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Thermally coupled moving boundary model for charge–discharge of LiFePO₄/C cells



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HIGHLIGHTS

- Electrochemical thermal model for cell with phase transforming electrode.
- Validation of charge–discharge voltage response and heat generation.
- Model analysis of electrochemical heat sources for optimal thermal design.
- Methodology to devise efficient fast charging protocol.

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ABSTRACT

Optimal thermal management is a key requirement in commercial utilization of lithium ion battery comprising of phase change electrodes. In order to facilitate design of battery packs, thermal management systems and fast charging profiles, a thermally coupled electrochemical model that takes into account the phase change phenomenon is required. In the present work, an electrochemical thermal model is proposed which includes the biphasic nature of phase change electrodes, such as lithium iron phosphate (LFP), via a generalized moving boundary model. The contribution of phase change to the heat released during the cell operation is modeled using an equivalent enthalpy approach. The heat released due to phase transformation is analyzed in comparison with other sources of heat such as reversible, irreversible and ohmic. Detailed study of the thermal behavior of the individual cell components with changing ambient temperature, rate of operation and heat transfer coefficient is carried out. Analysis of heat generation in the various regimes is used to develop cell design and operating guidelines. Further, different charging protocols are analyzed and a model based methodology is suggested to design an efficient quick charging protocol.

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1. Introduction

Characteristic high energy density of lithium ion battery comes at a cost of self-heating of this power source due to several inherent electrochemical processes. These electrochemical processes can be thermodynamically classified as dissipative and non-dissipative phenomena which lead to inevitable heating of batteries. Self-heating may lead to severe safety hazards and can lead to phenomenon like thermal run away. It provides the impetus to discern

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not only the physics of the dissipative thermodynamic processes but also the effect of it in on working of these batteries. In order to understand the thermal behavior in detail it is important to develop the fully coupled electrochemical thermal model. It may be noted that the thermal effects differ across lithium ion cells of varying chemistries due to the varying electrochemical processes [1]. Thermal stability is the key property that ensures safe operation and efficient thermal management. In this regard, lithium iron phosphate (LiFePO₄, LFP) is increasingly deployed as positive electrode material in lithium ion cells owing to its high thermal stability, in addition to cost effectiveness, non-toxic nature and long cycle life [2–6].

Modeling the electrochemical processes in a cell has been

predominantly based on a macro homogeneous approach wherein homogeneous equations are used to model the solid matrix and the electrolyte system [7–10]. Transport in the solid phase is modeled by considering diffusion in the individual particles constituting the electrode resulting in a pseudo two dimensional (P2D) model. The generalized structure of the governing partial differential equations (PDE) facilitates incorporation of thermal effects with the electrochemical model [11,12]. The general energy balance based on thermodynamic principles for an electrochemical system [13] assumes temperature uniformity within the cell. It has been successfully used to incorporate the macro homogeneous models in a single cell as well as a stack [14]. An alternate approach based on the local heat generation developed subsequently, [15,16] is proven to be equivalent to the thermodynamic approach. A thermal energy equation capable of describing the internal temperature distribution of the cell is developed using the volume-averaging approach [17]. These developments have resulted in various studies where a coupled electrochemical – thermal model is used to analyze the behavior of lithium ion cells [18–20]. Thermal coupling enables incorporation of the temperature dependence of thermodynamic [21] and transport properties of the electrochemical model based on experimental observations [22]. Further, electrochemical thermal models are developed and extended for lithium ion cells with planar electrodes [23] and spirally wound cells [24]. Coupled thermal–electrochemical models are also used to assess uneven heat generation in battery packs [25] and thermal effects on capacity fade [26] of lithium ion cells. Detailed 3D models are developed for large format lithium cells with the electrochemical–thermal coupling as a sub-model in the complete modeling framework [27,28]. It should be mentioned that, to describe the cell temperature rise in certain situations, lumped parameter thermal models [29,30] are also used. The electrochemical model is required to obtain information about the individual sources of heat from electrodes/electrolyte and the dependence of the heat generation rates on the operating conditions. Information about the controlling electrode and the optimum operating conditions are important for the design of thermal management systems.

