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Electrochemical Performance of Lithium Ion Batteries for Electric Vehicles

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To study the electrochemical performance of lithium ion battery for electric vehicles, this paper uses numerical simulation method combined with experimental data, to make a simulation study of one-dimensional voltage features, electrolyte concentration distribution and current density distribution of the lithium battery. The results show that the electrochemical performance of lithium ion battery for electric vehicle affects the stability of the lithium ion battery, and is closely related to the life of lithium ion battery. At last, it is concluded that the obtained data and conclusions have strong theoretical significance and guiding value for engineering application of lithium batteries.

1. Introduction

Energy and environment are two major challenges that the development of human civilization in the new century faces. The adoption of new technology to reduce vehicle emissions and energy consumption has become an important direction of the development of automobile technology (Candace et al., 2007, Yamada et al., 2001). And electric vehicles have achieved zero emissions of pavement and low energy consumption, which has become one of the most attractive solutions of energy saving and emission reduction work (Croce et al., 2001; Béatrice et al., 2004; Nian et al., 2014).
Lithium ion battery is the source of electric vehicle power, with the advantages of recyclable charge, compact structure and light weight (Boulet-Roblin et la., 2016; Huang, et al., 1995; Liang, et la., 2009; Marom et al., 2011). At present, the main research on methods used in power lithium-ion batteries at home and abroad mainly applies simulation research and experimental research (Szczech and Song, 2010; Reddy et al., 2010; Kim and Cho, 2008; Armstrong et al., 2006; Johnson et al., 2016; Fisher et al., 2008). For the simulation of lithium ion batteries, the relevant information of the micro level of electrode materials can be obtained firstly (Kim and Cho, 2008; Liu et al., 2014), and the different electrode materials are compared and analyzed by means of simulation, so as to reduce the development cost of electrode materials matching and the test cycle of materials (Hassoun et al., 2008). Secondly, the relevant data and rules which cannot be involved in the experimental research can be obtained, which can guide the design of lithium ion batteries and the matching of the whole vehicle (Luo et al., 2013). Thirdly, the simulation of lithium ion battery can further deepen the understanding of the cause and process of lithium ion battery heat production and heat dissipation, and provide reference for improving the safety of lithium ion battery (Hwang et al., 2011). Based on the battery thermal model established by the domestic and foreign scholars, we make full use of the test results to explore the electrochemical performance of lithium ion batteries for electric vehicles. The data and conclusions obtained have strong theoretical significance and engineering application guiding value for the research of lithium battery.

2. One dimensional simulation of lithium ion battery

The main reactions in lithium ion batteries are positive electrode transport, negative electrode transport and electrolyte transport. With the movement of lithium ions, the lithium ion battery is in accordance with the law of conservation of mass, charge conservation law, Fick's diffusion law and so on. When the Newman model is used for simulation, the following assumptions are made:

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Positive and negative electrode materials are spherical particles, and internal particle diffusion transport is in line with Fick's diffusion law;

The spherical particles in the positive and negative electrodes belong to the spatial uniform distribution; The concentration change and distribution of electrolyte accord with dilute solution theory;

Neglect the convection and radiation heat transfer inside the battery, but consider the heat conduction; The diffusion coefficient of lithium ion in solid phase and liquid phase does not change with the temperature; The current density will not affect the concentration of electrolyte;

In the one-dimensional simulation, the discharge time of the battery is set to 2000s, and the charging time is 2000s.

3. One dimensional calculation results and analysis of lithium ion battery

The lithium ion battery, in the set boundary conditions and initial conditions, is conducted with non steady state calculation. After procedure debugging, the final iteration is performed until the convergence. Then, we can obtain the voltage characteristic changes, electrolyte concentration distribution in the charging and discharging process of circulating charging and discharging lithium ion battery.

