Comparison and analysis of temperature distribution in pouch and cylindrical Li-ion battery by finite element thermal model

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Abstract

Li-ion battery is the most popular energy storage system for the propulsion of an electric vehicle since the Li-ion batteries are high energy storage device and high energy density. However, Li-ion battery performance is highly sensitive to the operational temperature. The aim of the present study was to comparison and analysis of temperature distribution between the pouch and cylindrical Li-ion battery. The solution in thermal equations to be solved by approximating in the form of the partial differential equations (PDE) by 3-D finite element method using that all the coded developed by MATLAB program and the mathematical model that is time dependent. The simulation results show that an increased discharge current rate from 1C to 5C results show temperature increased. An increase the surface area and the cross-section tab area under the same volume conditions. The simulation results in formation of temperature decreased caused heat generation decrease. Thus, the temperature distribution of the pouch Li-ion battery less than the cylindrical Li-ion battery.

Keywords: Li-ion battery, 3-D finite element method, thermal distribution, thermal model

1. Introduction

It this well known that the most popular energy storage system for the propulsion of an electric vehicle, Li-ion battery is considered as one of the major concerns, since the Li-ion batteries are high energy storage devices and high energy density. However, the Li-ion battery performance is highly sensitive to the operational temperature [1]. For example, Li-ion batteries often suffer severe power loss under temperatures below zero degrees Celsius and face the increased risk of a thermal runaway at extremely high temperatures [2]. Thus, a thermal management system is necessarily required to control the system temperature within a permitted range, and maintain the temperature uniformity throughout the overall system.

The above thermal analysis of heat transfer problems will be explained in the form of differential equations, which require the solution to be solved by approximating in the form of the partial differential equations (PDE) and the popular method of solving a partial differential equation is 3-D finite element method [3]. The aim of the present study was to comparison and analysis of temperature distribution between the pouch and cylindrical Li-ion battery by using a 3-D finite element method, which is controlled the Li-ion battery under the same volume conditions. To find a suitable model for using in electric vehicles and accurately predict their thermal behavior under convection conditions.

2. Mathematical Model of Temperature for Li-Ion Battery

Based on these assumptions, a Li-Ion battery 3-D heat transfer equation under the Cartesian coordinate is derived as Equation (1).
\[ \rho c \frac{\partial T}{\partial t} = k_x \frac{\partial^2 T}{\partial x^2} + k_y \frac{\partial^2 T}{\partial y^2} + k_z \frac{\partial^2 T}{\partial z^2} + Q \]  

(1)

Where \( \rho \), \( c \), \( t \) and \( T \) are the average density (kg/m\(^3\)), the average specific heat capacity (J/kg\(^\circ\)C), time (sec) and temperature (\(^\circ\)C) of the battery, respectively. \( k_x \), \( k_y \) and \( k_z \) represent the thermal conductivity (W/m\(^\circ\)C) of the battery in coordinate \( x \), \( y \) and \( z \) and \( Q \) represents the heat generation (W/m\(^3\)).

The Li-Ion batteries are made up of multiple layers of different materials. To simplify the calculation, the average density and the average specific heat capacity of Li-Ion battery can be calculated as [4]

\[
\rho_{\text{cell}} = \frac{\sum_i m_i}{\sum_i v_i} \quad \text{and} \quad c_{\text{cell}} = \frac{\sum_i \rho_i c_i v_i}{\sum_i m_i}
\]

Another important parameter is the thermal conductivity coefficient, which can be calculated as follows [4]

\[
k_s = \frac{V_{\text{cell}}}{\sum_i v_i} \quad \text{and} \quad k_p = \frac{\sum_i k_i v_i}{V_{\text{cell}}}
\]

Where \( k_s \) and \( k_p \) are the average heat conductivity coefficient in series and parallel respectively. During the discharge cycle, the heat generation is taken place caused by the flowing of current \( I \), through the cell. And the heat generation for the battery which was developed by reference [5-6] can be written as

\[
Q = Q_j + Q_s + Q_t = \frac{I}{V_{\text{cell}}} \left( U^o - U \right) - T \frac{\partial U^o}{\partial T} + \frac{I^2}{A_{\text{tab}}} \sigma_{\text{tab}}
\]

(2)

Where \( I \), \( V_{\text{cell}} \), \( U^o \), \( U \), \( A_{\text{tab}} \) and \( \sigma_{\text{tab}} \) are the battery operating current (A) (positive for discharging and negative for charging), the cell volume (m\(^3\)) of battery, open circuit potential (V), the cell potential (V), the cross-section tab area (m\(^2\)) and the electrical conductivity of tab (MS/m), respectively. The first term is the heat generation due to joule heating can be described as

\[
Q_j = \frac{I}{V_{\text{cell}}} \left( U^o - U \right) = \frac{I^2 R_m}{V_{\text{cell}}}
\]

