iJRASET
International Journal For Research in
Applied Science and Engineering Technology

INTERNATIONAL JOURNAL FOR RESEARCH

IN APPLIED SCIENCE & ENGINEERING TECHNOLOGY

Volume: 9 **Issue:** VII **Month of publication:** July 2021

DOI: https://doi.org/10.22214/ijraset.2021.36985

International Journal for Research in Applied Science & Engineering Technology (IJRASET)
ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 7.429
Volume 9 Issue VII July 2021- Available at www.ijraset.com

Simulation Methods Development for an EV Battery Pack in Terms of Thermal and Safety Aspects

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***Abstract:** This paper is the representation of our effort at modelling a LiFePO4 battery pack for an electric vehicle (EV) and further carrying out simulations on it. The process involves creating a single cell and then making a combination of these cells to form a battery pack. The simulations assist us in monitoring the thermal behaviour of the 60Ah battery pack after working for a stipulated amount of time at 1 and 2 C rates. It can be observed that the battery pack may experience thermal shock or thermal runaway leading to the failure of battery pack. Hence it is of paramount importance that we keep a check on the temperature range of the battery. The pack functions best when its temperature is maintained in the range of 288K-308K. This is a challenge in the absence of cooling. Hence, we used air and PCM (RT15 & RT31) as coolants to accomplish the objective of maintaining the temperature of battery pack within the optimum range.*

I. INTRODUCTION

A battery pack should address issues related to thermal stability, vibrations isolation and impact resistance at micro and macro levels. Hence, its continuous optimization for better performance becomes a necessity. Battery Management System (BMS) is an integral part for safety considerations in a battery pack. Thus, the development of Thermal Management System which is a part of BMS is extremely necessary as it improves the safety of Battery pack. Efficient temperature management systems contribute significantly to battery health and extend the overall lifespan. As the capacity and charge/discharge rate increase, battery security issues need more attention. Therefore, it is necessary to develop new TMS methods to meet the demand for higher power, faster charge rates, and improved driving performance.

The following literature review was conducted before the commencement of the design and simulation phase to fully understand the fundamentals and the complexities regarding the battery pack.

Lithium technology is mostly used in testing of battery because its specific power and energy density are highest, with low self-discharge ratio but its voltage by cell is high. So, Lithium battery has low overcharging tolerance. lithium-ion (Li-Ion) batteries can be classified among different categories based on other elements.

- NMC
- LFP
- LNMO
- NCA
- LMO
- LCO

Battery is the most important source for energy storage system (ESS) in HEV and EV. Lithium based battery have high voltage, good energy density, low self-discharge rate and good stability to become the major source for EV and HEV. Lithium battery has high calendar life and high energy density than conventional Nickel Metal Hydride (N-MH) and Lead acid batteries. Although Li batteries have high performance, they are sensitive towards thermal issues like continuous charging, discharging working under high temperature, it causes cell degradation and affects battery life and its performance.

1) *Li-ion Batteries:* The electro-chemical and electro-thermal performance of lithium-ion batteries has been the focus of many investigations in recent years, and the subject has been extensively treated analytically and numerically. A single lithium-ion battery cell consists of two current conductors, a negative electrode, a separator and a positive electrode. The electrodes are porous solids which consist of uniform size, spherical, active particles and additives. The separator is a porous polymer membrane. All components are immersed in an electrolyte. The electrodes and the electrolyte are involved in the charge and species balance that makes up the electro-chemical reaction. The current conductors provide a path for electrons to flow through an external circuit. These batteries are most extensively used in EV battery pack.

2) *Positive Electrode Chemistry:* Numerous commercially available lithium-based.

Electrode pairs have been identified. The positive electrodes utilize a lithiated metal oxide or lithiated metal phosphate as the active material. Three of the most commonly used positive electrodes chemistries are:

$LiCoO_2$
$LiMn_2O_4$
$LiFePO_4$.

