Numerical study on thermal runaway of lithium-ion batteries with liquid cooling

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Abstract—A number of fires broken out in electric vehicle in recent years have raised concerns about the thermal safety of batteries. Some cases of abuse, such as overcharge and overdischarge, nail penetration, and high temperature, can make the battery temperature exceed the control. Therefore, it is of great significance to study the occurrence and propagation mechanism of thermal runaway in batteries to improve the safety of batteries. In this paper, a micro-channel cooling system is established to study its cooling effect on the battery module. The electrochemical-thermal coupling model of the battery is established to analyze the heat transfer during the battery’s nail penetration process. Then a model of runaway propagation is established to analyze the heat transfer between batteries. The numerical simulation method is used to study the effect of the cooling system. The results show that the designed cooling scheme can prevent thermal runaway propagation between batteries.

1. Introduction

Lithium-ion battery has become the preferred power source for electric vehicles due to its high energy density and memory-free effect[1][2]. However, the inflammable battery materials bring greater safety risks to lithium-ion batteries. Especially in recent years, the occurrence of a number of electric vehicle fire incidents makes the safety of lithium-ion battery research be particularly important.

Domestic and foreign research institutions and automobile enterprises have done a lot of research on battery thermal runaway, caused by nail penetration, and liquid cooling BTM system. Based on the porous electrode theory, Chiu KuanCheng[3] established the electrochemical model of lithium ion battery and the electrochemical-thermal coupling model to simulate the battery’s nail penetration process by using the battery heat abuse equation combined with the temperature chamber experiment at
the same time. Santhanagoalan[4] studied the short-circuit behaviors in lithium-ion batteries by using the electrochemical - thermal coupling model, and they proposed four short-circuit forms: cathode - anode, cathode - anode collectors, cathode collectors - anode, cathode collectors - anode collectors. Fang Weifeng[5] established a 3D electrochemical - thermal coupling model for a lithium-ion battery with a capacity of 1Ah.

Chen Siqi[6] proposed a liquid-cooled battery temperature management system and adopted a multi-objective optimization method to obtain lower temperature and energy dissipation. Xu Jian[7] proposed a kind of micro-channel cooling system of battery module. The effect of liquid flow rate, nail penetration’s depth in the process of thermal runaway was studied. Lai Yongxin[8] proposed a compact and lightweight liquid-cooling BTM system, and the cooling effects of fluid mass, inner diameter, contact height and angle on the battery were studied.

In this paper, the electrochemical - thermal coupling model of a single cell is established to analyze the temperature change of the cell during the process of nail penetration. The thermal runaway propagation characteristics are studied by means of the micro-channel cooling system, and the effect of micro-channel cooling system is studied.

2. MODEL DESCRIPTION

2.1. Numerical model of battery

The established battery models include one-dimensional electrochemical model, one-dimensional internal short circuit model and three-dimensional heat transfer model, which are coupled with each other.

The one-dimensional electrochemical model is established based on the P2D model proposed by Newman[9] to describe the transport process of lithium ions and electrons between the cathode and anode of the battery, and it also follows the laws of mass conservation, charge conservation and energy conservation. Based on the porous electrode theory, Fick’s law and electrode dynamics, the P2D model ignores the difference between cathode and anode particles. The one-dimensional electrochemical model is composed of cathode, anode, separator, cathode collectors and anode collectors.

The conservation equations of mass and charge in the solid phase are

$$\frac{\partial c_s}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 D_s \frac{\partial c_s}{\partial r} \right)$$

(1)

$$\frac{\partial}{\partial r} \left( \sigma_{eff} \frac{\partial \phi_s}{\partial r} \right) = j$$

(2)

- $c_s$: Solid phase lithium ion concentration in electrode active particles;
- $t$: The time variable;
- $D_s$: Diffusion coefficient of solid phase lithium ion in electrode active particles;
- $r$: Radius distance inside spherical particle;
- $\sigma_{eff}$: Effective solid phase conductivity;
- $j$: Lithium ion diffusion flux per cross section of spherical particle surface;
- $\phi_s$: Solid phase voltage;

The conservation equations of mass and charge in the liquid phase are

$$\frac{\partial c_l}{\partial t} = \frac{\partial}{\partial x} \left( D_{eff} \frac{\partial c_l}{\partial x} \right) + \frac{1 - t^0}{F} j$$