(3)

The internal resistance \( R_m \) (~2 m\(\Omega \) [7]) during charge/discharge can be determined by Equation (4) [8]

\[
R_m = \frac{\left( U^o - U \right)}{I}
\]

(4)

And the second term is generated due to entropy change can be written as

\[
Q_s = \frac{I}{V_{\text{cell}}} \left( -T \frac{\partial U^o}{\partial T} \right) = -T \Delta S \frac{I}{nFV_{\text{cell}}}
\]

(5)

Where \( F \) is the Faraday constant (96,485 c/mol), \( n \) is the charge number of electron and taken to be equal 1. the entropy changes (\( \Delta S \) J/mol\(^\circ\)C) of LiNiMnCoO\(_2\) (NMC) and LiC\(_6\) (graphite) considered in this study are illustrated in Fig. 1. These data are taken from reference [9-10]. The entropy changes typically to a reduction reaction, which is the discharge reaction for a cathode in a full cell. Thus, the total change
in entropy for a cell during discharge is \[ \Delta S = \Delta S_c + \Delta S_a \] (6)

Where \( \Delta S_c \) represents the entropy change of the cathode material for reduction reaction, while \( \Delta S_a \) represents the entropy change of the anode material for the oxidation reaction.

Fig. 1. Entropy changes (J/mol·°C) under different state of charge (SOC): (a) LiNiMnCoO\(_2\) and (b) LiC\(_6\).

3. 3-D Finite Element Method

The 3.65V/20Ah pouch battery provided by the manufacturer can be found in [6]. In this battery cell, there are 18 cell assemblies. One such assembly consists of sub-layers are shown in Fig. 2. In a case study, a cylindrical battery on the right side was designed to compare the temperature distribution, which is controlled the Li-ion battery under the same volume conditions. The 3-D finite element method domain can be used linear tetrahedron elements, which a pouch cell model consists of 11,621 nodes and 53,204 elements, while a cylindrical battery consists of 10,565 nodes and 55,461 elements.

Fig. 2. Component of a pouch and a cylindrical Li-ion battery.
From Equation (1) the creating of finite element equations was applied to the method of weighted residual by the Galerkin method. And this paper was used the tetrahedron element for the shape function (three dimensions) for the finite element method. According to this method, Equation (7) and (8) are expressed corresponding with temperature [12].

\[
T(x, y, z, t) = T_1 N_1 + T_2 N_2 + T_3 N_3 + T_4 N_4
\]  

(7)

Where \(T_1, T_2, T_3\) and \(T_4\) are the temperature of node 1, 2, 3, and 4, respectively. And \(N_1, N_2, N_3\) and \(N_4\) are the element shape function, then

\[
N_n = \frac{1}{6V}(a_n + b_n x + c_n y + d_n z)
\]  

(8)

And \(V\) is the volume of the tetrahedron element, which can be found the determinants of the coefficient as follows (9).  

\[
V = \frac{1}{6} \begin{vmatrix} 1 & x_1 & y_1 & z_1 \\ 1 & x_2 & y_2 & z_2 \\ 1 & x_3 & y_3 & z_3 \\ 1 & x_4 & y_4 & z_4 \end{vmatrix}
\]  

(9)

The position coefficient defined by

\[
a_1 = x_4 \left(y_2 z_3 - y_3 z_2\right) + x_3 \left(y_4 z_2 - y_2 z_4\right) + x_2 \left(y_3 z_4 - y_4 z_3\right)
\]

\[
c_1 = x_4 \left(z_2 - z_3\right) + x_2 \left(z_3 - z_4\right) + x_1 \left(z_4 - z_2\right)
\]

\[
a_2 = x_4 \left(y_3 z_1 - y_1 z_3\right) + x_3 \left(y_4 z_1 - y_1 z_4\right) + x_1 \left(y_2 z_4 - y_4 z_2\right)
\]

\[
c_2 = x_4 \left(z_1 - z_3\right) + x_1 \left(z_3 - z_4\right) + x_3 \left(z_4 - z_1\right)
\]

\[
a_3 = x_4 \left(y_1 z_2 - y_2 z_1\right) + x_2 \left(y_4 z_1 - y_1 z_4\right) + x_1 \left(y_2 z_4 - y_4 z_2\right)
\]

\[
c_3 = x_4 \left(z_1 - z_2\right) + x_1 \left(z_2 - z_4\right) + x_2 \left(z_4 - z_1\right)
\]

\[
a_4 = x_3 \left(y_2 z_1 - y_1 z_2\right) + x_2 \left(y_1 z_3 - y_3 z_1\right) + x_1 \left(y_3 z_2 - y_2 z_3\right)
\]

