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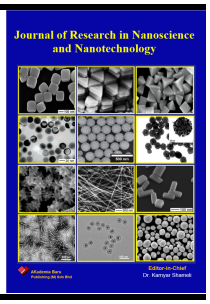

Enhancing Thermal Efficiency of Lithium-Ion Batteries Using Phase Change Materials: A CFD-Based Comparative Study

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ABSTRACT

Thermal management plays a vital role in the performance and safety of lithium-ion battery systems, addressing challenges such as overheating and efficiency loss. This study investigates the thermal performance of four different Phase Change Materials (PCMs)—Paraffin, Soywax, Lauric Acid, and Calcium Chloride Hexahydrate—using transient Computational Fluid Dynamics (CFD) simulations via ANSYS Fluent. Five simulation scenarios with iteration counts ranging from 100 to 500 were employed to evaluate heat distribution, phase transition behavior, and thermal and electrical efficiencies. The results demonstrate that Soywax exhibits superior performance with a thermal efficiency of up to 68% and an electrical efficiency reaching 98%. Paraffin also displays significant thermal buffering, achieving a thermal efficiency of approximately 64%. In contrast, Lauric Acid yields moderate thermal efficiency at around 55%, while Calcium Chloride Hexahydrate performs least effectively with a thermal efficiency of only 45% due to its slower heat response. The simulations confirm the necessity for a minimum of 300–400 iterations to capture accurate thermal behavior and ensure numerical stability. Consequently, the findings highlight Soywax and Paraffin as the most viable PCMs for improving battery safety and efficiency, presenting promising avenues for thermal regulation in electric vehicles and energy storage applications.

Keywords:
Phase Change Materials; CFD Simulation; Lithium-Ion Batteries; Thermal Management; Efficiency Analysis.

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1. Introduction

With the rapid development of electric vehicle (EV) technology and the increasing consumption of high-power electronic devices, the issue of thermal efficiency in energy storage systems, especially lithium-ion (Li-ion) batteries, has become a significant concern in the development of modern energy systems [1], [2]. Despite their advantages of high energy density and relatively long service life, Li-ion batteries are susceptible to temperature. Significant temperature increases during charging and

discharging can accelerate electrochemical degradation, reduce energy efficiency, and increase the risk of thermal runaway, which is dangerous to user safety. In this context, an effective thermal management system (TMS) is essential to maintain optimal performance and extend battery life, while ensuring overall system reliability and safety [3]. Although liquid or air-based active cooling systems have been widely used, these approaches often require additional energy consumption and complex maintenance. [4]. As a promising alternative, Phase Change Materials (PCM) are starting to be intensively developed for more efficient and energy-saving passive thermal management [5], [6].

PCM can absorb and release large amounts of latent heat energy during the phase change process (generally from solid to liquid), thereby stabilizing the temperature around its melting point [7], [8]. Thus, the PCM functions as a thermal buffer that keeps the battery temperature within optimal limits during the operational cycle [9]. However, the effectiveness of PCM is greatly influenced by its physical and thermal characteristics, such as melting point, specific heat capacity, thermal conductivity, and chemical and mechanical stability [10], [11].

This study aims to evaluate the thermal performance of four different types of PCMs, namely: Paraffin, Soywax, Lauric Acid, and Calcium Chloride Hexahydrate (CaCl_(2) 6H_2 O) in a lithium-ion battery-based energy storage system. These four materials were selected because they represent a combination of organic and inorganic materials with a wide variety of thermal characteristics, allowing for a comprehensive comparative analysis [12], [13].

Numerical simulations were performed using ANSYS Fluent software with a Computational Fluid Dynamics (CFD) approach to analyze temperature distribution, latent heat storage capacity, and thermal response of each PCM [14]. In this study, each simulation scenario was also varied based on the number of computational iterations, ranging from 100 to 500 iterations, to observe the consistency and convergence of the simulation results on the heat transfer dynamics that occur during the battery work cycle [15], [16].