3.1 Variation of voltage characteristics

The voltage characteristics of the lithium-ion battery directly affect the vehicle electrical design and vehicle power parameters matching. In the normal use of lithium batteries, the discharge should pay attention to the following two points:

The voltage loss at different time steps in the discharge process is shown in figure 1. The time steps are set to t=500s, t=1000s, t=1500s and t=2000s respectively. Along the length of the one-dimensional model (from positive to negative), the voltage shows a downward trend. Due to the change of Li ion migration rate and electrolyte concentration in the battery, the voltage loss extent is not the same, as shown in the gradient of 1~3 marked in figure 1. With the increase of time steps, the discharge speed is accelerated, and the voltage loss of the battery is greater. According to the relevant experimental results, the larger the discharge current is, the smaller the discharge capacity is and the faster the voltage drops. The voltage loss trend in the discharging process in the simulation is consistent with the daily use of lithium batteries and test.

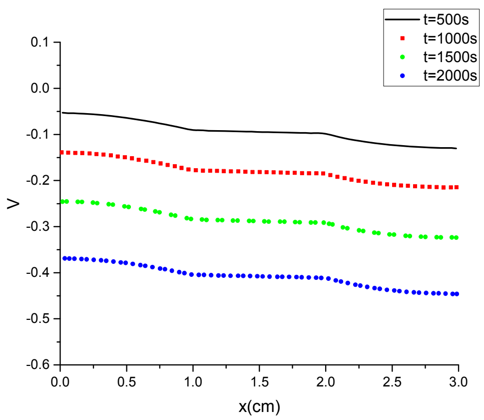

Figure 1: Voltage loss of battery in discharge process

3.2 Distribution trend of electrolyte concentration

The time steps are set to t=500s, t=1000s, t=1500s and t=2000s respectively. The overall change trend of the electrolyte concentration in the discharge process is shown in figure 2. In figure 2, the information is displayed on the cathode area, electrolyte area and anode area. The electrolyte concentration is gradually decreased, and the decrease trend is because, in the discharge process of Li ions, it moves from the cathode through the electrolyte to the cathode region, and the transport process leads to a decline in the concentration of electrolyte. In the electrolyte region, the trend of concentration decreases linearly, while in the positive and negative regions, it shows the curve change. This trend difference is because, in the electrochemical discharge process, the solution with the electrolyte area is consistent with the physical properties of dilute solution. With the migration of Li ions, dilute solution concentration decline curve is a straight line. Compared with the negative resistance region, the resistance (thermal) in the electrolyte region is much smaller, which is conductive for Li ions to rapidly migrate and move from the anode to the cathode, and thus it completes the discharging process. The change trend of electrolyte concentration in positive region, electrolyte region and negative electrode region during lithium ion discharge is shown in figure 3, figure 4 and figure 5. Although the region showed a downward trend, the decline that each time step corresponds to is not the same. With the increase of the concentration of time step, the concentration decline of each region has increased. The law of decline is in accordance with the slow firstly and rapid later in the actual discharging process.

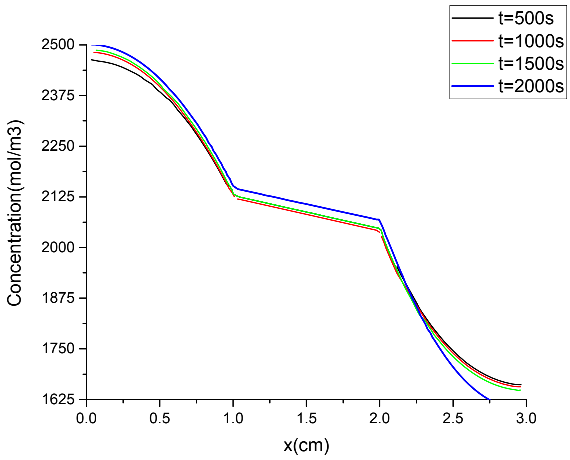

Figure 2: Variation trend distribution of electrolyte concentration in discharge process

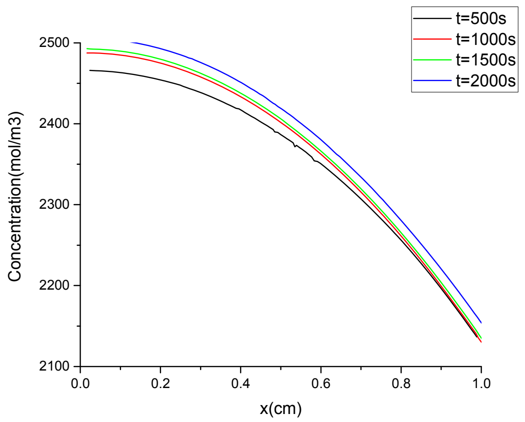

Figure 3: Concentration distribution of positive electrolyte in discharging process

