Experimental validation of a 0-D numerical model for phase change thermal management systems in lithium-ion batteries

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HIGHLIGHTS

- A 0-D thermal simulation is used to model a Li-ion battery pack built with phase-change composite material.
- The 0-D model results are compared against a 2-D thermal model and experimental data.
- Strong convective cooling is shown to produce temperature gradients in the pack.
- The 0-D model is most accurate when used in low convective cooling environments.

ARTICLE INFO

ABSTRACT

A lumped (0-D) numerical model has been developed for simulating the thermal response of a lithium-ion battery pack with a phase-change composite (PCC™) thermal management system. A small 10s4p battery pack utilizing PCC material was constructed and subjected to discharge at various C-rates in order to validate the lumped model. The 18650 size Li-ion cells used in the pack were electrically characterized to determine their heat generation, and various PCC materials were thermally characterized to determine their apparent specific heat as a function of temperature. Additionally, a 2-D FEA thermal model was constructed to help understand the magnitude of spatial temperature variation in the pack, and to understand the limitations of the lumped model. Overall, good agreement is seen between experimentally measured pack temperatures and the 0-D model, and the 2-D FEA model predicts minimal spatial temperature variation for PCC-based packs at C-rates of 1C and below.

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1. Introduction

Lithium-ion batteries continue to be a popular and growing energy storage technology across a variety of industries. Their high energy density along with good power density makes lithium-ion cells attractive for applications such as transportation, stationary energy storage, and personal electronic devices, among many others [1—4]. Regardless of the final end-use application, all Li-ion battery systems generate heat during use. The heat generated needs to be managed during battery operation to ensure the battery life is maximized and the safety of the system is not compromised by exposing the cells to unsafe temperatures. Elevated cell temperatures have been shown to decrease battery calendar and cycle life [5—9], accelerate aging mechanisms, and lead to increased risk of thermal runaway [10].

Typically, thermal management systems for large Li-ion batteries employ either an air or liquid-based coolant loop to extract heat away from the cells during operation. In the case of a vehicle-based battery, these cooling systems consume electrical power from the battery itself. The amount of power required for air cooling of a small hybrid electric vehicle battery was shown by Sabbah [11] to exceed 70 W during high power usage. Additionally, they noted that although temperature gradients in the pack increased at high levels of air cooling, the use of thermally conductive phase change materials could dampen these gradients and reduce total peak fan power needed to maintain a safe operating temperature. Pesaran [12] has highlighted the importance of minimizing temperature gradients in larger battery packs to maximize pack life. Rao and Wang [13] provided a survey of thermal management techniques for batteries, and also noted that for high power operation, liquid

cooled systems are prevalent, but care must be taken to avoid leakage, which could cause system damage.

Over the past several years, graphite-wax phase change composite (PCC™) materials have been successfully used as a stand-alone thermal management system for a variety of Li-ion batteries [14]. When in use, the PCC material in solid phase absorbs the heat generated by the Li-ion cells and undergoes phase change into liquid state, thus limiting the temperature rise of the battery. Upon cessation of use, the PCC material can reject heat to the environment, return through phase change to ambient temperature, and be ready for use again.

To illustrate the effectiveness and benefits of PCC as a thermal management strategy, this work presents a basic, 0-D numerical model for calculating the transient thermal behavior of a Li-ion battery pack utilizing PCC material (Section 2.1). To provide inputs to the model, a commercially available 18650 lithium ion cell is thermo-electrically characterized to provide data for cell heat generation (Sections 2.2 and 2.3). Additionally, three different PCC materials are characterized to capture their sensible and latent heat behavior by means of differential scanning calorimetry (Section 2.4).

A central goal of this work is to demonstrate that a relatively simple, 0-D model can accurately capture the heat generation and temperature rise of a small PCC-enhanced battery pack, thereby enabling thermal management system analysis of a battery pack without relying on sophisticated computational tools. The past decade has brought incredible growth and sophistication of Li-ion thermal models, up to a point where complete 3-D electro-thermal models utilizing porous electrode theory are becoming available to researchers and industry [15]. Although accurate, these types of simulations require large scale computing infrastructure to execute, as well as intricate knowledge of cell design and chemistry. The model described in this paper lends credence to others in the field [16–18] who have shown that 0-D models can accurately simulate single cell thermal behavior during operation.

