

T.R.
GEBZE TECHNICAL UNIVERSITY
GRADUATE SCHOOL

**THERMAL MODELING AND VERIFICATION OF A POUCH-TYPE
LITHIUM-ION CELL USING EQUIVALENT CIRCUIT MODELING AND
MACHINE LEARNING**

BELFUN ARSLAN

**A THESIS OF MASTER OF SCIENCE
DEPARTMENT OF CHEMICAL ENGINEERING**

ADVISOR: ASSISTANT PROFESSOR ÖZGÜN YÜCEL

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T.C.
GEBZE TEKNİK ÜNİVERSİTESİ
LİSANSÜSTÜ EĞİTİM ENSTİTÜSÜ

EŞDEĞER DEVRE MODELLEMESİ VE MAKİNE ÖĞRENMESİ
KULLANARAK KESE TİPİ LİTYUM-İYON HÜCRESİNİN TERMAL
MODELLEMESİ VE DOĞRULAMASI

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TEMMUZ 2024



MASTER of SCIENCE JURY APPROVAL FORM

A thesis submitted by Belfun, Arslan, defended on 09/07/2024 before the jury formed with the 04/07/2024 date and 2024/34 numbered decision of the GTU Graduate Administration Board, has been accepted as a MASTER of SCIENCE thesis in the Department of Chemical Engineering.

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To my Family

ABSTRACT

Lithium-ion batteries are widely used in energy storage systems and are notable for their high energy density. The performance, energy density, and cycle life of these batteries are directly influenced by operating conditions. The optimum operating temperature range of lithium-ion batteries varies between 15 °C and 35 °C, and exceeding this range can lead to accelerated reactions, increased heat production and the risk of thermal runaway. This study focuses on modeling and experimentally verifying the thermal behavior of a 5 Ah NMC-polymer cell using the ECM model in ANSYS FLUENT at 25 °C ambient temperature and discharge currents of 0.25C, 0.5C, and 1C. Experimental data showed temperatures of 27.58 °C, 30.65 °C, and 39.16 °C, while numerical results were 27.11 °C, 31.4 °C, and 39.65 °C, demonstrating good agreement. The thermal behavior of cell with water-cooled aluminum plates was examined, *Re* number was 4436.24 and therefore the flow is considered turbulent. For CFD simulation, a polyhedral mesh with 3220062 elements was created with ANSYS FLUENT MESHING. The results show that the cell temperature decreases at 1C discharge and a more homogeneous temperature distribution occurs. The study also employed machine learning methods, including Gaussian process regression (GPR), support vector machine (SVM), neural network (NN), and linear regression (LR), to predict maximum cell temperatures, with GPR yielding the closest results to actual values ($R^2=0.99$, MAE= 0.317, RMSE= 0.4686 and RAE= 0.2196). Overall, the ECM model proved effective in predicting cell temperature profiles for thermal management, offering a computationally efficient alternative to complex electrochemical-thermal models.

Keywords: Pouch type Li-ion cell, Thermal model, ECM model, CFD, Liquid cooling, Machine learning.

ÖZET

Lityum-iyon bataryalar, enerji depolama sistemlerinde yaygın olarak kullanılan ve yüksek enerji yoğunluğu ile dikkat çeken teknolojilerdir. Bu bataryaların performansı, enerji yoğunluğu ve döngü ömrü gibi özellikleri, çalışma koşullarından doğrudan etkilenir. Sıcaklık, lityum-iyon bataryaların performansını ve güvenliğini önemli ölçüde etkiler. Lityum-iyon bataryaların optimum çalışma sıcaklık aralığı 15 °C ile 35 °C arasında değişir ve bu aralığın üzerine çıkılması hızlanan reaksiyonlar, artan ısı üretimi ve termal kaçak riskine yol açabilir. Bu çalışma, 25 °C ortam sıcaklığında ve 0.25C, 0.5C ve 1C deşarj akımlarında ANSYS FLUENT'te ECM modeli kullanarak 5 Ah NMC-polimer hücresinin termal davranışını modellemeye ve deneysel olarak doğrulamaya odaklanmaktadır. Deneysel veriler sırasıyla 27.58 °C, 30.65 °C ve 39.16 °C sıcaklıklarını gösterirken, sayısal sonuçlar 27.11 °C, 31.4 °C ve 39.65 °C olarak bulunmuş ve iyi bir uyum göstermiştir. Su soğutmalı alüminyum plakalarla hücrenin termal davranışı incelendi, *Re* sayısı 4436.24 olarak hesaplandı ve bu nedenle akış türbülanslı olarak kabul edildi. CFD simülasyonu için ANSYS FLUENT MESHING ile 3220062 elemanlı bir poligonal mesh oluşturuldu. Sonuçlar, 1C deşarjda hücre sıcaklığının azaldığını ve daha homojen bir sıcaklık dağılımının oluştuğunu gösterdi. Çalışmada Gaussian process regression (GPR), support vector machine (SVM), neural network (NN) ve linear regression (LR) makine öğrenimi metotları kullanılarak maksimum hücre sıcaklıkları tahmin edilmiş ve GPR en yakın sonuçları ($R^2=0.99$, MAE= 0.317, RMSE= 0.4686 and RAE= 0.2196) vermiştir. Genel olarak, ECM modeli, hücre sıcaklık profillerini öngörmeye ve termal yönetimde etkili bir yöntem olarak, karmaşık elektro-kimyasal termal modellere kıyasla hesaplama açısından verimli bir alternatif sunmaktadır.

Anahtar Kelimeler: Kese tipi Li-ion hücre, Termal model, ECM model, CFD, Sıvı soğutma, Makine öğrenimi.

ACKNOWLEDGEMENTS

I would like to express my deepest appreciation to my supervisor, Dr. ÖZGÜN YÜCEL. I would like to thank my manager and my colleagues, at Mutlu Akü for their support. I am also grateful to my unique family.

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LIST OF SYMBOLS AND ABBREVIATIONS

V	: Voltage
V_{ocv}	: Open-Circuit-Voltage
V_1	: Concentration polarization voltage
V_2	: Activation polarization voltage
R_s	: Internal resistance
R_1	: First parallel resistance
R_2	: Second parallel resistance
C_1	: First parallel capacitance
C_2	: First parallel capacitance
ρ	: Density
D	: Diameter
μ	: Viscosity
Re	: Reynolds number
C_p	: Heat capacity
∇	: Gradient operator
k	: Thermal conductivity
T	: Temperature
$\dot{q}$	: Heat source per unit volume
$\dot{q}_{rev}$	: Reversible heat source per unit volume
$\dot{q}_{pol}$	: Polarization heat source per unit volume
$\dot{q}_{ohm}$	: Ohmic heat source per unit volume
$\bar{V}$	: Velocity
μ_t	: Turbulent viscosity
Pr	: Prandtl number
Pr_t	: Turbulent Prandtl number
q_a	: Heat emitted from battery cell to environment
h_a	: Heat transfer coefficient
T_{bm}	: Average temperature
T_a	: Ambient temperature
U_{ds0}	: Electrical conductivity
U_{ds1}	: Electrical conductivity
$Y_{i_{predicted}}$	: i th predicted by the model
$Y_{i_{observed}}$	: i th actual observed value
$\bar{Y}_{observed}$	: Mean of the observed value
y_i	: Actual observed value i th data point
$\hat{y}$	: Predicted value i th data point
s	: Total number of data point
GPR	: Gauss Process Regression
SVM	: Support Vector Machine
LR	: Linear Regression
NN	: Neural Network
HPPC	: Hybrid-Pulse-Power-Characterization
ECM	: Electric-Circuit-Modelling
SOC	: State-of Charge
BTMS	: Battery-Thermal-Management System
Δ	: Laplace operator

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1. INTRODUCTION

Energy crises and environmental pollution have become common problems faced by all countries in the world. The advancement and adoption of electric vehicles (EVs) and battery energy storage (BES) technology serve as potent measures to address these issues. Among the essential components of EVs and BES, the battery pack assumes a crucial role in energy storage [Periasamy vd., 2024].

Figure 1.1 shows the projections of global Li-ion battery cell demand between 2022 and 2030, categorized by regions and sectors. The demand, which was approximately 700 GWh in 2022, is expected to increase 27%, reaching around 4,700 GWh by 2030. Sector-wise, the mobility sector is expected to constitute the largest portion of the demand, followed by stationary storage and consumer electronics. These projections highlight the increasing importance of Li-ion battery technologies, driven by the proliferation of electric vehicles and renewable energy systems [Web 1].

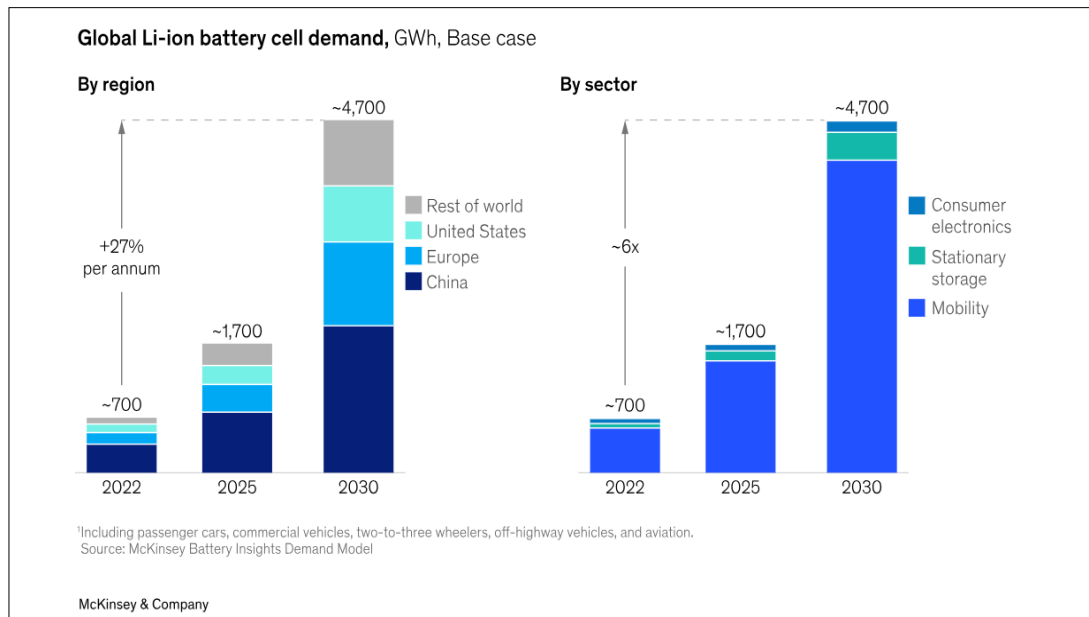


Figure 1.1: Projections of Global Li-ion Battery Cell Demand by Region and Sector.

The lithium-ion battery emerges as the preferred choice for battery packs owing to its numerous advantages, including long cycle life, a high voltage range, a low self-discharge rate, lightweight design, and absence of memory effect. However, lithium-ion batteries (LIBs) are sensitive to temperature variations during operation. **Figure**

1.2 shows that the ideal operating temperature for LIBs falls within the range of 15°C to 35°C. Temperatures exceeding 35°C intensify internal side reactions, leading to capacity deterioration and reduced battery lifespan. Additionally, incidents of fire or explosions in EVs due to overheating batteries are frequently reported, prompting significant concerns regarding EV safety. If the operating temperature falls below 0 °C, the reversible battery capacity is reduced due to the increased viscosity of the electrolyte and the slower interfacial kinetics. At higher temperatures, cycle stability deteriorates due to increased side reactions and strong SEI formation. As a result, the desired performance is achieved within an operating temperature range of 15-35 °C. Consequently, effective thermal management becomes critical for maintaining battery performance and ensuring safety throughout the battery's lifecycle [Yue et al., 2021].

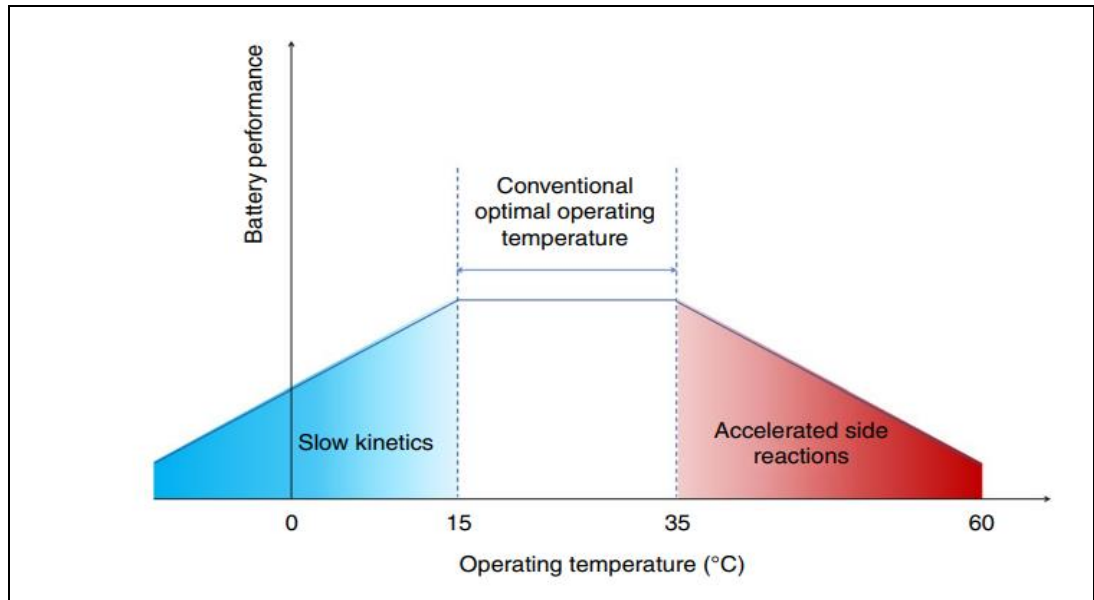


Figure 1.2: Effect of operating temperature on battery performance.

It is becoming increasingly important to model and simulate LIBs in order to improve battery thermal management systems and gain a fundamental understanding of their electrochemical performance and thermal properties. An equivalent circuit model (ECM), an electrochemical model, and a semi-empirical model are the three general methods used in a thermal model to describe the battery's thermal performance. The distribution of electronic and ionic currents, temperature gradients, and other intricate aspects of electrochemistry are disregarded in favor of the thermal behavior in the first two models. In addition, a combined electrochemical-thermal model that considers both thermal behavior and electrochemical phenomena offers important insights into

battery performance. This model offers comprehensive information about the electrochemical behavior and is helpful in the development of battery components. For thermal management purposes, however, it is not appropriate for the development of full cell scale batteries because of its high computational complexity [**Paccha-Herrera et al., 2020**].

Conversely, simulation programs are essential for simulating intricate systems and forecasting outcomes; however, they frequently necessitate substantial processing power and duration. Their practical application is limited by these lengthy calculations, which can be expensive. Recent developments in machine learning, however, present a viable remedy. By identifying patterns in data and producing predictions far more quickly than with conventional simulations, machine learning (ML) techniques can drastically cut down on processing times.

The purpose of this work is to use the ECM model in ANSYS FLUENT to generate a numerical model of the nickel-manganese-cobalt (NMC) lithium-ion cell and compare it with experimental data. Experimental and numerical methods were used to study the thermal behavior of the pouch-type polymer NMC lithium-ion cell at room temperature and current rates of 0.25 C, 0.5 C, and 1 C and results were validated. Then, the cell was discharged at various states of charge (SOC) range and current rates of 0.25 C, 0.5 C, 0.75 C, 1 C, and 1.5 C in the validated CFD model. Obtained maximum temperatures from model was used four machine learning models—Gaussian process regression (GPR) - Linear Regression (LR), Neural Network (NN), and Support Vector Machine (SVM)—and were compared in MATLAB. Finally, the cooling model of the cell with 25 °C water during discharge at 1C current rate was carried out numerically and experimentally and the results were interpreted.

This work focuses on industries like energy storage and the electric vehicle sector, where batteries are widely used. To remove restrictions on Li-ion battery use and increase battery lifetime in these industries, thermal management is crucial. By numerically analyzing the temperature of a commercially available NMC cell using an ECM model and lowering the computational cost through ML algorithms, the study seeks to assist in the identification of a workable thermal management system. The study provides a fresh viewpoint with this creative methodology.

2. LITERATURE REVIEW

2.1. Lithium-Ion Working Principle

The cathode, anode, separator, and electrolyte are the four primary parts of a LIB. In LIBs, energy storage and release are made easier by the cathode and anode's roles as charge carriers. While permitting the passage of lithium ions (Li^+), the separator physically divides these electrodes to stop internal short circuits. An essential part of this process is the electrolyte that conducts the ions, including Li^+ . Lithium ions travel between two electrodes in a lithium-ion battery—the cathode, which is typically made of lithium metal oxide, and the anode, which is typically made of graphite—to store and release energy. The anode releases electrons during the charging process, whereas the cathode absorbs electrons during the reduction phase.

On the other hand, after returning from the cathode, the anode releases electrons through an oxidation reaction, and the cathode absorbs electrons during discharge through a reduction reaction [Warner, J.T.2019]. **Figure 2.1** shows that ReDox operation of LIBs.