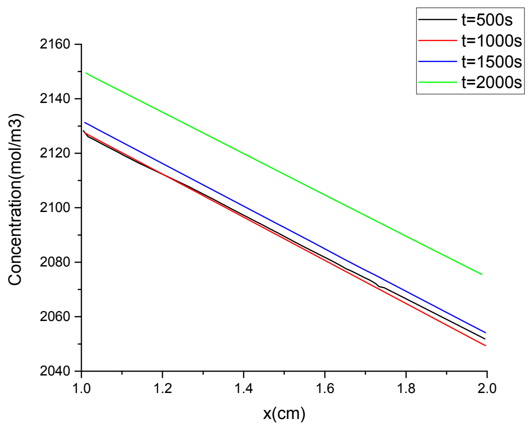

Figure 4: Distribution of electrolyte concentration in discharging process

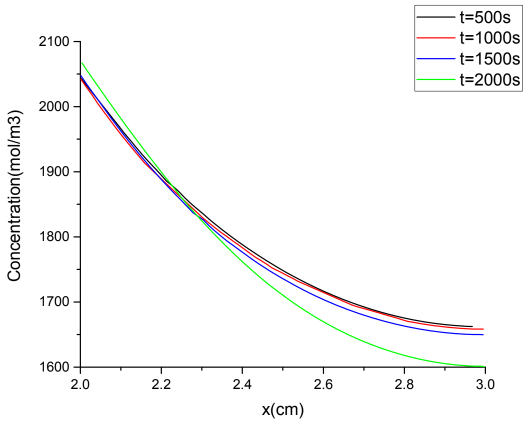

Figure 5: Concentration distribution of negative electrolyte in discharging process

The battery voltage characteristics is closely related with the distribution of the electrolyte. When the time step is in t=2000s~t=3000s charging, Ohmic losses occurred, and the voltage trend fluctuations. When the time step has reached the peak voltage at t=3000s~t=4000s, t=5000s~t=6000s reached a stable voltage after charging. The change of the concentration in figure 6 also conforms to the trend of voltage variation, and the electrolyte concentration increases gradually with the migration of ions during the charging process when the charge reaches the peak value of the voltage. This is due to the change of Ohmic internal resistance, and the related research data show that the heating capacity is much greater than the heating capacity during the discharging process. During the discharging process, the whole lithium ion battery will continue to heat, and the corresponding effective internal resistance will become larger.

From the distribution of positive electrolyte concentration in figure 7 in the process of charging, the increasing and following feature of electrolyte concentration is good in the time step of t=3000s and t=4000s. In the two time steps region, the electrolyte concentration distribution is more uniform than the time step in the t=5000s and t=6000s. In the time step region, the Ohmic effect is obvious, the electrolyte concentration has been gradually transited from the lowest concentration value in the discharging process to a constant value, and achieved slight balance in the change of direction from negative to positive electrode. In fact, the diffusion rate of products and reactants in the electrochemical process is far less than the rate of a chemical reaction, resulting in electrolyte solution concentration changes. The uneven distribution phenomenon of electrolyte concentration is known as concentration polarization. In the electrolyte region, there is a certain number of active substances, and the corresponding pores in the charging process also gradually expand, and the porosity increases. With the operation of charging, it is gradually close to the electrochemical reaction end point, namely the peak voltage charging curve. The porosity of active material is one of the reasons result in the change of electrolyte concentration.

