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Comparison of 1D and 3D Electrochemical-Thermal Model of Lithium-Ion Battery

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Abstract **-** Due to the increase in its application areas, Lithium-ion (Li-ion) batteries and their thermal behavior are considered in this study. The comparisons of the 1D/3D electrochemical (EC) modeling and 1D/3D thermal analysis are the aim of this study. In order to understand the advantages and disadvantages of the 1D and 3D electrochemical and thermal models, and their effect on heat generation on battery, firstly, 1D and 3D electrochemical analyses of lithium-ion cells are performed separately at 1C rate for 1 layered cell. By examining the electrochemical behavior of the 1 layered cell both in 1D and 3D, the heat generation is calculated, and secondly, by creating a thermal model, the heat generation is obtained from the electrochemical analysis that provides input as a heat source for the thermal model. Thirdly, 1D and 3D thermal models of 1 and 20 layered cells are generated. Finally, the thermal behavior and temperature distribution of both cell designs are examined. The comparisons of models include the computational time, thermal distribution of both 1 and 20-layered cells. The results showed that the computational time in 3D model is longer than 1D model. Besides the temperature distribution difference both 1D and 3D model was found to be almost the same.

Keywords**:** Li-ion battery, Electrochemical model, Thermal Model, Thermal Behavior

1. Introduction

The demand for energy storage technologies is increasing significantly, especially with the demand for electric vehicles. Batteries that convert chemical energy into electrical energy, which are the most widely used energy storage technologies, are used in many areas. Batteries are divided into two groups as rechargeable and non-rechargeable. Rechargeable batteries offer solutions for energy storage by using them again and again. Recent studies are focusing on renewable energy sources and electric vehicles for changing environmental regulations. Within the framework of zero carbon emission, innovative technologies and energy storage systems are developed accordingly. As compared and summarized in Fig. 1 in terms of their volumetric energy density and gravimetric energy density, li-ion batteries are a suitable battery system for both renewable energy sources and electric vehicle applications.

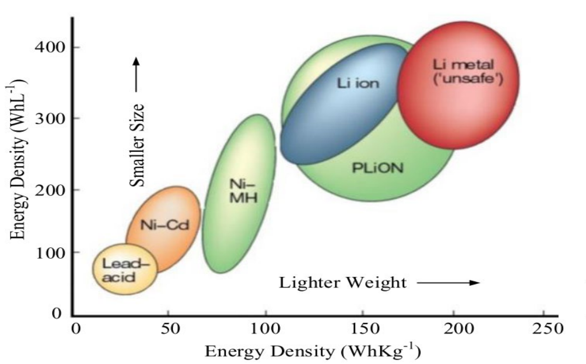

Fig. 1: Volumetric (Wh/L) and gravimetric (Wh/kg) energy density of various battery types [1].

In li-ion batteries, while chemical energy is converted into electrical energy during discharge, lithium ions (Li^+) come out from the negative electrode (anode) layers and settle in the positive electrode (cathode) layers. This process is called intercalation. During charging, the process is reversed, that is, the Li^+ have separated the layers of the cathode and settled in the layers of the anode. This process is called deintercalation. The lithium intercalation/deintercalation process, which occurs with ion flow through the electrolyte, is accompanied by a reduction/oxidation redox reaction of the electrode supported by the electron flow through the external circuit [2]. The separator allows the flow of ions while preventing the flow of electrons inside the cell. Fig. 2 shows the deintercalation of ions between the layers of the negative electrode and the intercalation between the layers of the positive electrode during discharge in a li-ion battery.

