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Numerical simulation on the temperature behavior of Cylindrical Lithium – Ion Battery

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ABSTRACT:
Electric vehicles represent the current development trend in the automobile industry. They are poised to play a key role in the transition to a low-carbon transport system.Lithium-ion batteries present a significant challenge for the electric car industry, as battery temperature greatly impacts both performance and lifespan. The increasing temperature during charge/discharge of Lithium-ion batteries may cause thermal runaway which can lead to a potential factor of igniting a very dangerous explosion and irreparable human injuries. Therefore, understanding the thermal behavior during charge/discharge of Li-ion batteries becomes even more necessary. In this study, the thermal behaviors of cylindrical Lithium-Ion Batteries at different discharge rates were analyzed based on numerical simulations using ANSYS Fluent software. The results showed that the maximum temperature of battery surface is proportional to the battery discharge rate, i.e., the higher the C-rate, the greater the cell surface temperature. The maximum temperature at discharge rates of 0.5C, 1C, 2C, and 3C are respectively 305.7^{o}K, 314.87^{o}K, 338.87^{o}Kvà 359.16^{o}K. Furthermore, it has been observed that the obtained model can be used in the design of a cooling system to eliminate non-uniform heat dissipation.

KEYWORDS: *Lithium-ion battery; thermal modelling; heat generation; Cylindrical type; Battery modelling, Heat distribution.*

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I. INTRODUCTION

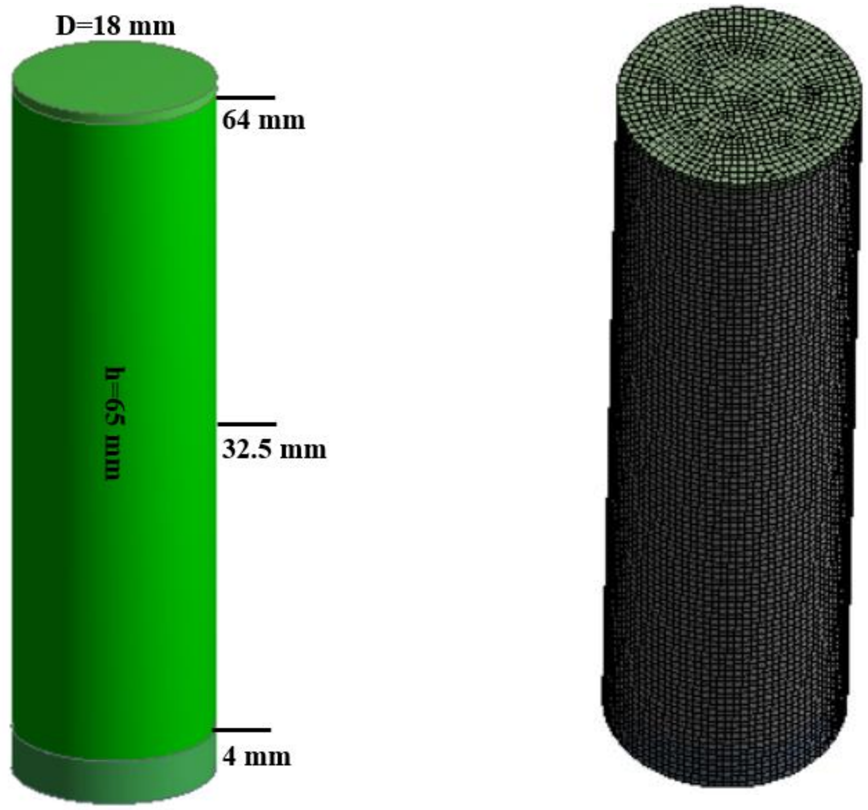
Electric vehicles represent the current development trend in the automobile industry, poised to play a key role in the transition to a low-carbon transport system.One of the most favorable power sources for these electric vehicles is a Lithium-ion battery, known for its long life cycle, safety and high durability. The lithium batteries contain lithium metal in their negative electrode. Currently, Li transition compounds such as LiCoO2, LiNiO2, LiMn2O4 and LiFePO4 are used as cathode material in battery cell production, demonstrating good performance during charge and discharge cycling. The recommended optimal operating temperature for batteries is between 0°C and 40°C[1], with the temperature difference between individual cells not exceeding 5°C [2]. However, the main drawback of the Lithium-ion batteries is that they generate a lot of heat due to ohmic and entropic reactions during charge/discharge [3]. This increasing temperature during charge/discharge of HEVs and EVs may cause thermal runaway which can lead to a potential factor of igniting a very dangerous explosion and irreparable human injuries[4]. Therefore, understanding the thermal behavior and discharge performance of Li-ion battery becomes even more necessary.