3) *LiFePO4:* $LiFePO_4$ is one of the most recent cathode materials to be introduced. Its olivine structure is very different from the layered and spinel structures of other lithium-ion chemistries. The intercalation mechanism is also different, involving phase changes. $LiFePO_4$ has a specific capacity of about 160 mAh/g and an average voltage of 3.3V. Recent developments have approached the theoretical discharge capacity. $LiFePO_4$ has the added advantage of being inexpensive and environmentally friendly. Due to these reasons $LiFePO_4$ has been selected by for the positive electrode.
4) *Negative Electrode Chemistry:* Negative electrode materials are typically carbonaceous in nature. It is important for the material to be able to hold large amounts of lithium without a significant change in structure, and have good chemical and electrochemical stability with the electrolyte. Furthermore, it should be a good electrical and ionic conductor, and be of relative low cost.
5) *Graphite:* Today, graphite in stacked layer is one of the most common anode materials in lithium-ion batteries. It is favoured for its small volume change during lithiation and delithiation. With graphite electrodes, high coulombic efficiencies of over 95% have been achieved, but they have a relatively low theoretical specific capacity of 362 mAh/g. Although this is already higher than the specific capacity of the commonly used cathode materials, higher specific capacity carbon-based electrodes are still desirable because they contribute to a lower overall battery density. Hence, we are using Graphite as the negative electrode.
6) *Electrolyte:* The choice of electrolyte in lithium-ion batteries is critical for the performance as well as the safety. The electrolyte is typically a lithium salt dissolved in a mixture of organic solvents. A good electrolyte must have low reactivity with other cell components, high ionic conductivity, low toxicity, a large window of electrochemical voltage stability (0-5V), and be thermally stable. For lithium-ion batteries utilizing liquid electrolytes, a mixture of alkyl carbonates such as ethylene carbonate (EC), diethyl carbonate (DEC), dimethyl carbonate (DMC), and ethyl-methyl carbonate (EMC) is used with $LiPF_6$ as the dissolved lithium salt. Many lithium salts are possible, but it is difficult to find one that is chemically stable, safe, and forms a high conductivity solution. $LiPF_6$ offers the best compromise between these criteria and has been the standard in lithium-ion batteries.
7) *Separator Materials:* Lithium-ion cells use microporous films to prevent physical contact between the positive and negative electrode while permitting free ion flow. The presence of a separator material can adversely affect battery performance as it increases electrical resistance and increases battery density. Therefore, care must be taken in selecting an appropriate material. All commercially available liquid electrolyte cells use microporous polyolefin materials, such a polyethylene (PE) or polypropylene (PP). Requirements for Li-ion separators include:

a) High machine direction strength to permit automated winding
b) Does not yield or shrink in width
c) Resistant to puncture by electrode materials
d) Effective pore size less than 1 µm
e) Easily wetted by electrolyte
f) Compatible and stable in contact with electrolyte and electrode materials.

8) *Current Collectors:* Current collectors comprise the component of the battery responsible for transferring the flow of electrons from the electrodes to an external circuit. There are several types of current collectors: mesh, foam, and foil. To minimize overall size and improve volumetric capacity of cells, metallic foils which are thin and light are preferred. Current collectors are an electrochemically inactive volume in the cell, but form the substrate that the electrochemically active materials are applied to. Active materials are applied onto the thin current collectors with a conducting agent and an adhesive binder. Hence, current collectors should possess high electrical conductivity to reduce cell resistance as well as chemical stability in contact with liquid electrolyte over the operation voltage window of electrodes.

ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 7.429
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Simulation Methods for EV battery pack: Electro-thermo coupled model electrical and thermal section

a) *ECM:* Scaled and discretised
b) *Scaled:* Considering that behaviour of each cell is the same
c) *Discretised:* Controlling and analysing each cell separately.

