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Conference Paper

Oral Presentation

Investigation of Thermal Behavior of Lithium Ion Batteries under Different Loads

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Abstract

Electric Vehicles (EV) has become very important for decade because of they reduce the threat of energy crisis and environmental pollution. But electric vehicles should still need to improve battery technologies. Lithium ion batteries are preferred in EVs due to their high energy and power density, long life and environmentally friendly properties compared to other batteries used. However, the low range problem of electric vehicles has become one of the negative features of these batteries as well as all these advantages. One of the ways to overcome this problem and improve its performance is to keep the lithium ion batteries in the specified temperature range. When these batteries go out of the specified operating range for high performance and safety, they are subject to thermal degradation and loss of capacity.

One of the reasons that cause performance degradation; the irregular distribution of heat accumulated in the battery. In lithium ion batteries, the heat generated as a result of chemical reactions during charge / discharge spreads faster than the inner surface of the battery on the outer surface of the battery. These differences lead to irregular distribution of heat and cause the battery to lose capacity. In addition to the temperature difference due to the position of the batteries in the package, the irregular distribution in a single cell shortens the life of the battery and adversely affect its performance. Therefore; In order to keep the temperature in the operating range, to prevent irregular temperature distribution and to increase the life and safety of the battery, the battery thermal management system (BTMS) is very important.

In this study, the thermal behavior and performance of pouch type Lithium-ion batteries which are used in hybrid electric vehicles (HEV) and EVs has been investigated at different discharge rates based on numerical simulations. Numerical simulation was performed through a traditional software package using the dual potential multidimensional multi-dimensional (MSMD) battery model to analyze the cell discharge behavior and investigate its thermal performance. When the battery load is increased, irregular thermal distribution and temperature rise has been observed. It has been seen that the model is accurate to be used in battery thermal management systems to ensure homogeneous thermal distribution of batteries.

Keywords: Electric vehicles, pouch type lithium ion battery, battery modelling, battery thermal management system, heat distribution

1. INTRODUCTION

Motor vehicles which are increasing in proportion to the world population and become an indispensable part of our lives for transportation cause environmental pollution by using fossil fuels. Gases of gasoline and diesel fuel vehicles released into the atmosphere; 65% have carbon monoxide, 55% has nitrogen oxide and 45% has hydrocarbon [1]. The fact that thousands of vehicles emit these toxic gases every day not only confront us with the fact of environmental pollution, but also threatens our health. On the other hand, with the limited amount of fossil fuel sources and mainly due to greenhouse gases, the problems are accepted by everyone. With more attention to renewable energy, scientists have developed environmentally friendly tools such as Electric Vehicle, Hybrid Electric Vehicles, to alleviate this problem and to control the amount of toxic gas emitted [2]. The lead-acid and nickel-cadmium batteries used in these vehicles have not been effective until today due to the long charging time, low range problem, high battery prices and lack of charging stations. But; Lithium ion batteries (LIB) which perform better than others today are used [3]. With the development of technology, portable electronic devices that enter our lives and make our lives easier, need a source of energy to work in a long and effective way. This energy source; reliable, long-lasting, easy to maintain, can be char-

ged in a short time and high-energy source lithium-ion batteries are encountered. Lithium ion batteries are known as rechargeable secondary batteries. The long shelf life, wide operating range, high power discharge capacity, lack of memory effect help the lithium-ion battery move higher among other batteries, but more preferable in the production of electric vehicles [4]. The most important disadvantage of these batteries is that they produce a lot of heat due to ohmic and entropic reactions during charge / discharge [5]. This increase in temperature during charging / discharging of HEVs and EVs can result in thermal leaks, explosions and injury to persons when they become irreparable and unstoppable [6].

