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Enhancing Battery Thermal Management in Li-ion-Powered Electric Vehicles using Phase Change Material-based Systems: A Multi-Scale CFD Simulation Study

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ABSTRACT

Electric cars (EVs) and hybrid electric vehicles (HEVs) are propelled by Li-ion batteries for a clean and sustainable future. Under harsh and abusive conditions, a battery pack generates a lot of heat, which could result in a disastrous thermal runaway. The current work suggests a Battery Thermal Management System (BTMS) based on Phase Change Material (PCM) to prevent thermal runaway. Using ANSYS's multi-scale, multi-dimensional Newman, Tiedemann, Gu, and Kim (NTGK) model, a 3D simulation of a single battery with PCM, is carried out. The thermal performance and discharge behavior of the battery pack is analyzed by the NTGK model. The solidification and melting model is combined with the NTGK for PCM-based BTMS. Under harsh and abusive circumstances, the effect of different discharge rates on the thermal performance of 26650 Li-ion cell with and without PCM is investigated. The PCM-based BTMS reduces the maximum battery temperature by 2.243 K, 1.44 K, and 2.5 K and increases temperature uniformity at 0.5C, 1C and 1.5C discharge rates, respectively. The data available from this research will be useful in the development of passive BTMS for EV applications.

1. Introduction

The major issue that the automobile industry is facing today is the increasing rate of pollutants that are emitted by automobiles. Several rules related to this have been issued to reduce the pollutants emitted. Stricter rules, decreasing reserves of conventional fossil fuels, imbalance distribution, and increasing energy demand highly contribute to automotive companies switching towards electric vehicles and hydrogen energy [1,2]. These electric vehicles offer the most efficient and cost-efficient solution to the above-mentioned problem. Today, the sales of electric vehicles have increased considerably as it is very convenient for customers. Batteries and play an increasingly

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important role in renewable energy storage [3]. The performance of an electric vehicle is majorly dependent on the output capacity of a battery [4]. The battery temperature is also a critical factor for battery operating performance. The charge/discharge rate as well as the lifespan of a battery is dependent on the temperature of the battery. This makes the thermal management system of an EV battery pack extremely important.

When it comes to electric vehicles, Lithium-Ion batteries are the optimum choice for energy storage for their technical features. They have a high energy density and propensity to self-heat once the electrolyte reaches a certain temperature (from 70° to 130° C), but lithium-ion batteries are naturally subjected to deterioration due to their operating condition and state of charge [5]. Currently available li-ion batteries have low efficiency due to excessive cost, low discharge rate, battery temperature issue, thermal runaway, and battery degradation. The complexity of liquid channels used to cool the battery is also a major issue for its increasing cost. There are two main sources of heat generated from the battery- 1) Electrochemical operation and 2) Joule heating due to the motion of electrons within the battery. Therefore, battery thermal management is crucial to ensure the reliable and safe operation of EV batteries. Its main aim is to maintain the battery temperature to its optimum operating temperature for the battery to work with top efficiency [6].

There are two types of battery thermal management system (BTMS) Active system: Here specific coolant such as water or air is circulated forcefully to maintain an optimum temperature. Air cooling: This type of cooling system uses air as a coolant. This air is used to either heat, cool, or ventilate within the battery pack to maintain an optimum temperature [7]. This intake air is either taken directly from the atmosphere or from is provided using a blower. Air has low heat capacity and low thermal conductivity which makes it not an optimal choice for cooling. Toyota Prius, Nissan Leaf. Liquid cooling: Here a liquid is used as a coolant. This system is found to be approximately 3500 times more efficient than an air cooling system. Liquid has higher thermal capacity and higher density than air therefore it is a better option than air cooling, but there are some drawbacks like higher cost, the complexity based on the type of coolant used, and the potential chances of leakage which would result in total failure of the battery system [8,9].

