Thermal Analysis of a Latent Heat Storage based Battery Thermal Cooling Wrap

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Abstract: This paper details the thermal analysis of a cylindrical lithium iron phosphate (LiFePO\textsubscript{4}) battery cell with a latent heat thermal cooling wrap. The model has been developed as a tool to study the cooling effects of the wrap on the battery cell during discharging. The study aims to provide insight to the proposed battery thermal management strategy based on a single cell, which can later be scaled up to a battery pack. The proposed latent heat storage based battery cooling wrap is used to passively manage the heat produced by the cell and absorbing and maintaining the battery temperature within operational temperatures and below thermal runaway temperature. The simulation results are validated by experimental results. The error is deemed to be minor and results show good agreement.

Keywords: Thermal simulation, Heat transfer, Cylindrical, Lithium-ion battery, Latent heat, Cooling wrap.

1. Introduction

The most common cause of lithium-ion battery failure is high temperature. Heat is produced from electrochemical reactions occurring in the cell during charging and discharging [1]. Improper and inadequate battery thermal management contributes to such temperature related failures. If the heat is allowed to build up, the battery will overheat and eventually fail catastrophically, also known as thermal runaway. In other cases, excessive built-up heat during operation significantly impacts the performance, safety and cycle life time of the cell [2, 3]. Therefore, it is crucial to maintain the battery temperature within the safe operating temperature range and under thermal runaway temperature.

Cylindrical lithium-ion batteries are widely used in our everyday commercial products ranging from laptop computers to electric vehicles. These batteries are often abused and require robust thermal management systems to keep the cells within healthy temperature range. In general, there are mainly two categories of thermal management techniques, namely, active and passive cooling. Active cooling involves a prime mover which moves the cooling medium around the heat source, for example, a forced air convection system or liquid cooling system. Whereas, passive cooling utilizes phase change materials (PCM) which stores heat energy via latent heat [4, 5]. Even though latent heat systems do not require additional or parasitic power, they require proper designing to be able to absorb the full load of thermal energy.

Hence, it is crucial to accurately model and predict the thermal behavior in lithium ion batteries. Thermal management system designers need to understand the thermodynamic and kinetic characteristics of the battery which can be costly and time-consuming by experimental methods [6-8]. An accurate battery model also aids in the ensuring the safe and optimal electrochemical performance of the cell [9].

Several studies have proposed different methods battery thermal management strategies using phase change materials. Ling et al. [10] and Greco and Jiang [11] proposed and developed a paraffin/expended graphite (EG) composite battery thermal management system which successfully cooled the cell down while the EG improved the thermal conductivity of the PCM. Other methods of improving thermal conductivity include the addition of carbon fibers [12], metallic fins [13] and copper foam [14]. These methods performed numerical and experimental analysis on their proposed designs for confirmation and validation.

Thermal simulation and analysis at the early stages of the design process can demonstrate the performance of the system and allow for corrective actions or optimization to be carried out. Computer aided simulations also provide visualisation of thermal distributions and identify hot spots which will require further attention.

In this paper, the battery cell with the latent heat wrap is modeled and simulated with COMSOL Multiphysics. The study aims to demonstrate the thermal management capabilities of the cooling wrap by lowering the maximum temperature achieved by
the battery cell during discharging. An experiment with the physical battery cell was carried out and used to validate the simulation results.

2. System and Description

The battery cell used for the study is the commercially available A123 LiFePO4 26650 cylindrical cell. The LiFePO4 electrochemistry of the cell, also known as LFP, compared to the more readily available and commonly used lithium cobalt oxide, LiCoO2, is superior in safety, thermal stability and life span. LFP batteries are often used in electric powered vehicles due to these key features. The battery cell and its specifications are shown in Figure 1 and Table 1.