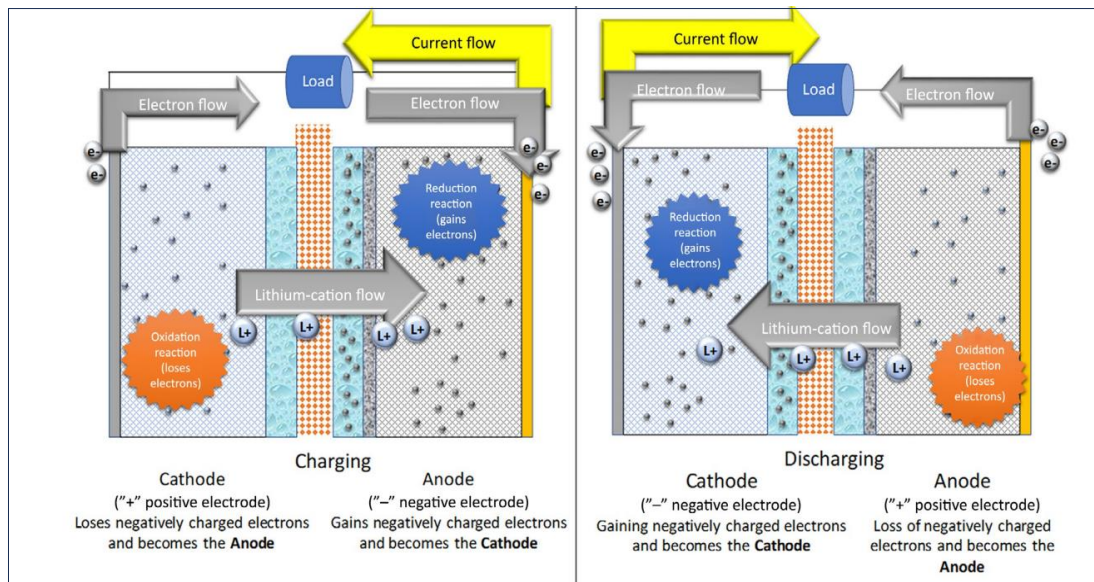


Figure 2.1: ReDox operations.

There have been numerous documented fires caused by LIBs over the past ten years. Changes in cell chemistry, the type of separator used, the active material, and the electrolyte selection can all affect how safe LIBs are. But in order to avoid catastrophic failures that could endanger users, the primary focus of lithium-ion battery safety is on safeguarding the cells within a system and keeping ideal temperature and voltage ranges.

A few potential reasons for cell failures are depicted in **Figure 2.2**. The causes on the left are shown as the consequences on the right, which typically result in thermal runaway. Three potential failure modes, internal short circuit, gassing, or impedance rise are typically the cause of cell failures. An internal short, for instance, may result from melting separator due to high temperatures, or it may be caused by production residue or dendritic growth entering the separator and shorting out the electrodes. Similar to the fingernail penetration test, a short circuit can also result from an object entering the cell. In the end, short circuits in these situations cause catastrophic failures [Warner, J.T.2019].

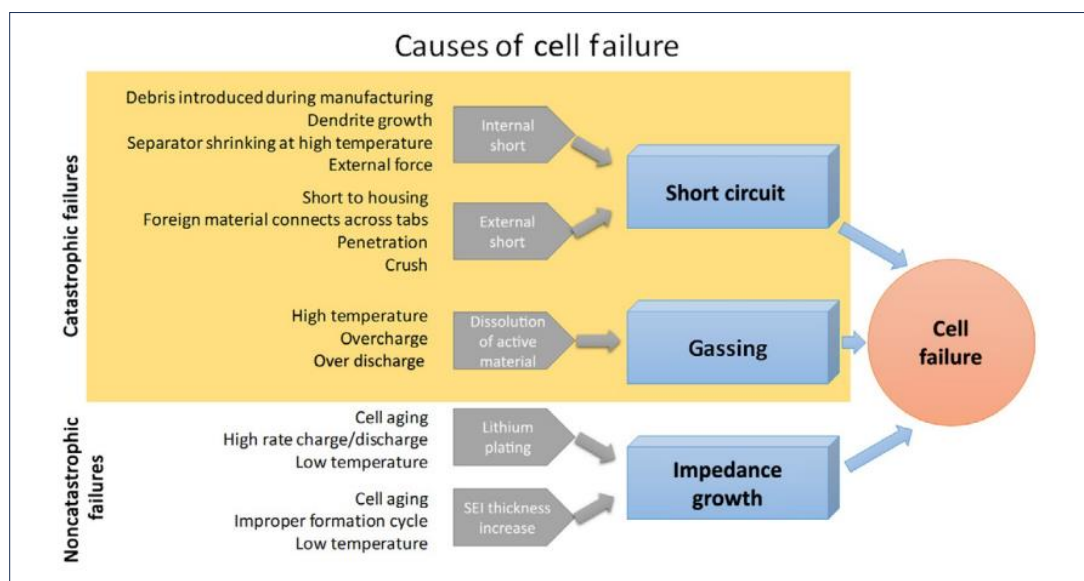


Figure 2.2: Cell failure types and causes.

A catastrophic short-circuit event is depicted in **Figure 2.3**. A cell may undergo an internal short circuit via a number of different pathways. An explanation for this could be that the cell gets hot. The development of lithium metal dendrites, which pierce the separator and establish an electrical connection between the anode and cathode, is

another frequent cause. Debris getting inside the cell during manufacturing can also result in internal short circuits [Warner, J.T.2019].

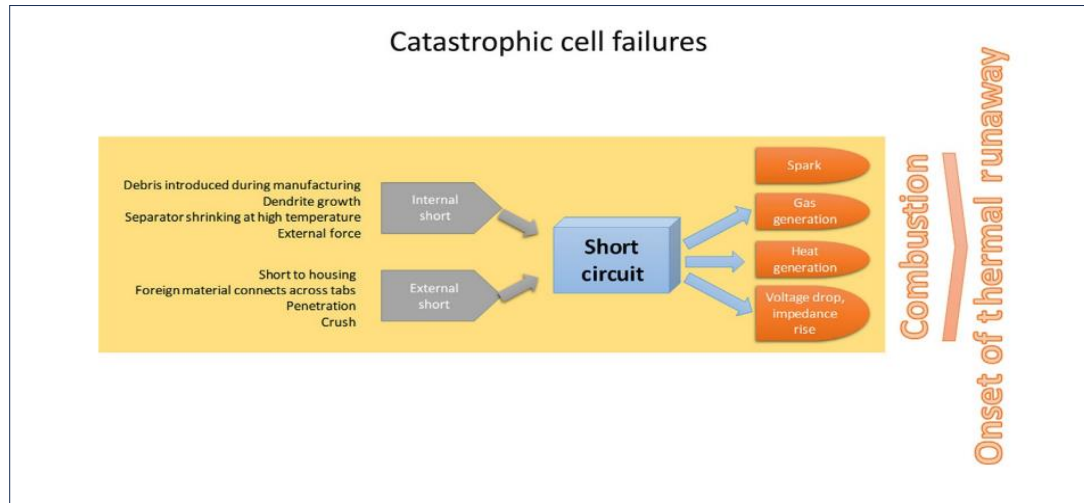


Figure 2.3: Catastrophic short circuit events.

An external short circuit is the other kind of short circuit. This happens when a conductive substance that is external to the cell simultaneously touches the positive and negative terminals or is added to the cell, connecting the electrodes electrically. Similar to an internal short circuit, an external short circuit can also fail by rapidly releasing energy at a single point, producing heat or gas, sparks, flames, explosions, and frequently the jelly roll ejecting from the cell housing [Warner, J.T.2019].

2.2. Electrical Circuit Model (ECM)

It is not necessary to have a thorough understanding of the electrochemistry of the battery cell in order to model batteries using equivalent circuit models (ECMs). Nonetheless, because ECMs can accurately mimic the dynamics of battery cells, they are frequently utilized in real-time applications like automotive battery management systems (BMS). Battery cells are typically represented by ECMs as electrical circuits made up of resistors and capacitors. A variety of ECMs, including the Rint model, the Thevenin-based electrical model, the impedance-based electrical model, and the runtime-based electrical model, are available in the literature, as **Figure 2.4** illustrates [Saldaña et al., 2019].

One of the most basic equivalent circuit models is the Rint model, as shown in **Figure 2.4 (a)**. The resistance (R_0) and open circuit voltage (V_{oc}) in this model account for

the variations in resistance values that occur during charging and discharging. The electrical model based on Thevenin expands upon the Rint model by incorporating a parallel RC network to replicate the battery's polarization effect. The Thevenin model is highly accurate in simulations and is comparatively simple. Nonetheless, the primary drawback of the Thevenin model is its assumption of constant parameters. The three components of the Thevenin model are equivalent capacitances, internal resistances, and open circuit voltage, as seen in **Figure 2.4 (b)** [He et al., 2011].

Figure 2.4 (c) displays impedance-based models. **Figure 2.4 (c)** fit the impedance spectra using a complex equivalent network structure after obtaining an AC equivalent impedance model in the frequency domain via electrochemical impedance spectroscopy. Equivalent circuit models based on impedance are limited to a specific SOC and temperature condition. As a result, they are unable to forecast the battery cell's DC behavior. To simulate the runtime and DC behavior at constant current, the runtime-based equivalent circuit model presented in **Figure 2.4 (d)** is too complicated. It can only model the transient response to a limited extent. For system design, integration, and optimization, Chen and Rincon-Mora have been developing a comprehensive model that combines the advantageous features of these equivalent circuit models.

This model integrates the propagation time data from propagation time-based models, the transient capabilities of Thevenin-based models, and the AC characteristics of impedance-based models. The suggested model has the ability to increase system efficiency and prolong battery life for portable electronic devices by accurately capturing both runtime and I-V power [Chen et al., 2006].

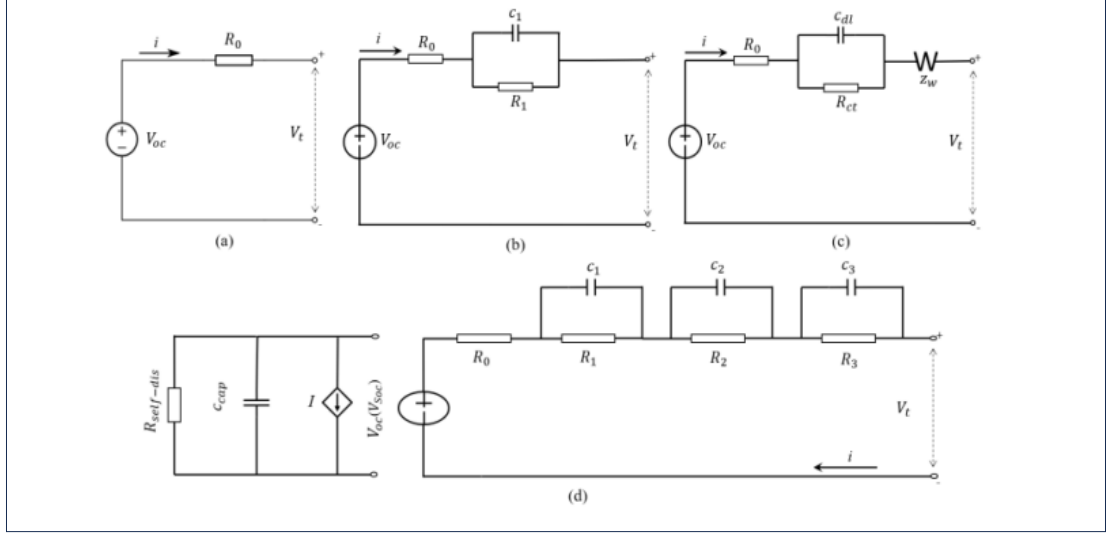


Figure 2.4: Commonly used equivalent circuit models; (a) Rint model, (b) Thevenin model, (c) impedance model, (d) operating time-based electrical circuit model.

Based on the work of Chen and Rincon-Mora, Ansys Fluent adopted the equivalent circuit model with 6 parameters (V_{oc} , R_s , R_1 , C_1 , R_2 , C_1) as seen in **Figure 2.5**.

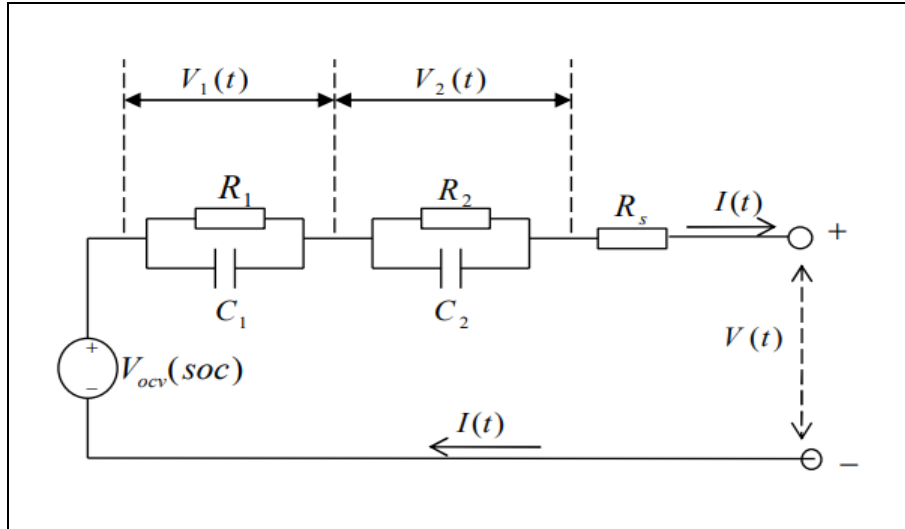


Figure 2.5: ECM model schematic representation.

An HPPC (Hybrid Pulse Power Characterization) test is conducted in the ECM model utilized in ANSYS FLUENT in order to gather the required battery data. One technique for figuring out a battery's dynamic performance characteristics is the HPPC test. The purpose of this test is to evaluate the cell's battery performance across the voltage range that is available. This test profile can be run under various temperature stressors and current loads, and it includes both discharge and regeneration pulses at

different SOCs. **Figure 2.6** displays the ECM model that represents the HPPC test pulses.

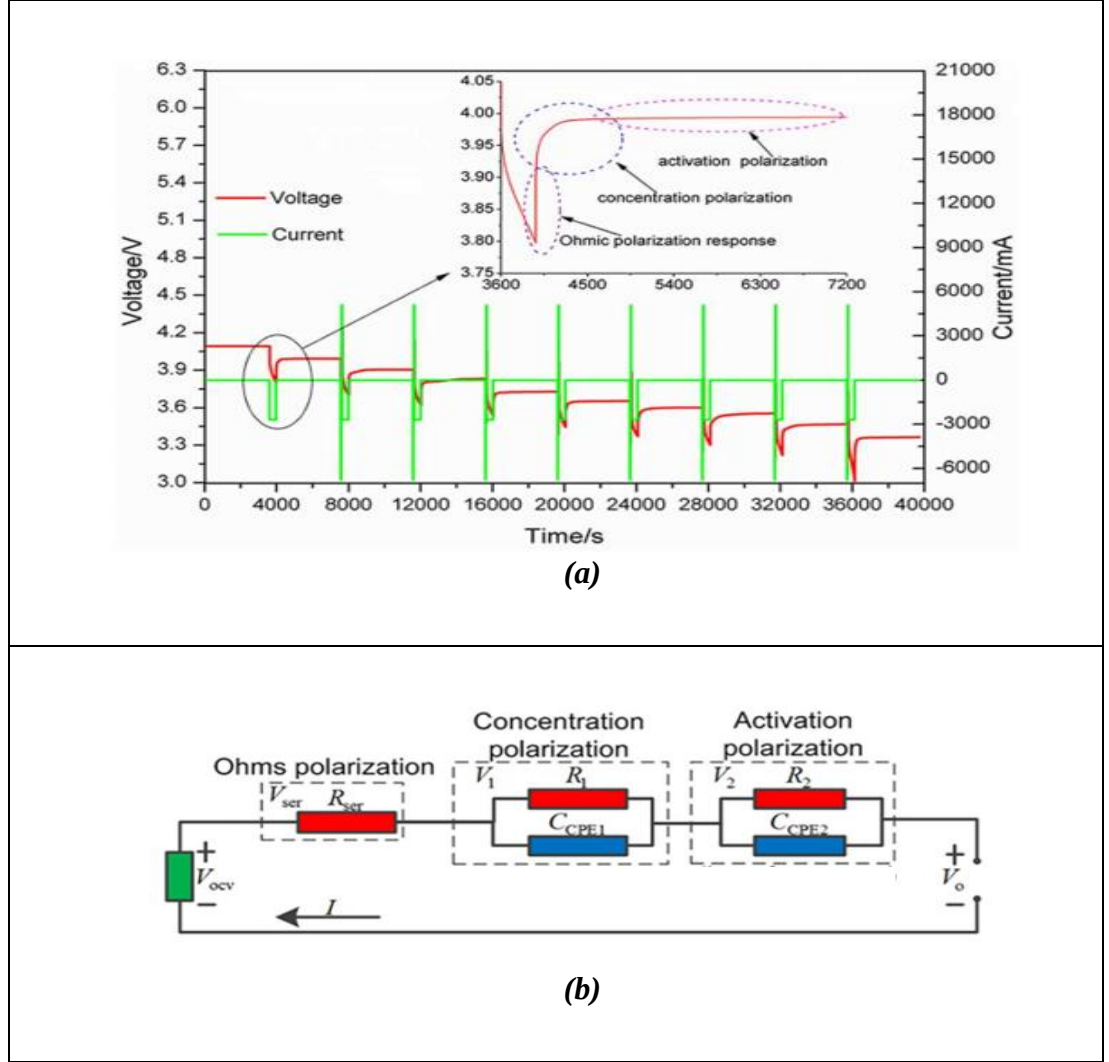


Figure 2.6: (a) HPPC test of lithium-ion battery; (b) Simplified lithium-ion battery ECM based on HPPC test.

$$V(t) = V_{ocv}(soc) + V_1 + V_2 - R_s(soc)I(t) \quad (2.1)$$

$$\frac{dV_1}{dt} = -\frac{1}{R_1(soc)C_1(soc)}V_1 - \frac{1}{C_1(soc)}I(t) \quad (2.2)$$

$$\frac{dV_2}{dt} = -\frac{1}{R_2(soc)C_2(soc)}V_2 - \frac{1}{C_2(soc)}I(t) \quad (2.3)$$

$$soc = soc_0 - \frac{\int_0^t I(t)dt}{3600Q_{Ah}} \quad (2.4)$$

2.3. Machine Learning Methods

Within the field of artificial intelligence (AI), machine learning (ML) allows computers to learn from data and gradually become more efficient over time without the need for explicit programming. It entails creating algorithms with pattern recognition and data-driven decision-making capabilities. Supervised learning, unsupervised learning, and reinforcement learning are the three categories of machine learning, as illustrated in **Figure 2.7**.

