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# Electrochemical–thermal analysis of 18650 Lithium Iron Phosphate cell

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ABSTRACT

A pseudo two dimensional electrochemical coupled with lumped thermal model has been developed to analyze the electrochemical and thermal behavior of the commercial 18650 Lithium Iron Phosphate battery. The cell was cut to obtain the physical dimension of the current collector, electrodes, separator, casing thickness, gasket, etc. The layer structure of the spiral wound, cylindrical casing, gasket and heat shrink wrapping were modeled to understand better the temperature distribution across the cell. Natural convection and radiation were used to reflect the heat dissipation on the side surface. Experimental study was carried out to validate the simulation results. The simulation results suggested that the cell temperature and total heat generation rate have a positive correlation with the $I_t$-rates and these were inline with the experimental results. Reaction heat was the main heat source and it contributed about 80–85% of the total heat generated during charging and discharging of the cell. Based on the simulation results, the final temperature of the cell surface was elevated to 59 °C using $10I_t$ of charging. The effect of electrical contact resistance between the connectors and terminals of the cell was also investigated. It was found that the electrical contact resistance caused a large temperature gradient across the cell. These effects are important and should be considered in the design of EV battery pack and thermal management system to reduce the maximum temperature and maintain the temperature uniformity of the cells.



## 1. Introduction

Depleting fuels source and increasing environmental awareness are some of the main challenges in the automotive industry. Electric Vehicles (EVs) and Hybrid Electric Vehicles (HEVs) are projected as one of the most sustainable solutions for future transport. However, the performance and thermal management of the battery pack with respect to the life cycle and related warranty cost are some of the significant challenges faced by automakers. The Lithium ion (Li-ion) battery which boasts of high power and energy density was used to replace Nickel Metal Hydride (NiMH) and lead acid batteries which have lower energy density and depth of discharge (DOD) in EVs and HEVs [1–4]. Various chemistries of the Li-ion battery are being studied. For example, different types of cathode material ($LiCoO_2$, $LiMn_2O_4$, $LiFePO_4$ and $LiVPO_4$), anode material (graphite, hard carbon, $Li_4Ti_5O_{12}$, $Li_{4.4}Si$ and $Li_{4.4}Ge$) and electrolyte ($LiPF_6$, $LiBF_4$ and $LiClO_4$) have been synthesized to produce different structural configurations of the battery such as spiral wound, elliptic and stacked plate [4–6]. At high charging/discharging rates, electrochemical reactions occur at faster rates and the cells are prone to extensive heat generation. Localized heat accumulation will lead to excessive temperature rise that can initiate electrolyte ignition resulting in thermal runaway and in the worst case-explosion. Therefore, the study on the thermal behavior of the Li-ion battery is necessary to ensure the safety and optimum electrochemical process in the battery.

Several researchers have developed the mathematical models to predict the electrochemical process occurring within the Li-ion battery, charging and discharging behavior and various thermal models have been established to explain the heat generated in the battery [7–20]. Most of the studies are focused on the $LiCoO_2$ [10–13] or $LiMn_2O_4$ [14–18] system using electrochemical–thermal models. The thermal models employed in these studies range from lumped models-treating the layer structure of the cells as homogeneous material with effective thermal properties, assuming a uniform cell temperature distribution, heat generation data obtained from experiments to detailed models that couple the electrochemical model with the thermal model using heat generation and temperature dependent physical properties. Most of these thermal models did not consider the outer can and the heat shrink wrapping present in commercially available batteries and the influence of contact resistance between the battery terminals and the external connectors. The dimensionality of the models range from one to three-dimensions depending on the complexity of the physical phenomenon considered. Most of the three-dimensional models do not consider the electrochemical phenomena and are purely thermal models based on the lumped capacity approach [19–25].