9) *Thermal Section:* A thermal ROM model is used. HTC (heat transfer coefficient) is obtained for each module containing a number of cells (98% accurate). Thermal abuse model. At elevated temperatures, exothermic reactions take place, Ansys uses two models for it: one equation model, NREL's four equation model.
10) *Thermal Issue for the Battery Pack:* Factors affected by temperature: electrochemical reactions, round trip efficiency, charge acceptance, power and energy capability, reliability, life cycle and cost. Excessive temperature degrades performance and a limited thermal dissipation can even produce burning in Li-ion battery cells; safety concerning heat accumulation due to the lithium flammability and explosiveness; non-uniformity in temperature of a cell pack favours localised deterioration in single battery elements.

a) *Electric Vehicle Battery Thermal Management System With Thermoelectric Cooling:* The developed battery thermal management system can be a combination of thermoelectric cooling, forced air cooling, and liquid cooling. Battery thermal management systems (BTMS) are developed to monitor and optimize the thermal status of batteries. The lifespan of batteries also greatly depends on the operating temperature. Under normal operating conditions, of −30 ◦C to 60 ◦C, the battery health varies significantly from the optimal battery temperature range. However, studies suggest that working at above 50 ◦C can be harmful to the lifespan of batteries. Efficient temperature management systems contribute significantly to battery health and extend the overall lifespan. Subsequently, various BTMS have been developed to meet the demand for higher power, faster charge rates, and improved driving performance. The cooling process is difficult to manage. Traditional active methods generally lead to forced circulation and circulation of specific cooling materials and substances such as water and air. The main issue is that the cooling effect can be very limited under certain circumstances. Thermoelectric coolers (TEC) which are employed nowadays by battery thermal management are comparatively new. These have strong cooling capacities and reliable working potential, and have attracted increasingly more attention for integration into BTMS. Thermoelectric coolers (TEC) are based on the conversion of voltage to the temperature difference.

After conclusion of the literature review phase, the actual task of modelling was started on SOLIDWORKS.

II. DESIGN AND SIMULATION METHODOLOGY:

Some geometry considerations are necessary to take into account depending on the model applied. The lumped model is formulated without solving spatial temperatures, except for the cell surface, where the temperature is uniform.

A. *Battery Specifications*

These specifications are not fixed, and were changed as per the need for different conditions. Above Specifications have been provided just for reference.

Specifications	Values
Cathode material	$LiFePO_4$
Anode Material	Graphite
Electrolyte	Carbonate based
Nominal Cell Capacity	20.00 Ah
Nominal Cell Voltage	3.3 V
Cell Dimensions	227mm X 160mm X 7.25mm
Cooling Jacket Dimensions	230mm X 180mm X 142mm
Busbar Dimensions	50mm X 39.85mm X 2.60mm

Table 1

B. *Battery Pack Model*

Types of battery modelling methods in Ansys:

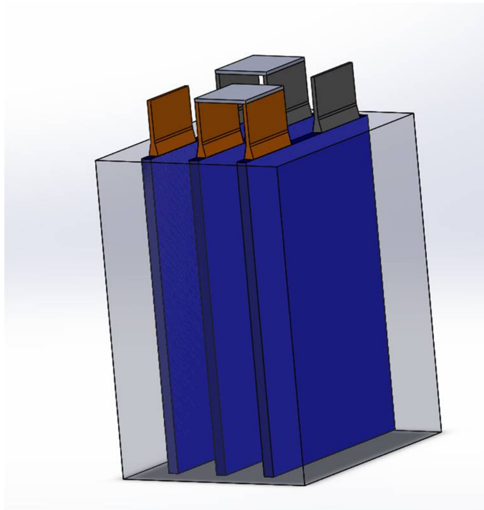

Figure 1 Battery Model

1) *MSMD Method:* The Single-Potential Empirical Battery Model (SPEBM) has a confined capability to investigate the whole variety of electrochemical phenomena in battery systems, particularly systems having intricate geometry. The ANSYS Fluent Dual Potential Multi-Scale Multi-Dimensional (MSMD) Battery Model (BM) solves these restrictions by utilizing a homogeneous model appertaining to a multi-scale multi-dimensional approach and deals with various physics in different solution domains. The MSMD method includes of three electrochemical sub-models as follows:

a) *The Newman, Tiedemann, Gu, and Kim (NTGK) Model:* Through employing the finite element method, the potential and current density distribution on the electrodes of a lithium-polymer battery were investigated by Kwon. The outcomes demonstrated that the aspect ratio of the electrodes and the size and locating of current collecting tabs have a considerable effect on the potential and current density distribution on the electrodes. The Newman, Tiedemann, Gu, and Kim (NTGK) model is a simple semi-empirical electrochemical model which was suggested by Kwon.

