Research on Key Technologies for Improving the Electro
catalytic Performance and Physical Properties of Lithium
Batteries in Electric Vehicles

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Abstract. Aiming at the uneven heat generation in various parts of the electric vehicle
lithium battery pack during the discharge process, the heat generation mechanism is
studied, and the lithium battery catalytic performance model is established to obtain the
current density and heat generation rate distribution law of the lithium battery cell on
the cell. The thermal model can simulate the thermal behavior of the battery under
application conditions. Study the laws of battery heat production, heat transfer, and heat
dissipation, and calculate the temperature changes inside and on the battery and the
temperature field information in real time to provide a basis for the design and
optimization of the battery and battery pack thermal management system. The
simulation results show that the established model can predict the heating distribution
and temperature field of the internal layered structure of the lithium-ion battery, which
is helpful for the subsequent analysis of key influencing factors.

Keywords: Lithium ion battery; electric vehicle thermal management; catalytic
performance; vehicle thermal management; safety

1. Introduction
Lithium-ion power batteries have the characteristics of high energy density and long cycle life, which
promote the rapid development of electric vehicles. However, safety issues such as fire and explosion
caued by battery thermal runaway still cannot be underestimated. It is very important to clarify the heat
generation mechanism of thermal runaway of lithium-ion batteries and explore the propagation
characteristics of thermal runaway in battery modules. Lithium-ion power battery is currently the power
source used in mainstream pure electric vehicles because of its high voltage platform, high-capacity
density, high specific power, many cycles, no memory effect, less self-discharge, and environmental
protection. Lithium-ion power batteries will generate a lot of heat due to electrochemical and physical
changes during use. If this heat cannot be monitored and controlled in real time to effectively dissipate
it, it will cause a large amount of heat between the battery cells [1]. Temperature difference, accelerated
generation of irreversible substances in the battery pack, thermal runaway, etc., reduce the service life
of the battery, and severely cause the battery pack to catch fire and explode, endangering the safety of
life and property. When the lithium-ion power battery is used under low temperature conditions, it will
cause a large reduction in charge and discharge capacity and an increase in internal resistance, which
will seriously affect the performance of the battery. Therefore, it is very necessary to analyze the thermal characteristics of the lithium-ion battery and the simulation analysis of the heat-generating temperature field and the heat-dissipating temperature field, and to effectively design the thermal management system of the lithium-ion power battery to make the lithium-ion power battery work in a suitable temperature range.

2. Model elaboration
Taking the 18650 cylindrical battery modules as the simulation research object, the positive electrode material is lithium manganate, the negative electrode material is graphite, the rated capacity is 2.5A·h, and the mass is 48g. The battery module has a 3×3 battery cell arrangement structure, and its exterior is a box, which simulates the heat transfer characteristics in a certain confined space, and its structure is shown in Figure 1. The batteries are sorted horizontally in order of No. 1-9 batteries [2]. If No. 1 battery is acupuncture, a local heat source $Q$ is given to simulate the Joule heat generated by the short circuit at the beginning of the thermal runaway, and then the No. 1 battery thermal runaway is simulated. When the No. 1 battery suffers from a thermal runaway, the temperature rises sharply, and the heat is mainly transferred to the surrounding battery cells through thermal conduction and thermal convection, which triggers the thermal runaway of other battery cells in the module to simulate the internal flow field of the battery module, The direction is from left to right, and the flow velocity is 0.1m/s. The initial temperature of the battery and the initial ambient temperature are both 25°C.

![Fig 1. Arrangement structure in battery module.](image)

2.1. Energy conservation equation
The energy conservation equation can be described as:

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot k \nabla T + Q$$

In the formula, $\rho$ is the battery material density, kg·m$^{-3}$; $c_p$ is the specific heat capacity of the battery material, J·kg$^{-1}$·K$^{-1}$; $T$ is the temperature, K; $t$ is the time, s; $k$ is the thermal conductivity, W·M$^{-1}$·K$^{-1}$; $Q$ is the heat generation rate per unit volume of each exothermic reaction inside the battery during use, W·m$^{-3}$. Table 1 summarizes the physical properties of battery materials, and Table 2 lists the volume fraction of each component in different areas of the battery.
Table 1. Physical properties of battery materials.