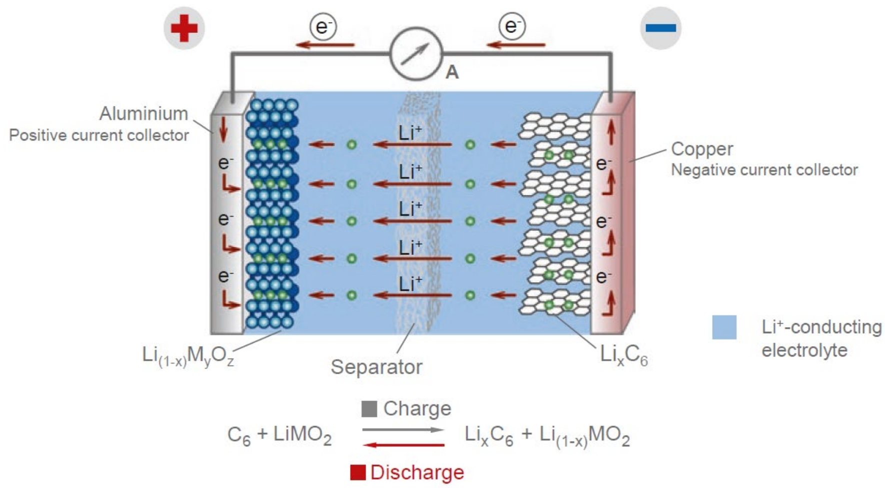

Fig. 2: Schematic representation of the movement of ions and electrons during discharge of a li-ion battery [3].

2. Numerical Model

Li-ion batteries are modeled with various methods by computer-aided programs. The electrical and electrochemical model is one of the main methods. When examining battery designs, the electrochemical model gives more precise results than the electrical model, as they show a clear relationship between electrochemical parameters and battery geometry [4].

The important task of li-ion battery simulations is to determine the li-ion battery characteristics obtained with various experimental data such as charge-discharge curves, lithium beam analysis, X-ray diffraction, and neutron diffraction. There are various simulation models to explain microscopic and macroscopic phenomena [5].

2.1. Electrochemical Model

There are several methods for electrochemical modeling. The most common of these is the Newman model. In the electrochemical model prepared by Newman and his research group, a model including conservation of mass, conservation of charge and electrochemical kinetic principles was developed based on concentrated solution theory and porous electrode theory. In this model, Doyle et al. [6] chose to model the galvanostatic charge/discharge behavior of the sandwich-shaped cell.

In this study the electrochemical model is used to model the electrochemistry model for the li-ion cell with the macroscopic model by using the Comsol Multiphysics program. In this model, the lithium ions are transported only in electrolytes whereas the electrons are transported only in solid materials, since the transport of lithium ions in liquid phase and electrons in solid phase is considered separately. The term lithium-ion source is determined by the chemical reaction on the surface of the active particles induced by the electrochemical potential gap between the particle surface and the electrolyte. Unlike many li-ion cell model, copper and aluminum current collector has been included in both 1D and 3D electrochemical li-ion cell model. In order to observe the potential and the current distribution on the electrode surface, 3D electrochemical li-ion cell model has been also modelled as well as 1D model. Schematic of 1D and 3D li-ion cell geometry shown as below.