In recent years,numerous investigations have focused on modeling lithium-ion batteries. Nicolas et al. [5]studied the thermal modeling of large prismatic LiFePO4/graphite batteries, developing coupled thermal and heat generation models for characterization and simulation. They proposed a parameter determination method based on a quasi-steady state assumption. Their approach considered battery heating during characterization, specifically the temperature variation due to heat generation during current pulses. This temperature variation is estimated by combining the coupled thermal and heat generation models. The electrical parameters are determined as functions of state of charge (SoC), temperature, and current. Finally, they experimentally validated their model with a precision of 10°C.Lundgren et al.[6]presented a detailed 3D electrochemical-thermal model with experimental validation of a prismatic cell.Pals et al. [7]introduced a one-dimensional model for predicting the thermal behavior of lithium polymer batteries.Simplified one-dimensional thermal modeling with lumped parameters was presented by Hallaj et al. [8]and others to simulate temperature distribution inside lithium-ion battery cells. Tourani el al.[9]proposed a multi-scale, multi-dimensional thermoelectrochemical model to study the thermal behavior of lithium-ion cells.

The purpose of this study is to investigate the thermal behaviors of cylindrical lithium-ion batteries at discharge rates of 0.5C, 1C, 2C, and 3C using the NTGK model in ANSYS Fluent. The results showed that the maximum surface temperature of the battery is proportional to the discharge rate, meaning that higher C-rates result in higher cell surface temperatures. Specifically, the maximum temperatures at discharge rates of 0.5C, 1C, 2C, and 3C were 305.7^{o}K, 314.87^{o}K, 338.87^{o}K, and 359.16^{o}K, respectively. Additionally, the model demonstrated potential for use in designing cooling systems to eliminate non-uniform heat dissipation.

II. COMPUTATIONAL DOMAIN AND GOVERNING EQUATIONS

The dimensions of the cylindrical lithium-ion battery calculation model, simulated using the software package, are presented in Fig. 1a. The computational domain of the lithium battery is discretized using structured hexahedral mesh elements, as shown in Fig. 1b.



(a) (b)

Figure 1: (a) Schematic of Lithium-ion battery cell applied in the simulation and (b) 3D meshing of Lithium-ion battery cell

In this study, a Dual Potential Multi-Scale Multi-Domain approach, incorporating an NTGK electrochemical sub-model, is utilized to analyze a Li-ion battery cell. The electrical and thermal field characteristics of the battery are resolved within the computational domain at the cell scale as detailed in [10]:

$$\frac{\partial_\rho C_p.T}{\partial t} - \nabla[k_c.\nabla T] = \sigma_{pos}\left|\nabla\emptyset_{pos}\right|^2 + \sigma_{neg}\left|\nabla\emptyset_{neg}\right|^2 + \dot{q}_{E_{ch}} + \dot{q}_{short} \quad (1)$$

$$\nabla\left[\sigma_{pos}\nabla\phi_{pos}\right] = -\left(j_{E_{ch}} - j_{short}\right) \quad (2)$$