The operating temperature range for Li-ion batteries is between -20 ° C and 60 ° C and the desired temperature range is between 15 ° C and 35 ° C to achieve high performance. [7]. Temperatures outside the desired range cause significant capacity loss. For this reason, an effective Battery Temperature Management System is required to distribute the heat generated in the battery pack. In addition to the irregular temperature distribution between cells, the temperature imbalance within a cell is also an important source of problem. Since a large proportion of electrochemical reactions occur at the electrodes, the rate of heat generation is not the same in different locations within a Li-ion cell. A LiCoO2 positive electrode is reported to produce up to four times the heat of the entire battery [8]. Therefore, the temperature increase is not correct within the cell. This can result in the deterioration of the battery caused by local distortion, which has a negative impact on the performance of the entire cell. That's why, understanding the thermal behavior of the Li-ion battery and its thermal performance during discharge is becoming even more important.

Many studies have been performed based on the modelling of lithium ion batteries. Chen and Evans developed two-and three-dimensional models and observed the thermal behaviour of the LIBS. They assumed that the heat generation rate was not altered throughout the cell [9-11]. Pals and Newman presented a one-dimensional model for a cell of lithium polymer batteries (LPBs) and predicted its thermal behavior [12].Verbrugge modeled three-dimensional flow and temperature distributions in LPB modules [13]. Botte et al. Used a mathematical model involving the carbon anode decomposition reaction to estimate the thermal behavior of LIBs under medium to high rate discharge conditions [14]. The simplified one-dimensional thermal modelling was presented by Al-Hallaj and others to observe the temperature distribution within the LIB cells. [15]. The electrochemical-thermal model for LPBs by combining a two-dimensional thermal model and a one-dimensional electrochemical model was developed by Song and Evans [16]. Gu et al. Developed a two-dimensional thermal and electrochemical model to analyze the thermal behavior of LIB cells [17-18]. A three-dimensional LIB model with convection and radiation-related boundaries was developed by Chen and his friends to examine different heat distribution performances

on all surfaces [5]. Two-dimensional thermal modeling based on potential and current density distributions was presented by Kwon et al. [19-20].

In this study, the model of pouch type lithium ion battery was formed and its thermal behaviors at discharge rates of 0.5C, 1C, 2C and 3C were analyzed. It has been observed that the obtained model can be used in the design of a cooling system to eliminate non-uniform heat dissipation.

2. MATHEMATICAL MODEL

In a lithium-ion battery, the anode and cathode are made of active materials coated on the surface of the metal foils. A polymer separator is placed between the opposite polar foils to prevent the electrons from passing through them. Two models are used to estimate the development of chemical, thermal and electrical processes in a battery: 1) Single Potential Empirical Battery Model 2) Dual Potential Multi-Scale Multi-Domain (MSMD) Battery Model. The Single Potential Empirical Battery Model is useful if the geometry of the current collector, electrodes and separator is fully resolved. This model is best suited for electrode scale estimates in a single battery cell. However, the model is limited in battery systems, in particular to study all electrochemical events in complex geometry systems. Even for a single battery cell it would be very expensive to solve all layers clearly. In addition, many industrial applications use a battery pack consisting of a plurality of cells connected in series or parallel. (MSMD) battery model exceeds these limitations using a homogeneous model based on a multi-scale multi-dimensional approach. In this approach, the whole battery is considered as an orthotropic continuum; therefore, the network is no longer limited by the microstructure of the battery. To suit various analysis requirements, there are three electrochemical sub-models in the model, 1) Newman, Tiedemann, Gu, and Kim (NTGK) empirical model, 2) Equivalent Circuit Model (ECM) and 3) Newman alts Pseudo 2D (P2D) model complexity level. The models offer the flexibility of examining physical and electrochemical phenomena emitted to various length scales in battery systems of various embodiments [21].

In This study, the reason for selecting the NTGK model is that it is simpler to calculate because it requires a minimum number of model parameters [21]. This has been shown to be an advantage when supplying the battery, due to the difficulty of obtaining technical information. At the same time, the NTGK model is semi-experimental and requires battery discharge performance data to determine the polynomial coefficients of its parameters.