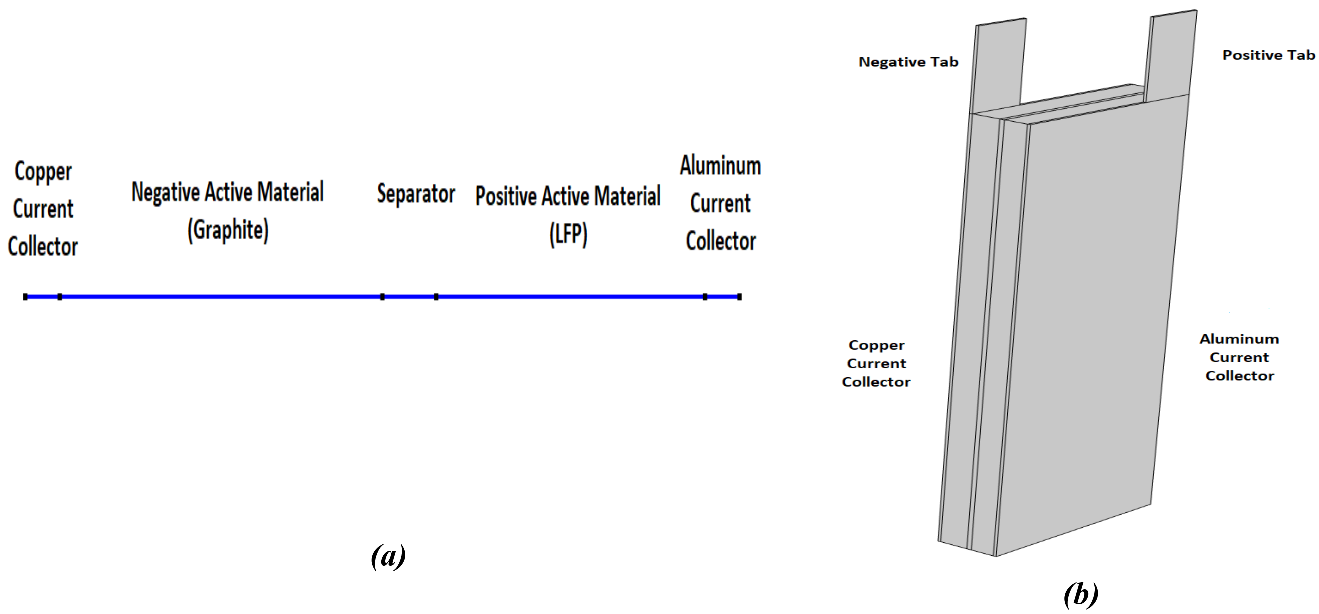

Fig. 3: Schematic of 1D (a) and 3D (b) li-ion cell geometry.

2.2. Thermal Model

The battery thermal model considers heat accumulation, convection, conduction, and heat generation. Battery heat generation is occurred due to activation, concentration, and ohmic losses.

A 3D thermal model can be developed using a heat transfer module with a design consisting of a core of the battery, positive and negative tabs, and a covered geometry with a rigid battery case. To simplify the calculations, the thermal model does not consider the layered structure of the battery interior. The energy conservation equation is the main equation in the thermal model and is illustrated in the equation below.

$$\rho c_p \frac{\partial T}{\partial t} = \nabla(\lambda \nabla T) + \dot{q} \tag{1}$$

$$\dot{q} = \dot{q}_{rev} + \dot{q}_{ohm} + \dot{q}_{act} + \dot{q}_{ex} \tag{2}$$

where $\dot{q}$ (W/m^3) is the heat generation rate of a battery consists of thermodynamic reversible heat (q_{rev} W/m^3) and irreversible heat ($\dot{q}_{irrev}$ W/m^3).

The reversible heat is caused by the change in the entropy of the electrode active material, which is triggered by the (de) intercalation of Li ions and occurs only in the porous electrodes. Irreversible heat includes ohmic heat ($\dot{q}_{ohm}$ W/m^3) and polarization heat ($\dot{q}_{act}$ W/m^3). The transport of charge in solid conductive material and electrolyte causes ohmic heat while the excess potential is responsible for polarization heat. However, the joule heat generated by the tabs can be neglected. Also, there is a small temperature difference between the battery surface and its surroundings. Therefore, radiation heat transfer can also be neglected and only convection should be considered as the thermal boundary condition. Thus, the heat transfer boundary condition based on Newton's cooling law is determined by $\dot{q}_{ex}$ in the thermal model [8, 9].

2.3. Electrochemical-Thermal Coupled Model

The average change in the temperature of the battery calculated by the thermal model is regularly coupled with the electrochemical model. As the discharge process, some temperature-dependent parameters change by the temperature. the obtained new heat generation is inserted into the thermal model as a heat source to obtain new temperature The schematic representation of the electrochemical-thermal coupled model is given in Fig. 4. As performed in this both the 1D and 3D electrochemical models are used to generate the thermal analysis as shown in Fig. 4. The interaction between the thermal model and the electrochemical model can be explained by the Arrhenius equation [8]:

$$\Phi = \Phi_{\mathrm{ref}} \exp\left[\frac{E_a}{R}\left(\frac{1}{T_{\mathrm{ref}}} - \frac{1}{T}\right)\right] \tag{3}$$

where Φ is a temperature dependent parameter, E_a ($Jmol^{-1}$) is the activation energy, R (8.314 $Jmol^{-1}K^{-1}$) is the gas constant, T (K) is the battery temperature, T_{ref} (K) is the ambient temperature.

In this study, 1D and 3D electrochemical models are created, and heat generation is obtained from these models. The obtained heat generation from electrochemical model is used in thermal model in order to find the temperature distribution at 1C rate. The above analysis is performed for both 1 and 20 layered cell. The computational simulation time and the temperature distribution obtained from the thermal model are compared for 1 and 20 layered cells which is modeled in 1D and 3D electrochemical model.