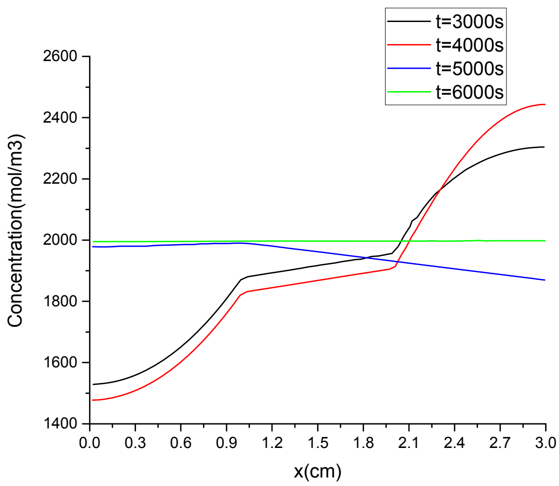

Figure 6: Distribution trend of whole electrolyte concentration in charging process

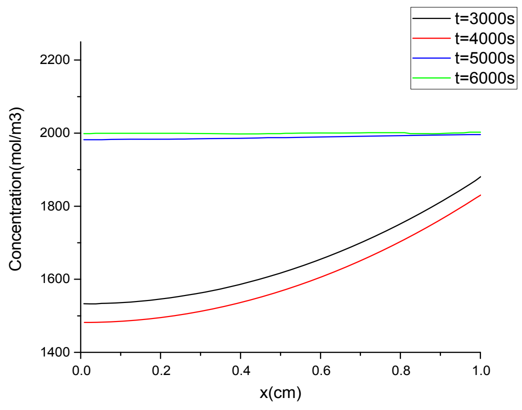

Figure 7: Concentration distribution of positive electrolyte in charging process

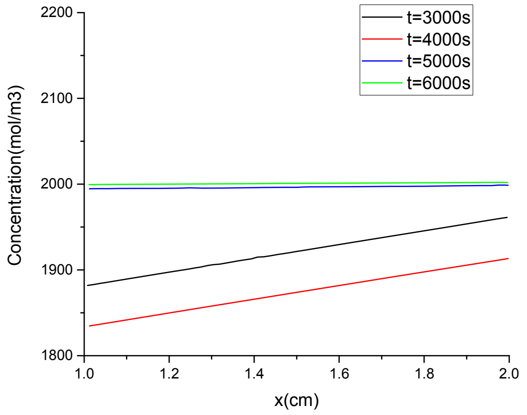

Figure 8: Concentration distribution of electrolyte in charging process

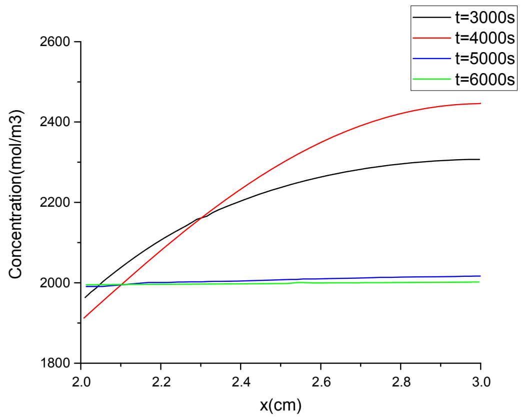

Figure 9: Concentration distribution of negative electrolyte in charging process

4. Conclusions

In the discharging process, the battery voltage drop meets the application trend of slow first and rapid later, and completes the discharge process. When the discharge process is finished, the battery is charged. Because of the Ohmic loss and the change of the concentration release of the electrolyte, the charging voltage will be stable at the set operating voltage after reaching the peak voltage, and the charging characteristic law is consistent with the actual charging process. With the increase of discharge time, the electrolyte concentration of anode region, electrolyte region and cathode region is gradually decreased. The decrease trend is because, in the discharging process of Li ions, it migrates from the cathode through the electrolyte to the cathode, and the transport process leads to a decline in the concentration of electrolyte. The change of electrolyte concentration during charging is closely related to the distribution of battery voltage characteristics. The tendency of the change of current density in discharge process is poor, which is caused by the change of charging current, Ohmic thermal resistance and active material and other factors. The conclusion of this study is that the electrochemical characteristics of lithium batteries, including voltage fluctuations, electrolyte concentration trends and current density distribution, are closely related to the stability and application life of lithium batteries.

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