b) *Equivalent Circuit Model (ECM):* The voltage-current correlation can be achieved by dissolving the following set of electric circuit mathematical equations. For a determined battery, the open circuit voltage, resistances of resistors and capacitances of capacitors are subordinates of the battery state of charge (SOC). These subordinates could be represented in two various procedures in ANSYS as a set of equations.

c) *Newman's Pseudo-2D (Newman's P2D) Model:* This model is based on the Newman's group investigations. Newman's research team, through utilizing concentrated solution theory, modelled the galvanostatic charge and discharge of a lithium anode/solid polymer separator/insertion cathode cell. Because the model is general and comprehensive, it can comprise a numerous span of polymeric separator materials, lithium salts, and composite insertion cathodes.

Interpolation of lithium into the active cathode material is simulated utilizing superposition, which simplifies the numerical computations.

For our analysis we have used the Equivalent Circuit Model (ECM) method.

C. *Battery cell Characteristics*

1) The battery cell characteristics are determined from the Hybrid Pulse Power Characterisation (HPPC) test.
2) The various required values are calculated from the graphs which are plotted using the experimental values.
3) To conduct this test, Thevenin's model is used with one series resistance and a pair of Resistance-capacitance circuit.
4) All the battery characteristics like cell voltage, current capacity, temperature-time relations can be known from the HPPC test.

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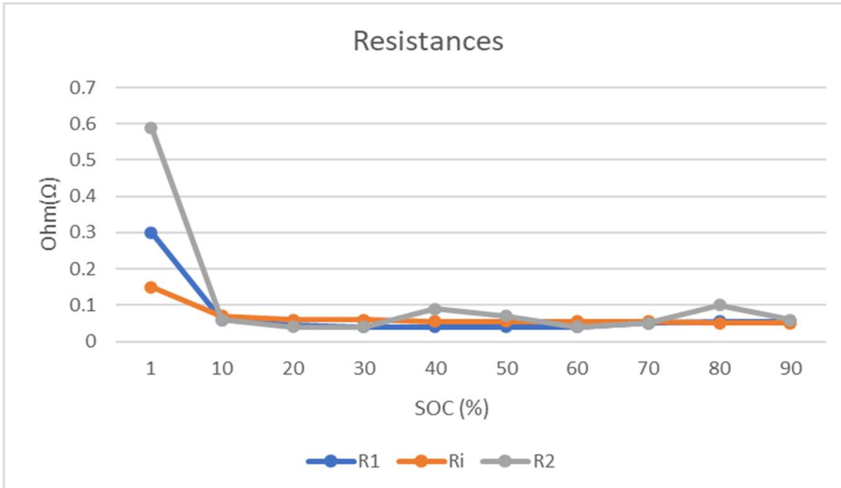
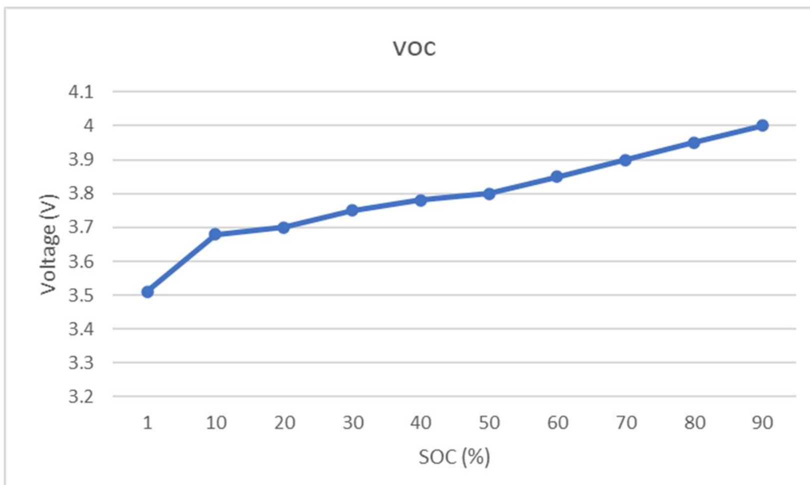
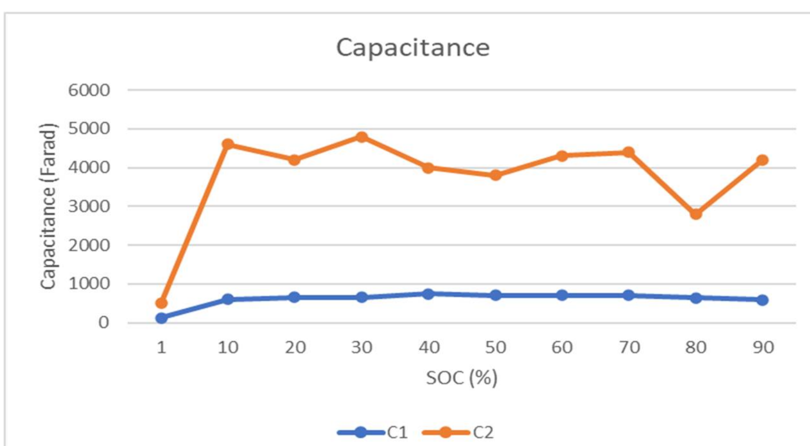
D. Simulation Parameters







