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Comparative Thermal Analysis of Paraffin-Based PCM and Graphite Composite PCM in Lithium-Ion Battery Packs

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Abstract

Introduction: Thermal regulation remains a critical challenge in lithium-ion battery systems used in electric vehicles, particularly under high load, fast charging, and prolonged operating conditions. Inadequate heat dissipation can accelerate battery degradation, reduce energy efficiency, and increase safety risks. Phase change materials (PCMs) have emerged as promising passive thermal management solutions due to their ability to absorb excess heat during phase transition. Among available PCMs, paraffin-based materials are widely used for their high latent heat capacity and cost effectiveness, while graphite composite PCMs offer enhanced thermal conductivity and structural stability. However, a direct comparative evaluation of these two materials under identical operating conditions remains limited.

Objectives: The primary objective of this study is to comparatively assess the thermal performance of paraffin-based PCM and graphite composite PCM when integrated into a lithium-ion battery module used in a Tesla Model S. The study aims to evaluate their effectiveness in controlling battery temperature, maintaining thermal stability, and regulating phase change behavior during operation.

Methods: A three-dimensional computational fluid dynamics (CFD) model of a single battery module containing 444 cylindrical 18650 cells was developed using CATIA and analyzed in ANSYS Fluent. Separate simulations were conducted for paraffin-based PCM and graphite composite PCM under identical boundary and operating conditions. Transient simulations were performed for 1800 seconds using a forced convection cooling approach. Key performance metrics, including volume-average PCM temperature, area-weighted average battery surface temperature, and volume-average liquid fraction, were evaluated to quantify thermal behavior and phase change characteristics.

Results: The results indicate that the paraffin-based PCM achieved slightly lower average battery surface temperatures, demonstrating effective short-term heat absorption and dissipation. In contrast, the graphite composite PCM exhibited a substantially lower liquid fraction throughout the operational cycle, indicating prolonged solid-phase retention and improved thermal stability. This behavior reflects the superior heat conduction capability of the graphite composite material during extended operation.

Conclusions: The comparative analysis reveals that paraffin-based PCM is more suitable for applications requiring rapid thermal response, such as fast charging or high-power demand conditions. Conversely, graphite composite PCM provides enhanced long-term thermal stability, making it advantageous for sustained driving and continuous operation. The findings highlight the importance of selecting PCM materials based on specific operational requirements to optimize battery safety, performance, and lifespan in electric vehicle applications.

Keywords: Electric vehicles, EV batteries, CFD simulations, Li-on batteries; Phase change material, Thermal management

1. Introduction

The transportation sector worldwide is recognized as a leading contributor to greenhouse gases, which harm human health and the environment[1][2]. This situation has considerable detrimental effects on human health and the environment because of the pollutants produced by vehicles operating on internal combustion engines[3]. Currently, the number of vehicles in operation across the globe is a staggering 1.2 billion. Furthermore, this figure is expected to reach approximately two billion by 2035[4]. The said conditions pose considerable concern, but it also represents a prime opportunity. With the advent of modern technology, the efficiency of these vehicles and their emission levels can be dramatically improved, reducing their toll on the environment[5]. One potential solution lies in electric vehicles, primarily powered by renewable energy sources [6][7][8]. These innovative modes of transport, driven by electricity instead of traditional fuels, oppose the harmful effects of car emissions[9]. The fundamental difference is that electric vehicles (EVs) operate without engines, which negates the need for gasoline. Consequently, they are at the forefront of environmental conservation[10].

An electric vehicle (EV) lithium-ion battery assembly involves cell preparation, module assembly, thermal management system installation, and performance testing, all of which affect the effectiveness and security of the automotive vehicle[11]. Battery packs may be overheated because of road conditions or climate shifts. However, air-cooling methods may not be sufficient, leading to reduced battery performance and potential safety risks[12]. Adequate cooling is achieved by integrating phase change material (PCM) components into thermal control systems[13]. PCMs absorb excess heat during phase changes[14], helping maintain optimal temperatures[14] [15]. Embedding PCMs within battery modules or utilizing PCM-based cooling jackets can result in more uniform heat distribution and improved heat absorption, enhancing battery performance[16] and safety compared with ordinary air-cooling methods[17]. Al-Hallaj and Selman [18] studied a large battery setup with cylindrical cells and PCMs between cells inside the module. They stated that PCMs have substantial potential for effectively managing temperature. They suggest that PCMs can function as passive thermal management systems (TMS) for batteries. Al-Hallaj et al. [19] explored the usage of battery modules featuring cylindrical Li-ion cells coupled with a PCM as a TMS. They established that these battery setups, including PCMs, tend to have longer lifespans. Additionally, authors indicated that approximately 90% of the battery's nominal capacity could be harnessed, thus enhancing the effectiveness of utilizing a PCM within the battery pack.

