collecting tabs, the positive electrode (PE), the separator and the negative electrode (NE). The whole is bathed in the electrolyte (2 mol/L LiPF6 in EC/DMC solvent) as illustrated in Fig. 1. The geometrical details such as the electrodes, separator and current collectors, tabs thicknesses and particle radius are included in Table 4. Several designs of single