\[
c_4 = x_3 \left(z_2 - z_1\right) + x_2 \left(z_1 - z_3\right) + x_1 \left(z_3 - z_2\right)
\]

\[
b_1 = y_4 \left(z_3 - z_2\right) + y_3 \left(z_2 - z_4\right) + y_2 \left(z_4 - z_3\right)
\]

\[
d_1 = x_4 \left(y_3 - y_2\right) + x_3 \left(y_2 - y_4\right) + x_2 \left(y_4 - y_3\right)
\]

\[
b_2 = y_4 \left(z_1 - z_3\right) + y_1 \left(z_3 - z_4\right) + y_3 \left(z_4 - z_1\right)
\]

\[
d_2 = x_3 \left(y_1 - y_3\right) + x_1 \left(y_3 - y_4\right) + x_3 \left(y_4 - y_1\right)
\]

\[
b_3 = y_4 \left(z_2 - z_1\right) + y_2 \left(z_1 - z_4\right) + y_1 \left(z_4 - z_2\right)
\]

\[
d_3 = x_4 \left(y_2 - y_1\right) + x_2 \left(y_1 - y_4\right) + x_1 \left(y_4 - y_2\right)
\]

\[
b_4 = y_3 \left(z_1 - z_2\right) + y_1 \left(z_2 - z_3\right) + y_2 \left(z_3 - z_1\right)
\]

\[
d_4 = x_3 \left(y_1 - y_2\right) + x_1 \left(y_2 - y_3\right) + x_2 \left(y_3 - y_1\right)
\]
After that used weighted residual by the Galerkin method and was applied to the differential equation (1), where the integrations were performed over the element domain \( V \).

\[
\int_V N_n \rho c \frac{\partial T}{\partial t} dV + \int_V \left( k_x \frac{\partial N_n}{\partial x} \frac{\partial T}{\partial x} + k_y \frac{\partial N_n}{\partial y} \frac{\partial T}{\partial y} + k_z \frac{\partial N_n}{\partial z} \frac{\partial T}{\partial z} \right) dV + \int_{\Gamma} N_n h T d\Gamma + \int_V N_n Q_s dV
\]

\[
= \int_{\Gamma} N_n h T_0 d\Gamma + \int_V N_n Q_j dV + \int_V N_n Q_0 dV
\]

From equation (10) can be expressed in matrix form

\[
[C] \{ T \} + [K_c + K_h + K_s] \{ T \} = \{ Q \}
\]

(11)

Where \([C]\) is the heat capacity matrix, \([K_c]\), \([K_h]\) and \([K_s]\) are the thermal conductivity matrix, the heat convection matrix, and the entropy change matrix, respectively. And \([Q]\) is the load vector for heat generation can be described as

\[
[C]_{4x4} = \rho c \frac{V}{20}
\]

(12)

\[
[K_c]_{4x4} = \frac{1}{36V} \left( k_x \left[ b_j b_k \right] + k_y \left[ c_j c_k \right] + k_z \left[ d_j d_k \right] \right) \quad j, k = 1, 2, 3, 4
\]

(13)

\[
[K_h + K_s]_{4x4} = \left( h + \Delta S \frac{I}{nFV_{cell}} \right) \frac{V}{20}
\]

(14)

\[
\{ Q \}_{4x1} = \{ Q_h + Q_j + Q_s \}_{4x1} = \left( h T_{amb} + \frac{I^2 R_m}{V_{cell}} + \frac{I^2}{A_{tab} \sigma} \right) \frac{V}{4}
\]

(15)

Where \( h \) is the heat convection coefficient (W/m\(^2\)∙˚C), \( T_{amb} \) is ambient temperature (˚C). In this paper, the simulation was set initial temperature equal to the ambient temperature (\( T_0 = T_{amb} = 25 \)˚C) and the heat convection coefficient was set to equal to 10 W/m\(^2\)∙˚C.

Equation (11) \( \{ T \} \) represents the temperature distributions depending on time. Thus, the backward difference method is used as shown in Equation (16) [13].

\[
\begin{align*}
\{ T \}^{t+\Delta t} &= \frac{\{ T \}^{t+\Delta t} - \{ T \}^t}{\Delta t}
\end{align*}
\]

(16)

For the calculation of all elements in the system of \( n \) nodes, the system equations are \( nxn \) matrix.
4. Dimension and Parameter of Li-ion Battery

The dimension of a pouch and a cylindrical Li-ion battery is shown in Fig. 4(a) and Fig. 4(b), respectively. The parameter of a pouch and a cylindrical Li-ion battery are provided in Table 1. [6].