Analyzing and testing PCM-based batteries in EVs is critical for optimizing thermal management [20]. Effective PCMs amplify heat absorption, balance temperatures to bolster battery productivity and longevity, and boost vehicle safety and reliability[21]. The said outcomes offer substantial insights into the evolution of EV technology, facilitating the meeting of rigorous performance criteria[22]. Software such as ANSYS Fluent aids scientists in exploring thermal regulation in EV batteries by replicating heat distribution and fluid movement[23]. The ANSYS software constructs a battery pack structure, incorporates PCMs, and mimics thermal loads to reflect the operational conditions. It evaluates the volume, average temperature, and liquid proportion of PCMs by utilizing these simulations to identify effective thermal control strategies[24]. It is observed that PCMs enhance heat absorption and dispersion, maintain suitable temperatures, and boost battery performance and durability. Rangappa and Rajoo [25] conducted a study on the application of PCM in Li-ion battery packs in EVs. They used computational fluid dynamics (CFD) in the ANSYS Fluent software to analyze the thermal management system. They tested active air cooling and PCM-based thermal management systems and mentioned that phase-change-material-based systems show better cooling efficiency than traditional air-cooling systems.

Khateeb et al. (2005) conducted an experimental study on different heat dissipation methods for Li-ion battery packs in electric scooters, which are both insightful and admirable. By focusing on natural convection cooling, an aluminum foam heat transfer matrix, and PCM-based materials, they discovered that PCM decreased the temperature by 50% compared to the control, thus promoting efficient cell operation. The simulation mirrored the experimental results almost perfectly, adding robustness to the study. Selokar [26] conducted an enlightening analysis of the PCM usage for Li-ion battery packs in EVs. They developed 3D model with CATIA v5 software, and thermal behavior examination using ANSYS Fluent software are commendable. They revealed that PCMs enhance the temperature distribution performance, thereby outperforming insulation materials. Yu and Tao [27] mentioned that paraffin-based PCM and graphite composite PCM are essential materials for efficient thermal management in EV battery packs. Paraffin-based PCM are cost-effective, whereas graphite composite PCM offers superior thermal conductance and stability, with the choice of material depending on the specific thermal management needs and performance demands[28].

Tesla Model S revolutionized EVs with cutting-edge lithium-ion battery packs. These batteries offer superb range, high performance, and energy efficiency[29]. Effective thermal management systems are vital for maintaining optimal temperatures, increasing battery lifespan, and delivering consistent performance. The ideal temperature range for lithium-ion batteries is 25-50°C. Maintaining battery temperatures within this range bolsters efficiency and cost-effectiveness by preventing overheating and excess cooling. Previous studies on PCM-based thermal management in EV batteries primarily focused on single-material applications, such as paraffin or graphite composites, but lacked direct comparative analyses of these materials. The present study uniquely contributes by comprehensively comparing paraffin-based PCM and graphite composite PCM, providing critical insights into their thermal efficiency, stability, and potential for improving battery performance. The present work planned to apply ANSYS Fluent software to lithium-ion battery packs on the Tesla Model S and to compare the thermal performance of paraffin-based PCM and graphite composite PCM.

2. Methodology

Emerging electric vehicles are working to eradicate fossil fuels in the transport industry, and batteries are critical to their functionality[30]. The Tesla Model S battery pack comprises 16 modules, all connected to a central bus bar through M8 bolt terminals. This bus bar collects electric current from every module, delivers it to a contactor, and then supplies it to the electric drive. A Model S battery pack produces 22.8 volts and 84 kWh (16x5.3 kWh). A typical model S battery pack is shown in Fig. 1 [31], and a single module is shown in Fig. 2.