Although various studies have examined the utilization of PCMs for battery thermal management systems, most of them are still limited to one type of material or do not evaluate the influence of simulation parameters, such as the number of iterations, on the final results [17], [14], [16]. This gap indicates the need for a more comprehensive comparative study with systematically varied numerical approaches. This study is significant because it compares four types of PCMs with different characteristics and sensitivity analysis to the variation of the number of simulation iterations. Therefore, the main objective of this study is to evaluate the thermal performance of Paraffin, Soywax, Lauric Acid, and (CaCl_(2) 6H_2 O) PCMs in a Li-ion battery-based energy storage scenario, through CFD-based numerical simulations in ANSYS Fluent, assess the effect of the number of iterations on the accuracy and stability of the simulation results.

Through this approach, the study is expected to provide a more comprehensive picture of the influence of PCM selection and simulation parameters on the effectiveness of battery thermal management. The results of this analysis are expected to be the basis for developing more efficient and applicable passive cooling systems in various future energy use scenarios, especially in electric vehicles and stationary energy storage systems.

Table I
Review of Recent Literature on The Use of PCM

Method	Materials	Research result	Reference
Laboratory experiments and thermal characterizations (DSC, SEM, LOI, TG-DSC)	Composite $CaCl_2 \cdot 6H_2O$ + CF, CNF, SCH	High-performance battery thermal management system for 0–120 °C range; improved cooling efficiency (50.7%), fire resistance (V0), and thermal runaway absorption (37,730 J).	[18]
Field experiment on Solar Air Heater (SAH) over 3 days	Paraffin, Soy Wax, Palm Wax	Paraffin achieved the highest energy efficiency (30–33.67%); palm wax provided the best exergy efficiency (up to 28.96%). Natural waxes are effective in solar-based agricultural drying.	[19]
Critical literature review	Paraffin, Paraffin/EG, Salt-based PCMs	PCMs are effective in passive battery cooling. Integration with structures like foam, fins, and aerogel enhances BTMS, but key challenges include thermal conductivity and leakage.	[20]
Battery cooling system design and simulation using CAD and thermal analysis	Paraffin (general PCM, not explicitly named)	Combined cooling plate and PCM system maintained max charging temp at 57.6 °C and discharging at 43.2 °C. Heat distribution improved; the system is better than no cooling.	[21]
Technical literature review and PCM classification	Paraffin, Paraffin/EG, Hydrated salts, Eutectic PCMs	Paraffin-based and composite PCMs are widely used in BTMS. Combinations with EG, metal foam, and heat pipes enhance cooling and temperature uniformity; thermal conductivity remains a key issue.	[22]

2. Methodology

2.1 Research Method

This study uses a Computational Fluid Dynamics (CFD) simulation approach through ANSYS Fluent software to analyze the thermal behavior of a lithium-ion battery system equipped with a phase change material (PCM) [10]. The primary focus of this study is to evaluate the thermal performance of four types of PCMs, namely Paraffin, Soywax, Lauric Acid, and Calcium Chloride Hexahydrate (CaCl_(2) 6H_2 O), which represent a combination of organic and inorganic materials, to identify the most effective materials for the passive cooling of lithium-ion batteries. Each PCM has different thermal characteristics, such as melting point, specific heat capacity, thermal conductivity, viscosity, latent heat, and solidus and liquidus temperatures [19], [20]. These parameters are the main inputs in the simulation, as shown in the flowchart. Thermophysical data from the PCM and system parameters are combined to build an accurate simulation model.

The simulation used a three-dimensional (3D) battery model with a PCM configuration surrounding the battery surface, resembling a passive thermal protection layer. The heat source in the battery was modeled as a heat generation process with a fixed value, and the initial system temperature was set at 307 K (equivalent to 33.85°C). The simulation was performed under transient thermal conditions to illustrate the temperature changes over time during the battery duty cycle. All simulation scenarios were run in ANSYS CFD, considering five variations in the number of iterations: 100, 200, 300, 400, and 500. The aim was to analyze the sensitivity of the simulation results to the number of iterations and ensure the convergence of the temperature distribution, which has still rarely been studied in previous studies.

All simulation scenarios use uniform boundary conditions (Figure 1). These boundary conditions represented a controlled and realistic simulation environment, ensuring consistency across all PCM material scenarios. Using a uniform time step and simulation duration allows for accurate comparison of temperature profiles and thermal responses, which are crucial for validating the effectiveness of each PCM type. Moreover, the thermophysical parameters were based on experimentally validated sources to increase the credibility and replicability of the simulation results.