$$\nabla\left[\sigma_{neg}\nabla\phi_{neg}\right] = \left(j_{E_{ch}} - j_{short}\right) \quad (3)$$

where $\emptyset$ is phase potential, σ is effective electric conductivity at electrodes, $\dot{q}_{E_{ch}}$ and $j_{E_{ch}}$ are the electrochemical reaction heat due to electrochemical reactions and volumetric current transfer rate respectively, $\dot{q}_{short}$ and j_{short} are the heat generation rate due to battery internal short-circuit and current transfer rate respectively. The suffixes pos, neg represents positive and negative electrode. The source terms $j_{E_{ch}}$ and $\dot{q}_{E_{ch}}$ are calculated based on the electrochemical sub-model which is NTGK in the present case. NTGK is a simple semi-empirical electrochemical model.

The volumetric current transfer rate is related to potential field by:

$$\mathrm{j} = \frac{C_N}{C_{ref} VOL} \mathrm{Y}\left[U - \left(\emptyset_{pos} - \emptyset_{neg}\right)\right] \tag{4}$$

where Vol is volume of active zone, C_{ref} is the battery capacity used to get U and Y parameter functions.

Deep of discharge (DoD) is calculated as follows:

$$\mathrm{DoD} = \frac{Vol}{3600 Q_{nominal}} \int_0^t j dt \tag{5}$$

Depending on Deep of discharge, the U and Y parameter functions are evaluated as follows:

$$\mathrm{U} = \left\{ \sum_{n=0}^{5} a_n (DoD)^n \right\} - C_2 \left(T - T_{ref}\right) \tag{6}$$

$$\mathrm{Y} = \left\{ \sum_{n=0}^{5} b_n (DoD)^n \right\} \exp\left(-C_1 \left\{ \frac{1}{T} - (1) T_{ref} \right\} \right) \tag{7}$$

Where C_1 and C_2 are constants for a particular battery and T_{ref} is the reference temperature.

The Electro-Chemical reaction heat is given by:

$$q_{ch} = j_{ch} \left[U - (\varphi_+ - \varphi_-) - T \frac{dU}{dT} \right] \tag{8}$$

The first term in this equation represents heat due to over potential, while the second term corresponds to entropy-based heat generation. The values of cell properties, material properties for the NTGK model, and the U and Y coefficients are presented in Tables 1 to 3, respectively.

Table 1. 18650 Li-ion cell properties

Parameters	Unit	Battery
Size/thickness	mm	18x65
Density	kg/m^3	2720
Heat capacity	J/(kg.K)	300
Nominal capacity	Ah	3.25
Nominal voltage	V	3.6
Charging voltage limit	V	4.2
Cut-off voltage	V	2.5

Table 2. Material properties for NTGK model

Properties	Active zone (Jelly roll)	Positive tab (Aluminium)	Negative tab (Steel)
Density (kg/m^3)	2939	2719	8030
Specific heat (J/kgK)	2400	871	503
Thermal conductivity (W/mK)	3	202.4	16.27
Electrical conductivity (S/m)	3.541x10^6, 9.83x10^5	3.541x10^6	8.33x10^6

Table 3. U and Y coefficients for NTGK model

U	a_0	a_1	a_2	a_3	a_4	a_5
	3.964894	0.875167	-8.31135	15.45835	-10.8806	1.756215
Y	b_0	b_1	b_2	b_3	b_4	b_5
	50.48632	-576.754	3022.293	-6947.46	7230.698	-2786.63

It is also important to note that the face of the cell directly exposed to the environment undergoes convection heat transfer. Due to this type of heat transfer, the heat generated inside the cell will dissipate into the atmosphere, as the ambient temperature is likely lower than the surface temperature of the cell in contact with the atmosphere. In this context, the rate of convection heat transfer must be defined using the following equation:

$$Q = Ah(T_s - T_\infty) \tag{9}$$

where Q is the rate of heat transfer out of the cell (W), h is heat transfer coefficient (W.m^{-2}K^{-1}), A is the surface area (m^2), T_S is the surface temperature of the disc (^{0}C), and T_∞ is the temperature of the environment (^{0}C). In this work, a natural heat convection transfer mode was considered with a coefficient of convection value equal to 5.