![Figure 1: A123 Systems LiFePO4 26650 battery cell](image)

Table 1: Battery cell specifications

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell Dimensions (mm)</td>
<td>Ø26 x 65</td>
</tr>
<tr>
<td>Cell Weight (g)</td>
<td>76</td>
</tr>
<tr>
<td>Cell Capacity (Ah)</td>
<td>Nominal: 2.5</td>
</tr>
<tr>
<td></td>
<td>Minimum: 2.4</td>
</tr>
<tr>
<td>Voltage (V)</td>
<td>Nominal: 3.3</td>
</tr>
<tr>
<td>Internal Impedance (mΩ)</td>
<td>&lt;6</td>
</tr>
<tr>
<td>Standard Charge Method</td>
<td>1C to 3.6V CCCV, 45 min</td>
</tr>
<tr>
<td>Maximum Continuous Discharge (A)</td>
<td>70</td>
</tr>
<tr>
<td>Maximum Pulse Discharge (A)</td>
<td>10 seconds</td>
</tr>
<tr>
<td></td>
<td>120</td>
</tr>
<tr>
<td>Cycle Life</td>
<td>&gt;1000 cycles</td>
</tr>
<tr>
<td>Operating Temperature</td>
<td>-30°C to 55°C</td>
</tr>
</tbody>
</table>

As seen in Table 1, the operating temperature of the battery cell should not exceed 55°C. Therefore, an appropriate melting range of phase change material should be selected. However, due to the lower discharge rate for this study, a PCM of lower melting range was selected.

The selected PCM is the commercially available RT28HC by RUBITHERM® Technologies GmbH that has a melting point of 28°C over a temperature range of 3°C. The benefits of using organic paraffin is its high latent heat, non-toxic and non-corrosive properties.

The proposed design consists of a PCM-soaked absorbent material which is wrapped around the battery cell. The latent heat cooling wrap is sealed and held in place by a plastic shrink wrap as seen in Figure 2.

![Figure 2: Proposed design](image)

The benefit of the simplistic design is the weight reduction in the latent heat battery thermal management strategy. The total weight of the wrap and plastic shrink wrap is 10 grams, which accounts for approximately 12% of the total weight of the battery. Additionally, the wrap only increases the diameter of the cell from Ø26mm to Ø30mm. The wrap covers 35mm of the cell which correlates to 54% of exposed surface area of the cell. This means the proposed design will not interfere with standard current battery connectors.

3. Theory

The laws of thermodynamics govern the thermal equilibrium within systems and hence, the heat transfer between systems till thermal equilibrium is achieved. In the presence of a temperature gradient, heat energy will be transferred from the heated medium to the cold medium.

Heat energy is transferred by conduction, convection and radiation. Conduction refers to energy being transferred between solids or stationary fluid by the movement of energized atoms and molecules. Whereas convection is the transfer of energy due to movement within a fluid and radiation is energy transferred by infrared electromagnetic waves.

In this study, the main source of heat transfer is conduction between the battery cell and the latent heat thermal cooling wrap. The heat is being absorbed via latent heat by the PCM in the cooling wrap and is considered a stationary fluid. At the meantime, natural convection cooling the battery cell has also been considered. Hence, effects of heat transfer via radiation have been ignored.
3.1. Battery Thermal Theory

When the battery cell is discharged, electrochemical reactions occurring in the cell produces and generates heat. As dictated by Arrhenius laws, as temperature rises, chemical reactions increase exponentially. The temperature rise also aid in electron and ion mobility, reducing internal impedance and increasing capacity. This suggests that a battery’s performance is increased when heated.

However, if the temperature is not controlled or allowed to bypass its upper limits, irreversible chemical reactions and/or loss of electrolyte could occur and permanently damage the cell. In the worst case scenario, the catastrophic failure of the cell also known as thermal runaway would occur.

Thermal runaway occurs when the rate of heat generation within the battery has exceeded its rate of heat removal. The process begins with high cell temperature which leads to the expansion of active chemicals and causing the cell to swell. The chemicals start to break down which produces flammable gases. The melting of separator causes a short which ignites the flammable gases. The cathode of the cell also breaks down due to the heat and generates oxygen which fuels the fire. The thermal runaway is a continuous degenerative cycle that should be avoided at all costs.

4. Governing Equations

The numerical simulation encompasses three main physics; (1) the heat generation model of the battery cell, (2) the heat transfer between battery cell and PCM and (3) the melting of PCM. The equations from COMSOL provide some insight and solution for these phenomena.

4.1. Heat Generation

The heat generation from the battery cell is derived from the coupling of the 1D cell model, which is used to model the battery cell chemistry and the 2D axisymmetric model which is used to model the temperature in the battery [15].