The internal structure of the pouch type battery consists of multiple positive and negative electrode layers, separators, positive and negative electrode current collectors and solid-state polymer electrolyte, which are made separately with the same shapes and structures. The outer layer of the battery cell is covered with aluminum plastic composite film. A porous separator is arranged between the positive
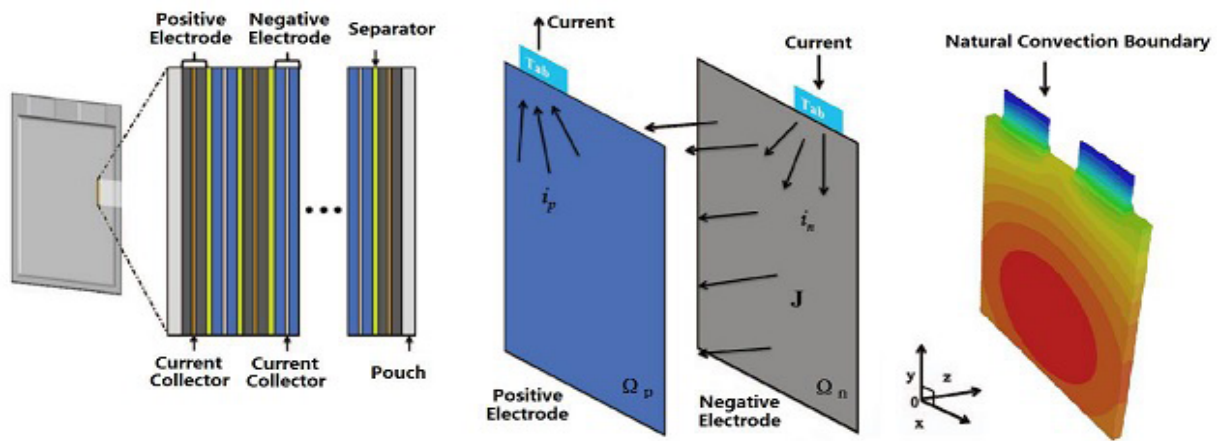
Figure 1: Schematic diagram of the modeling procedure of the pouch type battery cell a) Battery cell assembly b) 2D model c) 3D model [22]

and negative electrodes as shown in Figure 1 (a). Although the internal shape of the battery cell has a 3D structure, the discharge flow of the currents of each pair of electrodes appears as a 2D sandwich structure. It is time consuming to construct a mathematical model of the repeating electrical field, so the entire battery cell is simplified by generating only one pair of positive and negative electrodes, as shown in Figure 1 (b) [22]. In addition, the electric field parameters were obtained by the load protection equation. Finally, using a Computational Fluid Dynamics (CFD) method, the 3D mathematical model of the temperature field was obtained by combining the electric and temperature areas as shown in Figure 1 (c).

2.1 NTGK Model

The Newman, Tiedemann, Gu and Kim (NTGK) model is a simple empirical electrochemical model proposed by Kwon. In the model formulation, the volumetric flow transfer rate in Equation 1 relates to the potential field by the following algebraic equation:

$$j_{ECh} = aY[U - (\varphi_+ - \varphi_-)] \tag{1}$$

Where, a: represents the specific area of the electrode plate, the phase potentials for the and ϕ_- positive and negative electrodes represent the volumetric flow. U and Y are model parameters that show the functions of the discharge depth (DoD):

$$DoD = \frac{Vol}{3600 Q_{Ah}} \left(\int_0^t j dt \right) \tag{2}$$

Vol, battery volume and Q_{Ah} is total electrical capacity.

For a given battery, the voltage current response curve can be obtained by experimentation and then determined by the curve fitting the data. Kwon has adopted the following formulation for the proposed functions in [23]:

$$Y = \left(\sum_5^{n=0} a_n (DoD)^n \right) \exp\left[-C_1 \left(\frac{1}{T} - \frac{1}{T_{ref}} \right) \right]$$

$$U = \left(\sum^{n=0} b_n (DoD)^n \right) - C_2(T - T_{ref}) \tag{3}$$

Where, C_1 and C_2 are NTGK model's specific parameters.