Simulation tool used: ANSYS Fluent

Figure 2 HPPC data

Thermal and Physical properties of material used:
Air inlet velocity: 4m/s
Outlet pressure: zero-gauge pressure

Material	Density (Kgm^{-3})	Heat Capacity ($Jkg^{-1}K^{-1}$)	Thermal Conductivity ($Wm^{-1}k^{-1}$)	Emissivity	Melting Point (K)
Carbonaceous electrode	1347.33	1437.4	1.04		
Lithium electrode	2328.5	1269.21	1.58		
Al foil	2702	903	238		
Cu foil	8933	385	398		
PP separator	1008.98	1978.16	0.3344		
HDPE case	950	1886	0.42	0.9	
RT-31	890	2	0.21		304
RT-15	890	2	0.21		288

Table 2

Pure solvent melting heat (j/kg) =232700

60Ah LiFePO4 Battery Pack, Initial Temperature 300K, Max run-time 2.5Hrs				
Discharge Rate	Temperature Without Cooling	Temperature With Cooling		
		Air (Forced convection-4m/s)	RT15 PCM	RT31 PCM
1C	306K	302K	304K	302K
2C	316K	308K	309K	304K

Table 3

III. RESULTS AND DISCUSSION

A. Simulation with Air cooling

1) 1C Rate

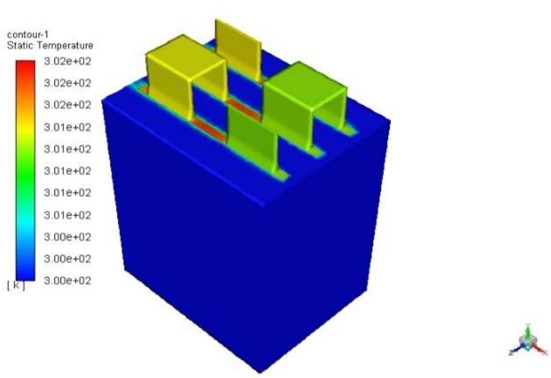


Figure 3.1

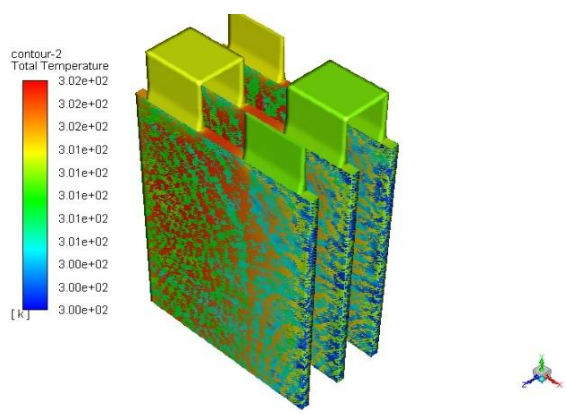


Figure 3.2

2) 2C Rate

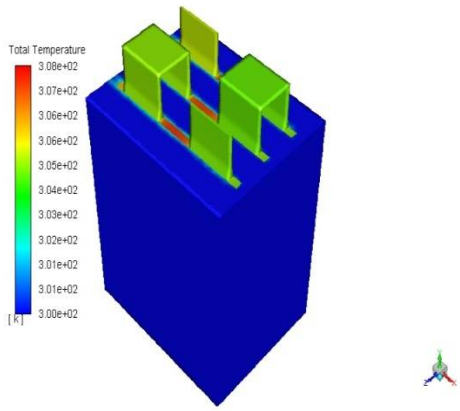


Figure 4.1

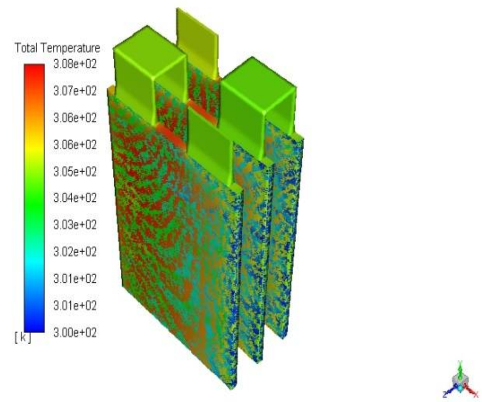


Figure 4.2

B. Simulation with PCM Cooling

1) RT15

For 1C rate

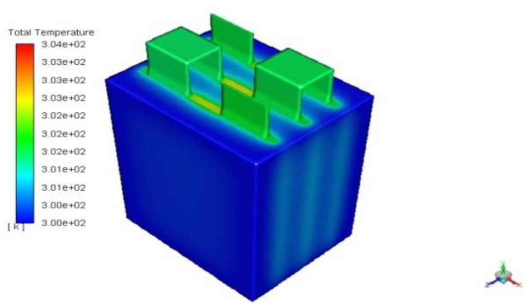


Figure 5.1

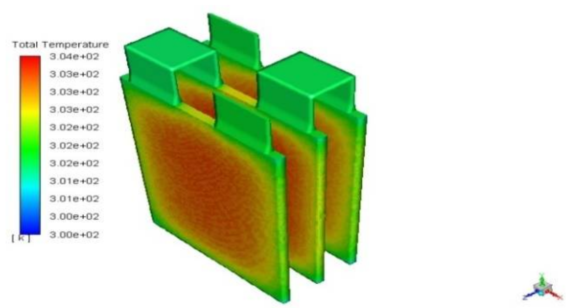


Figure 5.2

For 2C rate

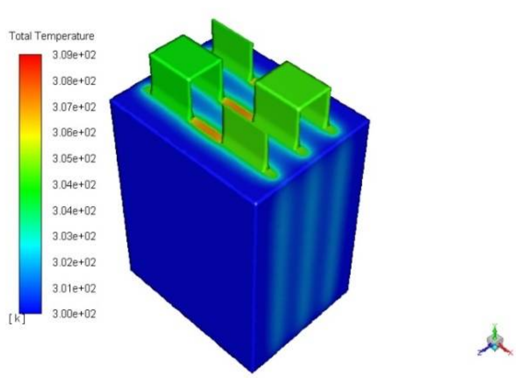


Figure 6.1

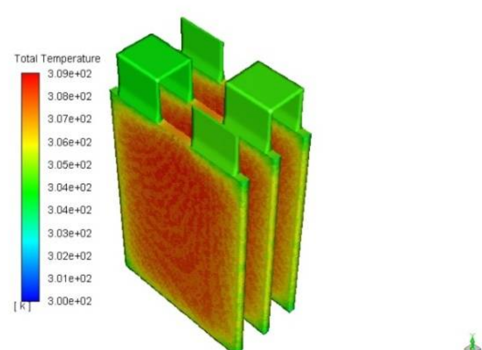


Figure 6.2

2) RT31

For 1C rate

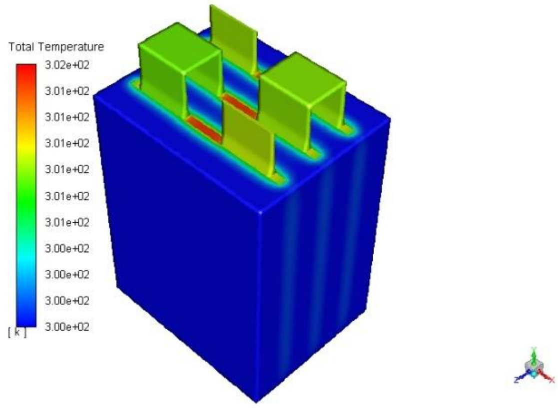


Figure 7.1

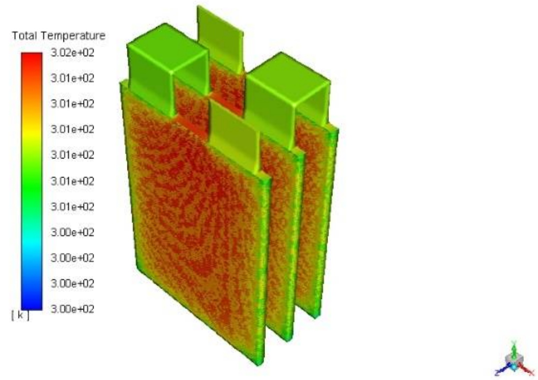


Figure 7.2

For 2C rate