| Parameter | \( r \) (kg·m\(^{-3}\)) | \( c_p \) (J·kg\(^{-1}\)·K\(^{-1}\)) | \( k \) (W·m\(^{-1}\)·K\(^{-1}\)) |
|-----------|-----------------|-----------------|-----------------|
| Negative  |                 |                 |                 |
| Copper    | 8900            | 385             | 398             |
| Graphite  | 2660            | 1437.4          | 1.04            |
| Indirect. | 1750            | 1120            | 0.12            |
| Separator |                 |                 |                 |
| PP/PE/PP  | 492             | 1978            | 0.334           |
| Positive  |                 |                 |                 |
| Aluminum  | 1500            | 903             | 238             |
| LiCoO\(_2\) | 2500          | 700             | 1.48            |
| Indirect. | 1750            | 1120            | 0.12            |
| Electrolyte | LiPF\(_6\)/EC+DMC+EMC | 1290        | 133.9           | 0.45 |

Table 2. The volume fraction of each component in the electrode and diaphragm.

| Volume fraction |
|-----------------|
|                |
| Anode           |
| Electrolyte     | 0.3            |
| Graphite        | 0.64           |
| Indirect.       | 0.006          |
| Separator       |
| Electrolyte     | 0.42           |
| PP/PE/PP        | 0.58           |
| Cathode         |
| Electrolyte     | 0.35           |
| LiCoO\(_2\)     | 0.59           |
| Indirect.       | 0.06           |

The heat dissipation methods of lithium-ion batteries include convection heat exchange and radiation heat exchange. In this paper, different heat dissipation methods are equivalent to convection heat treatment, so the heat exchange boundary conditions are unified as follows:

\[
q_{\text{conv}} = h(T_{\text{surf}} - T_{\text{amb}})
\]  

(2)

In the formula, \( h \) is the equivalent heat transfer coefficient, and the convection heat transfer and radiation heat transfer on the outer surface of the battery are equivalent to convection heat transfer; \( q_{\text{conv}} \) is the heat dissipation per unit area, W·m\(^{-2}\); \( T_{\text{surf}} \) is the temperature of the outer surface of the battery, K; \( T_{\text{amb}} \) is the temperature of the electric vehicle.

Due to the symmetry of the lithium-ion battery structure, this paper takes half of the battery as the research object. As shown in Figure 2, the left side of the model is the symmetry plane. In addition, considering the difference in the arrangement of the actual battery tabs, the calculation models are divided into three categories, as shown in Figure 2, where Figure 2(a) shows the symmetrical arrangement of the positive and negative tabs, and the upper surface is the positive tab. Figure 2(b) shows that the positive and negative pole tabs are arranged on the upper surface of the battery, and the positive pole tab is arranged in the middle; Figure 2(c) shows that the positive and negative pole tabs are symmetrically arranged on the upper surface of the battery [3]. In the calculation model of this paper, the convective heat transfer part is the outer surface of the right side of the battery and the positive and negative electrode tabs (width 10mm). All other outer surfaces are considered as adiabatic boundaries.
2.2. Thermal use reaction model
Regardless of the combustion reaction, during the thermal use of lithium-ion battery electric vehicles, possible exothermic reactions include solid-liquid membrane decomposition reaction, negative electrode material reaction with electrolyte, positive electrode material reaction with electrolyte, and electrolyte decomposition reaction. \( Q \) in formula (1) is calculated by the following formula:

\[
Q = \sum_i H_i W_i R_i
\]  

(3)

In the formula, \( H_i \) is the unit heat release of different exothermic reactions inside the battery during use, \( J \cdot kg^{-1} \); \( W_i \) is the carbon content of different areas inside the battery, \( kg \cdot m^{-3} \); \( R_i \) is the reaction rate of different exothermic reactions, \( s^{-1} \). The decomposition reaction of the solid-liquid membrane (SEI) occurs at the negative electrode, and the reaction temperature is in the range of 90–20°C, and the reaction rate:

\[
\frac{dc_{sei}}{dt} = -R_{sei} = -A_{sei} \exp \left[ -\frac{E_{a, sei}}{RT} \right] c_{sei}^{n_{sei}}
\]  

(4)

When the temperature is higher than 120°C, the lithium embedded in the negative electrode graphite material and the electrolyte directly undergo an exothermic reaction, and the reaction rate:

\[
\frac{dc_{neg}}{dt} = -R_{ne} = -A_{ne} \exp \left[ -\frac{t_{sei}}{t_{sei0}} \right] \exp \left[ -\frac{E_{a, ne}}{RT} \right]
\]  

(5)

Among them,

\[
\frac{dt_{sei}}{dt} = R_{ne}
\]  

(6)

When the temperature is higher than 170°C, the reaction rate of the positive electrode material and the electrolyte:
When the temperature is higher than 200°C, the decomposition reaction of the electrolyte may occur in the positive and negative electrodes and the isolation membrane area, and the reaction rate:

\[
\frac{d\alpha}{dt} = R_{pe} = A_{pe} \alpha^{m_{pe}-1} (1 - \alpha)^{n_{pe}-1} \exp \left[-\frac{E_{a,pe}}{RT}\right]
\]  