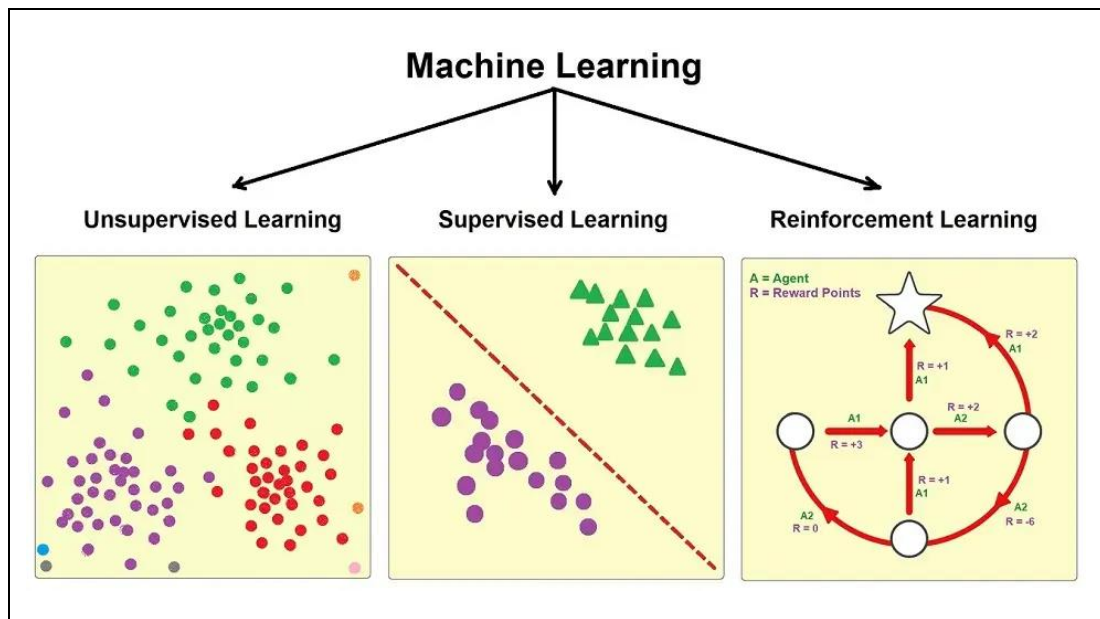


Figure 2.7: Classification of machine approaches.

Models are trained with labelled data in supervised learning; that is, an output identifier is assigned to each training pattern. By doing this, the model gains an understanding of the relationship between inputs and outputs and is able to forecast new, unobserved data with accuracy. Unlabeled data is used in unsupervised learning. Finding hidden structures or patterns in the data and classifying related elements into clusters are the objectives. This approach works well for tasks like identifying anomalies and segmenting customers. Another method for teaching an agent to make decisions by interacting with its surroundings is reinforcement learning. Agent learns to maximize the cumulative reward over time and is rewarded or punished based on its actions. This kind of learning is especially helpful in situations like autonomous vehicles, robotics, and games. Together, these three types of machine learning provide powerful tools for analysing data and making intelligent decisions in a wide range of applications

[Nasteski et al., 2017]. GPR, SVM, NN and LR are the most commonly used types of supervised learning.

The linear relationship between the input and output variables is assumed by LR. Consequently, it might not be effective for input variables and output to have a non-linear relationship. For instance, linear regression may not be able to adequately model scenarios where the data set contains a non-linear or parabolic relationship [Maulud et al., 2020].

GPR does not use parametric shaping to model the relationship between data points. The ability to record any relationship in the data set is made possible by this feature. GPR is capable of making uncertain predictions and adapting to any relationship between input and variables. Gaussian processes can therefore more accurately capture and predict parabolic or other non-linear relationships found in the data set [Sharifzadeh et al., 2019]. Figure 2.8 shows that representation of LR and GPR.

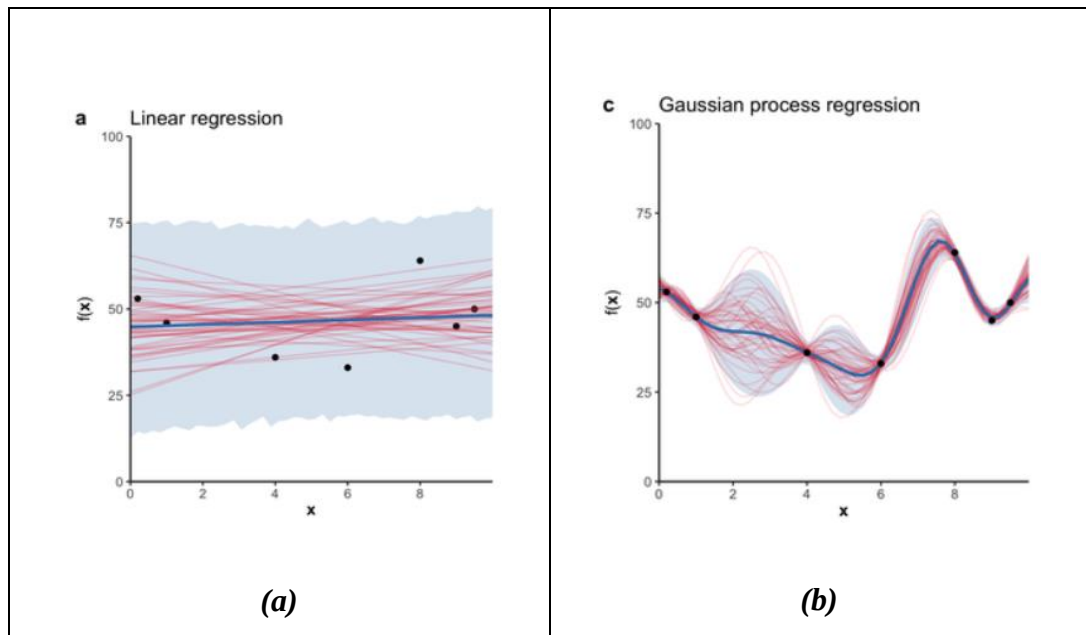


Figure 2.8: Representation of linear regression and gaussian process regression.

In a high-dimensional space, support vector machines (SVMs) identify the ideal hyperplane that minimizes classification error while separating classes with the greatest margin. By mapping the input data into higher dimensional domains where they are simpler to separate, kernel functions allow them to deal with non-linear relationships between input features. SVMs are frequently used in fields like image classification, text categorization, and bioinformatics because they perform well in

tasks with complicated decision boundaries. **Figure 2.9** shows that representation of SVM [Ghosh et al., 2019].

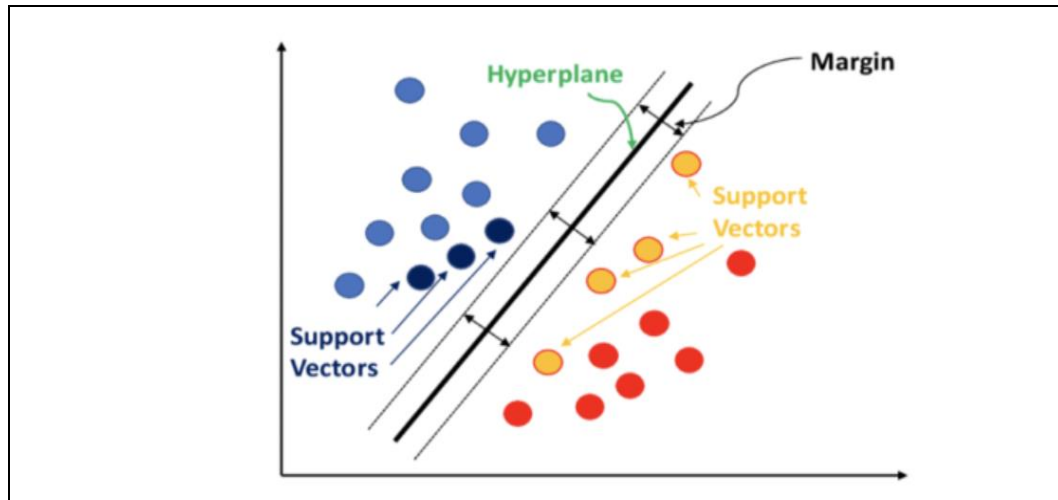


Figure 2.9: Representation of support vector machine.

Artificial neural networks (ANNs) are mathematical models that mimic how the human brain processes information. They are made up of artificial neurons. These networks use a system of weighted connections between neurons to process incoming data. Each layer uses activation functions to produce an output. Weights are modified during training to reduce error, typically through the use of backpropagation. The network picks up patterns from the data in this way, and it can utilize these patterns to forecast new data. Neural networks are an effective tool for complicated tasks like face and handwriting recognition and language translation [Chen et al., 2019]. **Figure 2.10** shows that representation of NN.

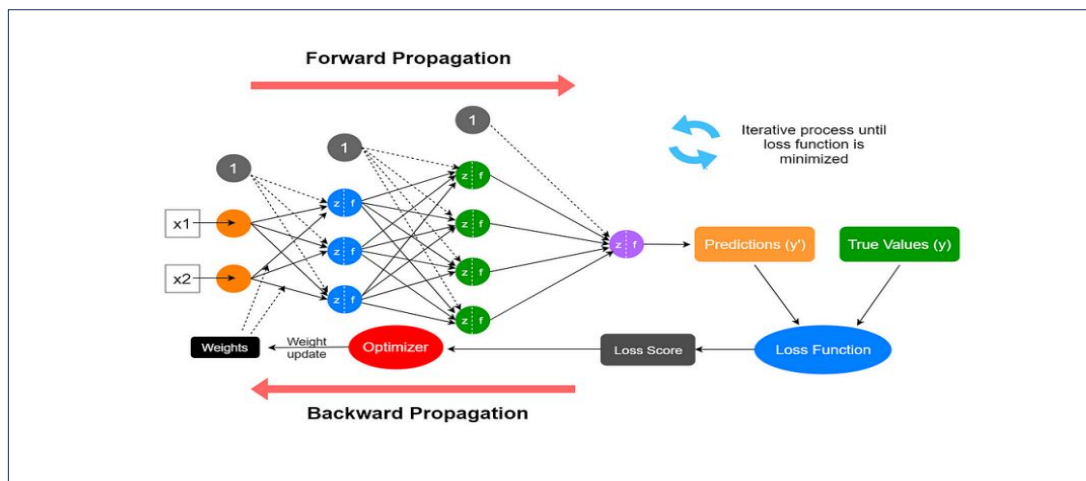


Figure 2.10: Representation of neural network.

2.4. Cooling Methods

Maintaining the battery pack's temperature within the designated range and minimizing temperature variations amongst the cells necessitates the use of an efficient battery thermal management system (BTMS). The battery pack's safe and effective operation is guaranteed by the BTMS, which is also in charge of controlling and dispersing the heat produced by the electrochemical reactions occurring in the cells. The battery system can make use of a variety of BTMS options. As shown in **Figure 2.11**, there are three primary BTMS techniques: passive, active and hybrid methods [Ghaeminezhad et al., 2023]. Subsequently, **Table 2.1** provides a comparison benchmark about the advantages and disadvantages of the above-discussed BTMS main techniques [Sadeghi, G., 2022].

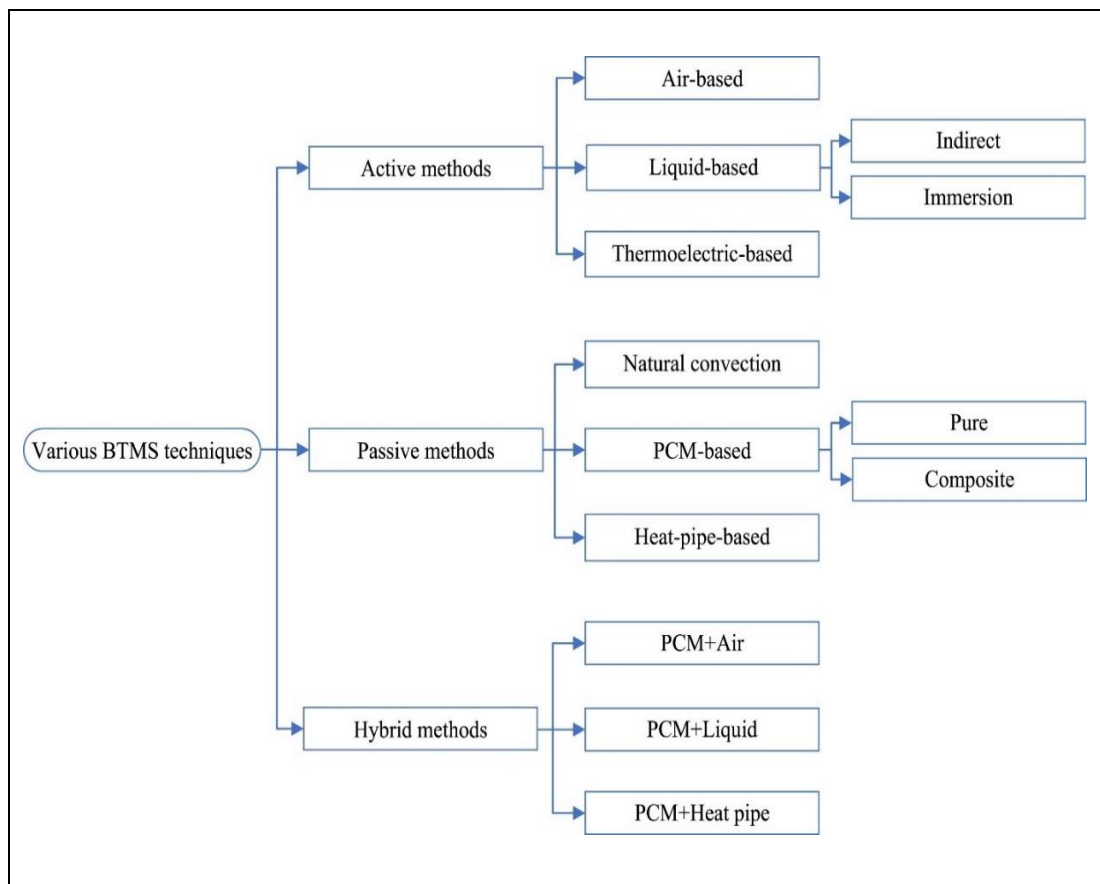


Figure 2.11: BTMs techniques.

Table 2.1: Advantages and disadvantages of the BTMS main techniques.

BTMS various techniques		Advantages	Disadvantages
Active	Air-based	Simple operation and configuration; easy maintenance; direct contact; low weight.	Low efficiency; low specific heat; expensive; difficult to distribute air evenly; additional fan required; high operating costs.
	Liquid-based	Improved efficiency; direct contact; relatively higher specific heat capacity.	Costly; short service life; large, occupied volume; complex structure; leakage problem.
	Thermoelectric based	Silent; requires no internal chemical reaction; is a static device; minimal maintenance costs; reliable and durable; no release of hazardous gases.	Additional power required; low efficiency.
Passive	Natural convection	Light weight; low initial and operating costs; simple configuration; direct contact; easy maintenance.	Difficult to achieve uniform air distribution; low efficiency; low thermal conductivity.
	PCM-based	High latent heat; compatibility with extreme conditions; relatively high efficiency; uniform temperature distribution; maintenance of long-term reliability; low cost.	Leakage problem; low thermal conductivity.
	Heat-pipe-based	Relatively high efficiency and thermal conductivity.	High complex structure; high initial and operational costs; leakage problem.
Hybrid		Combination of the advantages of an active and a passive system; good temperature distribution in the battery pack; simple configuration; additional option to dissipate the generated heat to the outside; excellent natural convection.	High complexity and cost.

3. MATERIAL AND METHODS

3.1. Experimental

Power-Xtra PX105080 NMC polymer Li-ion pouch type cell was used in the experiment. Current collectors for positive and negative electrodes are aluminum and copper respectively. Temperature tests were performed in an NUVE climatic test cabinet at 25°C with 0.25C, 0.5C and 1C constant discharge. NEWARE battery tester was used for charge and discharge tests.