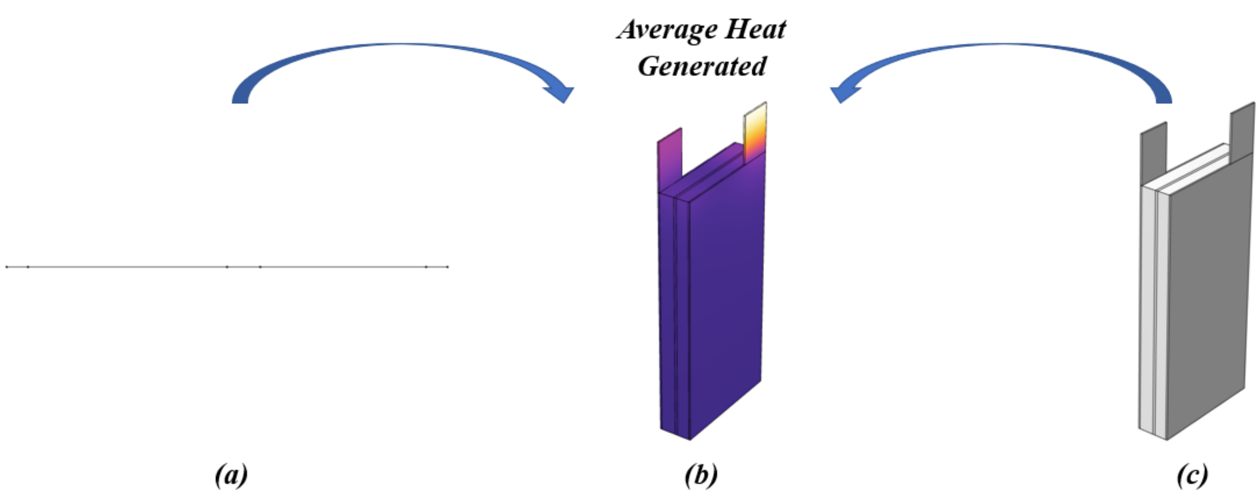

Fig. 4: Schematic representation of the 1D electrochemical model (a), 3D electrochemical model (c) and 3D thermal model as a coupled model (b).

3. Result and Discussion

As mentioned, the aim of this study is to compare the 1D and 3D electrochemical models on heat generation, thus the temperature distribution and on computational simulation time. In order to have these comparisons, the 20 Ah, 3.2 V, LFP pouch cell is considered. The model is created by using Comsol Li-ion battery design and Heat Transfer in Solids modules. The necessary battery parameters and material properties are taken from [9]. In both 1D and 3D electrochemical models, the same geometrical and chemical parameters are used. In addition, the same mesh quality is performed for both models to compare difference of temperature and computational time.

Electrochemical models of 1D and 3D has been created as single layered cell both since heat generation can be obtained from 1D layered cell and coupled with thermal model. In this model, the battery is charged at 1C under constant current (CC) as seen in Fig. 5. As seen from Fig. 5, initially the battery is empty (7 % SOC) and started to be charged at

1C rate, the voltage increases from 3 V to 3.4 V and stays remain at a constant 3.4 V, and at the end, the voltage increases to around 3.65 V (99 % SOC). After that the simulation is finished.

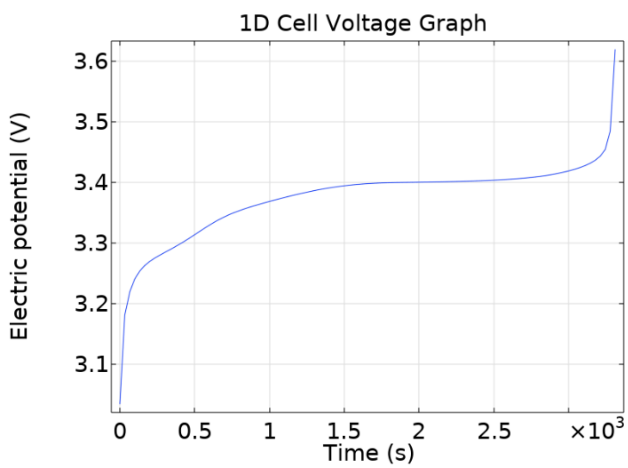

Fig. 5: 1D and 3D one layered cell voltage change at 1C charge.