When the temperature is higher than 200°C, the decomposition reaction of the electrolyte may occur in the positive and negative electrodes and the isolation membrane area, and the reaction rate:

\[
\frac{dc_e}{dt} = -R_e = -A_e \exp \left[-\frac{E_{a,e}}{RT}\right] c_{e, m_{e}}
\]

3. System simulation model

3.1. Analysis of temperature characteristics

3.1.1. Analysis of overall temperature rise characteristics. Lithium-ion battery discharge is a typical transient heat conduction process with a sometimes-varying internal heat source. Figure 3 shows the variation of the average temperature of each layer of a lithium-ion battery with discharge time. Figure 3 shows that as the discharge process progresses, the average temperature of the battery rises. However, the average battery temperature rise is not strictly linear [4]. This is because the increase in battery temperature will affect the change in heat generation, making it non-linear. In addition, the average temperature at the tabs of the positive and negative poles is slightly higher, and the average temperature of the other layers changes basically the same over time.

![Fig 3. The average temperature of each layer of a single cell varies with discharge time.](image)

3.1.2. Analysis of temperature non-uniformity. Figure 4 shows the variation of the difference between the maximum temperature and the minimum temperature of a single lithium-ion battery with discharge time. Figure 4 shows that the maximum temperature difference increases with the discharge process, and the temperature difference reaches the maximum at the end of the discharge. However, the maximum temperature difference is only about 0.3°C, indicating that the overall battery temperature is relatively uniform under the simulated operating conditions.
Fig 4. The temperature difference of a single cell changes with the discharge time.

3.2. The process of thermal runaway of single cell

220°C (the temperature at which the diaphragm collapses, and the thermal runaway can no longer be prevented) is used as the criterion for the thermal runaway to be triggered. Figure 5 shows the heat release of each part of the material under the thermal runaway of a single cell [5]. The analysis revealed that it only took about 30 seconds for the single battery cell to accelerate the release of heat to the end of the heat release of the material itself, that is, from the beginning to the end of thermal runaway, the characteristics of the rise in battery temperature can be analyzed from the perspective of heat.

Fig 5. The heat release curve of each material when the heat is out of control.

It can be seen from Fig. 5 that, firstly, the decomposition reaction of SEI begins in the 8th second, and the battery temperature rises sharply at about 200°C (related to the nature of the material itself). This is because the SEI film is in a meta-stable state and is very sensitive to temperature. The decomposition reaction occurs at a temperature of about 100°C, releasing heat, and at the same time, the negative electrode is in direct contact with the electrolyte. Secondly, around the 11th second, the
reaction between the positive electrode material and the electrolyte, the reaction between the negative electrode material and the electrolyte, and the decomposition reaction of the electrolyte are also activated in sequence, and the peak heat release reaches the order of tens of millions of watts, which in turn causes a step in the battery temperature. The rise of thermal runaway occurs.

3.3. Analysis of battery heat generation
At a low discharge rate, the total heating power $q$ changes with the change of the reversible heating power $q_r$. Under the $0.01C$ discharge rate in Fig. 6, this change is more obvious, and the reversible heat and total heating power curves almost coincide. This is because at low discharge rates, the reversible thermal power accounts for a larger proportion, and the fluctuations in the middle and late stages of the discharge are larger, while the irreversible thermal power and ohmic thermal power change smoothly and account for a small proportion. At a discharge rate of $0.01C$, the reversible heating power accounts for 87% of the total. At a high discharge rate, the total heating power $q$ varies with the liquid phase ohmic heating power $q_{je}$ and irreversible heating power $q_i$. Because at a high discharge rate, the liquid phase ohmic heating power and irreversible heating power increase with the depth of discharge, and the magnitude of the decrease gradually increases, and their proportion to the total amount gradually increases. At a discharge rate of $5C$, the liquid phase ohmic heating power and irreversible heating power account for 55% and 22% of the total, respectively, while the reversible heating power is only 12%.

![Fig 6. Changes of total heat generation power per unit volume and heat generation power of each part under different discharge rates.](image)

4. Conclusion
By studying the heat generation mechanism of the battery, the catalytic performance model of the battery was established, and then the heat generation law of the battery was obtained. It was found that the heat generation rate near the positive and negative ears was greater than other parts, and the heat generation rate near the positive electrode was the highest. Based on the heat generation law and the thermophysical parameters of the battery module, a battery water cooling and heating management system is designed, and the calculation method of the water flow rate of the cooling system is given; the simulation results of battery modules with different thicknesses of heat conducting plates are compared and the heat conduction is found. When the thickness of the plate is 0.5mm, the overall cooling effect of the battery module is the best.
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