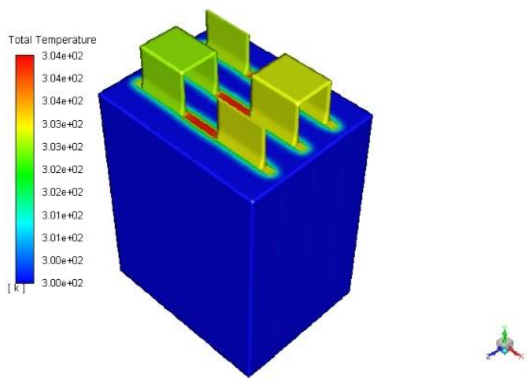


Figure 8.1

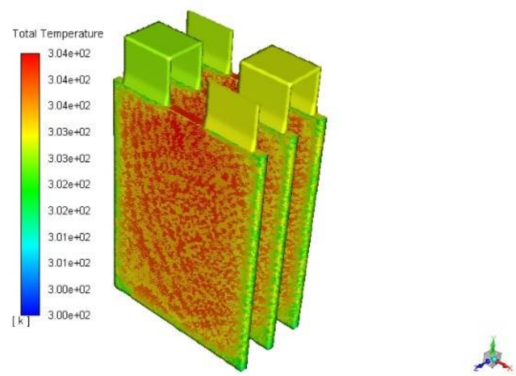


Figure 8.2

IV. CONCLUSION

Fundamental thermal properties of the LiFePO4 cell and battery, along with the heat generation characteristics, have been studied. The rate of heat generation, along with the total heat generated by the cell, increased with the increase in the current rate. The effectiveness of

several cooling materials used in a passive thermal management system to maintain lower cell surface temperature and low surface temperature gradient has been studied. The results notify that PCM cooling using the RT31 coolant is the most effective and the desired temperature range of 288K-304K can be achieved using the same. Air can also prove to be an effective coolant if higher air flow velocity is used.