(3)

$$\frac{\partial}{\partial x} \left( \kappa_{eff} \frac{\partial c_l}{\partial x} \right) + \frac{\partial}{\partial x} \left( \kappa_{eff} \frac{\partial \ln c_l}{\partial x} \right) + j = 0$$

(4)
ε_e: Porous electrode electrolyte phase volume fraction;
C_e: Electrolyte phase lithium ion concentration;
D_e^{eff}: Effective diffusion coefficient of liquid lithium ion;
\( \dot{i}_e \): Number of lithium ion migration;
K_{eff}: Effective rate constant;

The establishment of a one-dimensional short-circuit model in cathode and anode can be used to study current transport of electrons during nail penetration process. This model only includes cathode and anode of the battery, and the amount of short-circuit current can be described by the number of broken diaphragms. In this model, the density of short-circuit current is calculated as in (5)

\[
i_{\text{short}} = n_f \sigma_{\text{short}} \frac{\partial \Phi_s}{\partial x}
\]  

\( i_{\text{short}} \): short-circuit current;
\( n_f \): Number of broken diaphragm layers;
\( \sigma_{\text{short}} \): The conductivity between the positive and negative electrodes;
\( \Phi_s \): The cathode voltage;

The heat at the short circuit location is described by the joule heat law as in (6)

\[
q_{\text{short}} = n_f \sigma_{\text{short}} \left( \frac{\partial \Phi_s}{\partial x} \right)^2
\]  

\( q_{\text{short}} \): Heat at short circuit;

When establishing the three-dimensional heat transfer model of the battery, the specific structure of the battery is neglected and the battery is simplified into an integrated structure. In order to calculate the heat generation during battery acupuncture, the one-dimensional electrochemical model, one-dimensional internal short circuit model and three-dimensional heat transfer model should be coupled in pairs.

2.2. The heat transfer model

Purified water is used as coolant for lithium-ion battery modules. The energy conservation equation of the liquid in the cooling plate can be expressed as

\[
\frac{\partial}{\partial \tau} \left( \rho_w c_w T_w \right) + \nabla \cdot \left( \rho_w c_w \bar{\nu} T_w \right) = -\nabla \cdot \left( \lambda_w \nabla T_w \right)
\]  

(7)

The momentum conservation equation of the coolant can be expressed as

\[
\frac{\partial}{\partial \tau} \left( \rho_w \bar{\nu} \right) + \nabla \cdot \left( \rho_w \bar{\nu} \bar{\nu} \right) = -\nabla P
\]  

(8)

The continuous equation of the coolant can be expressed as

\[
\frac{\partial \rho_w}{\partial \tau} + \nabla \cdot \left( \rho_w \bar{\nu} \right) = 0
\]  

(9)

\( \rho_w \): The density of the coolant;
\( c_w \): Specific heat capacity of coolant;
\( T_w \): The temperature of the coolant;
\( \vec{V} \): The velocity vector of water in cooling plate;
\( \lambda_w \): The thermal conductivity of the coolant;
\( P \): The static pressure;

2.3. Thermal abuse model
Thermal runaway refers to the rise of battery temperature caused by various cases of abuse. When the temperature reaches a certain range, it will cause the failure of various materials in the battery, resulting in a series of violent side reactions. The accumulated energy accelerates the rate of temperature rise, which finally loses control. Among them, the most important reactions include the decomposition of SEI, the reaction between cathode material and electrolyte, the reaction between anode material and electrolyte, and the decomposition of electrolyte. The heat of the four major side reactions of the battery can be expressed as

\[
Q_{\text{tot}} = Q_{\text{sei}} + Q_{\text{neg}} + Q_{\text{pos}} + Q_{\text{ele}}
\]  

(10)

\( Q_{\text{tot}} \): The four side reactions produce the sum of the heat;
\( Q_{\text{sei}} \): Heat generation by SEI decomposition;
\( Q_{\text{neg}} \): The anode active material reacts with the electrolyte to produce heat;
\( Q_{\text{pos}} \): The cathode electrode active material reacts with the electrolyte to produce heat;
\( Q_{\text{ele}} \): Decomposition of the electrolyte produces heat;

