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# Electrochemical-Thermal Simulation of Cell Lithium-Ion Battery of Electrical Vehicle

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## 1. Introduction

Full Electric Vehicles (FEVs) will replace Internal Combustion Engine Vehicles (ICEVs) in the future. Batteries are the energy supply units that act as the driving forces of these electric vehicles. Among rechargeable batteries, lithium-ion batteries are more preferable in electronic devices due to high energy density (almost two times the nickel-cadmium battery), lighter weight, less volume (almost 3 to 5 times other batteries), fast charging capability, low self-discharge rate (less than 10% per month), and high durability (more than 500 cycles). Lithium-ion batteries work based on the movement of lithium-ion between positive and negative electrodes. The cell of these battery consist of a positive current collector, a negative current collector, a positive electrode, a negative electrode, a separator, and an electrolyte solution that fills the space between two electrodes. In the discharging cycle, lithium ions move from the negative electrode to the positive electrode and do the opposite in the charging cycle. This process generates heat and electric current. The challenges of using lithium-ion batteries include increasing efficiency, safety, and durability. Hence, an accurate Battery Management System (BMS) is required for the battery to function properly.

In this article, a single prismatic lithium-ion battery cell is simulated during the discharge cycle at different rates using the electrochemical-thermal method. The simulations are performed in AVL FIRE software using 3D computational fluid dynamics. Using a single cell reduces computation time as well as simplicity in changing battery parameters, which can eventually be extended to a lithium-ion battery stack. The innovation of this study is the use of the electrochemical-thermal method which by considering the electrochemical reactions between the electrodes and the electrolyte and also by simultaneously solving the electrical, chemical and thermal equations, makes the simulations much more accurate than most previous studies. Since the electrochemical-thermal method requires a large number of input parameters and also has a very high computation time, this method has been used less inn previous studies. Another innovation of this study is calculating the features of lithium batteries like State of Charge (SOC), which can be calculated directly at any time by solving equations. In other researches, SOC estimation methods like Kalman filter method that has a relatively high cost and computational error have often been used.

## 2. Battery Specifications

In this research, a single cell of ePLB C020 lithium-ion polymer prismatic battery is used to simulate the lithium-ion battery. The above-mentioned battery is made by EiG Corporation from South Korea with a nominal and a maximum capacity of 20Ah and 21Ah, respectively. Each stack of this battery contains 34 individual cells, which are connected in parallel. The positive electrode is made of Lithium Nickel Manganese Cobalt Oxide ( $\mathrm{Li[NiMnCo]O_2}$ ), the negative electrode is made of graphite, the positive current collector is made of aluminum, and the negative current collector is made of copper. The type of electrolyte used in the battery is lithium hexa fluoro phosphate ( $\mathrm{LiPF_6}$ ), which is a combination of ethylene carbonate and dimethyl carbonate.

## 3. Validation of Simulation Results

To validate the results of the electrochemical-thermal simulations, the voltage vs. capacity curve of simulation and experimental data are compared to each other. The voltage vs. capacity curve is shown in Figure 1 at constant current discharge rates of 1C, 2C, 3C, and 5C. As can be observed, a good agreement is obtained between experimental and numerical simulation results. The maximum error values are compared to the experimental results at rates of 1C, 2C, 3C, and 5C are 1.22%, 1.37%, 1.49%, and 1.65%, respectively.

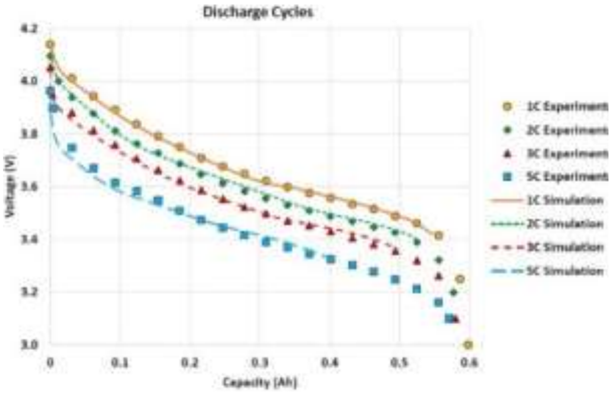

**Figure 1. Voltage variations vs. capacity of battery at different discharge rates in simulation (lines) and experiment (symbols)**

For further validation of the simulations, the variations in average battery surface temperature are calculated in terms of battery capacity during the discharging cycle. These results are then compared to experimental results. Figure 2 shows the mentioned diagram, which is in good agreement with the experimental results.