In Heat Transfer in Solids Multiphysics, the three-dimensional form of both the 1D and 3D electrochemical models is created for 1 layered cell. The temperature distribution of 1 layered cell by using 1D and 3D electrochemical models is represented in Fig. 6. As seen from the figure, the average temperature of the cell increases from ambient temperature which is at 303.15 K to 316 K and 317 K for the 1D and 3D electrochemical model, respectively. Also, in order to analyse the effect of the number of cell layer on thermal distribution, the cell layer is increased to 20 layers and the temperature distribution for 20 layered cell are performed. The temperature distribution of 20 layered cell of 1D and 3D electrochemical models is demonstrated in Fig. 6. As seen from the following figure, the average temperature increases from ambient temperature which is at 303.15 K to 316 K and 317 K for the 1D and 3D electrochemical models, respectively.

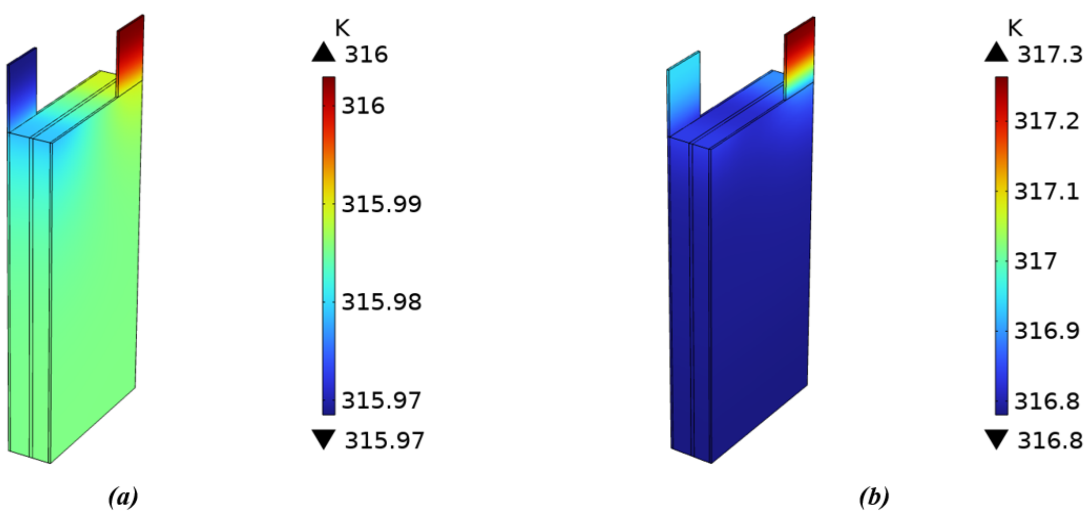

Fig. 6: 1 layered cell temperature distribution at the end of 1C charge, (a) 1D EC, (b) 3D EC.

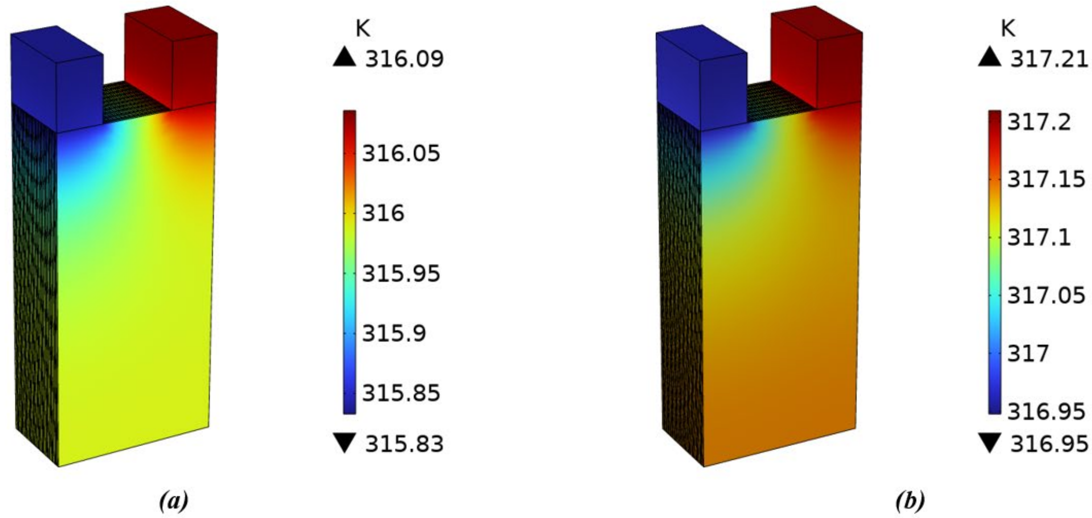

Fig. 7: 20 layered cell temperature distribution at the end of 1C charge, (a) 1D EC, (b) 3D EC.