Based on the type of coolant used, this system is divided into two types, Direct liquid cooling system: In this method, the battery is immersed in the coolant. The coolant is in complete contact with the battery. This provides uniform cooling of the battery pack and provides better performance of the cell. The coolant to be used should be dielectric with high thermal capacity, high thermal conductivity, and low viscosity. Due to its inflated cost and liquid proofing this system is not widely used in the EV segments. It is majorly used by high-performance cars such as Koenigsegg's Regera and Aston Martin's Valkyrie. Indirect Liquid Cooling System: Here a duct layout is built between and around the cells. The coolant used here does not get in contact with the cells. This liquid should have high heat conductance to reduce the temperature of the cells. Thermally conductive but electrically isolated liquids are used. The conductivity of the liquid can also be enhanced by using different designs of cooling channels [10]. Different cold plates like thickened cooling fin design, sandwich cooling plate design, and intercepted cooling plat design are used based on the requirement. It is considered a safer option as it does not have chances of electrical conduction [11].

Passive system: Heat pipes and phase change systems (PCM) are used to have zero power consumption and thus improve the discharge rate of the vehicle [12]. They are:

- (i) Direct refrigerant cooling: the refrigerant/ evaporator in the cooling circuit uses a direct heat exchanger to cool the battery. It is an effective method in a nominal temperature range but as the temperature increases the performance of the cooling system decreases.
- (ii) Phase change material cooling.

- (iii) Thermoelectric cooling: it works on the effect of the Peltier-Seebeck effect, it converts electric voltage into temperature difference and vice versa. As the temperature increases, voltage across the nodes also increases these nodes are connected with a fan whose voltage also increases and provide forced cooling of the battery.
- (iv) Heat pipe cooling: Phase change materials are those materials that have high latent heat. This substance absorbs/releases sufficient heat during phase change and therefore acts as a major source of reservoir. They are a very innovative idea when it comes to battery thermal management systems. Because of their high latent heat, they absorb much of the heat from the battery and help it to run at its ideal temperature for a long time [13].

Air cooling uses more energy because it has a lower specific heat capacity, which raises parasitic power and lowers thermal efficiency. In contrast, liquid cooling uses more parts, which adds weight and complexity. Additionally, there is a potential for leaking. Dielectric fluid is needed for direct liquid cooling, which raises the price. Heat pipes are large, heavy, and have intricate designs. They also require extensive maintenance and degrade in performance with time. Since PCM is a passive cooling method, it uses no additional power. It can keep the battery at a safe operating temperature because it can absorb large amounts of latent heat. For BTMS applications, organic PCM is typically utilized. However, PCM has very little mechanical structure and very little heat conductivity. Because of this, its commercial fame is not as great [14].

However, there are certain drawbacks to PCM. If the surrounding temperature is too high, the PCM will eventually melt. Low thermal conductivity as a result will serve as a heat barrier. The PCM will function as a thermal mass and prevent the battery from operating in the preferred temperature range if the temperature is too low. Air cooling requires more power to operate due to its lower specific heat capacity, which raises parasitic power. Consequently, less cooling. On the other side, liquid cooling calls for more components, which adds weight and complexity. Additionally, there is a potential for leaking. Dielectric fluid is needed for direct liquid cooling, which raises the price. PCM heat pipes are large, heavy, and have intricate designs. They also need maintenance and perform poorly over time. Large, hefty, and featuring elaborate decorations are PCM heat pipes. They require upkeep and degrade with time in performance [15].

Grimonia *et al.*, [16] numerically investigated the cooling performance of capric acid and hexacosane PCM on an 18650 Li-ion cell, with a thickness variation of 3mm, 6mm, and 9mm. It was discovered that hexacosane with a 9mm has the best performance and can lower temperature by 6.54 K. Hexacosane remains solid up to a temperature of 327 K before transitioning to a liquid form above 329 K [16]. In an experimental study, Wang *et al.*, [17] discovered that epoxy can be used as a plasticizer to cure paraffin's low melting point and stop leaks. He employed three different forms of PCM, including PCM1—pure paraffin, PCM2—EG 20%, paraffin 80%, PCM3—EG 3%, epoxy 47%, and paraffin 50%. PCM 2 was discovered to have a melting point of 64.79 °C and a melting temperature of 59.79 °C With an increase in discharge rate, a lithium-ion battery produces more heat [17]. Zhao *et al.*, [18] employed copper foam with paraffin as a PCM coupled with liquid cooling since pure PCM is not very effective at transferring heat by heat conductivity. Most of the heat generated during discharging is located close to the battery surface, which is determined to be 39 °C. Due to its high latent heat and minimal sub cooling [18]. Hasan [19] discovered through experimentation that even steric acid can be employed as a PCM for thermal energy storage in home applications. A straightforward tube-in-tube system is best positioned horizontally since it produces the best results. The heat is directed both radially and axially due to its melting effect in convection [19].