![Figure 3: Coupling between cell and thermal model](image)

4.2. Heat Transfer

The time dependent heat transfer equation is as follows:

\[
\rho C_p \frac{\partial T}{\partial t} + \rho C_p u \cdot \nabla T = \nabla \cdot (k \nabla T) + Q \tag{1}
\]

Where, \( \rho \) is the density \((kg/m^3)\), \( C_p \) is the heat capacity at constant pressure \((J/kgK)\), \( T \) is the temperature \((K)\), \( u \) is the velocity field \((m/s)\), \( k \) is the thermal conductivity \((W/mK)\) and \( Q \) is the heat source \((W/m^3)\).

4.3. Phase Change

The melting process takes place through the latent heat energy equation. The governing equation for latent heat is as follows:

\[
q = m\Delta H_f \tag{2}
\]

Where, \( H_f \) is the latent heat of fusion \((kJ/kg)\) \( m \) is the mass \((kg)\) and \( q \) is heat power \((W)\). Latent heat of fusion is the amount of energy to change a gram of a substance from one phase to another and does so without changing its temperature;

The method used to simulate the phase change effect in COMSOL is also known as the apparent heat capacity method. It assumes a smooth transition over the temperature gradient with a phase mass fraction \( \theta \).

\[
\rho = \theta \rho_{phase1} + (1 - \theta) \rho_{phase2} \tag{3}
\]

Based on the enthalpy, the specific heat capacity is modified to include the effect of latent heat.

\[
C_p = \frac{1}{\rho} \left( \theta_1 \rho_{phase1} C_{phase1} + \theta_2 \rho_{phase2} C_{phase2} \right) + L \frac{d\alpha}{dT} \tag{4}
\]

Where,

\[
\alpha = \frac{1}{2} \cdot \frac{\theta_2 \rho_{phase2} - \theta_1 \rho_{phase1}}{\rho} \tag{5}
\]

Where, \( \alpha \) is the phase volume fraction, \( \theta \) is the phase mass fraction, \( \rho \) is density \((kg/m^3)\) and \( C_p \) is the specific heat capacity \((J/kgK)\).
5. **Numerical Model**

The electrochemical-thermal numerical battery and latent heat thermal cooling wrap model consist of a 1D lithium-ion battery module was used to simulate the electrochemical heat generation in the cell; and a 2D heat transfer module with phase change to simulate the heat transfer between the battery cell and the latent heat cooling wrap and the melting of PCM.

The 2D axis-symmetrical model is shown in Figure 4. The model consists of the battery cell and the latent heat cooling wrap of 2mm thickness.

![Battery model with cooling wrap](image)

**Figure 4: Battery model with cooling wrap**

5.1. **Boundary Conditions**

The main boundary conditions of the analysis are as follows:

- Lithium-Ion Battery (1D)
- Heat Transfer in Solids (2D)
  - Solid
  - Phase Change Material
  - Heat Source (from 1D)
  - Boundary Heat Flux (convective cooling)
- Time-dependent
- Simulation time of 1800 seconds with 5 second step size
- Initial temperature of 296K (23°C)
- Initial pressure of 1 bar
- PCM melting temperature of 301K (28°C)
- Battery discharge rate of 2C (5A)

The material properties used in the simulation are shown in Table 2.

<table>
<thead>
<tr>
<th></th>
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</tr>
</thead>
<tbody>
<tr>
<td>Graphite Electrode</td>
<td>Solid</td>
<td>1</td>
<td>881</td>
<td>-</td>
<td>2270</td>
</tr>
<tr>
<td>LiPF6 Electrolyte</td>
<td>Liquid</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>LFP Electrode</td>
<td>Solid</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>4140</td>
</tr>
<tr>
<td>Steel</td>
<td>Solid</td>
<td>44.5</td>
<td>475</td>
<td>7950</td>
<td>7850</td>
</tr>
<tr>
<td>Nylon</td>
<td>Solid</td>
<td>0.26</td>
<td>1700</td>
<td>-</td>
<td>1150</td>
</tr>
<tr>
<td>PCM</td>
<td>Liquid</td>
<td>0.2</td>
<td>2000</td>
<td>240</td>
<td>880</td>
</tr>
</tbody>
</table>

The electrical properties of the electrodes and electrolyte can be found in the COMSOL material library.

5.2. **Assumptions**

A few assumptions were used to simplify the simulation and reduce computational cost but still maintain its accuracy. These assumptions are as follows:

- The green plastic shrink wrap over the battery cell had been neglected.
- The clear plastic shrink wrap over the latent heat cooling wrap and the battery cell had been neglected.
- Heat lost due to conduction of battery connectors and wiring was not considered.