During discharge, temperature values were measured with Pt100 temperature sensors at 5 points marked in **Figure 3.1**. Temperature data were recorded on the JUMO LOGOSCREEN nt device. Cell properties are given in **Table 3.1**.



Figure 3.1: NMC polymer Li-ion cell.

Table 3.1: Cell Properties.

Cell Properties	Value	Unit
Cell-Capacity	5	Ah
Nominal-Voltage	3.7	V
Charging Cut-off Voltage	4.2	V
Discharging Cut-off Voltage	2.75	V
Standard – Charging Current	0.2	C
Standard-Discharging Current	0.2	C
Anode material	Graphite	
Anode current collector	Copper foil	
Cathode material	Lithium nickel manganese cobalt oxide	
Cathode current collector	Aluminum foil	

The aluminum cooling plate shown in **Figure 3.2** was used in the liquid cooling test. 25 °C tap water was used as coolant. The pump was not used for water circulation. The outlet water was discharged from the plate into to sink during testing. Inlet water velocity was calculated by debimeter as 0.56 m/s.



Figure 3.2: Aluminum cooling plate.

Figure 3.3 and **Figure 3.4** show the experimental setup inside and outside the climate chamber, respectively.

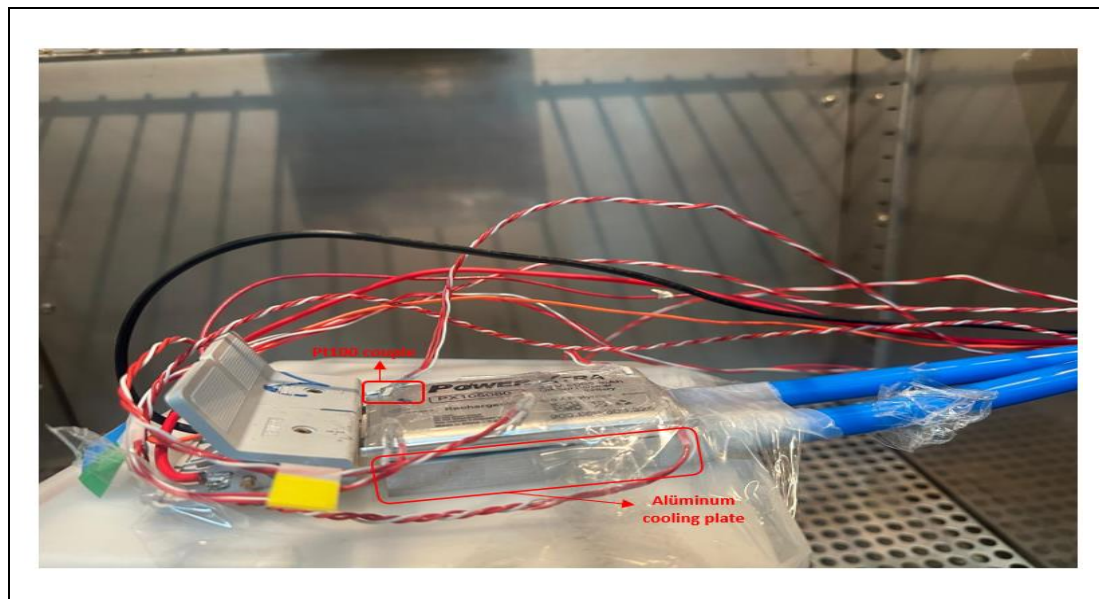


Figure 3.3: Experimental set-up for inside of climatic test cabinet.

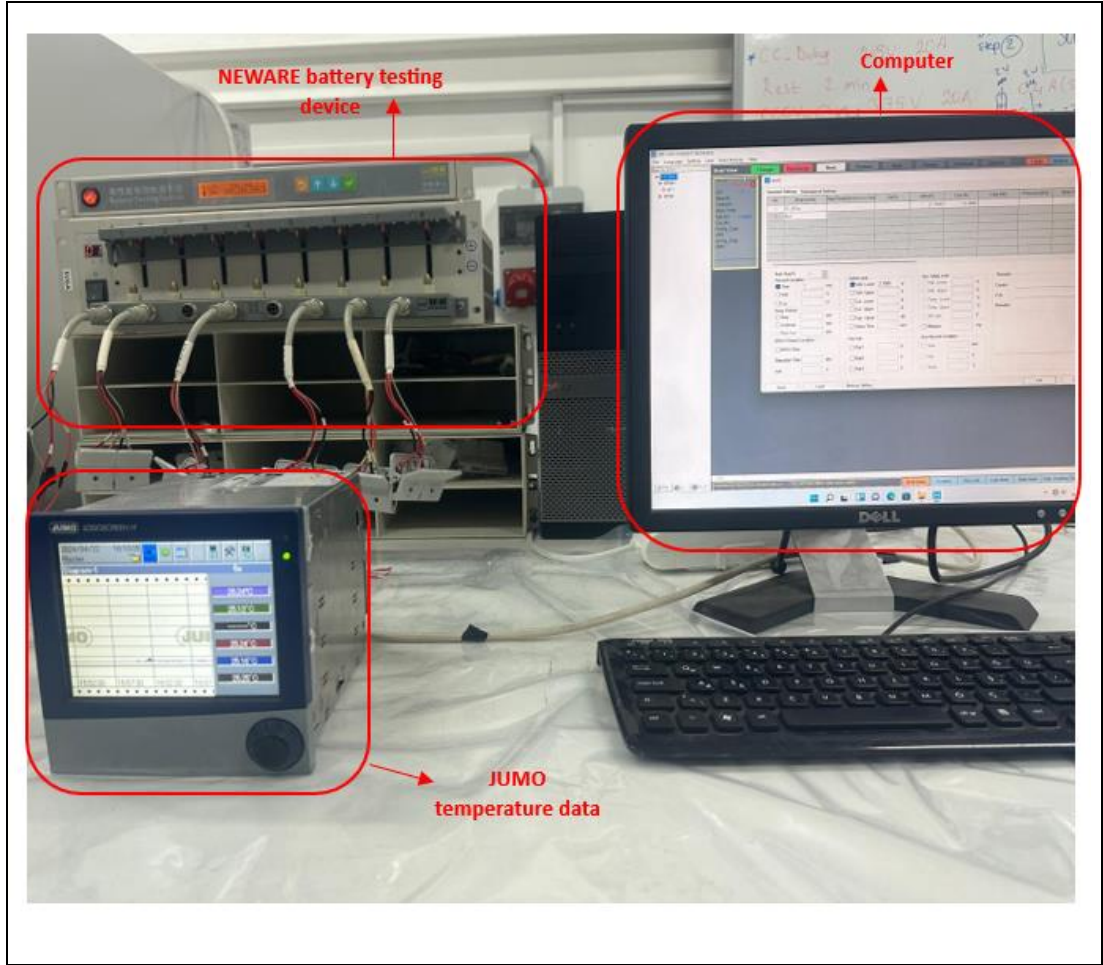


Figure 3.4: Experimental set-up for inside of climatic test cabinet.

In this research, the flow inside the cold plates is turbulent and therefore for turbulence model in ANSYS Fluent was used. The Reynolds number is used to determine the flow regime (laminar or turbulent) and was defined as shown in Eq. (3.1). In this study, $Re = 4436.24$ and therefore the flow is considered turbulent. Calculation of Reynolds number of water was shown below.

Density of water at 25 °C (ρ) = 998 kg/m³

Diameter of water inlet (D) = 0.007 m

Viscosity of water at 25 °C (μ) = 0.00089 Pa.s

Calculated water velocity ($\vec{V}$) = 0.56 m/s

$$Re = \frac{\rho \times \vec{V} \times D}{\mu} = \frac{998 \frac{kg}{m^3} \times 0.56 \frac{m}{s} \times 0.007 m}{0.00089 Pa.s} = 4436.24 \quad (3.1)$$

3.2. Mathematical Modelling

The mathematical models used in this thesis are mentioned in this section.

3.1.1 Battery Model Equations

Heat is produced in a lithium-ion battery cell as a result of electrochemical reactions brought on by charging and discharging. Different amounts of heat are produced as a result of these reactions in the battery's electrodes, current collector, and separator [Kantharaj et al.,2019]. Ohmic resistance causes the electrons to produce heat as they pass through the current collectors. When lithium ions diffuse from the electrolyte into the separator structure and pass through the microporous structure of the separator, they encounter resistance, which causes heat to be produced. The active region, where electrochemical reactions occur, experiences activation and concentration polarizations, which result in heat generation at the electrodes [Kantharaj et al.,2019]. Thus, heat generation in lithium-ion batteries is caused by multiple processes, such as phase change heat, heat of mixing (related to concentration gradients in the electrolyte and active material), and irreversible and reversible heat [Farag et al., 2017]. The primary heat sources that contribute to heat generation in the cell, however, are reversible and irreversible heat [Chen et al., 2017]. The energy balance equation can be written as follows.

$$pC_p \frac{\partial T}{\partial t} = \nabla(k\Delta T) + \dot{q} \quad (3.2)$$

Where p is the density, C_p is the heat capacity ($\text{Jkg}^{-1}\text{C}^{-1}$), T is the temperature ($^{\circ}\text{C}$), t is the time (sec), and k is the thermal conductivity ($\text{W m}^{-1} \text{ }^{\circ}\text{C}^{-1}$), $\dot{q}$ (W/m^3) is the heat source per unit volume in the battery.

$$\dot{q} = \dot{q}_{\text{rev}} + \dot{q}_{\text{pol}} + \dot{q}_{\text{ohm}} \quad (3.3)$$

$\dot{q}$ is equal sum of reversible heat ($\dot{q}_{\text{rev}}$) and irreversible heats: polarization heat ($\dot{q}_{\text{pol}}$), and ohmic heat ($\dot{q}_{\text{ohm}}$). In which, $\dot{q}_{\text{rev}}$ is caused by the entropy change of electrode materials, $\dot{q}_{\text{pol}}$ is related to the polarization voltage during discharge process, and

$\dot{q}_{ohm}$ is derived by the electrical ohmic heat in the solid phase as well as ionic ohmic heat in the electrolyte [Song et al., 2014].

3.1.2 Fluid Flow Equations

As was previously mentioned, the RANS equations (Reynolds Averaged Navier Stokes) are used to model the turbulent flow in this study. This CFD study's primary goal is to produce findings that can be confirmed by experimental measurements. The CFD technique offers a comprehensive data space that complements the experimental results, as the experimental technique only provides point data. The energy equation is also solved since the temperature field is of interest [Panchal et al., 2017]. The governing equations are:

$$\nabla x \bar{V} = 0 \quad (3.4)$$

$$\rho \left[\frac{\partial \bar{V}}{\partial t} + (\bar{V} \cdot \nabla \bar{V}) \right] = -\nabla \bar{p} + (\mu \nabla^2 \bar{V} - \varphi) \quad (3.5)$$

$$\frac{\partial \rho T}{\partial t} + \nabla x [\rho \bar{V} T] = \nabla x \left[\left(\frac{\mu}{Pr} + \frac{\mu_t}{Pr_t} \right) \nabla T \right] \quad (3.6)$$

where ∇ is gradient operator, $\bar{V}$ is the average velocity (m/s), $\vec{V}$ is speed (m/s), P is the pressure (Pa), φ is the Reynolds stress, Pr is the Prandtl number, μ_t is turbulent viscosity (Pa.s), and Pr_t is turbulent Prandtl number.

3.3. Hybrid Pulse Power Characterization (HPPC)

HPPC testing was carried out according to the following steps after the CCCV charging step until 0% charge state and the testing scheme is shown in **Figure 3.5**.

- 1h rest
- Pulse discharge with 0.5C for 10s
- 10min rest
- Pulse charge with 0.5C for 10s
- 10min rest
- 0.2C discharge until lost 5% capacity of cell's capacity

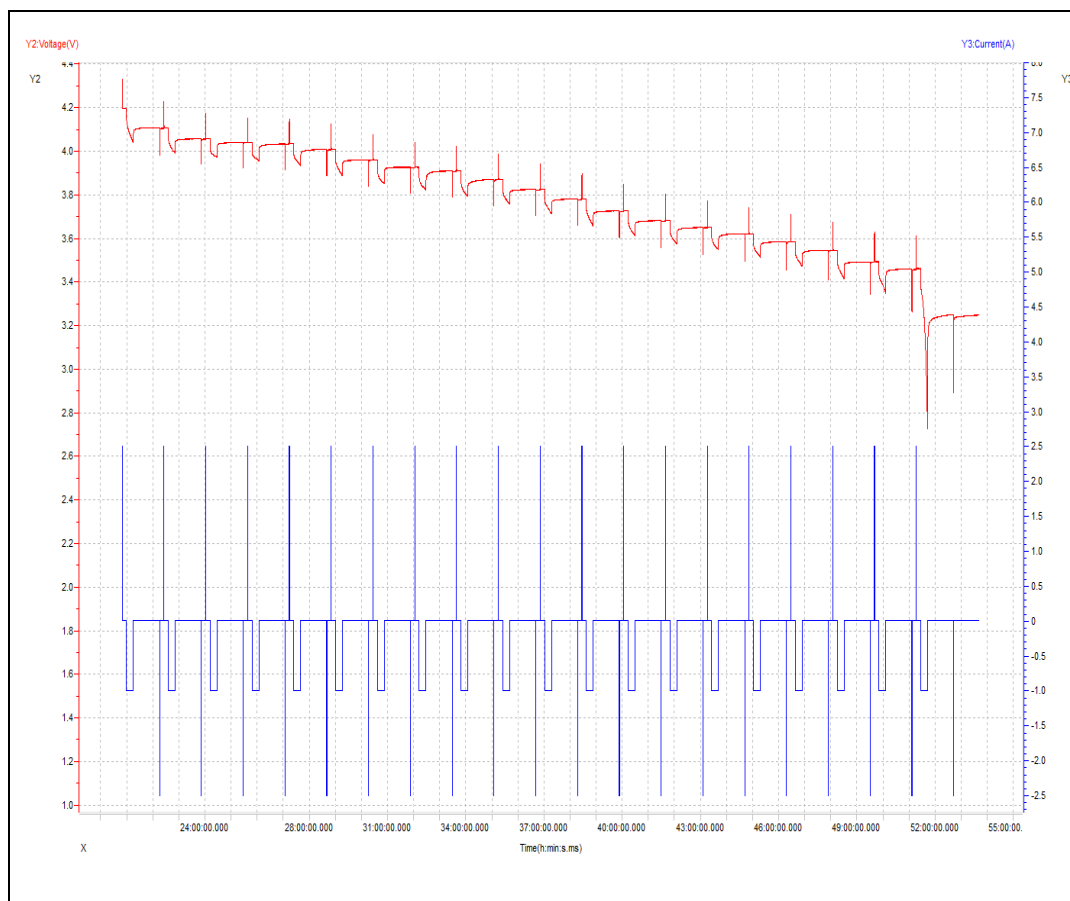


Figure 3.5: HPPC test result.

The pulse discharge with 0.5 C for 10s step performed at 0.99 state of charge is shown in **Figure 3.6** as an example.

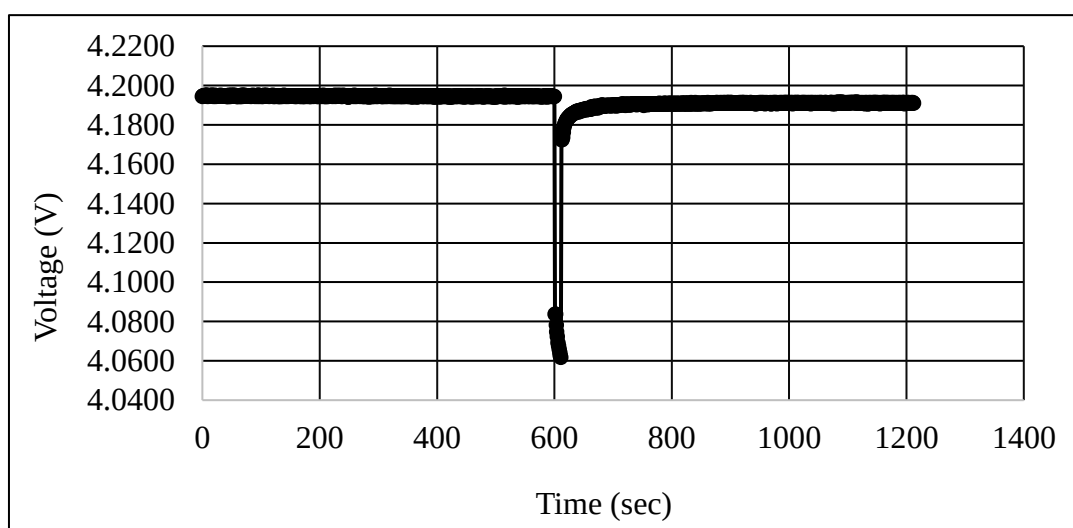


Figure 3.6: Pulse discharge with 0.5C for 10s at 0.99 state of charge.

R_s (ohmic polarization) data obtained from the HPPC test as a function of state of charge is shown in **Figure 3.7**. Resistance is highest at 0.001% charge state. It is interpreted from the graph that the internal resistance is highest at 0.001% SOC.