There are several methods to enhance the thermal conductivity of a PCM, and due to its low heat transfer, several methods are adopted. The enhancement techniques are analyzed numerically, and

their effectiveness is assessed for both constant surface heat flux and constant surface temperature conditions. They are fins, insertion of high conductive material or particles, carbon Nanotubes, carbon brushes, metallic rings, and multi-tube configuration.

Another great PCM is graphene-coated nickel foam that has been saturated with paraffin wax. Hussain *et al.*, [20] experimentally discovered that this mixture increases the thermal conductivity of pure paraffin by 23 times. Comparing this mixture to pure paraffin, the latent heat of paraffin is reduced by 30%. This is caused by a drop in the mass fraction of pure paraffin inside the nickel with the graphene coating. In comparison to pure paraffin, the specific heat capacity of graphene-coated nickel that has been soaked with paraffin wax is 35% lower [20,21]. For composite PCM to conduct heat effectively, carbon fibers must be distributed uniformly. The thermal performance of the combination is greatly influenced by the particle size and carbon fiber weight percentage. The pace at which batteries' internal temperatures rise and fall is slowed down by carbon. The most effective carbon fiber for heat transfer has a mass fraction of 0.46% and a length of 2mm [22].

Sanker *et al.*, [23] experimentally investigated that copper foam is preferable to nickel foam because copper foam with 97% porosity performs better in terms of thermal conductivity. Because it offers superior cooling performance than the traditional system, the addition of metal mesh, particularly copper, is thought to be a very promising alternative. The battery temperature was seen to drop by 10 °C during discharge when copper mesh was added to the PCM. Aluminum mesh can be utilized as a protective barrier around the battery because it has been discovered to be amazingly effective at lowering the battery's surface temperature [23]. A variety of techniques, including metallic fillers, metal matrix construction, and finned tubes, are suggested to improve the heat passage in a latent heat thermal energy storage system.

Batteries with thermal management systems frequently use phase change materials (PCM). It is a viable option because it has a high latent heat capacity and conductivity. To replace liquid-cooled BTMS, PCM-based BTMS must first improve in both mechanical structure and thermal conductivity. The type of battery utilized, the battery's maximum operating temperature, and the kinds of thermal conductivity improvement techniques employed all play a very important role in the PCM selection process. Therefore, the primary objectives of this project are the development of a single lithium-ion cell and a PCM-based BTMS for that cell. As a result, the current study will concentrate on selecting the best PCM for a selected Li-ion cell and applying a simple technique to enhance its thermal conductivity.

2. Methodology

A CFD model of 26650 Lithium Cobalt Oxide (LiCoO₂) cell is developed in this study. The thermal analysis of li-ion battery is done using a dual potential Newman, Tiedemann, Gu, and Kim (NTGK) formulation using Ansys design modeler. The simulation is performed at the three different battery discharge ratings of 0.5C, 1C and 1.5C.

2.1 Battery Geometry and Meshing

The battery in use has a diameter of 26 mm and a length of 65 mm as shown in Figure 1. The cathode, the anode, and the electrolyte are the three components that make up this cell. Graphene carbon is employed as the anode, and lithium cobalt oxide is the cathode. Here, the positive and negative tabs are passive zones, and the cell is an active zone.