(1) The decomposition of SEI

\[
Q_{\text{sei}} = H_{\text{sei}} \cdot W_{\text{sei}} \cdot A_{\text{sei}} \cdot \exp \left( \frac{-E_{a,\text{sei}}}{RT} \right) \cdot c_{\text{sei}}
\]  

(11)

\[
\frac{dc_{\text{sei}}}{dt} = -A_{\text{sei}} \cdot \exp \left( \frac{-E_{a,\text{sei}}}{RT} \right) \cdot c_{\text{sei}}
\]  

(12)

(2) The reaction between cathode material and electrolyte

\[
Q_{\text{neg}} = H_{\text{neg}} \cdot W_{\text{neg}} \cdot A_{\text{neg}} \cdot \exp \left( \frac{-E_{a,\text{neg}}}{RT} \right) \cdot c_{\text{neg}}
\]  

(13)

\[
\frac{dc_{\text{neg}}}{dt} = -A_{\text{neg}} \cdot \exp \left( \frac{-E_{a,\text{neg}}}{RT} \right) \cdot c_{\text{neg}}
\]  

(14)

\[
\frac{dz}{dt} = A_{\text{neg}} \cdot \exp \left( \frac{-E_{a,\text{neg}}}{RT} \right) \cdot c_{\text{neg}}
\]  

(15)

(3) The reaction between anode material and electrolyte

\[
Q_{\text{pos}} = H_{\text{pos}} \cdot W_{\text{pos}} \cdot A_{\text{pos}} \cdot a \cdot (1 - a) \cdot \exp \left( \frac{-E_{a,\text{pos}}}{RT} \right)
\]  

(16)

\[
\frac{da}{dt} = A_{\text{pos}} \cdot a \cdot (1 - a) \exp \left( \frac{-E_{a,\text{pos}}}{RT} \right)
\]  

(17)

(4) The decomposition of electrolyte

\[
Q_{\text{ele}} = H_{\text{ele}} \cdot W_{\text{ele}} \cdot A_{\text{ele}} \cdot \exp \left( \frac{-E_{a,\text{ele}}}{RT} \right) \cdot c_{\text{ele}}
\]  

(18)
\[ \frac{dc_{ele}}{dt} = -A_{ele} \cdot \exp \left( \frac{-E_{a,ele}}{RT} \right) \cdot c_{ele} \]  \tag{19}

\( H \): Heat generation per unit mass of the reactants;
\( W \): Carbon per unit volume of reactants;
\( A \): Frequency factor;
\( E_a \): Activation energy;
\( c_{sei} \): The proportion of unstable Lithium ion in the diaphragm;
\( z \): The ratio of SEI film thickness to particle size of active material;
\( c_{neg} \): The proportion of Lithium ion in the anode material that can react with the electrolyte;
\( a \): The proportion of positive electrode materials involved in the reaction;
\( c_{ele} \): The percentage of unreacted electrolyte;
\( R \): Gas reaction constant;
\( T \): Temperature of battery;

2.4. The geometric model

The micro-channel cooling model is shown in Fig. 1. The battery is NCM lithium-ion battery, the positive electrode material is Li(NiCoMn)O2, the negative electrode material is graphite, and the size is 130×68×13 mm. The cooling plates are placed on one side of the four parallel batteries. The size of the cooling plate is 130×52×6 mm, and the section size of the cooling channel is 4×4 mm. The section figure of the cooling channel is shown in Fig. 2. In addition, the length of the nail is l=107 mm, and diameter is φ=3 mm.

![Figure 1. The microchannel cooling model](image1)

![Figure 2. The section figure of the cooling channel](image2)
3. RESULT AND DISCUSSIONS

3.1. Thermal runaway in a single battery

In nail penetration process of battery, the cathode is connected to the anode. Due to the resistance of nail is small, only about a few milliohm, so in a short period of time, the nail in the battery becomes a huge production of heat, which makes the temperature of nail area increase fast. And the generated heat can quickly spread to the surrounding. When the temperature reaches a certain level, four side reactions will occur, which in turn makes the battery generate more heat. In the last, the temperature of battery will be out of control.

The temperature change of the battery within 300s after nail penetration is shown as Fig. 3. As can be seen from Fig. 3, thermal runaway happens in a short period of time. The temperature of the battery rises slowly before 30 s, and the heat comes from the short-circuit of the cathode and anode during the process of nail penetration, which generates a large amount of joule heat. After 30s, four side reactions of the battery are triggered and the temperature rises rapidly, reaching a maximum temperature of 620℃. Finally, the overall temperature of the battery starts to drop, because the battery materials has been constantly worn away.