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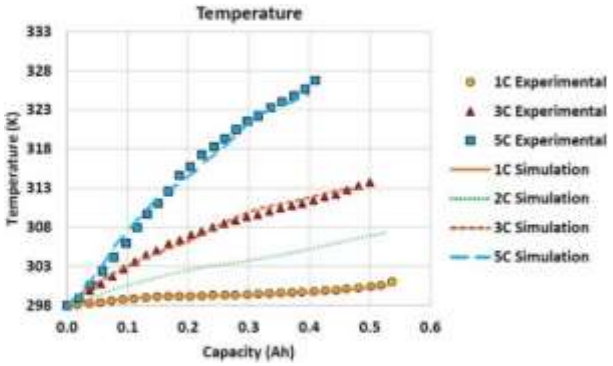

**Figure 2. variations of average battery surface temperature vs. capacity at different discharge rates in simulation (lines) and experiment (symbols)**

## 4. Discussion

After validating the simulation results, other features of the battery are determined. The results of 3D electrochemical-thermal simulation of a single ePLB C020 lithium-ion battery cell are obtained using computational fluid dynamics at constant current discharge rates of 1C, 3C, and 5C. One of the most important results is the SOC of battery. Figure 3 shows the SOC of a single lithium-ion battery cell in a constant current discharge cycle. As can be seen, the SOC started to decrease from the initial value of 1 (100%) with an almost constant slope at all three discharge rates of 1C, 3C, and 5C. It is also observed that at a certain capacity, a lower SOC can be obtained by reducing the discharge rate. At discharge rates of 1C, 3C, and 5C, the battery SOC is reduced to the values of 0.176, 0.325, and 0.528, respectively.

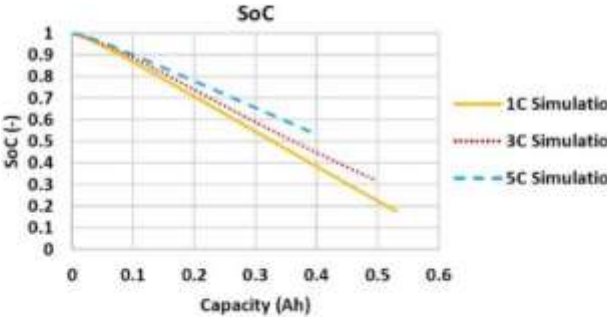

**Figure 3. Battery SOC vs. capacity at different discharge rates**

Variations in lithium-ion concentration at different discharge rates in the positive electrode of the lithium-ion battery are presented in Figure 4. As can be seen, when the discharge cycle begins, lithium-ions move from the negative electrode to the positive electrode, and the lithium-ion concentration in the positive electrode increases with an almost constant slope.

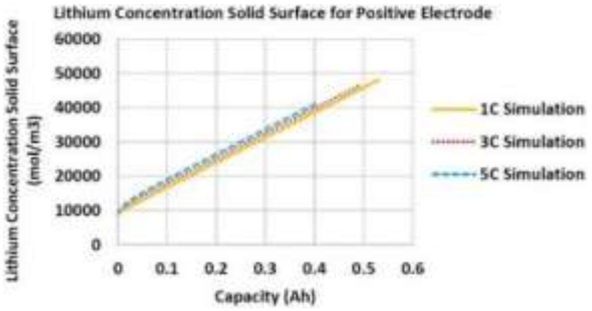

**Figure 4. Variations of Li-ion concentration in the positive electrode vs. battery capacity at different discharge rates**

## 5. Conclusion

In this article, the 3D numerical simulation of a single prismatic lithium-ion battery cell is performed by the electrochemical-thermal method. Using a single cell reduces computation time as well as simplicity in changing battery parameters, which can eventually be extended to a lithium-ion battery stack. In this research, electrochemical-thermal method was used by considering electrochemical reactions between electrodes and electrolyte. The electrochemical-thermal method increases the accuracy of the results by solving the electrical, chemical, and thermal equations simultaneously, and can calculate parameters such as SOC accurately at each moment. In the simulations, three constant current discharge cycles was performed at 1C, 3C and 5C rates. A good agreement is obtained between experimental and numerical simulation results at all three discharge rates. Finally, the parameters of lithium-ion battery such as SOC, electrical potential distribution in current collector, lithium-ion concentration in the positive electrode, average temperature distribution at battery surface, and heat generation during discharge cycle are determined at different rates.