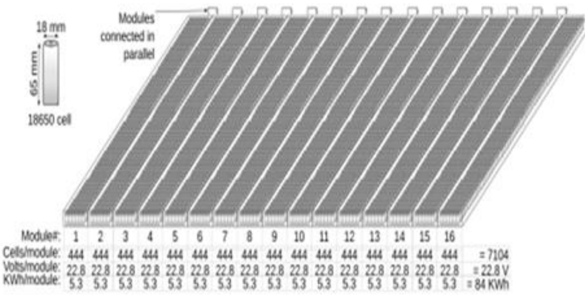

Fig. 1 Schematic diagram of Tesla S model battery pack

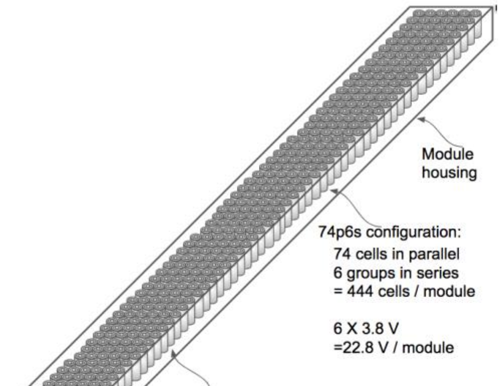

Fig. 2. Showing single module of battery pack [31]

Because vehicles traverse various routes and diverse road conditions, their batteries may generate heat, necessitating control or reduction. This is crucial to ensure the smooth and efficient operation of the vehicle. In the present work, a strategic developmental approach utilizes two variants of Phase Change Materials (PCMs), specifically paraffin and graphene, integrated within the battery unit of Tesla Model S. This integration primarily aims to provide efficient heat dispersion and enhance thermal management, thereby extending the battery lifespan.

Sharma et al. [31]mentioned that the initial battery pack has been meticulously designed using the specific features of the CATIA v5 R20 software and is characterized by a diameter of 0.18 m and a height of 0.65 m. This model boasts 18650 cells, which are carefully arranged into 16 different modules, with 444 cells within each module. The battery pack measurements encompassed a length of 3400 mm, a width of 1945.82 mm, and a height of 85 mm.

2.1 Simulation steps followed in ANSYS fluent software.

The present work involves analyzing a single module in ANSYS Fluent software. For the investigation, a battery pack was designed using CATIA software and imported into ANSYS software for further study.

i. Materials Selection

Choosing a paraffin-based PCM is beneficial because of its remarkable latent heat and affordability, making it preferable for thermal management. Graphite composite PCM, which is known for its improved thermal conductivity, aids in heat dissipation and stability. Assessing these materials sheds light on optimizing LIB packs' thermal functionality and material efficiency.

ii. CFD Simulation Setup

Geometry and Materials: A single module of the battery pack designed in CATIA v5 was imported to

ANSYS Fluent, and the image is shown in Fig. 3. Module 1 has 444 cells, and PCM solid is kept holding the battery pack. The properties of the paraffin-based PCM and graphite composite PCM are listed in Table 1, and the same was used as the input properties. The energy mode, sonification, and melting options are kept on, as it is a thermal problem.

Table 1. Materials properties of paraffin-based PCM and graphite composite PCM

Material / Properti	Density	Specific heat	Thermal conductivity	Latent heat
Paraffin based PCM	880	2000	0.236	134200
Graphite based PCM	789	1980	16.6	123000

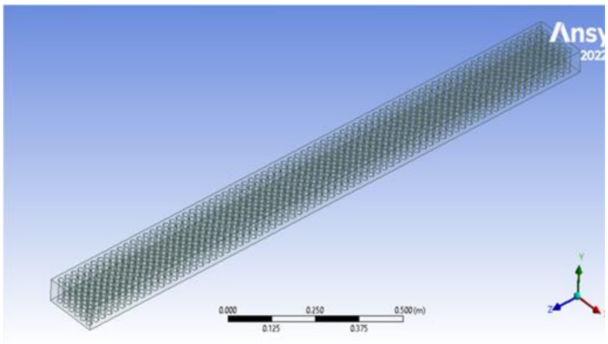

Fig. 3. Showing single battery pack having 444 cells

iii. Meshing

The battery pack model was designed using CATIA, which illustrates the Tesla Model S setup, consisting of 16 modules with 18,650 cells. Phase-change materials (PCMs) have been included for efficient temperature regulation. With the help of ANSYS Fluent, a detailed thermal interplay between the battery cells and PCM is achieved. Meshing is performed, as depicted in Fig. 4.