Lithium ion batteries with LFP as positive electrode are known to give non-monotonic discharge response owing to its crystallographic phase transformation. The large scale interest in LFP as the positive electrode has resulted in various studies on the thermal behavior of these batteries [30–32]. Electrochemical–thermal models for LFP based cells are developed to study the effect of contact resistances and heat sources [33,34], and for assessing safety limits [5]. 3D models [35,36] and cycle life models to study the capacity fade mechanisms [37–39] are also developed. As mentioned earlier, the phase transformation in LFP also incurs thermal effects which are not accounted for in these studies. It is reported that by accounting effect of characteristic phase transformation in an electrochemical model [40] results in correct representation of charge discharge asymmetry [41], tangential front propagation [42], phase separation as well as path dependent response [43]. Given that LFP electrodes exhibit multi-phase coexistence, its effect on the thermal behavior is yet to be studied in detail and is attempted in this manuscript.

In this work the intent is to develop on the generalized moving boundary model for LFP/C cells [43] to include the non-isothermal behavior. This is achieved by incorporating the effect of heat due to phase transformation using an equivalent enthalpy approach, along with other principle electrochemical sources of heat from the anode, separator and the cathode, as a source term in the governing energy balance equation. The electrochemical processes are in turn coupled by incorporating the temperature dependences of the mass and charge transport properties [34–36]. In the Section 2 of

this work the governing equations and the material properties are introduced and elaborate description of different heat sources for LFP/C cell is explained in subsections. Further, in Section 2.4 the definitions of performance indicators are provided. Several case studies based on model simulations are presented in Section 3. The non-isothermal model thus developed is validated with experimental data. As these cells are used as energy source in various applications, it is important to understand the dependence of heat generation on operating conditions in order to conceive appropriate cooling concepts resulting in efficient battery pack design. In this regard, the dependence of the heat released on the ambient temperature is investigated. Analysis of the effect of ambient temperature of LFP/C cells is not reported earlier, to our knowledge. In a battery pack, the single cell interacts with the surrounding cooling medium through the heat transfer coefficient. Hence, the dependence of the rate of heat generation on this quantity is studied in detail. The insights obtained from this analysis are used to obtain optimal operating conditions that minimize thermal losses and extend battery life. This study enables to conceive appropriate cooling concepts when cells are used as energy source in automobiles and provide key insights in the design of an efficient battery thermal management system.

Research interest in generating and assessing fast charging protocols for lithium ion batteries is gaining momentum. Therefore, different case studies dealing with this aspect are addressed in the Section 3.6. It is known that faster charging times can be achieved by increasing the magnitude of the current during the constant current (CC) mode in the conventional charging scheme [44]. Other schemes involve multi-stage constant current (MSCC) [45], boost charging [46], constant power charging [44], pulsed current charging [47], linearly and non-linearly decreasing current [48] charging. It is shown that from a thermal view point the pulsed charging protocol [35] is not efficient and a multi-stage constant current (MSCC) or linearly decreasing current (which is a limiting case of infinite stage MSCC) are more suitable candidates for quicker charging [34,47,48]. An increase in the magnitude of the charging current however, can be detrimental due to higher heat generation. The effect of heat generation on fast charging protocols have started to receive attention recently [34] but a systematic electrochemical thermal analysis is lacking. Detailed analysis of quicker charging protocol carried out in the present work with focus on the effect of operating conditions in the Section 3.7 of the manuscript.

2. The coupled electrochemical thermal model

In this section the model equations for cell with phase change electrode is discussed. This is followed by the introduction of the various performance indicators that can be computed from the model. LiFePO_4 is known to undergo crystallographic structural phase transformation from lithiated triphylite structure (denoted by β) to de-lithiated heterosite (denoted by α) structure during reversible extraction of lithium. The details of the multi – phase coexistence is discussed in detail elsewhere [43], and the basic application to modeling is detailed in the next subsection.

2.1. Thermal electrochemical model

The electrochemical model for lithium ion cell is mathematically described by the following governing PDEs [8,9].

These consist of mass transport equation,

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