The electrochemical reaction temperature is as follows;

$$\dot{q}_{ECh} = j_{ECh} \left[U - (\varphi_+ - \varphi_-) - T \frac{dU}{dT} \right] \tag{4}$$

The first term here is heat from over-voltage; the second term is heat from entropic heat.

2.2 Model Parameters

The dimensions of the 14.6 Ah LiMn2O4 LIB which are modeled in the package software program and the mesh size of this 3D geometry designed to be 0.005 m are shown in Figure 2.
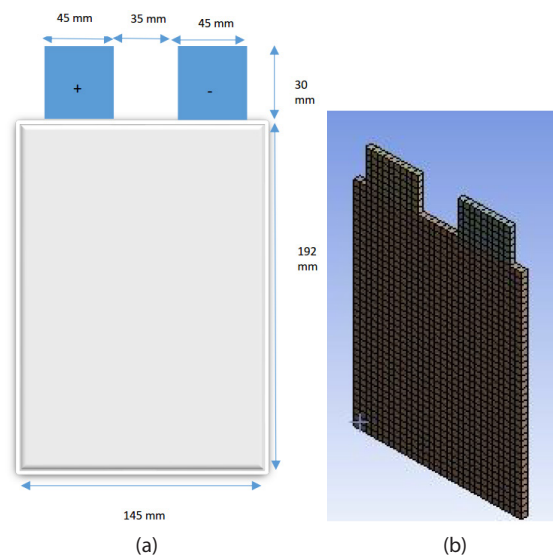
Figure 2: a) 14.6 Ah LiMn2O4 LIB dimensions b) Mesh image of the designed model

The default parameters used in NTGK model were taken in the studies in [24] and are shown in Table 1. The study was used to obtain the discharge curves parameters of the typical 3.7 V lithium ion battery in [25]. Given that the NTGK model adjusts the capacity of the modeled battery cell, it is found that the default parameters for this research are sufficient.

Table 1: MSMD Battery Module Input Parameters

MSMD battery module parameters		
Parameter	Value	Units
Electrical parameters		
Nominal Cell Capacity	14.6	Ah
C-Rate	0.5,1,2,3,5	-
Min. Stopping voltage	3	V
Max. Stopping voltage	4	V
NTGK model polarization parameters		
Initial DoD	0	-
Capacity reference	14.6	Ah
U constants:		
a0,a1,a2,a3,a4,a5	4.12,-0.804,1.075,-1.177,0,0	
Y constants:		
b0,b1,b2,b3,b4,b5	1168.59, -8928, 52504.6, -136231, 158531.7, -67578.5	
Temperature corrections:		
C1,C2	1800, -0.00095	
Cell materials		
Density	2092	Kg/m^3
Specific Heat (Cp)	678	J/kg-K
Thermal conductivity	18.2	w/m-K
UDS-0	1.19e+06	Kg/m-s
UDS-1	9.83e+05	Kg/m-s
Electrical conductivity	3.541e+07	Siemens/m
Pole Materials		
Density	8978	Kg/m^3
Specific Heat (Cp)	381	J/kg-K
Thermal conductivity	387.6	w/m-K
UDS-0	Model parameters	Kg/m-s
Electrical conductivity	1e+07	Siemens/m

3. SIMULATION STUDY

The Simulations were obtained through the analysis program, which includes the finite element method using the mathematical methods and parameters shown in Chapter 2. Firstly, the MSMD battery has been selected according to the electrical parameters of the 14.6 Ah-LIB battery. Here, the minimum and maximum stopping voltages are shown as 3 V and 4 V respectively. This is because; The potential difference in charging or discharge of the battery does not damage the battery. It is under control that it does not fall below 3 V during Discharge, and does not exceed 4 V during charging.