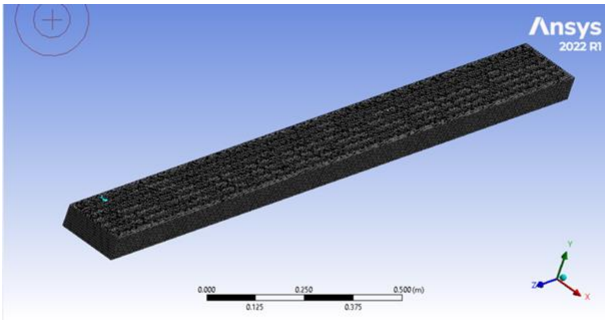

Fig.4 Meshing of 1 module of the battery pack

iv. Boundary Conditions

The simulation of thermal loads imitates the normal operational circumstances of the Tesla Model S battery pack, such as charging and discharging routines. Forced convection cooling imitates the actual cooling conditions, guaranteeing a precise depiction of the thermal management efficiency in the simulations. The boundary conditions for the battery temperature were selected as 308 K, the wall solid temperature was 300 K, and the convection value had a heat-transfer coefficient of 10 W/m^{2}k.

v. Solution initialization

The solution is initialized by computing from the solid wall preset at a temperature of 300 K, which aids in evaluating the thermal distribution within the solid. The material may be paraffin-based or a PCM graphite composite and this evaluation offers valuable insights into its specific thermal performance.

vi. Run calculation

The model operates for half an hour, which is 1800 s. Temperature and liquid proportion measurements occur at one-second intervals to closely observe the paraffin-origin or graphite composite PCM's thermal features and phase alteration patterns throughout the simulation.

2.2 Analysis of Metrics

i. Volume Average Temperature of PCM

During the simulation, the temperature data for each cell within PCM were collected each time. Volume average temperature is calculated using Eq.1.

$$T_{avg} = \frac{\sum(Ti*Vi)}{\sum Vi} \qquad (1)$$

where T_i is the temperature of the ith cell and V_i is the volume of the ith cell. The volume average temperature is calculated in each step to understand the temperature distribution at the battery surfaces, and results are given in Table 2.

ii. Area-Weighted Average Temperature at Batteries

The temperature data were collected at the surface of each battery cell, where the PCM was in contact. The area-weighted average temperature at the batter temperatures is measured using Eq.2.

$$T_{area\_avg} = \frac{\sum(Ti*Ai)}{\sum Ai} \qquad (2)$$

Where, T_i is the temperature of the ith surface element and A_i is the volume of the ith surface element. The temperature was calculated and is listed in Table 2 for each step to understand the temperature distribution at the battery surfaces.

iii. Volume Average of Liquid Fraction

The liquid fraction data for each cell within the PCM volume were collected at each step. The volume average of the liquid fraction is calculated using Eq. 3.

$$f_{Liguid \quad average} = \frac{\sum(fi*Vi)}{\sum Vi} \qquad (3)$$

where f_i is the liquid fraction of the ith cell, and V_i is the volume of the ith cell. The liquid fraction was calculated at each time step to monitor the phase-change behavior over the simulation period, and the results are presented in Table 2.

3. Results and discussion

A simulation experiment was conducted to examine the changes in the temperature of the volume average for the PCM and battery surfaces, along with the variations in the volume averages of the liquid fraction throughout their operational cycles. This was performed using Fluent software, and the derived results are presented in Table 2.

Table 2. Simulation results of Paraffin-based PCM and Graphite composite PCM

Material/properties	Paraffin-based PCM	Graphite composite PCM
Volume average temperature of the PCM	306.5	306.92
Area-weighted average temperature at the battery surfaces	307.19	307.53
Volume average of the liquid fraction during operational cycles	0.81	0.46

Table 2 shows a noticeable difference in the volume average temperatures between the paraffin-based phase change material (PCM) and the graphite composite PCM. The obtained results indicate that the temperature of the paraffin-based PCM is slightly lower than that of the graphite composite PCM and it also suggesting more effective at absorbing and disseminating heat throughout its volume.

Results of the area-weighted average temperature at battery surfaces, as depicted in Table 2, show that the area-weighted average temperature at the battery surfaces is lower for the paraffin-based PCM compared to graphite-based PCM. It suggests that the paraffin-based PCM provides better heat removal from the battery surfaces, leading to slightly cooler battery temperatures and potentially enhancing the battery's performance and longevity.

Table 2 presents the average volume of the liquid fraction for paraffin-based and graphite-based PCM. According to the results in Table 2, the graphite composite PCM has a significantly lower volume average of the liquid fraction value compared to the paraffin-based PCM. A lower liquid fraction indicates that the PCM remains in its solid phase for longer, suggesting that the graphite composite PCM has a higher heat absorption capacity and is more effective in maintaining thermal stability during operational cycles.