6. **Experimental Set-up**

The aim of the experiment is to validate the simulation results. The experimental set-up is shown in Figure 5.

![Battery with latent heat cooling wrap](image)

**Figure 5: Battery with latent heat cooling wrap**

The experimental set-up consists of the LFP 26650 battery cell wrapped with the latent heat cooling wrap. The battery cell is discharged to a programmable electronic load and its temperature is monitored with a K-type thermocouple, attached to the middle of the cell. The thermal data is logged, analysed and displayed graphically. The experimental sequence is shown in Figure 6.
The battery cell is discharged at 2C (5A) to the electronic load for 1800 seconds (30 minutes). A thermocouple is attached on the surface of the battery cell, as seen in Figure 7, beneath the cooling wrap which measures and transmits the analog data to the data acquisition unit. The analog data is converted in the DAQ to digital data to be analysed in various analytic software.

Figure 7: Thermocouple location

The central location of the thermocouple effectively captures the peak surface temperature of the cell.

7. Results and Discussion

7.1. Thermal Simulation Results

The thermal simulation shows the peak surface temperature of the battery cell. The simulation was also performed on a bare cell model without the latent heat cooling wrap for comparison purposes. The simulation results of the model are shown in Figure 8.

As seen in Figure 9, the peak temperature for the bare cell and cell with cooling wrap has been captured. The cell with cooling wrap has a more gradual increase in temperature after 28°C, which is the melting temperature of the PCM. This indicates that the PCM is absorbing the heat produced by the battery cell.

Hence, the cell with the cooling wrap recorded a lower temperature than the bare cell. The latent heat cooling wrap was able to reduce the cell peak temperature from 35.9°C to 30.9°C.

7.2. Experiment Results

The experiment was carried out to validate the accuracy of the numerical simulation performed in COMSOL Multiphysics. The experimental results are
displayed graphically as shown in Figure 10.

![Figure 10: Experimental Results](image)

As seen in Figure 10, the maximum temperature for the bare cell and cell with cooling wrap reached 36.0°C and 31.3°C respectively. Comparing the two curves, the temperature of the cell with the cooling wrap maintained a temperature approximately to that of the melting temperature of the PCM. However, it was also observed that there is a dip in temperature of the bare cell from 700s to 1200s even though there was no latent heat wrap to cool the cell. This is due to the negative entropic heat contribution, which is characteristic of a lithium-ion type battery.

### 7.3. Comparison of Results

The experiment and simulation results are compared for validation purposes and it has been observed that the simulation results match closely to the experiment results as shown in Figure 11.

![Figure 11: Simulation vs. Experiment Results](image)

The results obtained for the bare cell yield a root mean square (RMS) error of 0.77. The main discrepancy occurred from 0s to 800s, which relates to the initial heat generation of the cell. This difference is also observed in the cell with the cooling wrap.

The cell with cooling wrap produced a RMS error of 0.60. The main discrepancy observed was between 0s to 600s, which relates to the initial heat generation of the cell. This could also be due to the heat flux which is meant to simulate natural convection. Another possible reason is the difference in heat generating electrochemical reactions in the cell as compared to the real battery cell.

![Figure 12: Bare Cell - Experiment vs. Simulation](image)

![Figure 13: Cooling Wrap - Experiment vs. Simulation](image)

Figure 12 and Figure 13 are the comparison graphs between the bare cell and the cell with cooling wrap for both experiment and simulation.

### 8. Conclusions

The results obtained from the study demonstrate the feasibility of the proposed battery latent heat thermal cooling wrap as a passive battery thermal management system. The inclusion of the cooling wrap successfully brought the cell temperature down by approximately 5°C. The battery was also maintained within safe operating temperature.
The experimental result agrees to the simulation results with a small and acceptable error. Hence, the developed LFP electrochemical-thermal lithium-ion battery model can be used to predict cell thermal behaviors and validate the proposed battery thermal management strategy.

For future works, the thermal conductivity of the latent heat thermal cooling wrap can be improved with the addition of thermally conductive materials. However, addition of these materials might affect the heat storage capability of the wrap and increase its weight. Therefore, a study could be carried out to explore these effects and weigh its pros and cons.

References

15. COMSOL Multiphysics 5.2a, Thermal Modeling of a Cylindrical Lithium-ion Battery in 2d.