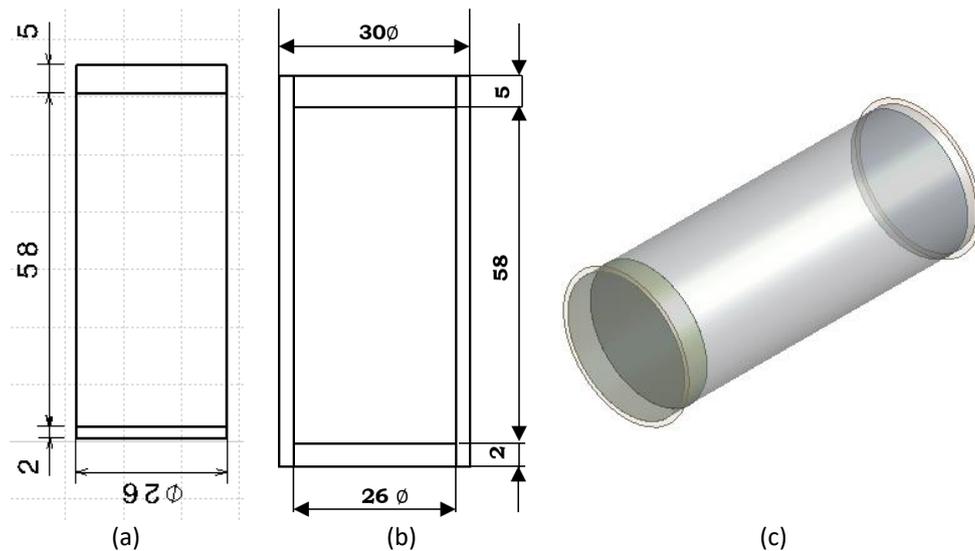


Fig. 1. NTGK Li-ion cell details (a) Single cell dimension (b) Cell with PCM dimension (c) Single cell battery model with PCM cooling

A geometrical model of a cooling system for a single cell 26650 Li-ion battery is developed using Ansys design modeler. A substance that undergoes phase shift surrounds this cell. Composite paraffin wax is the phase-change substance utilized in the analysis. The PCM in use has a cylindrical dimension of 2 mm in width and 65 mm in length, enclosing the cell entirely. Figure 1(b) displays the geometric model. The phase change material needs to be treated as a fluid domain when the cell's geometry is being modeled. Mesh independence study have been carried out to solve the NTGK single cell model with PCM cooling at a constant discharge current of 6 Amperes. The maximum temperature rise is used as the parameter of interest, and 1.15 mm is found to be the ideal mesh size for each scenario. Therefore, for the single cell NTGK model with cooling, a mesh with 67145 elements and 76824 nodes is selected for the study. In Table 1, mesh metrics are given for the above-mentioned mesh size.

Table 1
 Mesh Metrics for Single Cell with PCM

Parameter	Maximum	Minimum	Average
Element Quality	0.99787	0.38521	0.89752
Aspect Ratio	2.9768	1.0763	1.4782
Skewness	0.47091	1.5752e-005	9.3322e-002
Orthogonality	1	0.66917	0.98232

2.2 Equations Used in Numerical Analysis of the BTMS

In the present work, the Dual Potential Multi Scale-Multi Domain approach with NTGK electrochemical sub-model is adopted for analysis of li-ion battery cell. The electrical and thermal field characteristics of the battery are solved in the computational domain at the battery's cell scale as discussed in Paccha-Herrera *et al.*, [24]. The energy equation below describes how the PCM's heat absorption process works [15]:

$$\frac{\partial(\rho_{PCM}H)}{\partial t} = \nabla(K_{PCM}\nabla T) + S_h \quad (1)$$

$$H = h + \Delta H \quad (2)$$

$$\Delta H = \beta H \tag{3}$$

$$\beta = 0, T > T_m \tag{4}$$

$$\beta = 1, T < T_m \tag{5}$$

where sh is the rate of heat production, H is the PCM enthalpy, Δh is the PCM latent heat, h is the PCM sensible heat, K_{PCM} is the PCM's thermal conductivity, ρ_{PCM} is the PCM's density, β is the PCM's liquid fraction, and T_m is the PCM's melting point, or liquidus temperature. Eq. (1) supports the PCM's potential ability to absorb a total amount of heat. The PCM with a high melting temperature, density, specific heat, and thermal conductivity experiences significant absorbed heat. These circumstances can be used as a guide when selecting a quality PCM. The Li-ion cell specifications and cooling system material properties are listed in Table 2 and Table 3 respectively.

Table 2
 Cell Specification

Anode	Graphite Carbon
Cathode	Lithium Cobalt Oxide
Length	65 mm
Diameter	26 mm
Initial DoD	0
Reference Capacity	4.3 ah
Minimum Stopping Voltage	2.75 V
Maximum Stopping Voltage	4.2 V
System Current	6 A

Table 3
 Properties of phase change material

Parameter	Value
Density (Kg/m ³)	950
Specific Heat (J/kg K)	3000
Thermal Conductivity (W/m K)	7
Viscosity (kg/ (m s))	0.015
Pure Solvent Melting Heat (J/ kg)	146000
Solidious Temperature (K)	315.15
Liquidus Temperature (K)	317.15

2.3 Boundary Conditions for BTMS

The boundary condition has been applied on the interface between the complete cell (positive tab, negative tab, and the jelly roll) and the phase change material. The type of thermal boundary condition used is convection. The value for the heat transfer coefficient is considered [25]. Table 4 gives the value for the thermal boundary condition.