![Fig. 4. Dimension of Li-ion battery: (a) pouch cell and (b) cylindrical cell.](image)

![Table 1. Material and geometric properties of the Li-ion battery](table)

| Material                                      | $\rho$ (kg/m$^3$) | $k$ (W/m°C) | $c$ (J/kg°C) | $\sigma$ (MS/m) | thickness (µm) |
|-----------------------------------------------|-------------------|-------------|-------------|-----------------|----------------|
| Positive tab (Al)                             | 2.702             | 238         | 903         | 37.8            |                 |
| Positive electrode (NMC)                      | 2.895             | 1.58        | 1,270       | 70              |                 |
| Positive current collector (Al)               | 2.702             | 238         | 903         | 21              |                 |
| Negative tab (Cu)                             | 8.933             | 398         | 385         | 59.6            |                 |
| Negative electrode (graphite)                 | 1.555             | 1.04        | 1,437       | 79              |                 |
| Negative current collector (Cu)               | 8.933             | 398         | 385         | 12              |                 |
| Separator (PP)                                | 1.017             | 0.34        | 1,978       | 25              |                 |
| The cell core of pouch cell (mixture of the separator, the electrode, and the current collector) | 2,258.79 | $k_x = k_y = 26.58$ (parallel) | $k_z = 0.973$ (series) | 1,225.36 |
| The cell core of the cylindrical cell         | 2,258.79 | $k_x = k_y = 0.973$ (series) | $k_z = 26.58$ (parallel) | 1,225.36 |

5. Result and Discussion

The 3-D finite element method based simulation is coded with MATLAB programing for calculation of temperature distribution inside the Li-ion battery. At the beginning of discharge, the most heated region is located at the positive tab. Thus, the region of the battery core, which is adjacent to the positive tab is more heat than the rest, Superior heat generation at the aluminum positive tab compared to the copper negative tab is due to the lower electric conductivity, which can be described in Equation (17). Whereas, the heat generation in the battery core is one order of magnitude smaller than the tabs, which is shown only 5C-rate in Fig. 5(a). As the discharge progresses, the battery core, the positive tab and the negative tab increase to high temperature as shown in Fig. 5(b).

$$Q_t = \frac{I^2}{A_{tab} \sigma_{tab}}$$

(17)

Fig. 6(a) shows the most heated region is located at the cell core. Thus, the region near of the cell core...
is more heat than the rest. If comparison of area between the cell core and tab. Results show the temperature of the tab less than the cell core because thickness of tab less than the cell core in Fig. 5 under the same volume. In the end of discharge, the battery core, the positive tab and the negative tab increase to high temperature as shown in Fig. 6(b).

Fig. 5. The temperature distribution (°C) of the center section at 5C-rate: (a) 360 sec and (b) the end of discharge.

Fig. 6. The temperature distribution (°C) of cylindrical battery at 5C-rate: (a) 360 sec and (b) the end of discharge.

Fig. 7. The temperature curve of batteries under different rates: (a) max. temp. of core and (b) ave. surf. temp.

Fig. 7. shows the comparison of temperature distribution between the pouch and cylindrical Li-ion battery under the same volume conditions. Fig. 7(a) show the maximum temperature within the cell core of various discharge current rate, while Fig. 7(b) show the average surface temperature of various discharge current rate. These data confirm that an increased discharge current rate from 1C to 5C results
show temperature increased. The temperature of the cylindrical Li-ion battery more than the pouch Li-ion battery, because the surface area of the cylindrical battery received heat transfer from the air less than the surface area of the pouch battery. And show the temperature results in Table 2.

Table 2. Maximum and the average surface temperature under different C-rates of the Li-ion battery

| Temperature results (°C) | 1C     | 3C     | 5C     |
|--------------------------|--------|--------|--------|
| Max. temp. of core (pouch) | 26.52  | 35.69  | 48.45  |
| Max. temp. of core (cylindrical) | 28.31  | 39.80  | 51.92  |
| Ave. surf. temp. (pouch)   | 26.48  | 35.05  | 46.12  |
| Ave. surf. temp. (cylindrical) | 28.05  | 38.66  | 49.89  |

6. Conclusion

This work study was to comparison of temperature distribution between the pouch and the cylindrical Li-ion battery by 3-D finite element method. It may be concluded from the present study that the discharge current, the cross-section tab area, the electric conductivity, and the surface area has a significant influence on heat generation of the Li-ion battery. The simulation results show that an increased discharge current rate from 1C to 5C results show temperature increased. An increase the surface area and the cross-section tab area under the same volume conditions, the simulation results in formation of temperature distribution decreased caused heat generation decrease. Thus, temperature of the pouch Li-ion battery less than the cylindrical Li-ion battery.

Conflict of Interest

The authors declare no conflict of interest.

Author Contributions

Pao-la-or conducted the research; Somphong analyzed the data; Pao-la-or and Somphong wrote the paper; all authors had approved the final version.

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