The discharge velocity parameters were applied as 0.5 C, 1 C, 2 C and 3 C respectively. The NTGK model polarization parameters are the default parameters for the model of the software package. Material information has been entered into the system as cell material and polar material. Although polar materials are chosen differently for positive and negative materials some studies, this study has been chosen the same for does not make a big difference. Since the boundary conditions are very small in the extremes of the poles, it is assumed that there is no heat loss. The boundary conditions for Poles and cells were taken from the ambient temperature 300 K and the heat transfer coefficient (h) 5 w/m^2 K.

Figure 3 shows the temperature distributions in the discharge rates of 0.5 C, 1C, 2 C and 3 C respectively. It is seen that the temperature rises gradually depending on the discharge rates. While the temperature is higher at the center of the cell, the temperature decreased to the poles. In 0.5 C, the battery was discharged in 3000 seconds, although the average temperature was 300 K, up to 302 K in 1 C. The battery has been discharged 1600 seconds in 2 C, 1200 seconds at 3 C and the temperatures increased to 308 K and 314 K.

Figure 4 shows discharge curves in the discharge rates of 0.5 C, 1C, 2 C and 3 C respectively. As the discharge rate increases, the discharge time in the battery has been decreased. At the 0.5 C discharge rate, the battery voltage decreased from 4.10 V to 3.86 V in 3000 seconds, at 1 C discharge rate battery dropped from 4.10 V to 3.50 V in same time, at 2 C discharge rate battery voltage decrease from 4.10 V to 3.30 V in 1600 seconds, at 3 C discharge rate battery voltage decrease up to 3.20 V at 1200 seconds.