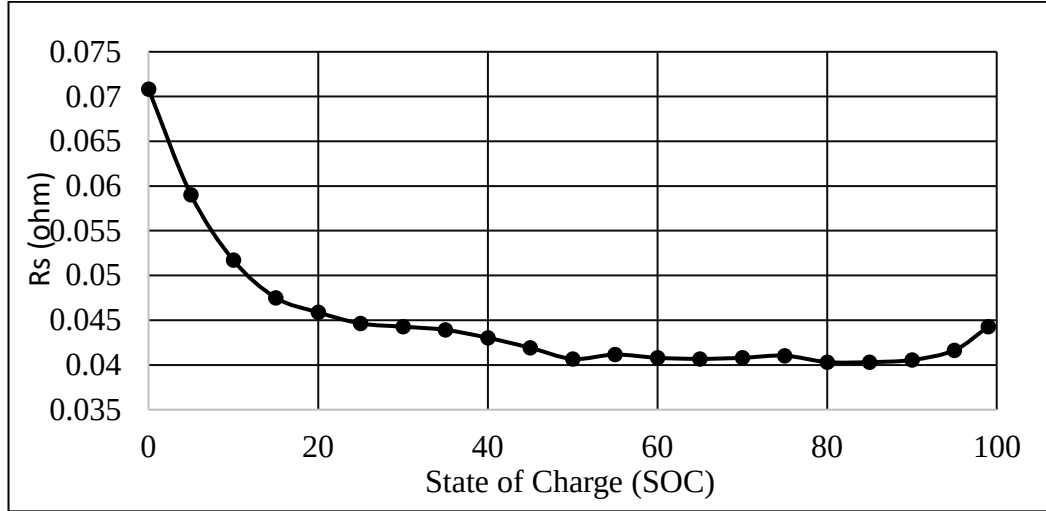


Figure 3.7: R_s values of NMC-polymer Li-ion cell according to SOC.

3.4. Cell Geometry and Thermal Management System Design

In this study, the thermal analysis of a 5 Ah capacity NMC cell at different discharge rates (0.25C, 0.5C and 1C) was carried out in Ansys Fluent software using the ECM model. It is assumed that the ambient temperature and the initial temperature of the battery cell are equal, and its value is 25 °C. In the simulations carried out for the verification study, polyhedral elements were preferred as the numerical mesh structure, and the maximum skewness quality value is 0.28 and the minimum orthogonal quality value is 0.4 with 183050 element size.

The cell is divided into two regions: active and passive. The active region is the part where electrochemical reactions occur. The active area of the battery cell consists of NMC cathode, graphite anode and electrolyte and the cell size are 75x 50x10 mm. The passive region is the part where electricity is transferred. The passive zone consists of battery cell terminals. The size of the terminals is 11.25x 4 x 0.15 mm. The negative terminal material is copper, and the material of the positive terminal is aluminum. Geometric details of the cell are shown in **Figure 3.8**.

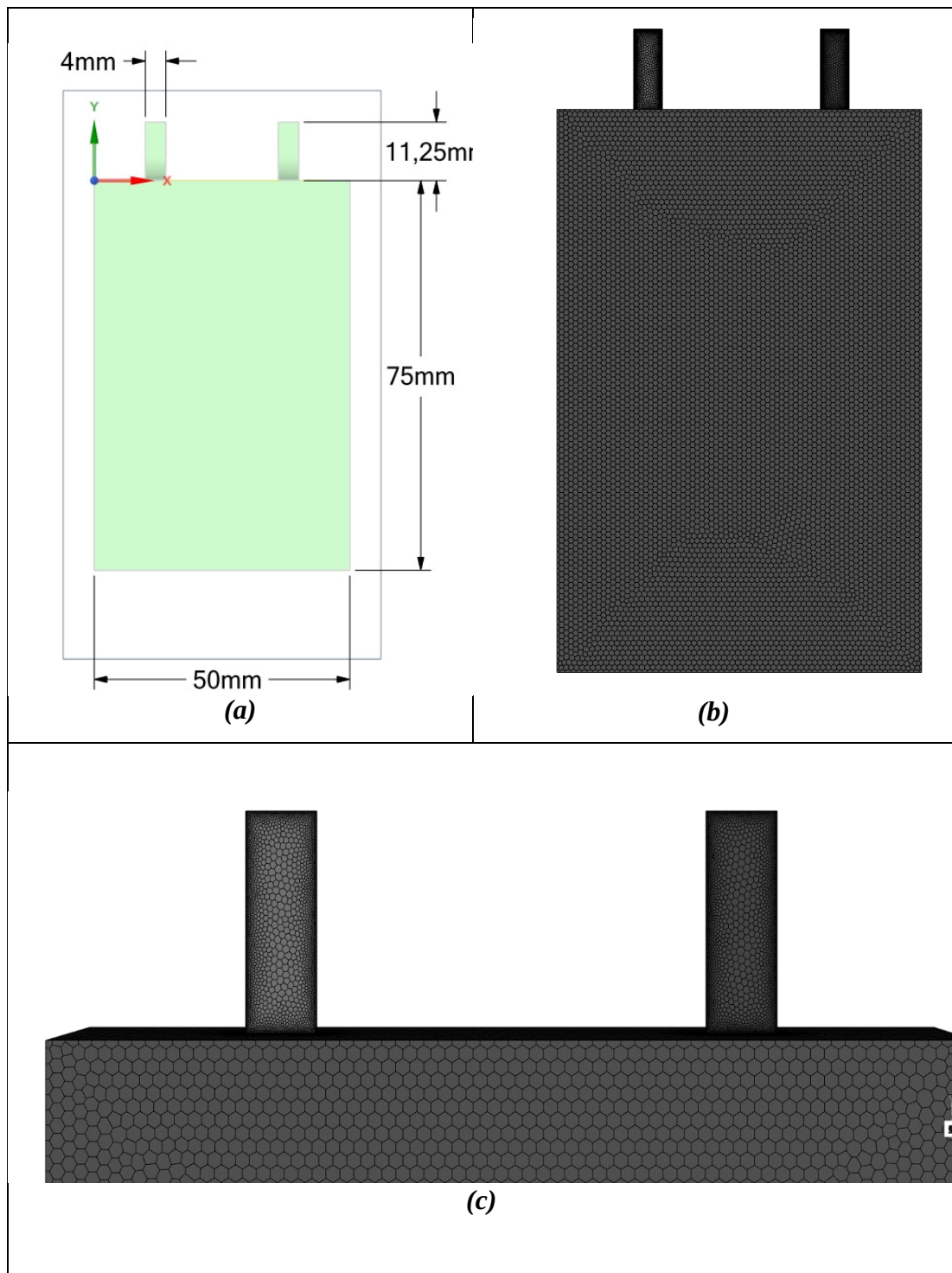


Figure 3.8: Geometric details of cell (a) cell geometry; (b) mesh structure of cell; (c) mesh structure of terminals.

An aluminum cooling plate was used to cool the cell. Geometric details of the cooling plate are given in **Figure 3.9**.

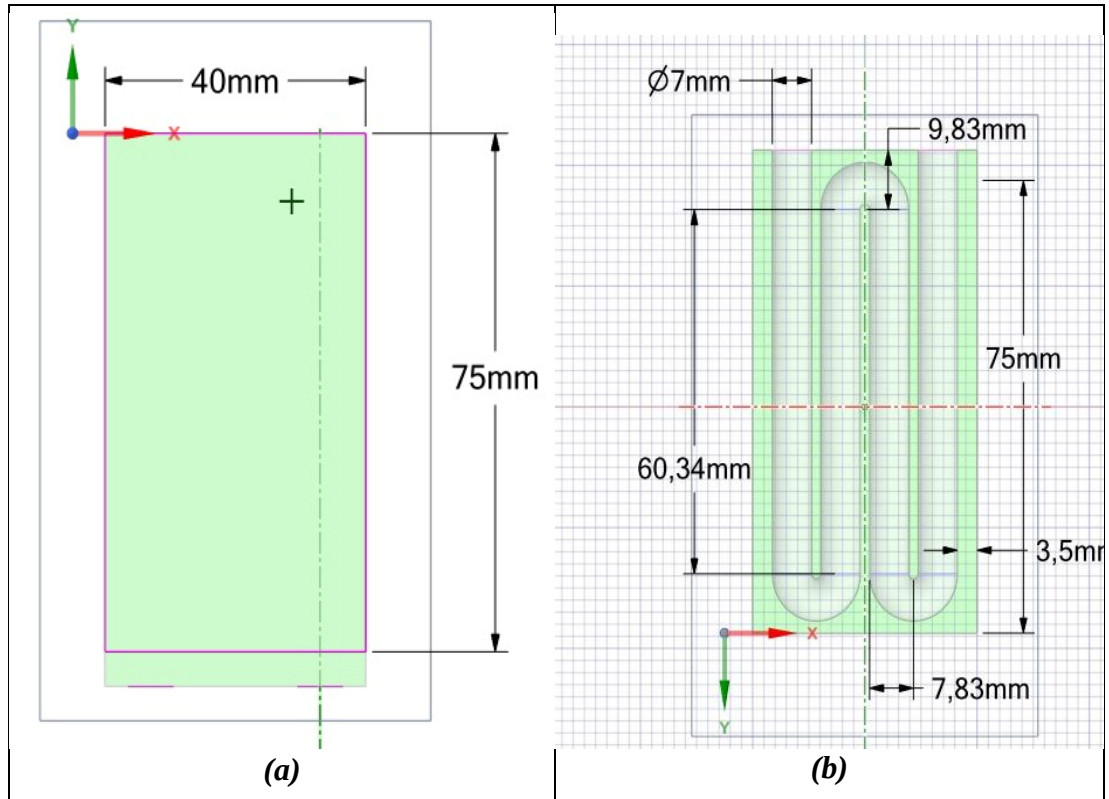


Figure 3.9: Geometric details of the aluminum cooling plate.

Mesh structure and independence study are that one of the most important issues affecting the accuracy of the results in computational fluid dynamics. Our results may vary depending on the number and quality of the mesh we have created. However, creating more than necessary mesh increases our computational cost. To prevent this situation and to eliminate the dependency of the results on the mesh, an independence study from the numerical mesh was carried out and the optimum number of numerical mesh ranges were determined. Ansys Fluent Meshing module was used to create a numerical mesh on the geometry. The most distinctive feature of Fluent meshing is that it creates a local polyhedral mesh type. For this reason, polyhedral mesh technology was used in the battery thermal management geometries studied within the scope of this thesis. The advantage of this element type is that there is more information exchange with neighboring cells, the number of elements is less, and it provides convergence in a shorter time with fewer iterations. However, although it reduces the number of elements, it requires more computer resources because it increases RAM consumption, which is a disadvantage of this element type. In numerical studies, the quality of the mesh is also very important, as well as the number. For this reason, we need to take care that the mesh we create are within certain quality

values. In general, orthogonal and skewness quality criteria express the skewness of our mesh structure.

The mesh independence study for liquid cooling was carried out at a constant discharge rate of 1C in five different element numbers, considering the situation in which water was used as the cooling medium, and the highest temperatures occurring on the cell were compared. The results of the study are given in **Table 3.2**, and the quality criteria of each mesh are summarized.

Table 3.2: Mesh indepenence study results.

Element number	Min Orthogonal	Max.Skewness	Max. Temperature
541791	0.502	0.382	30.99
652245	0.501	0.389	30.85
960383	0.501	0.389	30.85
1634691	0.502	0.378	30.85
3220062	0.503	0.38	30.85

In the analyzes performed on different element numbers, it is seen that the highest temperature value on the cell does not change after the number of elements 652245.

Figure 3.10 and **Figure 3.11** and **Figure 3.12**. shows the polyhedral mesh structure of BTMS with liquid having 3220062 elements.

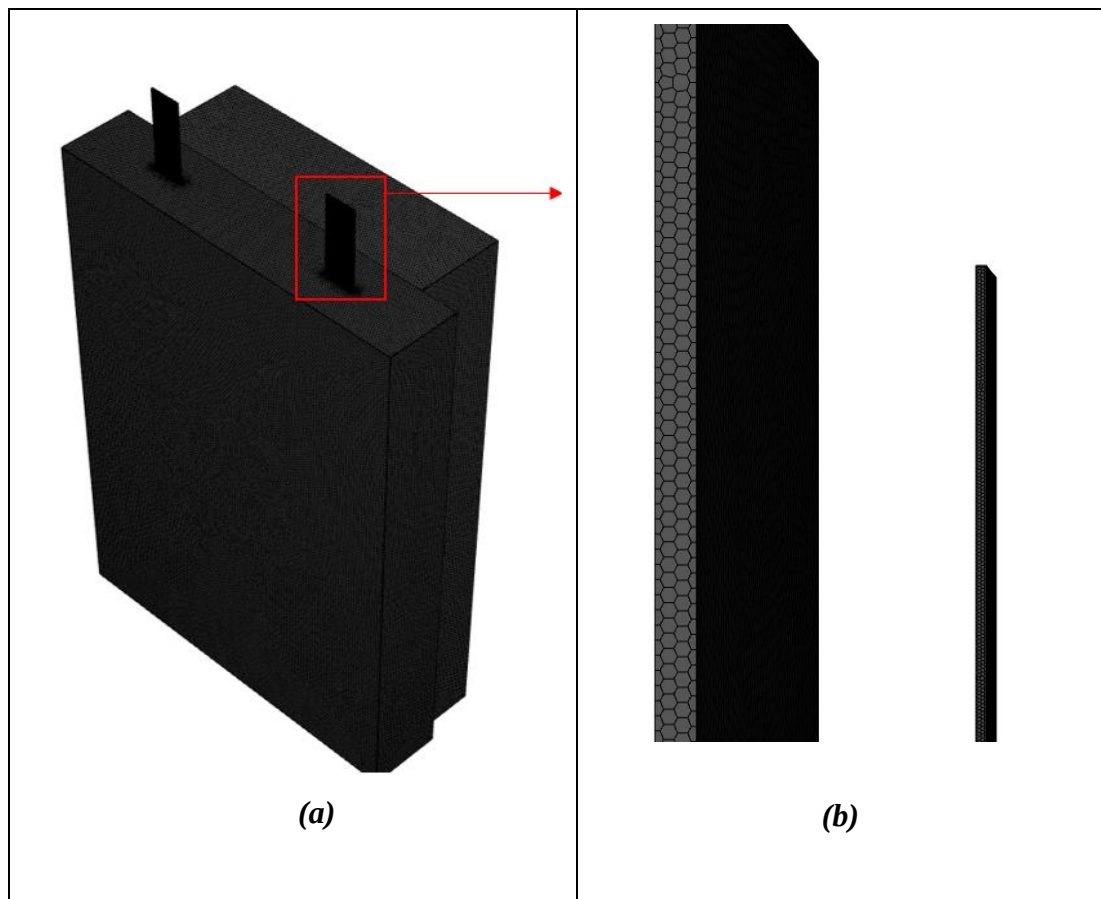


Figure 3.10: Polyhedral mesh structure of BTMS (a) BTMS mesh structure; (b) terminal's mesh structure.

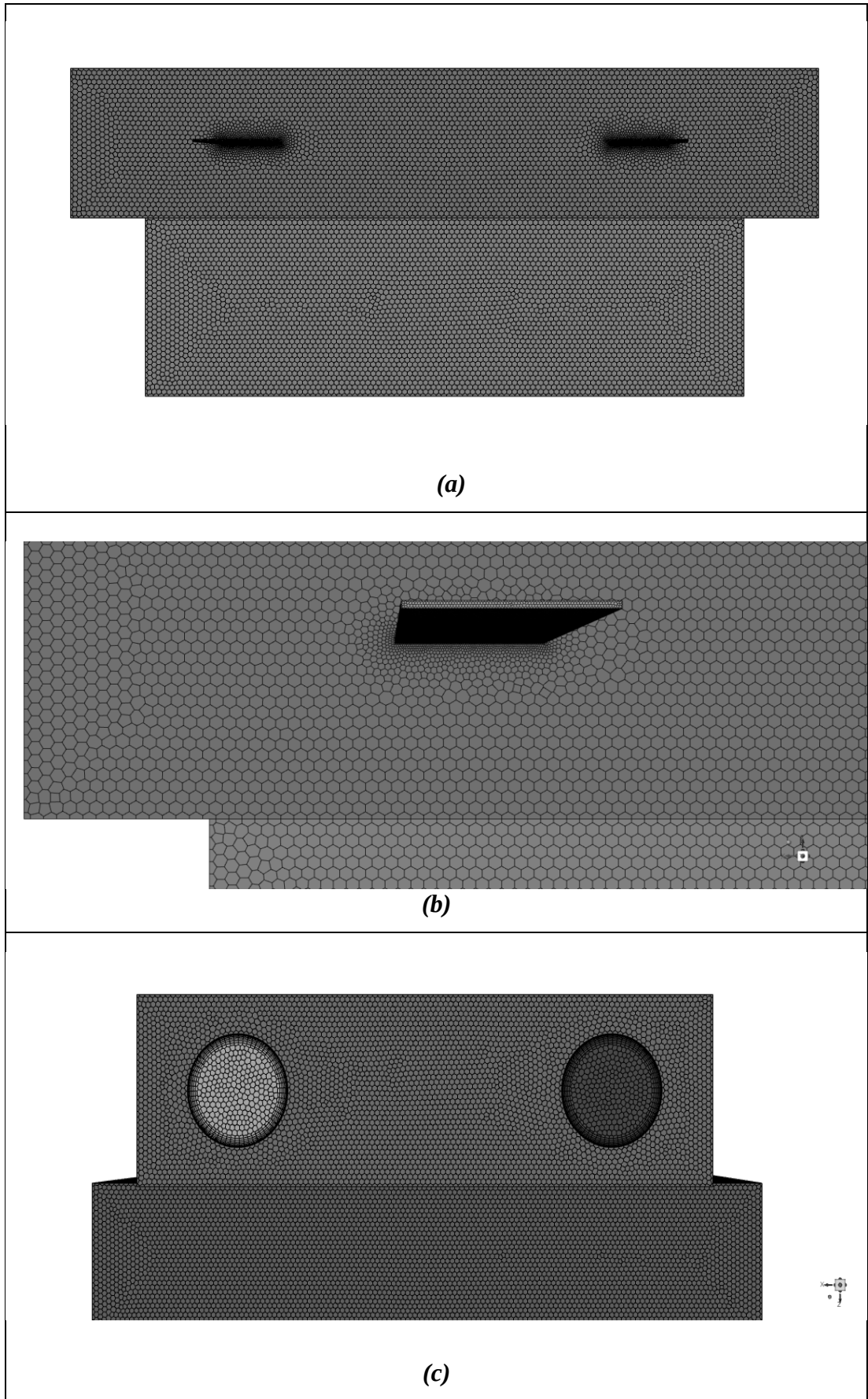


Figure 3.11: Polyhedral mesh structure of BMTS (a) top; (b) terminal's top; (c) bottom .