![Figure 3. Temperature variation of battery](image)

The consumption of internal materials in the process of thermal runaway is shown in Fig. 4. It can be seen from Fig. 4 that the initial reaction of thermal runaway is the decomposition of the SEI. At about 30s, the curve describing the csei begins to decline. Losing the SEI’s protection, the anode’s active material begins to react with the electrolyte, with cn and z changing. Then the value of the state variable a, which represents the reaction between the cathode and the electrolyte, begins to increase, and the value of the state variable ce, which represents the decomposition reaction of the electrolyte, begins to decrease rapidly. At about 40s, the reaction rates of such state variables as cn, z, a and ce reach the maximum value, and the temperature of the battery rises the fastest.

![Figure 4. The change curve of the materials](image)
3.2. Thermal runaway propagation in some batteries

The structure of series and parallel group makes the performance and reliability of the battery group depend on the weakest and most unstable cell. Once thermal runaway occurs in a single battery, the huge energy released by the battery is likely to lead to thermal runaway propagation and eventually the complete failure of the entire power battery system, which seriously threatens the safety of the persons and electric vehicles.

The thermal runaway propagation of the battery module is shown in Fig. 5. The thermal propagation of the battery model within 400s is studied. The temperature curve in the Fig. 5 describes the average temperature of each battery. The temperature of battery-1 reaches the peak of 600℃ at 50s. During this period, a large amount of heat generated by battery-1 rapidly spreads to the surrounding areas, and part of the heat is transferred to battery-2 in the form of heat conduction, making the temperature of battery-2 rise at a rapid speed. At 90s, the temperature of battery-2 rises rapidly, with the highest temperature reaching 860℃. Meanwhile, the temperature of battery-1 increases slightly, which is caused by the heat generated by battery-2 transferring to battery-1. At about 125s, the temperature of battery-3 rises rapidly, with the highest temperature reaching 900℃. The reason why the peak temperature of battery-3 is higher than battery-2 is that battery-3 has been heated by battery-1 and battery-2. At the same time, the temperature of battery-2 also shows a small increase. Finally, at 175s, thermal runaway happens on battery-4, the highest temperature of which reaches 605℃. The reason why the temperature of battery-2 and battery-3 is higher than battery-1 and battery-4 might be battery-2 and battery-3 are in the middle of the module and have less contact with the outside environment. In addition, it can be seen from the Fig. 5 that the time interval of thermal runaway of battery-2 and battery-3 is shorter than that of battery-1 and battery-2 or battery-3 and battery-4. Therefore, the heat dissipation of the battery module is very important for the safety of the battery.

![Figure 5. Thermal runaway propagation](image_url)

3.3. The effect of micro-channel cooling system

Based on the results of thermal runaway propagation, the effect of micro-channel cooling on thermal runaway propagation is studied. Water is used to be coolant, and initial temperature is 25℃, and side cooling is adopted, and flow rate is 6×10⁻³ kg/s.

The temperature of batteries in thermal runaway propagation with micro-channel cooling system is shown in Fig. 6. As can be seen from the Fig. 6, battery-1 still suffers from thermal runaway during the process of nail penetration, but the remaining three batteries do not suffer from thermal runaway, and the maximum temperature also decreases in order, indicating that the designed micro-channel cooling system can prevent thermal runaway to some extent.

![Figure 6. The effect of micro-channel cooling system](image_url)
Figure 6. Thermal runaway propagation with micro-channel cooling system

4. CONCLUSION
In this paper, the thermal management system of power cell based on micro-channel cooling is studied by numerical simulation. The thermal runaway model of single battery and the thermal runaway propagation model of battery model are established successively to analyse the heat production of battery during the process of nail penetration. Then the influence of micro-channel cooling system on thermal runaway propagation is studied. The results show that, although the micro-channel system cannot prevent the thermal runaway of the first battery, it can prevent the thermal runaway of other batteries under the condition of flow rate of $6 \times 10^{-3}$ kg/s. Therefore, in the design of the battery module, the thermal runaway propagation can be prevented by improving the micro-channel cooling system or combining it with other cooling schemes.

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