In addition, to enhance the accuracy of the CFD results, proper mesh refinement was applied around the battery-PCM interface area, where significant thermal gradients were expected to occur. This ensures that the heat transfer mechanisms, especially conduction and phase transition, can be captured effectively within the simulation domain. Mesh independence tests were also conducted before the main simulation phase to confirm that element size does not significantly influence the results.

Furthermore, the governing equations used in the simulation, including the energy conservation equation, were solved using a transient solver with second-order accuracy. The enthalpy-porosity technique was employed to model the phase change process of PCM, allowing for the tracking of melting and solidification behaviors during the battery's operation cycle.

Through this modeling setup, the study aims to provide a comprehensive and robust analysis of passive thermal regulation using PCMs under various operational conditions. This methodological framework (Figure 1) lays the foundation for the subsequent discussion on result validation and performance comparison among PCM types.

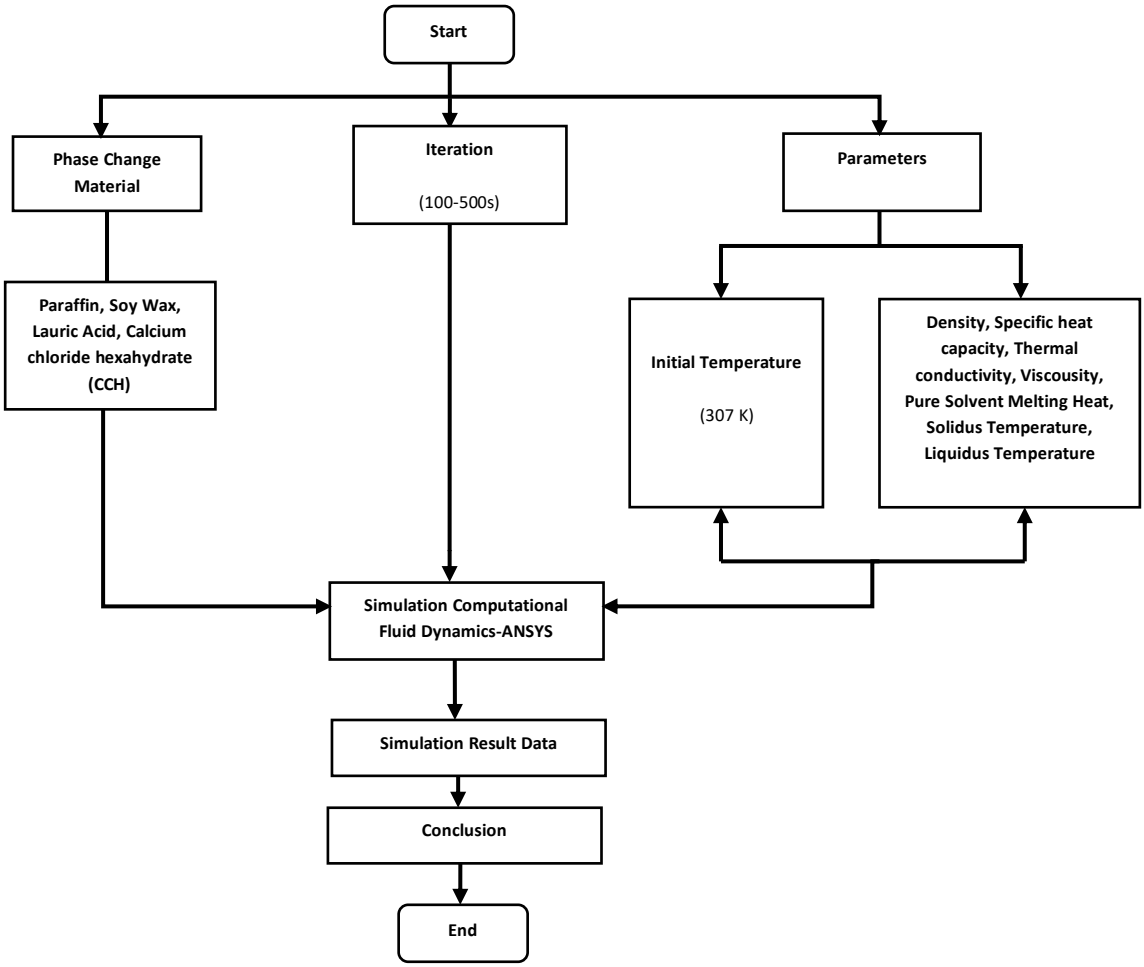


Fig. 1. Research Flowchart

2.2 Equations

To support Computational Fluid Dynamics (CFD) simulations in analyzing the thermal behavior of lithium-ion battery systems with phase change materials (PCMs), a series of basic mathematical equations describing the conservation of mass, momentum, and energy are used [23], [24]. These equations form the basis of numerical modeling implemented in the ANSYS Fluent software [25]. Simulations are performed under transient thermal conditions, considering the effects of heat conduction, fluid convection, and phase change phenomena on the PCMs used. The enthalpy-porosity approach is used to model the melting and freezing processes, which takes into account the contribution of latent heat [26], [27]. In addition, internal heat generation from the battery is modeled as a constant heat source.

The following are the equations used in the simulation:

2.2.1 Continuity Equation (Mass)

For incompressible fluids:

$$\nabla \cdot \vec{v} \tag{1}$$