Table 4
 The boundary condition for a single cell with PCM

Heat Transfer Coefficient [w/m ² k]	18
Free Stream Temperature [K]	297

3. Results

NTGK model are used to compute how cells behave when discharged at various speeds. Figure 2 illustrates the growth in cell temperature. With an increase in discharge rate, the temperature tends to rise. When compared to the experimental findings, the simulation results for a single cell without cooling are determined to be well within the allowable limit [18].

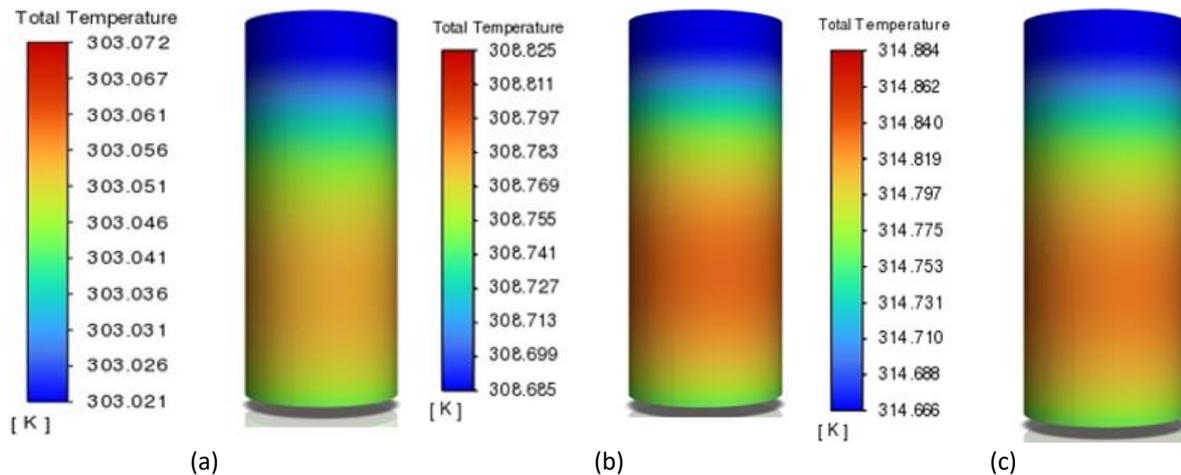


Fig. 2. Cell temperature profile at various discharge rates (a) 0.5 C (b) 1 C (c) 1.5 C

3.1 Single Cell without Cooling

The C-rate for three distinct discharge modules—0.5 C, 1.0 C, and 1.5 C—has been examined on the LiCoO₂ 26650 Li-ion battery using the Ansys Workbench. The cell's highest temperature was measured to be 314.88 K, 308.82 K, and 303.07 K for discharge rates of 1.5 C, 1.0 C, and 0.5 C, respectively. Figure 2 displays the temperature contours in the cell for various discharge currents. As an electrochemical reaction occurs inside the battery cell over time, the temperature of the cell rises as a result of increased internal heat generation. Due to the high current being drawn over a relatively short period of time, a 1.5 C discharge rate is determined to provide the cell's highest maximum temperature. As demonstrated in Figure 2, as the rate of discharge increases, the battery temperature rises and the amount of time that may be used drops dramatically. Figure 4 compares the voltage drop at three different discharge modules. The graph shows that temperature and voltage loss rise as the discharge rate does Figure 3. Due to high internal resistance, it has been reported that the cell's maximum temperature at 1.5 C discharge rate is 314.88K, and at the same discharge rate, the charge is completely drained in 2500 seconds.