Figure 5 shows the total heat generation at discharge rates of 0.5 C, 1 C, 2 C and 3 C, respectively. As shown in Figure 5, the total heat generation source was seen from the bottom of the cell to the upper layer of the cell. This is because the total flux density during charge and discharge is concentrated in the part of the cell towards the poles. As the rate of discharge rates increased, total heat production was observed to increase.
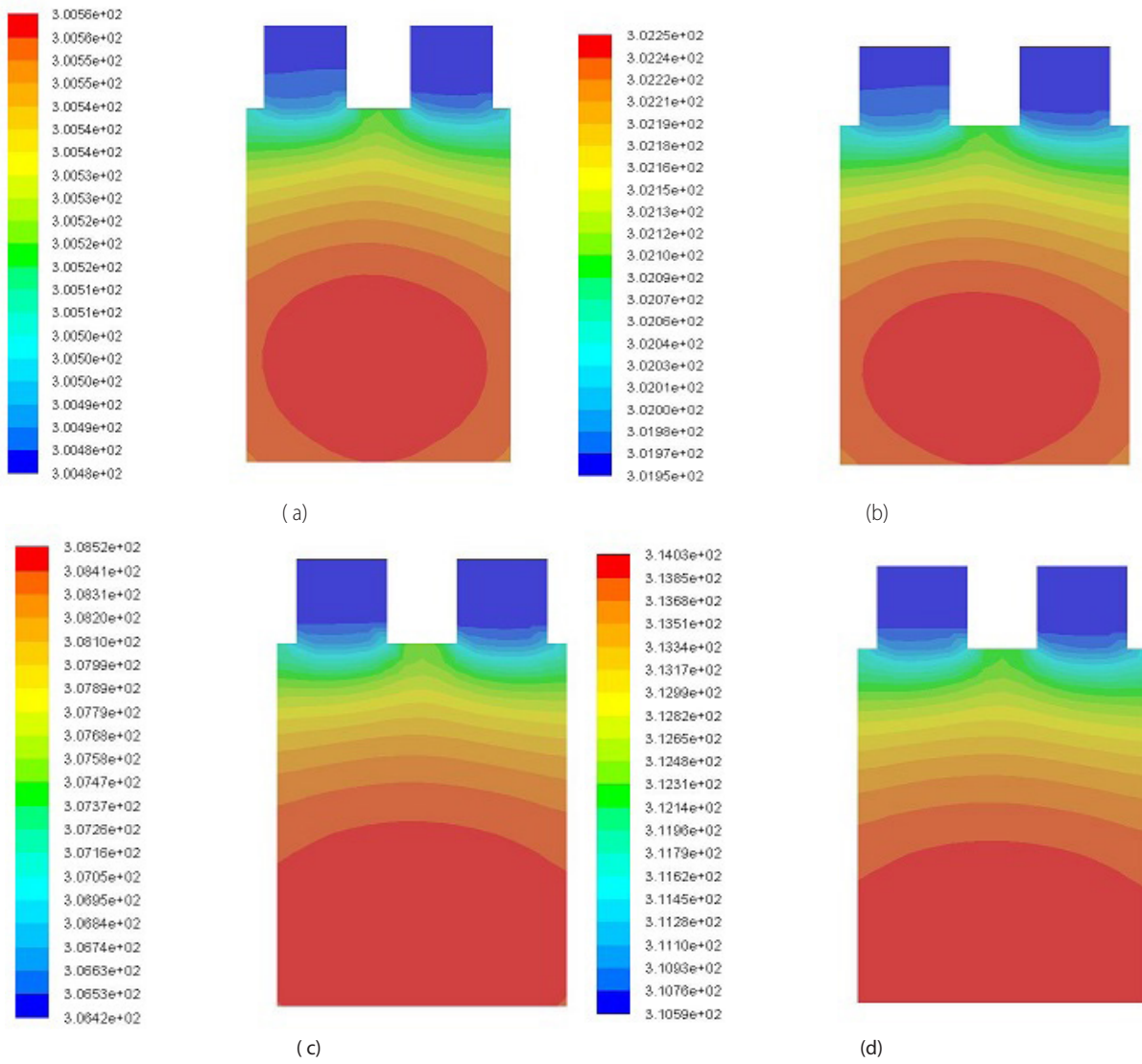
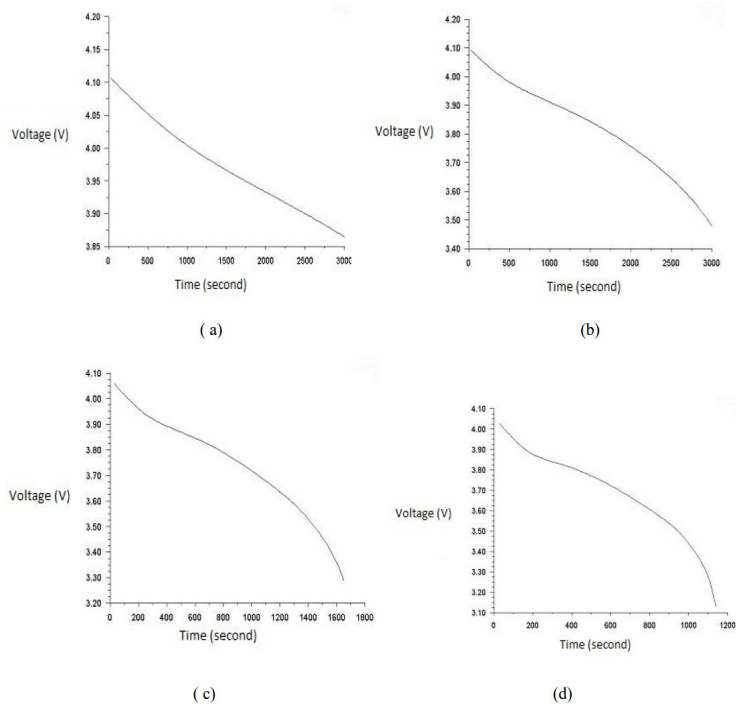Figure 3: Temperature distributions at a) 0.5C b) 1 C c) 2C d) 3C discharge rates