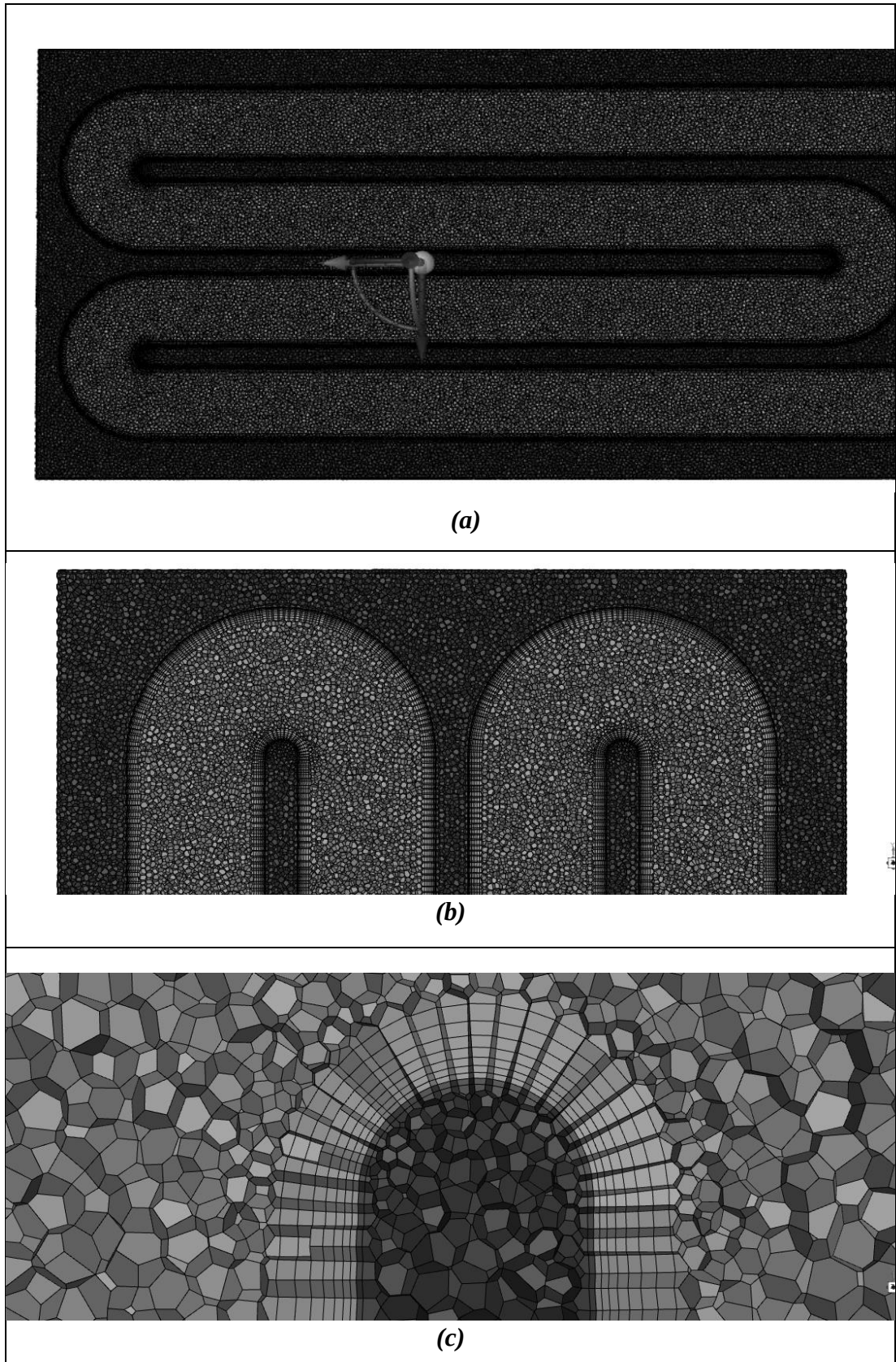


Figure 3.12: Polyhedral mesh structure of serpentine flow channel (a) channels; (b) return section; (c) mesh structure in flow and solid-regime transition.

3.5. Boundary Conditions

In this thesis study, coupled algorithm is used as the solution method. Coupled algorithm refers to the solution algorithm used to solve equations of flow, heat transfer, and other physical phenomena such as chemical reactions or multiphase flows. The coupled solution algorithm solves equations for different physical events simultaneously rather than separately or sequentially. In other words, it solves continuity equations based on momentum and pressure together. This situation better expresses the interaction between different physical events. This can lead to more accurate results but also requires more computational resources. However, simulations were carried out by choosing second-order discretization of pressure and other discretization schemes.

The flow variables are averaged at all scales of the turbulence to be modelled using a RANS-based modeling approach. Fluent provides two fundamental turbulence models based on RANS: K-Omega and K-Epsilon, in that order. The most widely used turbulence model is the K-Epsilon model because of its simplicity and resilience. The standard K-Epsilon model, the Realisable model, and the Renormalization Group (RNG) model are the three primary K-Epsilon model variations that are offered by Fluent. Their differences include the methods of calculating the production and destruction terms in the epsilon equation, the determination of turbulent Prandtl numbers, and the techniques for calculating turbulent viscosity. The Standard model uses fixed parameters, while the Realizable model uses dynamic and more realistic parameters, and the RNG model performs more detailed and precise calculations [Khasow et al., 2014].

The standard K-omega model and Menter's shear stress transport model (SST) are two additional variations of the K-omega turbulence model. The transport equations for k and ω are the same in both models. The SST model, however, deviates from the standard model in two significant ways: (1) it considers the transport effects of the fundamental turbulent shear stress, and (2) it smoothly moves from the inner to the outer region of the boundary layer.

The dimensionless parameter y^+ calculates the separation between the surface and the first grid cell. The value of y^+ must lie between 1 and 30 in order to accurately simulate turbulent flows. The first grid cell is outside the viscous sublayer, or too far away from

the solid surface, if the value of y^+ is greater than 30, which causes errors when documenting the flow behavior within the boundary layer. On the other hand, an incorrect simulation of the turbulent behavior near the boundary layer may occur if the y^+ value is less than 1, because the first grid cell is too close to the solid surface and is located within the laminar sublayer [Panchal et al., 2017]. In this study, a y^+ value of 2 was chosen, with the first grid cell height set at 0.043 mm.

The parameters chosen for the model development are as follows; viscous model: k-epsilon, Realizable, Enhanced wall treatment; thermal effects: turbulent intensity of 1%, ; solver: type: pressure based; velocity: absolute velocity; residuals convergence variables: X-velocity, Y velocity, Z velocity, energy, continuity equation; convergent criteria: 0.000001 residual; 1st - 2nd order: 2nd order; enhanced wall treatment (y^+)=2; solution method: Coupled.

The external walls of the battery cell are subject to a convective boundary condition. The heat emitted from the battery cell to the environment per unit area q_a (W.m⁻²) is calculated with the following equation 3.7, using Newton's cooling law.

$$q_a = h_a(T_{bm} - T_a) \quad (3.7)$$

T_{bm} represents the average temperature, T_a represents the ambient temperature and h_a represents the heat transfer coefficient. For this study, the heat transfer coefficient is accepted as 10 (W.m⁻². K⁻¹) and the ambient temperature is 25 °C.

Analyzes of the battery cell were carried out using the ECM model. In this study, the battery cell with a nominal capacity of 5 Ah was solved at three different discharge rates: 0.25 C, 0.5 C and 1 C. **Table 3.3** summarizes the details of the ECM model parameters [Sacchetti et al., 2020].

Table 3.3: ECM model parameters.

Model Properties	Value	Unit
Electrical Conductivity for Uds0 ; Uds1	$3.774.10^7$; $5.998.10^7$	[S/m]
Through and In Plane Thermal Conductivity	30.04 and 1.70	[W/Mk]
Density	1853.2	[kg/m ³]
Heat Transfer Coefficient	10	[W/m ² K]
Heat Capacity	987.01	[J/kgK]

3.6. Machine Learning Methods

Five statistical indices, including R^2 , MAE, RMSE and MSE, were used comparison of the results. 5-fold cross-validation was selected.

R-squared (R^2) is a measure of how well a regression model explains the variance (predicted value) of the dependent variable. It basically shows how well the model fits the data. The R^2 value varies between 0 and 1.

The mean square difference between the actual observed results and the results predicted by the model is measured by the Mean Square Error, or MSE. The squaring of the differences makes it penalize larger errors more severely.

The square root of the mean square error is known as the root mean square error, or RMSE. calculates the forecast errors' standard deviation (residuals). Because RMSE is expressed in the same unit as the original values, it is easier to understand.

The average magnitude of prediction errors within a range is measured by the Mean Absolute Error (MAE), which does not take direction into account. The mean of the absolute discrepancies between the actual and anticipated values is what it is. Equations (3.8) to (3.11) describe the formulation of R^2 , MAE, RMSE and MSE [Moayedi et al., 2020].

$$R^2 = 1 - \frac{\sum_{i=1}^s (Y_{i_{predicted}} - Y_{i_{observed}})^2}{\sum_{i=1}^s (Y_{i_{observed}} - \bar{Y}_{observed})^2} \quad (3.8)$$

$$MAE = \frac{1}{N} \sum_{l=1}^s |Y_{l_{observed}} - Y_{l_{predicted}}| \quad (3.9)$$

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^s [(Y_{i_{observed}} - Y_{i_{predicted}})]} \quad (3.10)$$

$$MSE = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y})^2 \quad (3.11)$$

4. RESULT AND DISCUSSION

Within the scope of this research, the average temperature of the 5 Ah capacity NMC polymer cell, measured from 5 different places during the discharge process, was numerically analyzed using the computational fluids software called Ansys Fluent and compared with experimental solutions. The maximum temperature data obtained because of the discharge process performed at different current rates and charging ranges were collected in Ansys Fluent and tried to be estimated using different machine learning algorithms. Then, in liquid cooling using an aluminum cooling plate, the focus was on the optimum operating temperature range required for the safe and healthy operation of the cell. For this purpose, various analyzes were carried out with different parameters and finding are explained in detail in this section.

4.1. Thermal Performance of Battery Cell

In this section, the thermal behavior of a 5 Ah NMC polymer cell without a cooling strategy under different discharge rates of 0.25C, 0.5C and 1C was examined.

4.1.1 Effect of Discharge Rate on Battery Cell Temperature

Figure 4.1 shows that change of temperature in the battery cell over time under different discharge-Crates in experimental and numeric studies. C rate is defined as a measure of the discharge rate of a battery relative to its capacity. In other words, the higher the C ratio, the more current is drawn and therefore the battery cell discharges in a shorter time. On the other hand, at higher discharge rates, losses (polarization and IR) will increase as more current is extracted from the battery cell. For this reason, as the discharge rate increases, the maximum temperature in the battery cell increases.

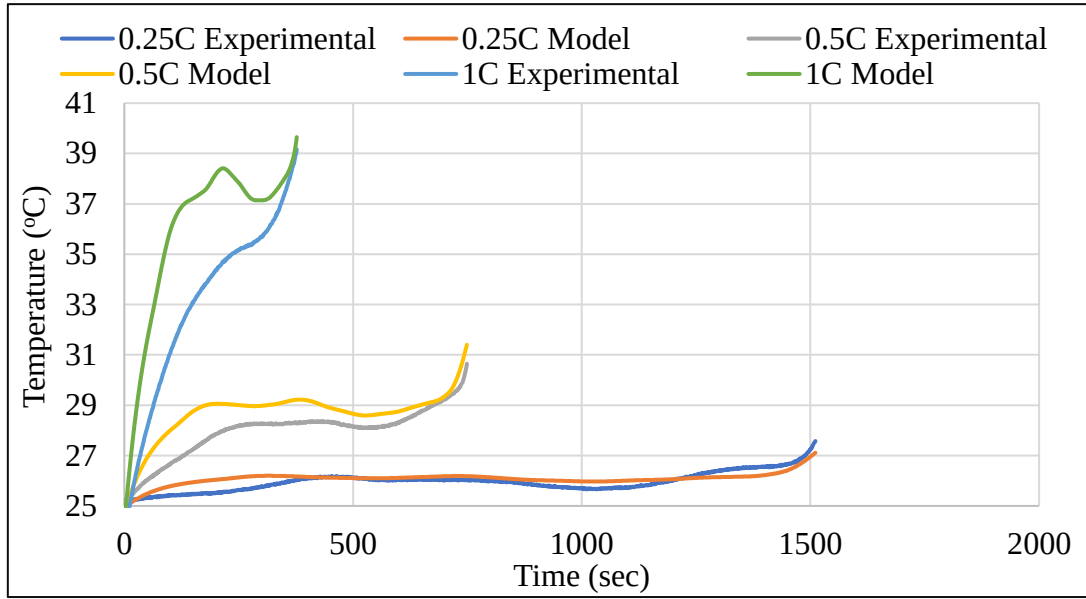


Figure 4.1: Temperature changes of NMC-polymer cell during discharge.

Figure 4.2 shows that change of voltage in the battery module over time under different discharge rates in experimental and numerical studies.

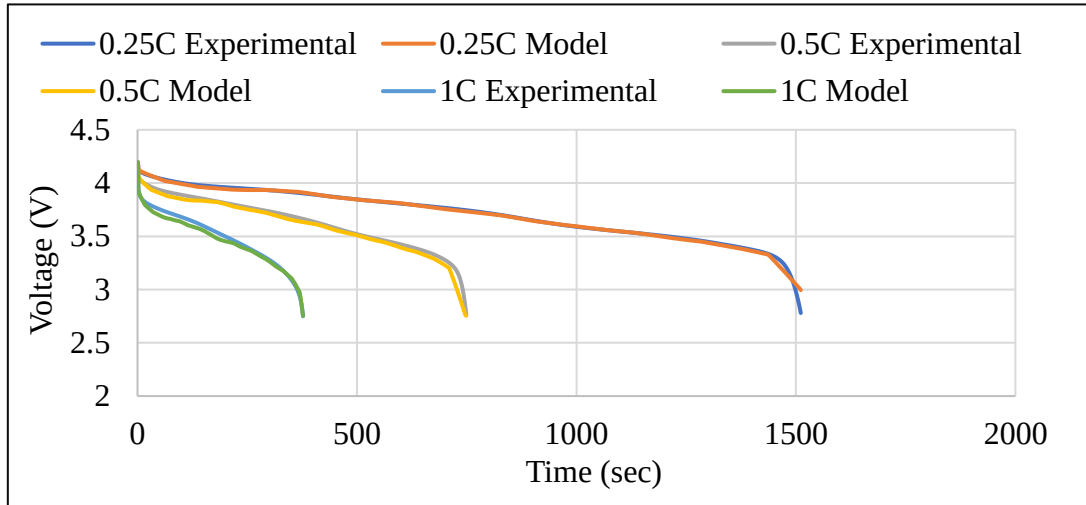


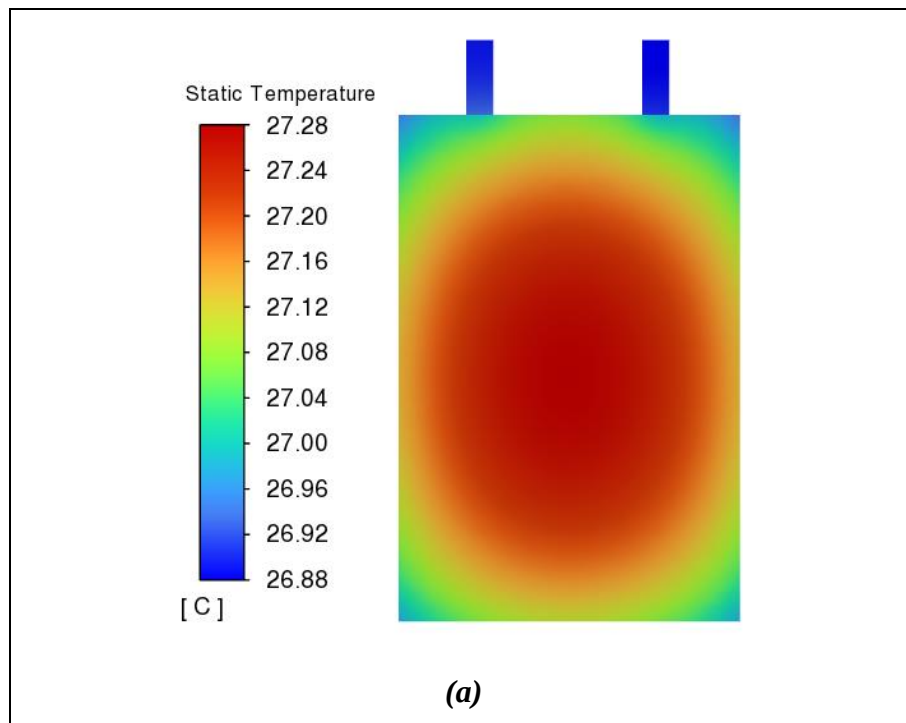
Figure 4.2: Voltage changes of NMC-polymer cell during discharge.