2.2.2 Navier-Stokes equations

For fluid flow considering viscosity:

$$\rho\left(\frac{\partial_{\vec{v}}}{\partial_t} + \vec{v}\cdot\nabla\vec{v}\right) = -\nabla p + \mu\nabla^2\vec{v} + \vec{F} \quad (2)$$

2.2.3 Energy Equation

For fluid flow considering viscosity:

$$\rho C_p\left(\frac{\partial T}{\partial t} + \vec{v}\cdot\nabla T\right) = \nabla\cdot(k\nabla T) + S_h \quad (3)$$

2.2.4 Phase Change Model

Used to model the melting or freezing of PCM: Total Enthalpy:

$$h = h_{sens} + h_{latens} = \int_{T_{ref}}^{T} C_p dT + \beta L \quad (4)$$

Liquid Fraction (β):

$$\beta = \begin{cases} 0, \\ 1, \end{cases} \frac{T - T_{solidus}}{T_{liquidus} - T_{solidus}} \quad (5)$$

2.2.5 Heat Generation from the Battery

$$S_h = q_{gen} \quad (6)$$

3. Results

3.1 Thermal Distribution of Paraffin PCM

The thermal behavior of the lithium-ion battery using paraffin as the phase change material (PCM) was evaluated under transient simulation using several iteration steps: 100, 200, 300, 400, and 500. The temperature distribution results are visualized in Figure 2, showing a distinct color gradient ranging from blue (low temperature) to red (high temperature), representing the total temperature field in Kelvin. At 100 iterations (Figure a), the lowest observed temperature at the outer layer of the PCM is 300.57 K, indicating the beginning of the heat propagation process. As the iteration count increases to 200 and 300 (Figures b and c), the outer temperature of the PCM gradually rises to 302.12 K and 303.39 K, respectively. These changes highlight the dynamic heat transfer between the battery core and the surrounding paraffin PCM, where heat is absorbed and gradually distributed outward. At 400 and 500 iterations (Figures d and e), the temperatures increase to 304.34 K and 305.04 K, respectively. The consistent growth in surface temperature signifies that the paraffin is effectively absorbing the latent heat, supporting its role as a thermal buffer. The red-colored region remains concentrated at the battery's core, indicating that the battery continuously acts as the primary heat source. At the same time, the surrounding PCM undergoes a gradual phase change from solid to liquid.