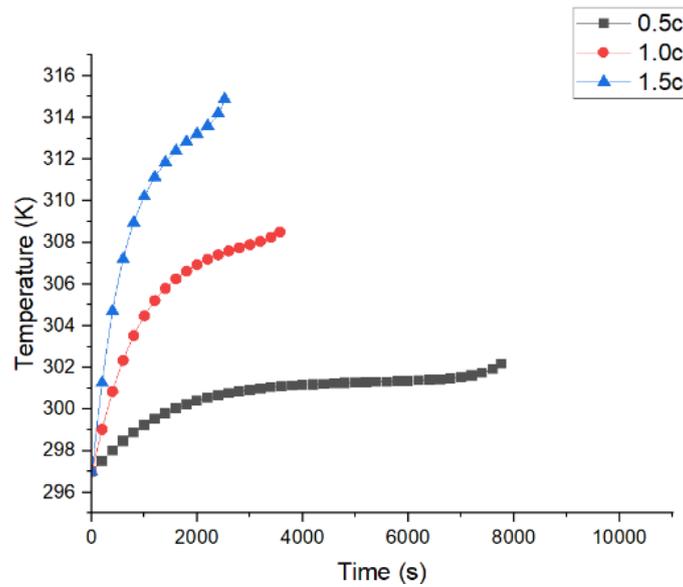


Fig. 3. Cell temperature profile at various discharge rates (a) 0.5 C (b) 1 C (c) 1.5 C

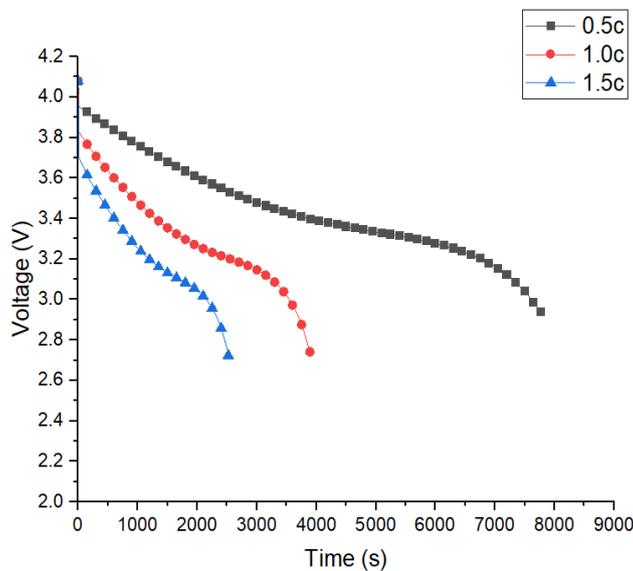


Fig. 4. Cell voltage profile at various discharge rates (a) 0.5 C (b) 1 C (c) 1.5 C

3.2 Single Cell with Phase Change Material

Through computational analysis of 26650 Li-Cobalt oxide cell surrounded with composite paraffin wax of width 2mm enclosing the cell, the maximum temperature of the cell has been computed. Using the PCM the maximum temperature of the cell with discharge rate of 0.5C, 1C, and 1.5C is found to be 300.82K, 307.41K, and 312.37K respectively as shown in Figure 5. The discharge time for cell with discharge rates of 0.5C, 1C, and 1.5C is 10000s, 3600s, and 2500s respectively. It can be seen that using a PCM around the cell, the temperature of the cell has reduced, which helps the battery to discharge for a longer duration and helps in increasing the battery life. Figure 5 shows the temperature contour of a cell with PCM, with discharge rate of 0.5C, 1C, and 1.5C respectively. From the contour, it can be concluded that the overall cell temperature is uniform.