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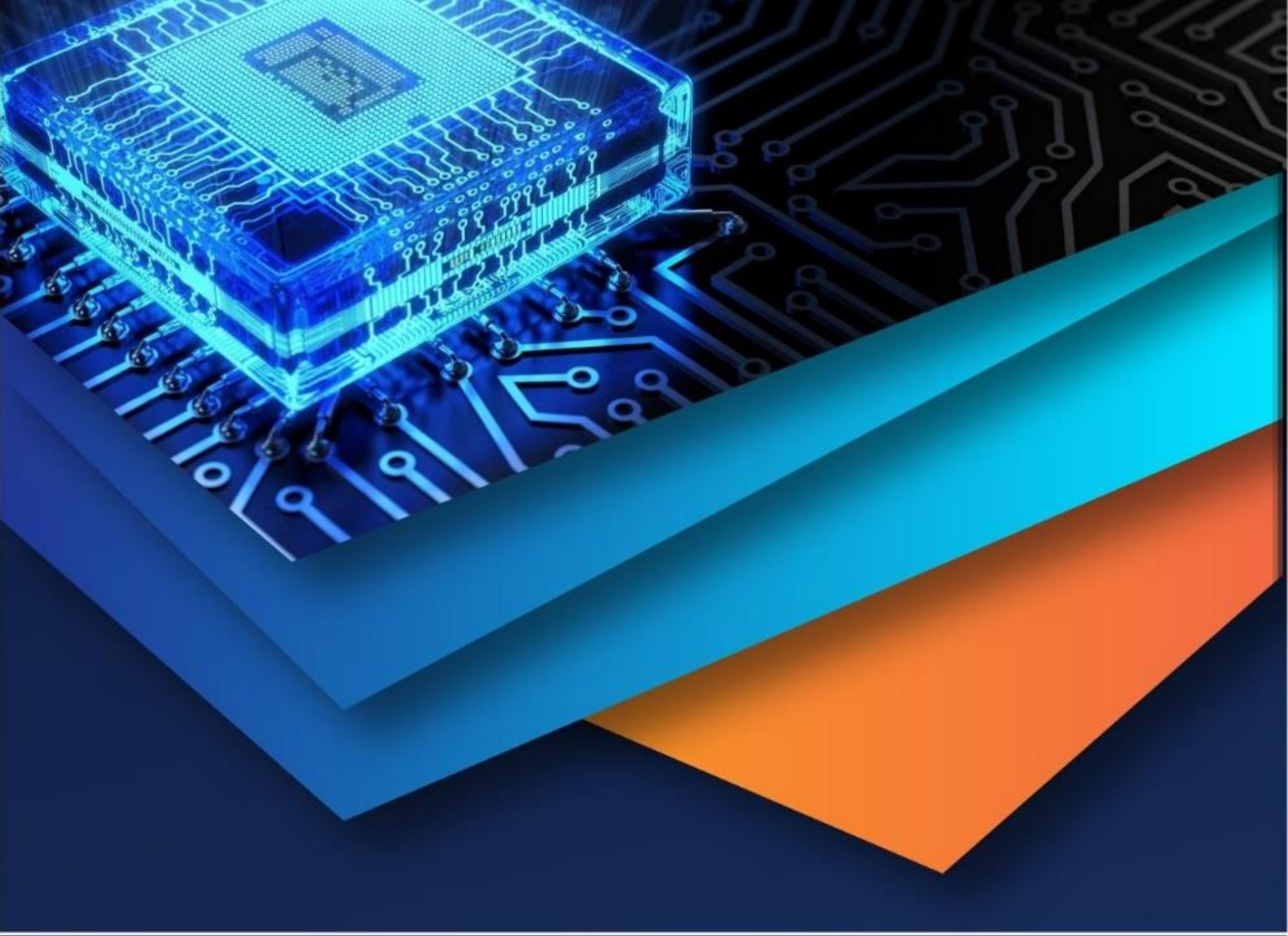

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