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**Nomenclature**

| | |
|---|---|
| $a$ | specific interfacial area of the electrode, $m^{-1}$ |
| $c$ | lithium concentration at the electrode/electrolyte interface, mol $m^{-3}$ |
| $A_{cc}$ | electrical connector contact area on the terminal, $m^2$ |
| $C_{dl}$ | electrical double layer capacitance, F $m^{-2}$ |
| $C_p$ | specific heat capacity for the active battery material, J $kg^{-1}$ $K^{-1}$ |
| $C_{bp}$ | theoretical capacity of the battery, Ah |
| $D$ | diffusion coefficient of Li-ion, $m^2$ $s^{-1}$ |
| $E$ | emissivity |
| $E_{eq}$ | open circuit voltage, OCV, V |
| $E_{0,ref}$ | equilibrium potential at reference temperature, V |
| $\frac{\partial E_{eq}}{\partial T}$ | temperature derivative of equilibrium potential, V $K^{-1}$ |
| $F$ | Faraday's constant, C $mol^{-1}$ |
| $f$ | mean molar activity coefficient of the electrolyte |
| $h$ | convective heat transfer coefficient, W $m^{-2}$ $K^{-1}$ |
| $I^k_{dis}$ | discharge current, A |
| $i$ | current density vector in a phase, A $m^{-2}$ |
| $i_{ioc}$ | transfer current density of a reaction at the electrode/electrolyte interface, A $m^{-2}$ |
| $i_0$ | exchange current density of an electrode reaction, A $m^{-2}$ |
| $j$ | transfer current resulted from the intercalation or de-intercalation of Li, A $m^{-3}$ |
| $k$ | electrochemical reaction rate constant, m $s^{-1}$ |
| $k_T$ | effective thermal conductivity of the active battery material, W $m^{-1}$ $K^{-1}$ |
| $L$ | thickness of the different layers of the cell, m |
| $R$ | universal gas constant, J $mol^{-1}$ $K^{-1}$ |
| $R_{SEI}$ | solid/electrolyte interfacial film resistance, Ω $m^2$ |
| $R_{cc}$ | contact resistance, Ω $m^2$ |
| $r_s$ | radius of the spherical particle, m |
| $T$ | absolute temperature, K |
| $T_\infty$ | free stream temperature, K |
| $T_{dis}$ | discharge time, h |
| $t_+$ | transport number |
| $Vol$ | volume of the cylindrical cell, $m^3$ |
| $z$ | $\frac{c_s}{c_{max}}$ |
| $\alpha$ | charge transfer coefficients |
| $\sigma$ | electric conductivity, S $m^{-1}$ |
| $\varepsilon$ | volume fraction of a phase |
| $\eta$ | activation over-potentials of an electrode reaction, V |
| $\xi$ | porosity of the specimen |
| $\phi_s$ | electric potential, V |
| $\phi_l$ | electrolyte potential, V |
| $\rho$ | effective density of the active battery material, kg $m^{-3}$ |
| $\sigma_{sb}$ | Stefan-Boltzmann constant, W $m^{-2}$ $K^{-4}$ |

*Subscripts*

| | |
|---|---|
| $a$ | negative electrode |
| $c$ | positive electrode |
| $ang$ | angular direction |
| $eff$ | effective |
| $f$ | filler volume fraction |
| $i$ | different layer of active battery material |
| $l$ | electrolyte phase |
| $max$ | maximum |
| $r$ | radial direction |
| $ref$ | reference state |
| $s$ | solid phase |
| $SEI$ | solid electrolyte interface |
| 0 | initial value |

$LiFePO_4$ (LFP) electrode with olivine structure is a promising candidate electrode material for electric vehicle battery. The LFP batteries have high thermal stability, nontoxic and less expensive as compared to other cathode materials such as $LiCoO_2$, $LiMn_2O_4$, $LiNiO_2$, etc. Besides, LFP also differs from other cathode materials with a phase change associated with various stage of lithiation and do not release oxygen at elevated temperatures which will cause thermal runaway of the cell [4,5,26]. Very few modeling works have been carried out to investigate the behavior of LFP [5,21,27].

Apart from studies on a single cell, energy management studies are conducted on battery packs as well. Minimization of the energy loss in the cells assemblies to allow maximization of the energy harvesting in the battery pack is very crucial in the energy management. The effect of the electrical contact resistance at the contact interface of the cell terminal and the bus bar has been overlooked. High electrical contact resistance will cause difficulty in the cell balancing, large variation of the cell temperature, reduce the storage capability of the cell and lead to localized heating and in the extreme case lead to cell explosion. A recent study established that the electrical contact resistance due to imperfect surface features between the connectors and cell terminal will cost about 20% loss in the total energy flow in and out of the battery [28]. Panasonic has changed the design of the NiMH module current collector to reduce the hot spots and improved the cell performance [29]. However, the current studies is based on electro-thermal model with single internal resistance value of the cell and neglect the transient behavior of the electrochemical changes in the battery during the charging and discharging [29].

In view of the above, the aim of this work is twofold: First, to investigate the electrochemical and thermal behavior of a commercially available 18650 LFP battery using mathematical modeling and experiments and seconds to apply the developed model to study the effect of contact resistance between the cell terminals and external connectors. A pseudo two-dimensional electrochemical model is coupled with a lumped three-dimensional thermal model to predict the electrochemical and thermal behavior of spirally wound LFP battery. The model predictions are compared with experimental data. The models are useful to provide fundamental understanding of the internal transport of the Li-ion and theoretical reference for the battery cooling system design for fast charging battery in EVs or HEVs applications.

## 2. Mathematical model

### 2.1. Pseudo two-dimensional electrochemical model

A schematic diagram of the 18650 LFP cell electrochemical model is shown in Fig. 1. The cell was cut to obtain the physical dimension of the current collector, electrodes, separator, casing thickness, gasket, etc as shown in Fig. 2. The thickness of the current collectors, electrodes, separator, outer can and heat shrink wrap are measured using LEICA DM 2500 M optical microscope. The height and length of the electrodes are measured with the stainless steel ruler. The dimensions and parameters used in modeling are tabulated in Tables 1 and 2. During the charging process, the lithium ions intercalate into solid particles of the negative electrode and de-intercalate from solid particles of the positive