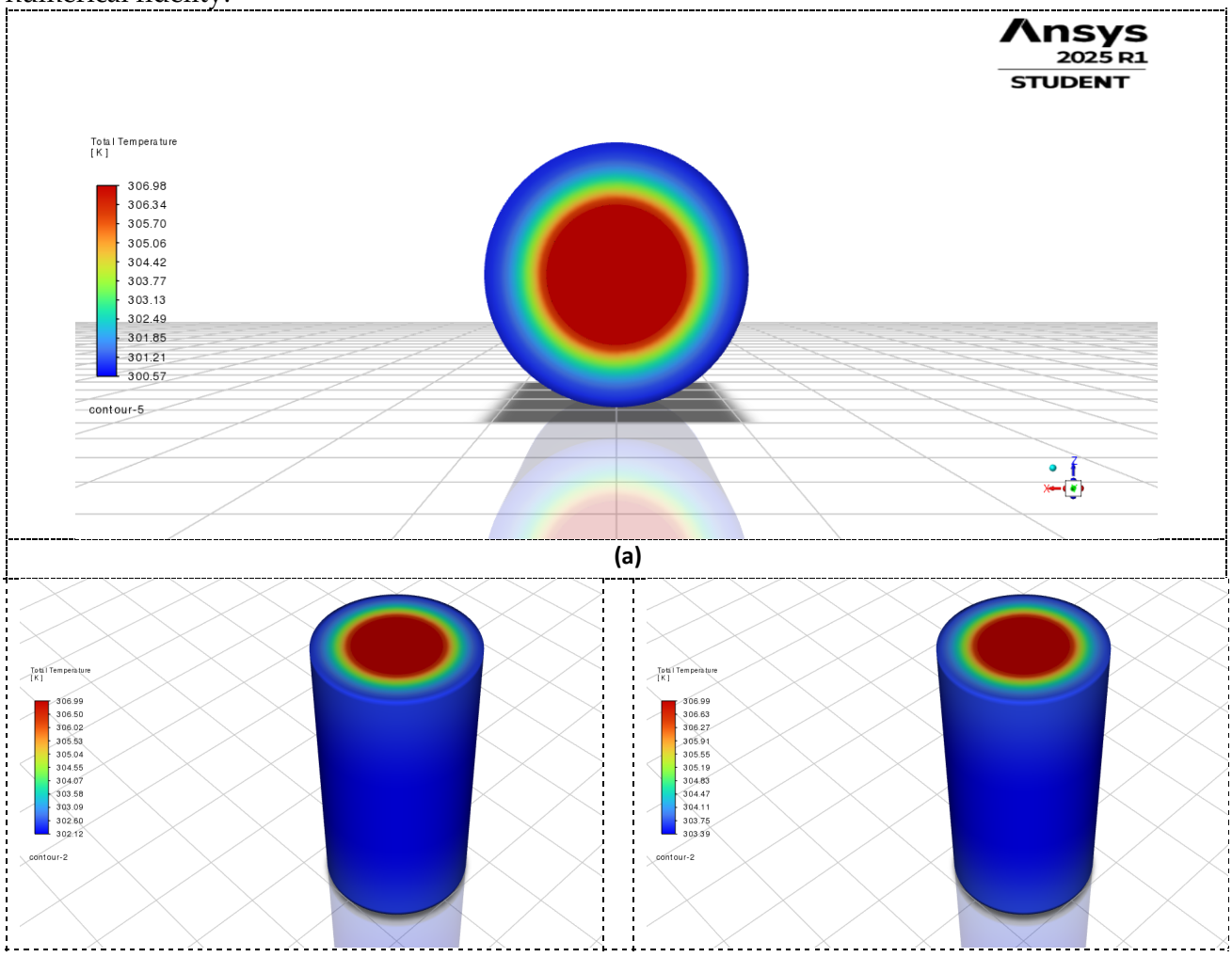
This progression also implies that more iterations yield a smoother and more stabilized temperature field, which is crucial for capturing the complete thermal response of the PCM during the battery operation cycle.

3.2 Scaled Residuals and Convergence Behavior

The convergence behavior of the simulation was assessed using scaled residuals, shown in Figure Y. Each line represents the residuals of key flow and thermal variables (continuity, velocities, energy, turbulence parameters) over 500 iterations. It can be observed that the energy equation shows rapid convergence, dropping to the order of 1e-06 before 100 iterations and stabilizing afterward. Meanwhile, residuals for velocity components (x, y, z) continue to decline steadily but remain higher than energy residuals, which is typical in conjugate heat transfer problems involving solid and PCM domains.

Notably, the continuity residual exhibits a sharp decrease, reaching below 1e-20, indicating that the simulation achieved numerical stability and mass conservation. The small oscillations in the early iterations reflect initial turbulence stabilization and mesh adjustment, which smooth out as the solution progresses.

These results confirm that 500 iterations provide sufficient steps to reach stable and physically meaningful outcomes. The use of paraffin as a PCM demonstrates its ability to delay temperature rise effectively, while the simulation setup successfully captures the phase transition process with high numerical fidelity.