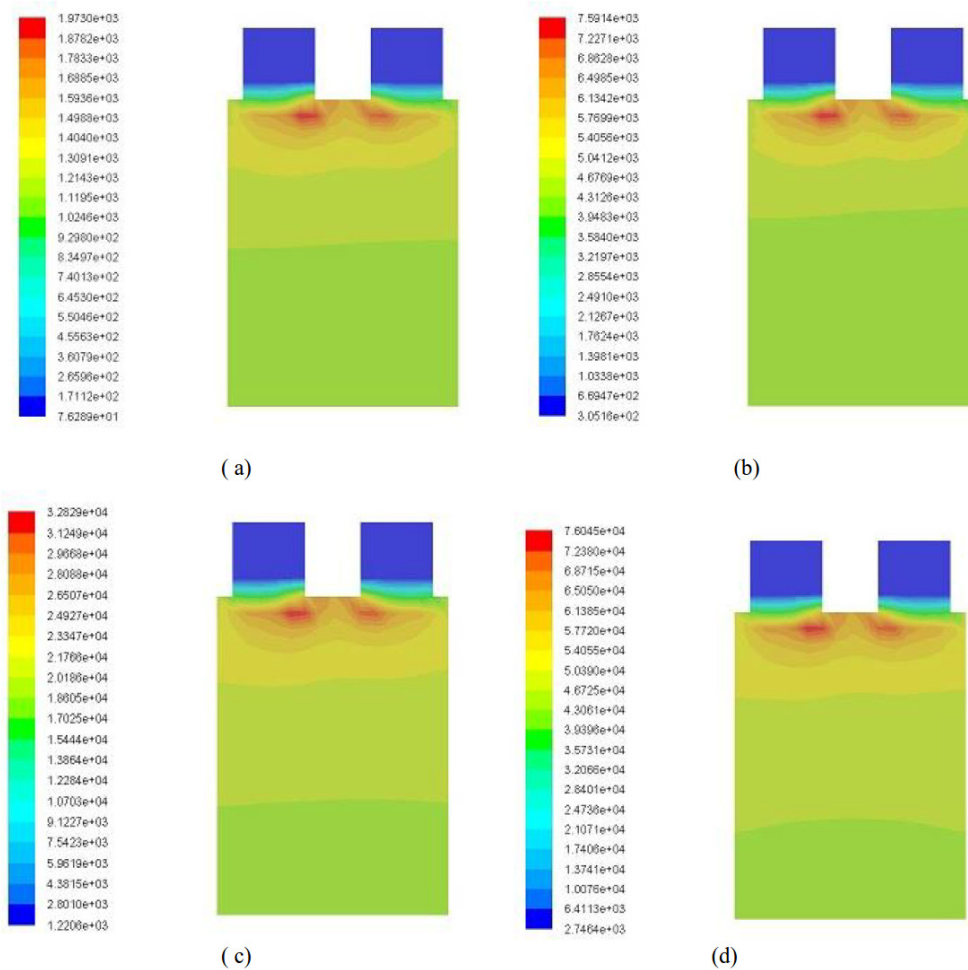Figure 4: Discharge curves at a) 0.5C b) 1 C c) 2C d) 3C discharge rates

Figure 5: Total heat generation at a) 0.5C b) 1 C c) 2C d) 3C discharge rates

4. CONCLUSIONS

Because of the increasing popularity of electric vehicles, the batteries used in these vehicles have attracted the attention of the researchers. Despite the high cost compared to other batteries, one of the reasons for reducing the life of lithium-ion batteries with high power and current density advantages is the high temperature and the explosion of heat leakage when it cannot be avoided. Therefore, temperature control has gained importance in both manufacturers and researchers.

In this study, the thermal behavior of 14.6 Ah LIB at 0.5 C 1 C 2 C and 3 C discharge rates were analyzed. It was observed that the total heat and temperature increased as the discharge time decreased at high discharge rates. This temperature was lower in the center of the cell and decreased towards the poles. Since the non-uniform distribution of the temperature also causes loss of capacity of the cell, a cooling system is needed to eliminate this irregularity. This study was a preliminary study for the design of the cooling system and was carried out to observe the thermal behavior of the battery in different discharge loads.

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