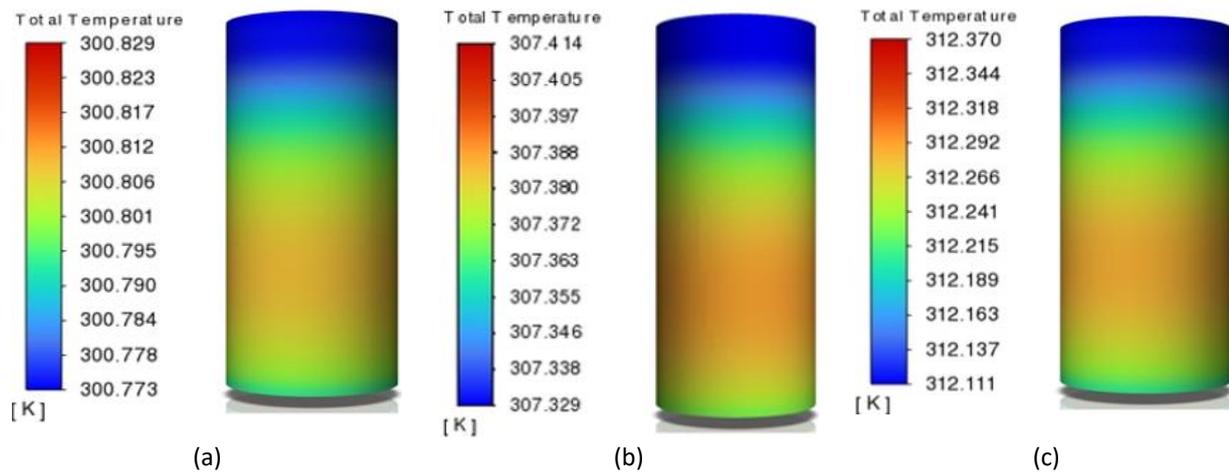


Fig. 5. Cell temperature profile at various discharge rates (a) 0.5 C (b) 1 C (c) 1.5 C

3.3 Comparison between the Maximum Temperature of Cell with and without PCM

For discharge rates of 1.5 C, 1.0 C, and 0.5 C, respectively, Figure 6, Figure 7, and Figure 8 show the variation of cell temperature with time. These data indicate that a single cell battery integrated with PCM cooling results in a considerable shift in temperature. All of these elements help to lower battery temperature, which lengthens battery life. A mechanism like this aids in preventing thermal runaway of the battery. In each of these scenarios, the battery begins at a base temperature of 297 K. The maximum temperature that the cell would reach without cooling is determined by the battery's programmed discharge rates. Before complete discharge, cell temperature rises with increasing discharge rates.