Three-dimensional physical models of the cell are employed for all computational models in this study. To assess mesh independence, three mesh sizes are examined: 40926, 85200, and 180491 elements, with the mesh density nearly doubling with each refinement. Figure 6 illustrates the findings of the grid independence study, depicting the maximum temperature over time for various numbers of elements. The second size (85200 elements) is utilized in the simulation.

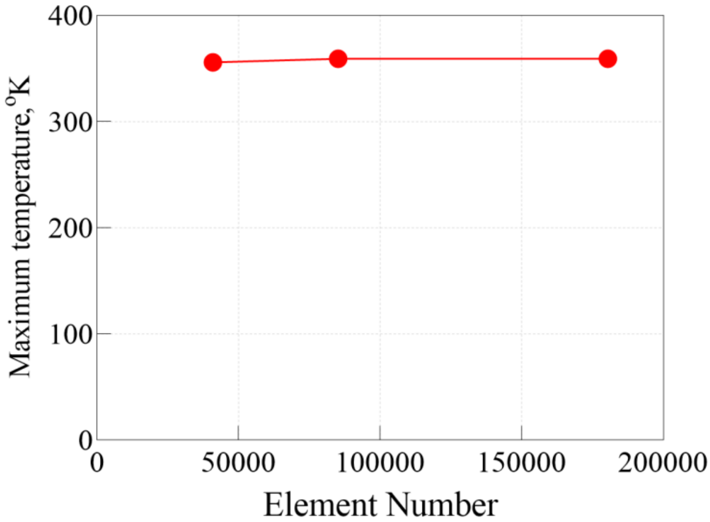


Figure 2. Grid independency test

III.RESULTS AND DISCUSSION

The temperature behavior of the cell under various discharge rates is computed using the NTGK model. The temperature rise in the cells is shown in Figure 3, indicating that the temperature increases gradually with higher discharge rates. As illustrated, the maximum battery cell surface temperatures are 305.7^{o}K, 314.87^{o}K, 338.87^{o}K, and 359.16^{o}K for 0.5C, 1C, 2C, and 3C discharge rates, respectively. While the maximum temperature of the cell increased by about 24 degrees for 2C compared to 1C, it increased by about 20 degrees for 3C compared to 2C. The maximum cell surface temperature reached 359.16^{o}K, which represents an increase of 64.2 degrees compared to the initial battery temperature at the beginning of the simulation (295 K). This clearly shows that the influence of high C-rates on maximum temperature is greater than their impact at moderate or low C levels.