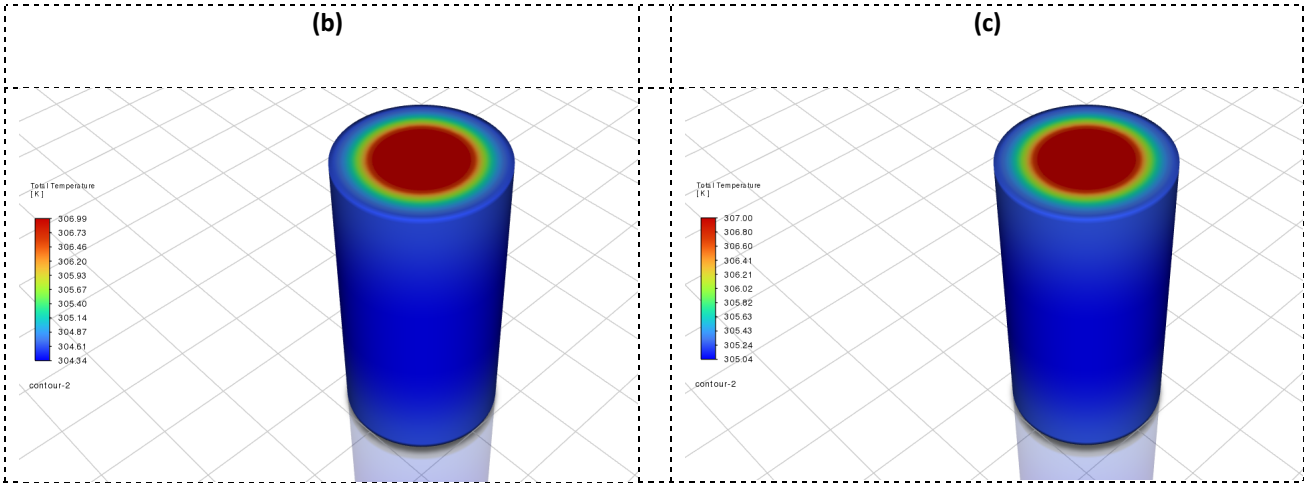


Fig. 2. Paraffin with Iterations: (a) 100s, (b) 200s, (c) 300s, (d) 400s, (5) 500s

3.3 Thermal Distribution of Soywax PCM

The thermal performance of lithium-ion batteries using soywax as a phase change material (PCM) was investigated through transient simulations using iterative time steps: 100, 200, 300, 400, and 500 iterations. The temperature distribution outcomes are visualized in Figure 3, exhibiting a transparent temperature gradient from blue (lowest temperature) to red (highest temperature), reflecting the overall thermal field in Kelvin.

At 100 iterations (Figure a), the outermost PCM region exhibits a minimum temperature of 300.54 K, indicating the onset of heat diffusion from the battery core to the surrounding PCM. The battery emits heat, while the soywax retains its solid form and begins absorbing energy primarily through conduction. As the iteration count increases to 200 and 300 (Figures b and c), the outer PCM temperature gradually rises to 302.60 K and 303.33 K, respectively. This progression marks the initial phase transition from solid to liquid in the PCM as latent heat is absorbed. The thermal gradient becomes smoother, with the blue regions beginning to fade, suggesting effective heat transfer throughout the soywax layer. At 400 and 500 iterations (Figures d and e), the PCM outer temperatures reach 304.28 K and 304.98 K, respectively. The increased temperature distribution and reduced blue regions imply that a larger portion of the PCM has melted, enhancing the heat absorption capacity of the soywax. The core of the battery consistently remains the hottest zone (around 306.99–307.00 K), shown in red, confirming its role as the dominant heat source.

Moreover, soywax exhibits excellent thermal inertia, meaning it can store a considerable amount of energy as latent heat without a dramatic increase in temperature. This property makes it ideal for managing transient thermal loads during high-demand periods such as rapid charging or discharging.