According to increasing discharge C-rate, temperature and voltage datum obtained from experimental and numerical are shown in **Table 4.1**. The test was repeated three times for each C-rate. The numerical model shows good agreement with experimental test data.

Table 4.1: Test results.

	Average Temperature (°C)		Voltage (V)		Standard Deviation
C-rate	Experimental	Numeric	Experimental	Numeric	Experimental
0.25	27.58	27.11	2.77	2.99	0.2
0.5	30.65	31.4	2.76	2.75	0.3
1	39.16	39.65	2.75	2.75	0.2

The uneven distribution of temperature inside the battery cell is another significant factor that influences how well batteries operate. This results in power reduction, performance loss, electrical imbalances in the battery, and a shorter lifespan. **Figure 4.3** displays the temperature distribution on the battery cell. The middle points of the active zone of the battery cell have the highest temperature. Additionally, it has been noted that as the discharge rate increases, the temperature difference within the battery cell also increases. It can be observed that the temperature distribution in the battery cell becomes more irregular as the C ratio rises.



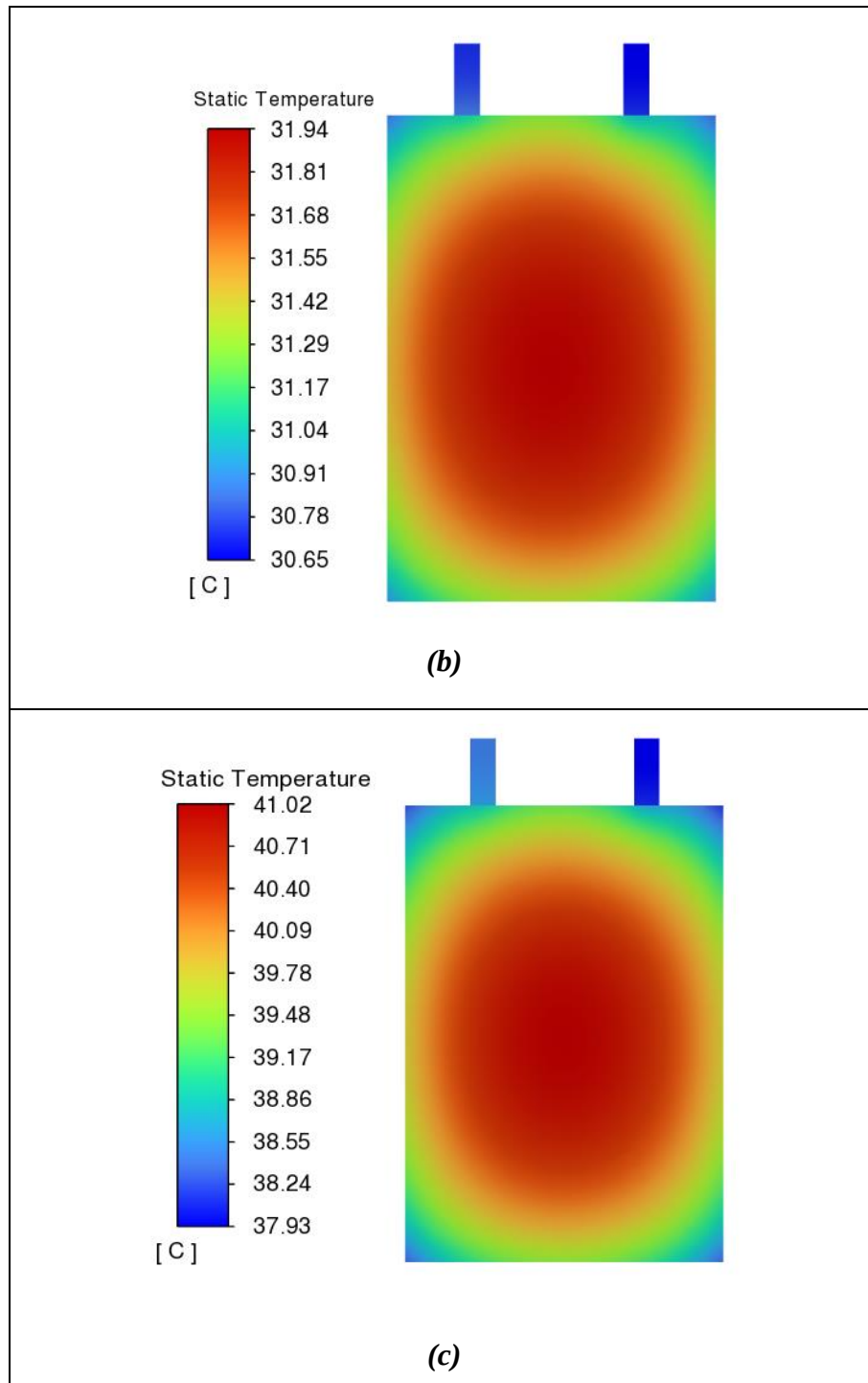
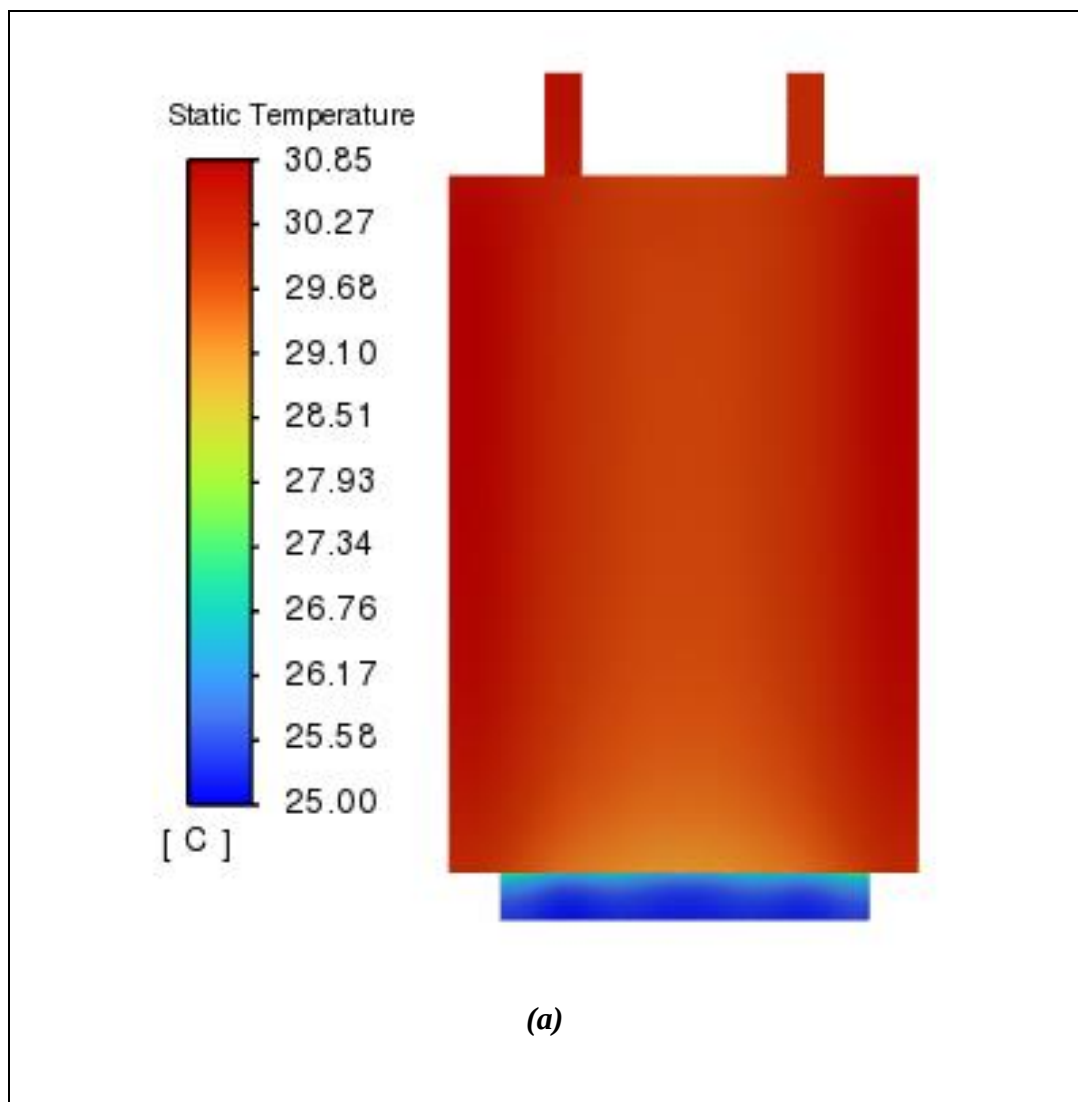


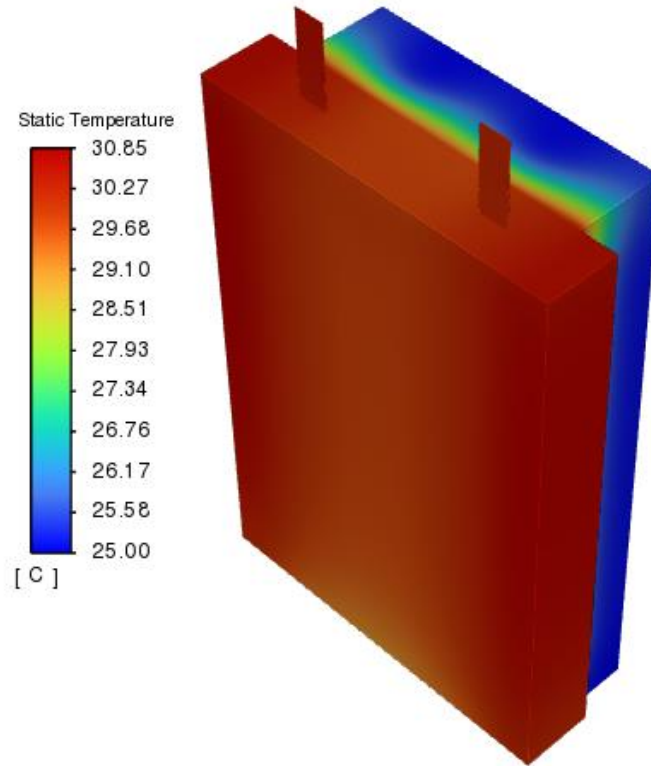
Figure 4.3: Temperature distribution of battery module at different discharge rates (a) 0.25 C; (b) 0.50 C; (c) 1C.

4.1.2 Effect of Liquid Cooling System on Battery Cell Temperature

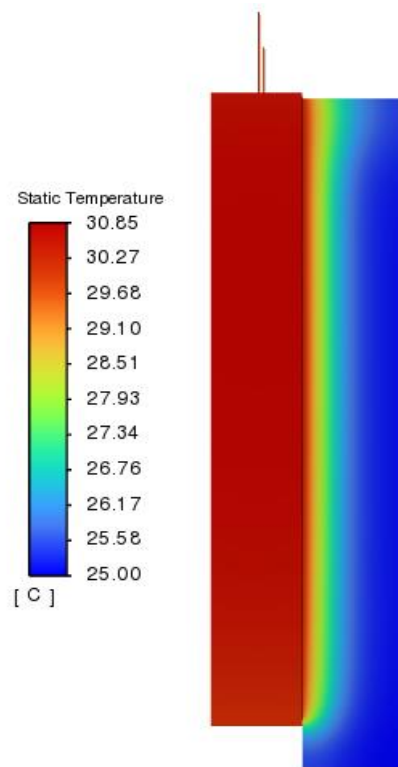
A liquid cooling and battery thermal management system was designed and its cooling performance was examined in order to maintain the 5 Ah capacity NMC polymer cell in the ideal operating temperature range during 1C discharge. In this section, the research findings are presented in detail.

Figure 4.4 shows that effect of liquid cooling and battery management system on the temperature distribution on the cell. A more uniform temperature distribution was obtained on the cell.





(b)



(c)

Figure 4.4: Liquid cooling system performance on battery cell temperature.

The velocity and wall shear vector profiles of water passing through serpentine channel in the aluminum cooling plate are shown in **Figure 4.5**. It is seen that the velocity and wall shear parameters increase in the return section of the serpentine channels.

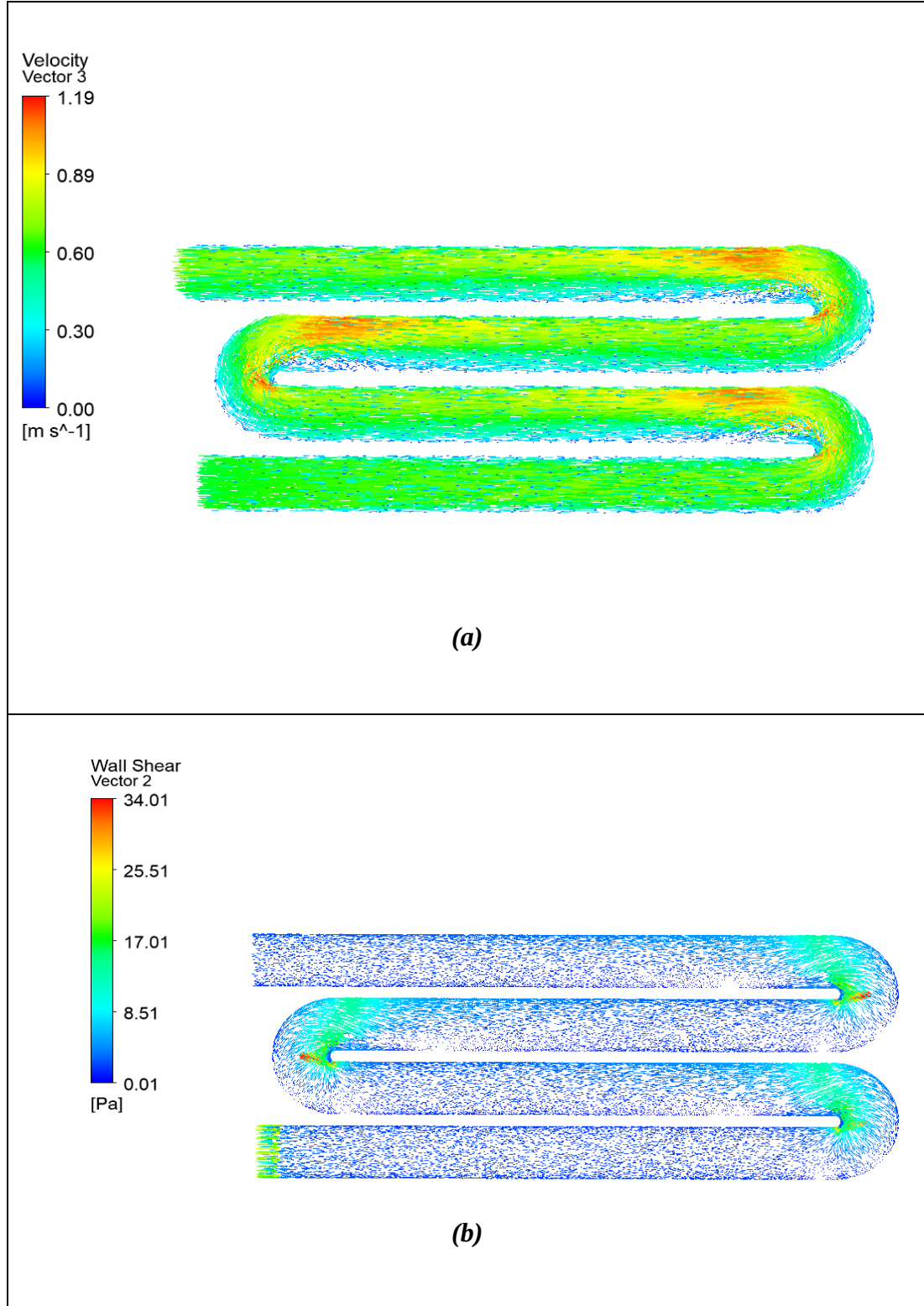


Figure 4.5: Flow characterization in serpentine channels (a)velocity; (b)wall shear vector.