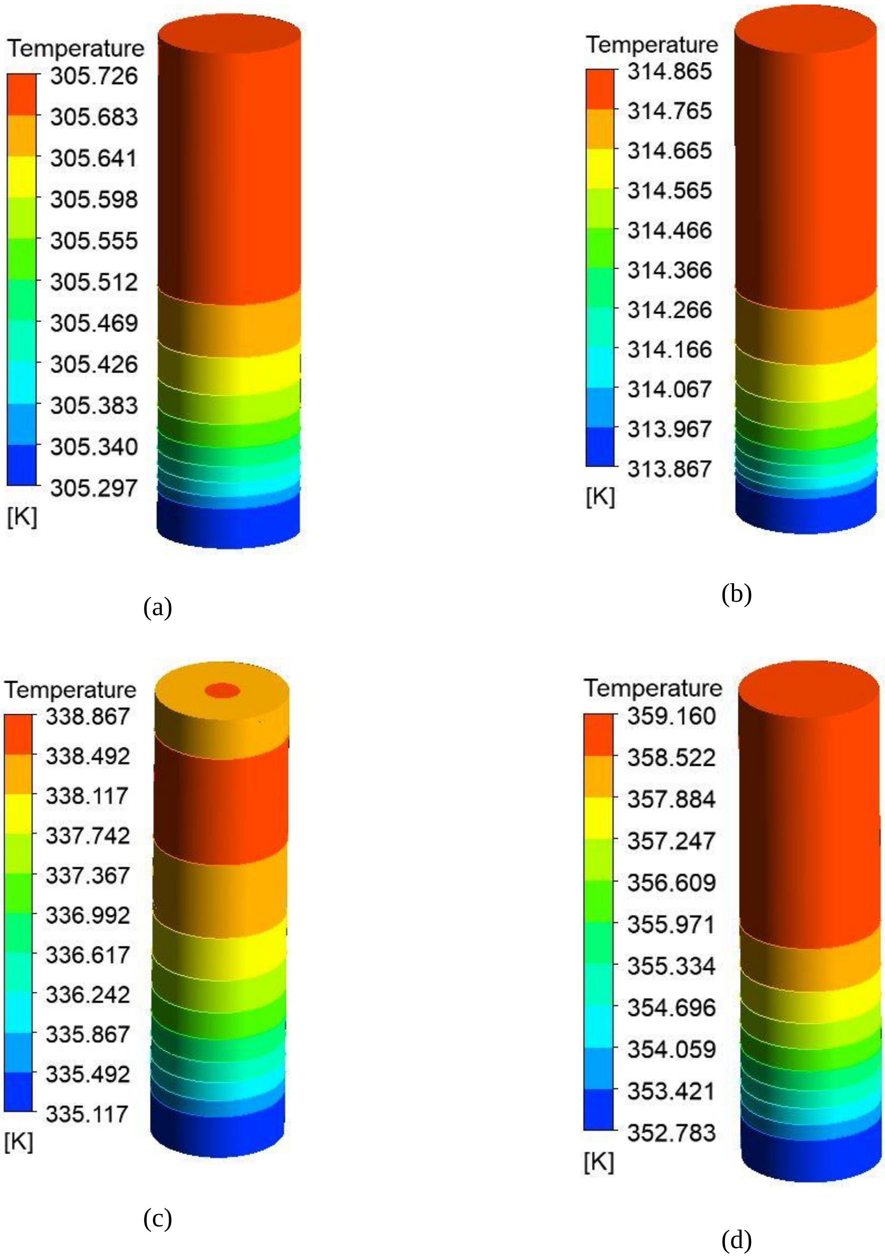


Figure 3. Surface temperature contour ofthe lithium-ion battery at different discharge rate: a) 0.5 C, b) 1 C, c) 2 C, d) 3C

The evolution of the maximum temperature achieved during the four discharge cycles is illustrated in Figure 4. As shown, the cell temperature increased each time the discharge current rate increased. The maximum temperature during a 0.5C-rate discharge cycle was 32.64°C, while this temperature increased to 41.68°C, 64.73°C, and 84.68°C at discharge rates of 1C, 2C, and 3C, respectively.