3.1 Discussion on thermal performance

The paraffin-based PCM demonstrated a marginally lower mean temperature on the battery surface, indicating better short-term thermal control than the graphite composite PCM. It is observed from the study that paraffin-based PCM offers improved heat absorption and dissipation, making them effective in preventing battery overheating during rapid energy discharge or charging cycles. Immediate reduction in surface temperature can enhance battery efficiency by maintaining optimal operating conditions, contributing to prolonged battery life and performance stability in electric vehicles.

From a broader design perspective, obtained results indicate that integrating paraffin-based PCM into battery packs could improve the overall thermal management system, reducing the need for active cooling mechanisms and contributing to energy efficiency. However, while paraffin PCM offers short-term advantages, the longer solid-phase duration and superior thermal conductivity of graphite composite PCM may provide more sustainable heat regulation in extended driving scenarios. Both materials offer unique benefits that can be tailored to specific EV performance requirements, balancing efficiency and battery longevity.

3.2 Discussion on liquid fraction analysis

The graphite composite PCM's significantly lower volume-averaged liquid fraction indicates that it remains in the solid phase for longer, providing superior thermal stability. It is also indicated that the graphite composite PCM can effectively manage heat over extended periods, ensuring the battery operates at lower temperatures during prolonged driving cycles. Staying solid for extended periods, it absorbs and distributes heat more consistently, reducing the likelihood of temperature spikes and preventing battery degradation.

From a broader perspective, using graphite composite PCM in EV battery packs could extend battery life by minimizing thermal stress during continuous operation. Enhanced thermal stability allows for more consistent energy output, improving the overall vehicle efficiency, especially in long-range or high-performance EVs. Additionally, reducing the liquid fraction could lower reliance on external cooling systems, potentially reducing energy consumption and improving the overall energy efficiency of the vehicle. Thus, graphite composite PCM offers valuable benefits for enhancing EV performance and battery longevity.

3.3 Discussion on implications for EV Battery design

While the paraffin-based PCM demonstrated slightly better immediate temperature control due to its rapid heat absorption and dissipation, the graphite composite PCM exhibited long-term thermal stability due to its lower liquid fraction. The stability can enhance battery safety, reduce the risk of thermal runaway, and prolong battery life by minimizing the thermal stress during extended operations. The choice of PCM material has broader implications for EV performance and design.

For applications requiring quick heat dissipation, such as high-speed acceleration or fast charging, paraffin-based PCM may be more suitable for providing immediate cooling to prevent overheating. On the other hand, for sustained driving conditions or long-range EVs, the ability of the graphite composite PCM to maintain lower operational temperatures over extended periods makes it a better option for ensuring battery longevity and consistent performance. Incorporating the right PCM based on operational needs can enhance overall vehicle efficiency, reduce energy consumption from active cooling systems, and optimize both short-term performance and long-term battery health, directly impacting the cost-effectiveness and reliability of EVs.

4. Conclusion

The present study investigated the thermal management of a lithium-ion battery pack in a Tesla Model S using two different PCMs: paraffin-based PCM and graphite composite PCM. Through CFD simulations performed using ANSYS Fluent software, we evaluated the thermal performance of a single battery pack module designed in CATIA v5. The simulations, conducted separately for each material, provide clear insights into their respective capabilities. The findings showed that paraffin-based PCM offer superior immediate thermal management**,** maintaining a lower average temperature on the battery surface and solid walls. This makes it more suitable for applications requiring rapid heat dissipation, such as rapid acceleration or fast charging cycles. However, the graphite composite PCM demonstrated a significantly lower liquid fraction (0.46) than the paraffin-based PCM (0.81), indicating superior long-term thermal stability**.** This long-term stability makes the graphite composite PCM more effective for extended operational cycling. It is ideal for continuous driving conditions and high-performance EVs where sustained thermal regulation is critical. Thus, the choice of these two materials depends on specific thermal management needs: paraffin-based PCM is better for short-term heat control, while graphite composite PCM exhibits long-term thermal stability, contributing to enhanced safety and extended battery life in electric vehicles.

5. Future scope of work

Future studies could explore alternative PCM composites, such as metal-based or hybrid materials, to enhance the thermal conductivity and stability of EV battery packs. Additionally, testing the thermal management performance of these materials in different EV configurations, such as compact or high-performance electric vehicles, would provide broader insights. Investigating the effects of varying operating conditions, such as extreme weather or rapid charging cycles, could also lead to more effective and adaptive thermal management strategies for diverse EV applications.

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