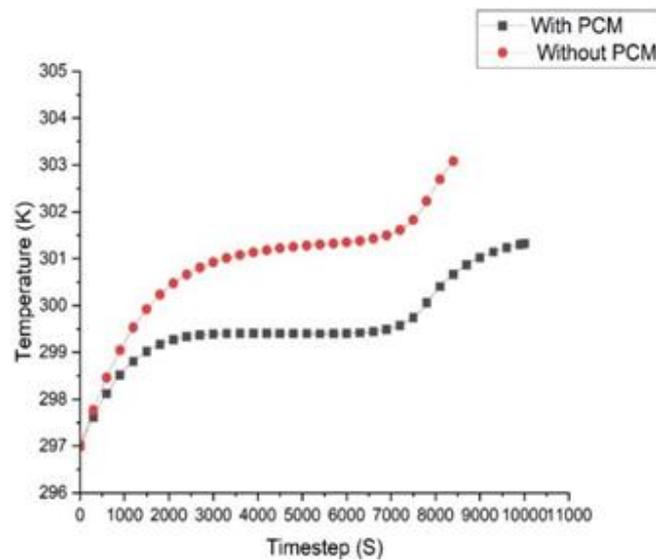


Fig. 6. Comparison of Cell temperature at 0.5C discharge rate

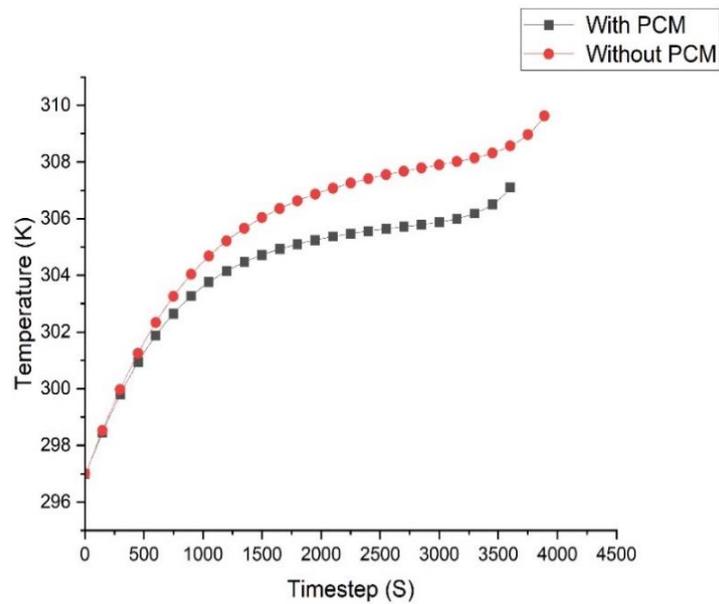


Fig. 7. Comparison of Cell temperature at 1C discharge rate

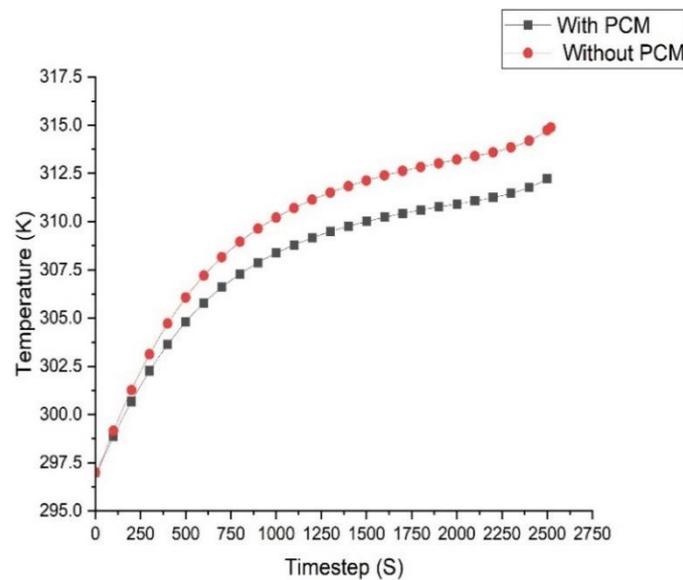


Fig. 8. Comparison of Cell temperature at 1.5C discharge rate

The maximum temperature of the cell at a discharge rate of 1.5 C is 314.88 K without cooling, and it would be closer to 312.37 K with the use of BTMS. The highest temperatures reached by cell without cooling at discharge rates of 1.0 C and 0.5 C are also determined to be 308.825 K and 303.027 K, and with cooling 307.414 K and 300.829 K. Utilising a thermal management system will reduce the highest temperature reached by 2.5 K, 1.4 K, and 2.2 K, respectively, for discharge rates of 1.5 C, 1.0 C, and 0.5 C. Table 5 lists the highest temperatures measured in a single cell with and without cooling.

Table 5
The boundary condition for a single cell with PCM

Discharge rate (C)	Initial temperature (k)	Without PCM (k)	With PCM (k)	Difference in temperature (k)
0.5	297	303.07	300.82	2.24
1	297	308.82	307.41	1.41
1.5	297	314.88	312.37	2.51

3.4 Limitations of Present Work

The present work is the modeling of a single cell with PCM cooling. The proposed PCM here is capable of maintaining a single cell within a safe operating range of temperature. The effect of varying ambient temperature on the PCM can be studied in the future. Different methods can be used to improve the thermal conductivity of PCM.

4. Conclusion

In the present work CFD analysis of 26650 LiCoO₂ cell has been carried out using dual potential NTGK model for EV application. The deviation of voltage and cell temperature with time for a single cell without cooling has been evaluated at different discharge rates of 2A (0.5 C), 4A (1.0 C), and 6A (1.5 C). Furthermore, a PCM is used as a coolant to control the maximum temperature attained by the cell. At different constant current discharge rates, the maximum temperature reached by the cell with and without cooling has been simulated. The results of the simulation study is summarized below

- (i) At discharge rates of 1.5 C, 1.0 C, and 0.5 C, respectively, a single cell without cooling reaches maximum temperatures of 314.88 K, 308.82 K, and 303.07 K.
- (ii) The discharge time of 0.5C, 1C and 1.5C are 7760s, 3890s and 2520s respectively.
- (iii) The maximum temperature attained by the cell with a phase change material, having a discharge rate of 0.5C, 1C and 1.5C is 300.82K, 307.41K and 312.37K.
- (iv) At discharge rates of 1.5 C, 1.0 C, and 0.5 C the cell with PCM decreases the highest temperature reached by 2.52K, 1.41K, 2.24K when compared to the bare cell, indicating that the BTMS used in the current study is effective.
- (v) The discharge time for cell with discharge rate of 0.5C, 1C and 1.5C is 10000s, 3610s and 2520s respectively.

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