Figure 4.6 and **Figure 4.7** show that change in voltage and temperature in the cell over time under 1C discharge rate in experimental and numeric studies, respectively. 2.75 V and 29.88 °C were obtained from experimental study. 2.65 V and 29.63 °C were obtained from numeric study. The test was repeated three times. Standard deviation is 0.1. The numerical model shows good agreement with experimental test data.

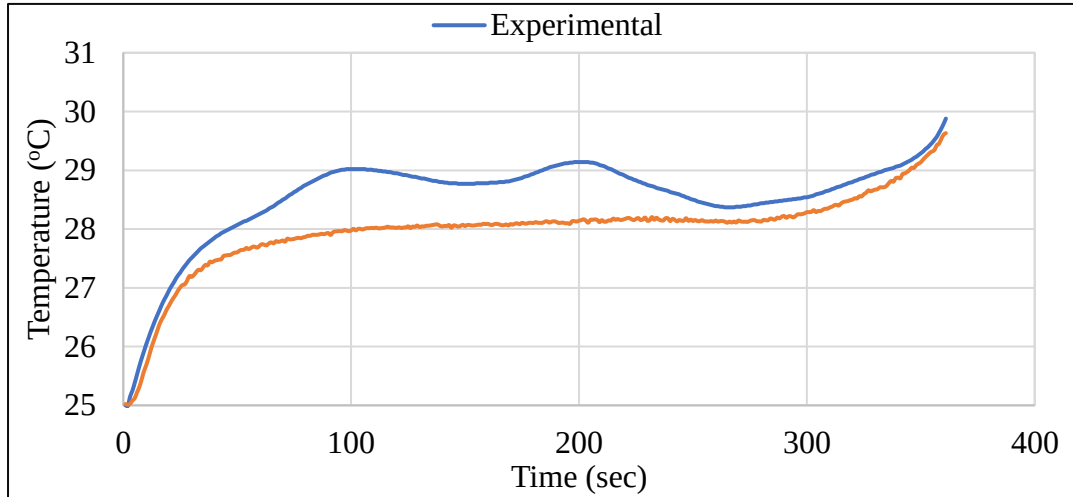


Figure 4.6: Temperature change result during discharge with liquid cooling system.

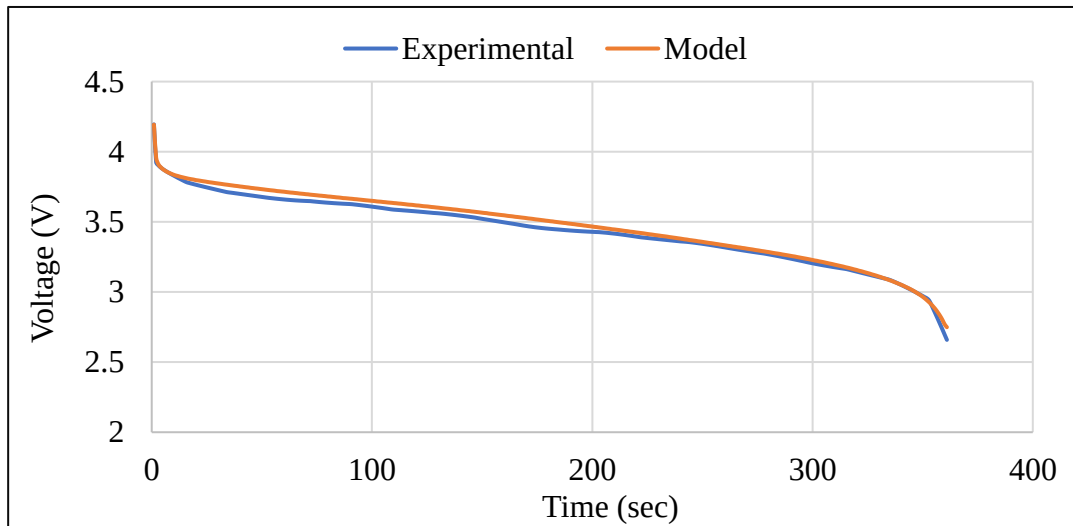


Figure 4.7: Voltage change result during discharge with liquid cooling system.

4.1.3 Temperature Estimation of Battery Cell at Different C-rate and SOC

Table 4.2 shows maximum temperature on cell from FLUENT at different C rate and SOC.

Table 4.2: Maximum temperature of battery cell at different C-rate and SOC.

No.	Akim (X1)	MAX SOC (X2)	MIN SOC (X3)	MAX TEMP (Y1)
1	0.25	0.99	0.0	27.28
2	0.25	0.99	0.1	26.28
3	0.25	0.90	0.0	27.08
4	0.25	0.90	0.1	26.27
5	0.25	0.90	0.2	26.15
6	0.25	0.90	0.3	26.06
7	0.25	0.80	0.0	27.1
8	0.25	0.80	0.1	26.27
9	0.25	0.80	0.2	26.15
10	0.25	0.80	0.3	26.06
11	0.25	0.70	0.0	27.12
12	0.25	0.70	0.1	26.27
13	0.25	0.70	0.2	26.16
14	0.25	0.70	0.3	26.06
15	0.25	0.60	0.0	27.14
16	0.25	0.60	0.1	26.27
17	0.25	0.60	0.2	26.16
18	0.25	0.60	0.3	26.06
19	0.25	0.99	0.2	25.96
20	0.25	0.99	0.3	26.06
21	0.5	0.99	0.0	31.94
22	0.5	0.99	0.1	29.35

Table continues

23	0.5	0.90	0.0	30.71
24	0.5	0.90	0.1	29.32
25	0.5	0.90	0.2	28.93
26	0.5	0.90	0.3	28.84
27	0.5	0.80	0.0	30.78
28	0.5	0.80	0.1	29.32
29	0.5	0.80	0.2	28.94
30	0.5	0.80	0.3	28.83
31	0.5	0.70	0.0	30.84
32	0.5	0.70	0.1	29.33
33	0.5	0.70	0.2	28.93
34	0.5	0.70	0.3	28.8
35	0.5	0.60	0.0	30.91
36	0.5	0.60	0.1	29.33
37	0.5	0.60	0.2	28.91
38	0.5	0.60	0.3	28.7
39	0.5	0.99	0.2	28.96
40	0.5	0.99	0.3	28.82
41	0.75	0.99	0.0	35.99
42	0.75	0.99	0.1	33.94
43	0.75	0.90	0.0	35.48
44	0.75	0.90	0.1	33.86
45	0.75	0.90	0.2	33.31
46	0.75	0.90	0.3	33.43
47	0.75	0.80	0.0	35.66
48	0.75	0.80	0.1	33.87
49	0.75	0.80	0.2	33.28
50	0.75	0.80	0.3	33.32

Table continues

51	0.75	0.70	0.0	35.83
52	0.75	0.70	0.1	33.86
53	0.75	0.70	0.2	33.2
54	0.75	0.70	0.3	33.11
55	0.75	0.60	0.0	36.01
56	0.75	0.60	0.1	33.8
57	0.75	0.60	0.2	32.98
58	0.75	0.60	0.3	32.56
59	0.75	0.99	0.2	33.34
60	0.75	0.99	0.3	33.42
61	1	0.99	0.0	41.02
62	1	0.99	0.1	38.92
63	1	0.90	0.0	40.58
64	1	0.90	0.1	38.8
65	1	0.90	0.2	38.24
66	1	0.90	0.3	38.65
67	1	0.80	0.0	40.7
68	1	0.80	0.1	38.79
69	1	0.80	0.2	38.1
70	1	0.80	0.3	38.3
71	1	0.70	0.0	40.94
72	1	0.70	0.1	38.68
73	1	0.70	0.2	37.83
74	1	0.70	0.3	37.71
75	1	0.60	0.0	40.98
76	1	0.60	0.1	38.45
77	1	0.60	0.2	37.22
78	1	0.60	0.3	36.42

Table continues

79	1	0.99	0.2	38.32
80	1	0.99	0.3	38.73
81	1.5	0.99	0.0	50.92
82	1.5	0.99	0.1	45.47
83	1.5	0.90	0.0	49.66
84	1.5	0.90	0.1	45.27
85	1.5	0.90	0.2	44.36
86	1.5	0.90	0.3	45.06
87	1.5	0.80	0.0	49.82
88	1.5	0.80	0.1	45.21
89	1.5	0.80	0.2	44.17
90	1.5	0.80	0.3	44.63
91	1.5	0.70	0.0	49.9
92	1.5	0.70	0.1	45.05
93	1.5	0.70	0.2	43.78
94	1.5	0.70	0.3	43.75
95	1.5	0.60	0.0	49.91
96	1.5	0.60	0.1	44.66
97	1.5	0.60	0.2	42.88
98	1.5	0.60	0.3	41.81
99	1.5	0.99	0.2	44.46
100	1.5	0.99	0.3	45.14

This section focuses primarily on evaluating how well four common machine learning tools—GPR, SVM, LR, and NN—estimate the maximum battery cell temperature. Three input factors—the maximum, minimum, and C-rate SOC values—were chosen for this purpose. The ANSYS FLUENT supplied the input database. The calculated values of R^2 , MAE, RMSE and MSE for estimating the response are tabulated in **Table 4.3**

Table 4.3: The results of proposed networks based on several statistical indexes.

Proposed models	Network results			
	R2	MAE	RMSE	MSE
GPR	0.9956	0.317	0.4686	0.2196
NN	0.9945	0.3262	0.5247	0.2753
SVM	0.9896	0.5818	0.7212	0.5202
LR	0.9776	0.8491	1.0489	1.1003

The GPR technique can be introduced as the outstanding model, due to the results obtained for it. Also, NN can be introduced as the second accurate model, respectively. Furthermore, The lowest training rate is obtained for the LR model due to its lowest testifying outputs.

Also, the correlation between the predicted and true values of responses is depicted in **Figure 4.8**. According to **Figure 4.8**, the GPR solution produced the outputs that are closest to the actual values of responses in dataset ($R^2=0.99$) phases.

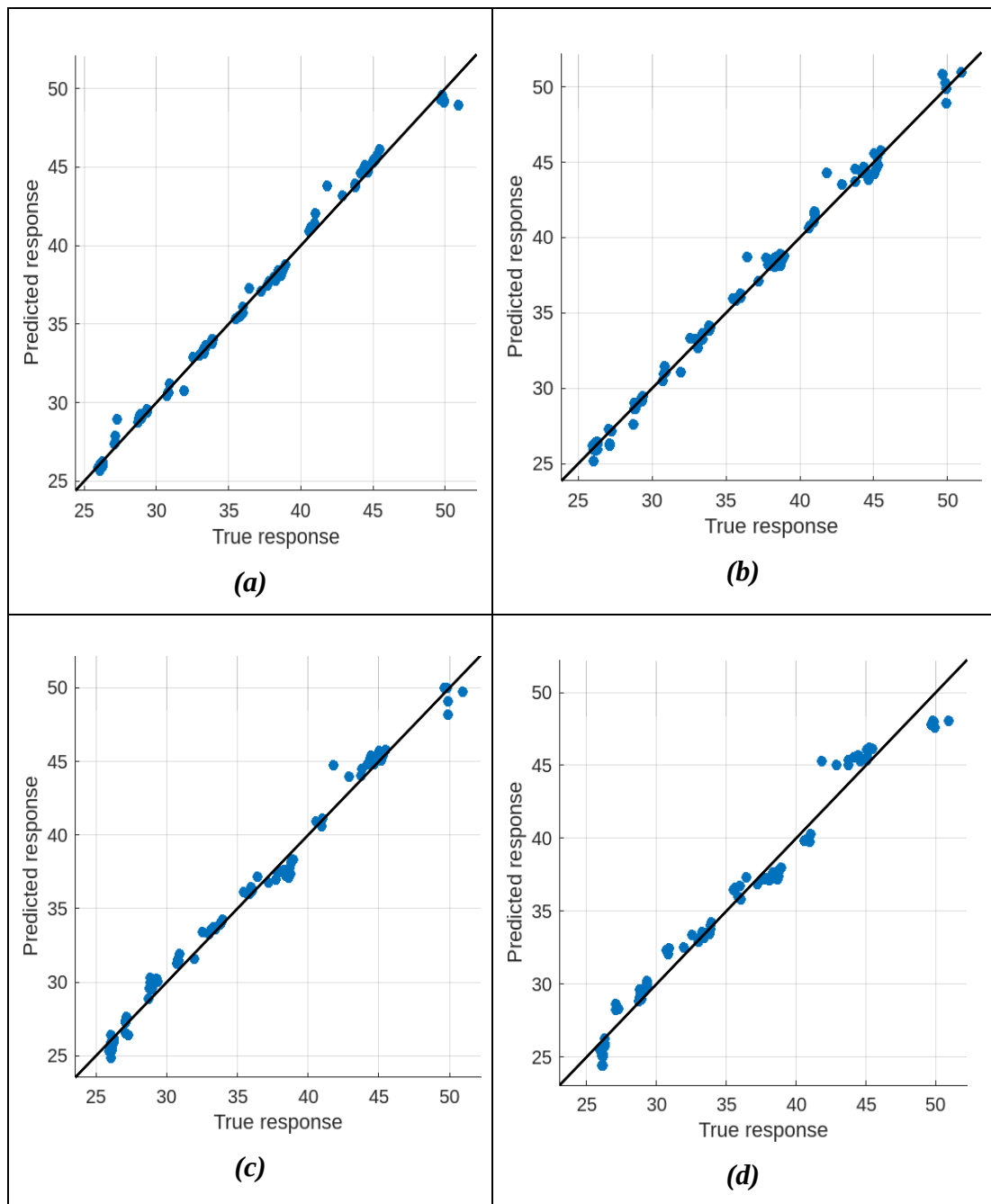


Figure 4.8: Correlation between the predicted and true values of responses.

5. CONCLUSION

One of the elements influencing lithium-ion battery performance is temperature. Higher or lower temperatures have a significant impact on battery performance. The ideal operating temperature range is between 15 °C - 35 °C. Thermal runaway can occur when lithium-ion batteries undergo misuse or are exposed to high temperatures, as these conditions accelerate various reactions and increase heat generation. When thermal runaway happens in a single battery, it is simple to spread the heat to the other batteries. Eventually, the battery pack as a whole fails, catches fire, or even explodes. Consequently, effective thermal management becomes critical for maintaining battery performance and ensuring safety throughout the battery's lifecycle. Thermal behavior of the energy storage system before use or production can be simulated using ANSYS FLUENT. Unfortunately, the chemical recipe of commercially purchased energy storage systems is unknown, which may limit modeling. However, the character of the system can be determined with HPPC testing and the system can be simulated with the ECM model. On the other hand, simulating in CFD takes a long time. ML based models such as neural networks have gained validity in predicting complex multi-parameter, linear and nonlinear problems with large amounts of relevant available data.

This study modeled and experimentally verified the thermal behavior of 5 Ah NMC-polymer cell at 25 °C ambient temperature and 0.25 C, 0.5C and 1C discharge currents using the ECM model in ANSYS FLUENT. According to increasing discharge C-rate, temperature values obtained from experimental data are 27.58 °C, 30.65 °C and 39.16 °C. The temperature values obtained from numerical data are 27.11 °C, 31.4 °C and 39.65 °C. The numerical model shows good agreement with experimental test data. The results obtained show that the non-uniform temperature distribution on the cell increases with increasing discharge current; It shows that the positive tab heats up more than the negative tab, and the highest temperature at the end of discharge is obtained in the center of the cell. Thermal behavior of NMC cell with water-cooled aluminum plate at 25 °C ambient temperature and 1C discharge current was modeled and experimentally verified. The cooling water is 25 °C and the inlet velocity of the liquid is 0.56 m/s. In this study, Re was 4436.24 and therefore the flow is considered

turbulent. For CFD simulation, a polyhedral mesh with 3220062 elements was created with ANSYS FLUENT MESHING. The created mesh has 0.38 max skewness and 0.503 min orthogonal quality values. 29.88 °C were obtained from experimental study while 29.63 °C were obtained from numerical study. The results obtained show that the liquid cooling system used successfully reduces the cell temperature increase at 1C discharge and at the same time creates a more uniform temperature profile than the uncooled system.

In order to reduce the simulation cost, the maximum temperature reached by the NMC polymer cell at different discharge current and charging ranges was calculated by ANSYS FLUENT and collected as data. The collected data were used in GPR, SVM, NN and LR ML methods in MATLAB. Five statistical indices, including R^2 , MAE, RMSE and RAE, were used comparison of the results. GPR solution produced the outputs that are closest to the actual values of responses in dataset ($R^2=0.99$, MAE= 0.317, RMSE= 0.4686 and RAE= 0.2196).

In a conclusion because the coupling of a complex electro chemical-thermal model is computationally expensive, the ECM model can be effective in predicting the cell temperature profile for thermal management.

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Belfun Arslan completed her undergraduate education in the Department of Chemical Engineering at İzmir Institute of Technology. She enrolled in the master's program in Chemical Engineering at Gebze Technical University in 2022. She has been working as a research and development engineer at Mutlu Akü Since 2021.

PUBLICATIONS AND PRESENTATIONS FROM THE THESIS

Arslan, B., Yücel, Ö., Yılmaz, C. H. (2024), ‘‘Thermal equivalent circuit modelling and experimental validation of pouch-type lithium-ion cell’’, Proceedings of the 9th World Congress on Momentum, Heat and Mass Transfer (MHMT'24), London, United Kingdom, 11-13 April.