As justification for the lumped approach, the 0-D model is validated against data collected from a small Li-ion battery pack composed of 18650 cells and PCC thermal management material (experimental Sections 2.6 and 2.7, results in Sections 3.1 through 3.4). Further justification for the 0-D model is obtained by performing a 2-D FEA thermal simulation, and the results from both numerical models are compared to the experimental data (Sections 2.8, 3.2). Good agreement is seen between the lumped model and experimental data, despite the non-dimensionality and relatively simple approach of the model. The 2-D model confirms low amounts of thermal non-uniformity in the battery for C-rates below 2C and limited convective cooling (Section 3.3). Finally, the 0-D model is used to explore the effect of different PCC phase change temperatures and the effect of charging on the thermal behavior of the battery pack (Sections 3.5 and 3.6).

2. Methodology

2.1. Lumped numerical model − overview and governing equations

The 0-D model developed for this work calculates Li-ion cell heat generation of an arbitrarily sized battery pack and estimates the thermal response of the cells and PCC material. When PCC material is integrated with cylindrical Li-ion batteries, such as 18650 or 26650 form factors, the resulting composite structure looks similar to Fig. 1. In order to keep complexity to a minimum and allow the model to run on a variety of computers, Microsoft Excel was chosen as the platform for the model.

The inability to spatially resolve temperature gradients in this model is permissible because small cylindrical Li-ion cells have
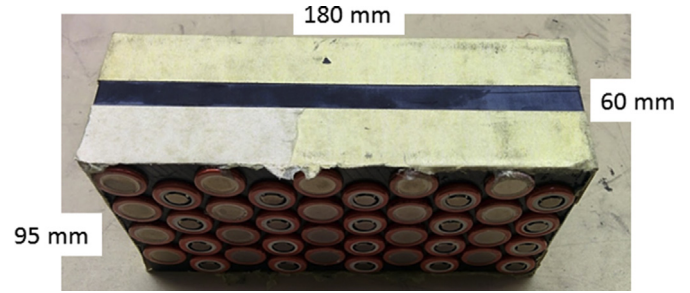

Fig. 1. 18650 Li-ion cells embedded in phase-change composite matrix.

been shown to have small Biot numbers, typically less than 0.05 [19,20], leading to minimal temperature variance inside the cells at moderate (<2C) rates. Additionally, the PCC material exhibits a high degree of thermal conductivity ($5 < k < 25$ W m^{-1} K^{-1}), allowing good temperature uniformity under low convective cooling conditions [19]. These two system properties support the use of a lumped approach, provided that high levels of external forced cooling are not present.

While in operation, a battery will generate heat while delivering or absorbing electrical power. This heat has been shown by Bernardi [21] to come from 5 possible sources: irreversible ohmic heating, reversible entropic heating, heat from phase change of the active materials, heat from mixing, and reaction heat. For the purposes of this work we will simplify the heat generation model to account for the irreversible ohmic heating and reversible entropic heat only, as done by Al-Hallaj [22], Wu [23] and Onda [24]. Additional heat sources can include cell electrical interconnections as well as monitoring and control electronics. Those sources are not included in this work due to their low overall fraction of total heat generation in the battery pack.

The 0-D model considers the cells and PCC to have no spatial dimensions, only a mass (m_{cells} and m_{PCC}), specific heat capacity (cp_{cells} and $cp_{PCC}(T)$), surface area (A), and an h value used to calculate convective heat loss. Combining the irreversible ($\dot{Q}_{irr}$) and reversible ($\dot{Q}_{rev}$) sources of heat generation, convective heat loss (h), and cell and PCC thermal masses yields the following expression for the energy balance of the battery system, shown in Eq. (1).

$$N_{cells}\left(\dot{Q}_{irr} + \dot{Q}_{rev}\right) - hA(T - T_{amb})$$
$$= \frac{\left(m_{cells}c_{p,cells} + m_{PCC}c_{p,\,PCC}(T)\right)dT}{dt} \quad (1)$$

2.2. Irreversible heat generation

The irreversible heat generated by the cell during charging or discharging can be calculated as follows in Eq. (2) or Eq. (3):

$$\dot{Q}_{irr} = I_{cell}(V_{OCV} - V_{Measured}) \quad (2)$$

$$\dot{Q}_{irr} = I_{cell}^2 R_{cell} \quad (3)$$

V_{ocv} is defined to be the open circuit voltage of the cell when at rest. The difference between V_{ocv} and $V_{measured}$ is the cell over-potential. The overpotential value is the sum of irreversible losses in the cell arising from the electronic resistance of the current collectors and cell terminals, the electronic resistance of the active materials and binders in the positive and negative electrodes, and the ionic ohmic resistance of the electrolyte to the flow of Li-ions during use. Additionally, activation polarization at the solid-