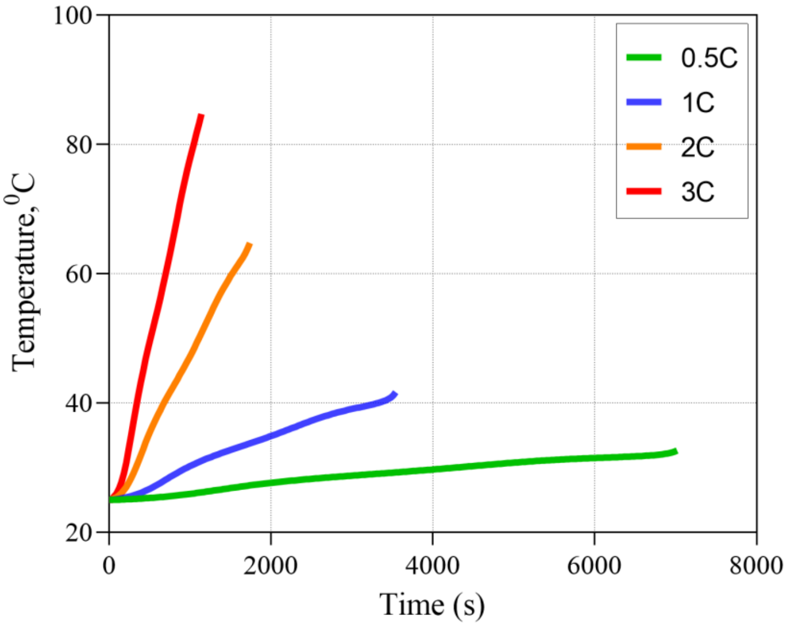


Figure 3. Temperature curves over time for the lithium-ion battery at different discharge rate

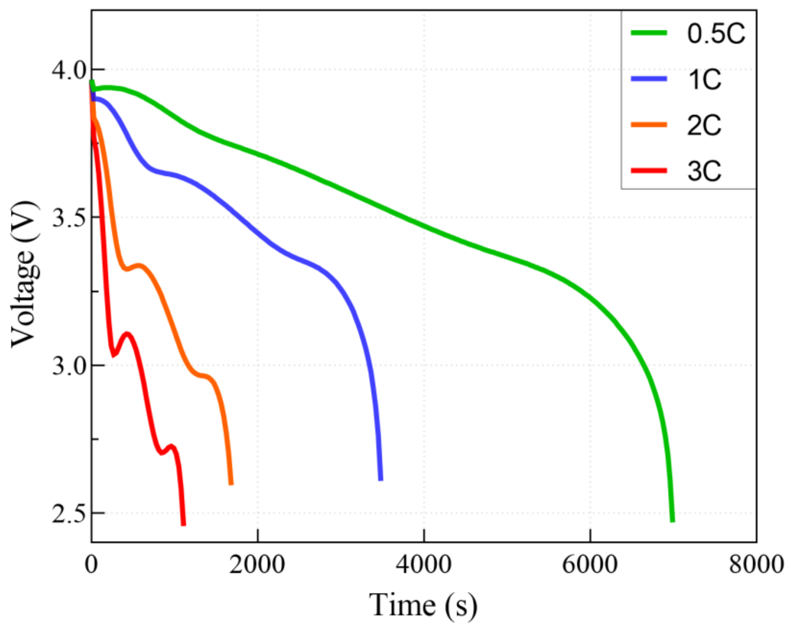


Figure 5. Evolution of the voltage of the lithium-ion battery during 4 different discharge rates

Figure 5 shows the evolution of the voltage of the cell during the different discharge rate, and as it is noticed the cut-off voltage limit was achieved faster with higher discharge rates applied. Ittook 3540 seconds tocompletely discharge the cell at 1C, while this value decreased to 1140 seconds at a C-rate of 3.

V. CONCLUSION

A numerical study was conducted to determine thermal behavior of cylindrical lithium-ion battery at different discharge rate of 0.5 C, 1 C, 2C, and 3C, usingThe NTGK model in ANSYS Fluent for simulation. The main conclusions of this work can be summarized as follows.

- The maximum temperature of battery surface is proportional to the battery discharge rate, i.e., the higher the C-rate, the greater the cell surface temperature.
- The maximum temperature at discharge rates of 0.5C, 1 C, 2 C, and 3 C are respectively 305.7^{o}K, 314.87^{o}K, 338.87^{o}K và 359.16^{o}K.
- Furthermore, a non-uniform thermal distribution has been observed with increased discharge rates. This non-uniform thermal distribution causes a loss of capacity and performance in the battery. Therefore, an accurate and effective cooling system is required to eliminate non-uniform temperature distribution. These results are a preliminary preparation for cooling system design.
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