The computational simulation time comparisons are also summarized in Table 1 for 1D and 3D electrochemical models and 1 and 20 layered cell. The computational time is generated by using the same mesh quality and the same local machine. As seen from Table 1, the computational time of 1D EC-3D thermal model for 1 and 20 layered cell are 27 and 65 seconds, respectively whereas 3D modelling computational time for both EC and thermal model is more than 1D EC-3D thermal model which computational times are 111 and 204 seconds for 1 and 20 layered cell, respectively.

Table 1: The comparison of 1D-3D model/1-20 layered computational time.

Computational Time	**1 Layered Cell**	**20 Layered Cell**
1D EC - 3D Thermal Model	27 seconds	65 seconds
3D EC - 3D Thermal Model	111 seconds	204 seconds

4. Conclusion

Due to the increase of application areas, li-ion battery thermal modeling is becoming more important. Even though there are many models for the simulation of the thermal model and the comparison of their simulation time, and their preciseness is not compared in detail in the studies. Thus, in this study, 1D and 3D electrochemical model on temperature distribution at 1C charge rate of 20 Ah, 3.2 V LFP pouch cell is taken into consideration. After validation, all parameters used in the simulation are taken as the same for both 1D and 3D electrochemical models. Later, the thermal model for both models is generated with the same mesh distribution and quality. The 1 layered and 20 layered cell structures are compared in terms of computational simulation time and temperature distribution.

In conclusion, the results of 1D and 3D models showed us that almost same temperature increasing. Therefore, 1D model can be preferred while obtaining heat generation from electrochemical model in order to save computational time. However, 3D modelling of cell can be important for observing the potential and current density distribution on the cell surface to analyze the electrochemical cell behaviour.

References

[1] M. A. Hannan, M. M. Hoque, A. Hussain, Y. Yusof, and P. J. Ker, “State-of-the-Art and Energy Management System of Lithium-Ion Batteries in Electric Vehicle Applications: Issues and Recommendations,” *IEEE Conf.*, pp. 19362–19378, 2018, doi: 10.1109/ACCESS.2018.2817655.

[2] G.-A. Nazri and G. Pistoia, *Lithium Batteries: Science and Technology*. Springer, 2009.

[3] R. Korthauer, *Lithium-ion batteries: Basics and applications*. Springer, 2018.

[4] A. Samba, N. Omar, H. Gualous, O. Capron, P. Van Den Bossche, and J. Van Mierlo, “Impact of Tab Location on Large Format Lithium-Ion Pouch Cell Based on Fully Coupled Tree-Dimensional Electrochemical-Thermal Modeling,” *Electrochim. Acta*, vol. 147, pp. 319–329, 2014, doi: 10.1016/j.electacta.2014.08.115.

[5] Y. Kato, Z. Ogumi, and J. M. Perlando Martin, *Lithium-Ion Batteries Overview, Simulation, and Diagnostics*. Pan Stanford Publishing Pte. Ltd., 2019.

[6] M. Doyle, T. F. Fuller, and J. Newman, “Modeling of galvanostatic charge and discharge of the lithium-polymer-insertion cell,” *J. Electrochem. Soc.*, vol. 140, pp. 1526–1533, 1993.

[7] H. Li *et al.*, “Electrochemical and thermal characteristics of prismatic lithium-ion battery based on a three-dimensional electrochemical-thermal coupled model,” *J. Energy Storage*, vol. 42, no. October 2020, p. 102976, 2021, doi: 10.1016/j.est.2021.102976.

[8] W. Mei, H. Chen, J. Sun, and Q. Wang, “Numerical study on tab dimension optimization of lithium-ion battery from the thermal safety perspective,” *Appl. Therm. Eng.*, vol. 142, pp. 148–165, 2018, doi: 10.1016/j.applthermaleng.2018.06.075.

[9] M. Alipour, E. Esen, and R. Kizilel, “Investigation of 3-D multilayer approach in predicting the thermal behavior of 20 Ah Li-ion cells,” *Appl. Therm. Eng.*, vol. 153, no. July 2018, pp. 620–632, 2019, doi: 10.1016/j.applthermaleng.2019.03.020.