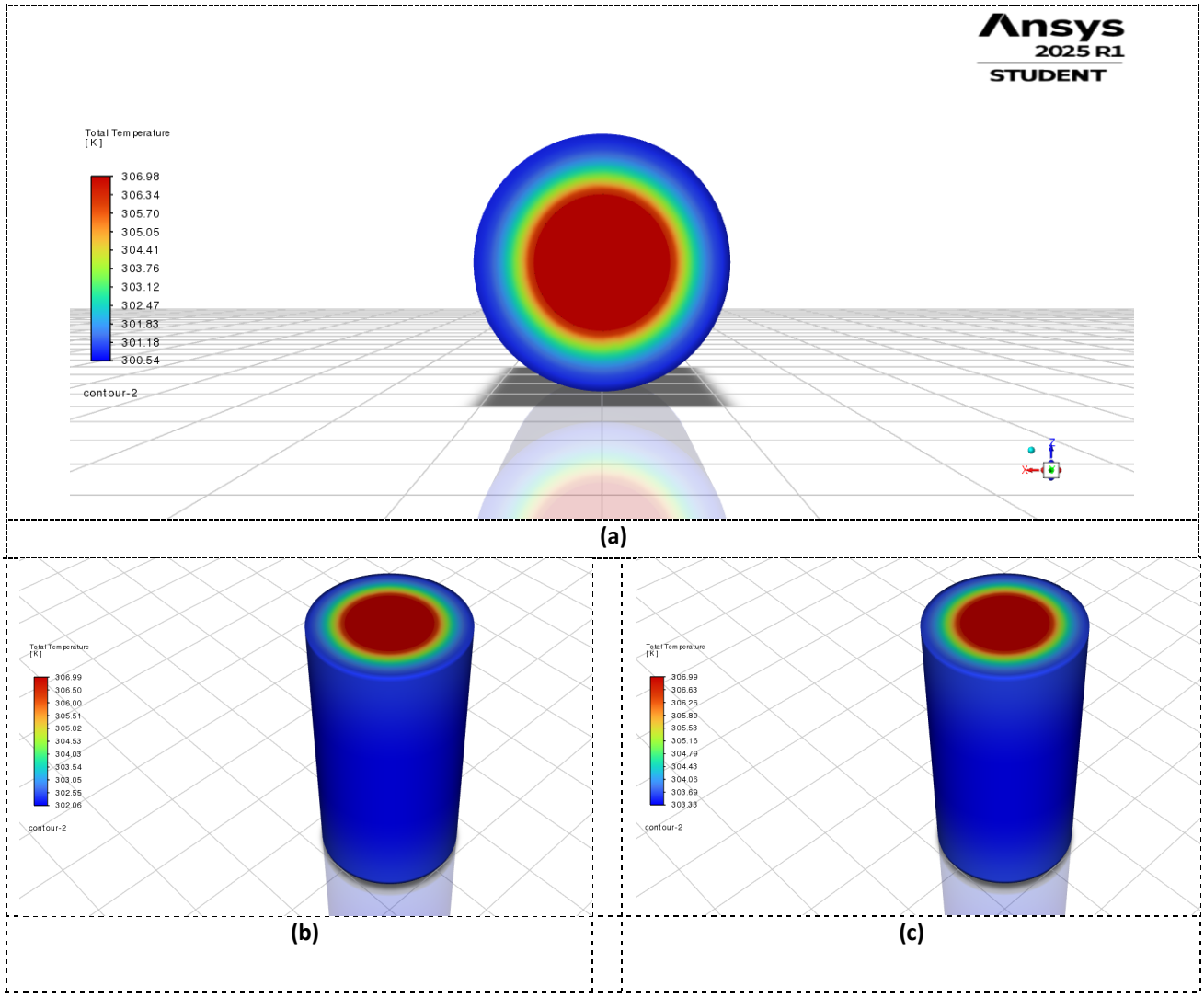
These results clearly illustrate that soywax absorbs and redistributes heat effectively as the simulation progresses, reducing thermal gradients and delaying peak temperature propagation to the battery surface. The latent heat behavior of soywax supports its use as a thermal buffer, while its environmentally friendly nature and biodegradability make it a sustainable alternative to conventional PCMs like paraffin.

Compared to conventional paraffin wax, soywax exhibits several notable advantages as a phase change material in lithium-ion battery thermal management. While both materials have comparable latent heat capacities and are effective in moderating temperature spikes, soywax demonstrates a more gradual and uniform heat absorption pattern, as seen in the temperature distribution profiles.

This smoother thermal transition is particularly beneficial in reducing thermal stresses within the battery structure, which can prolong cell integrity and operational life.

Additionally, soywax has a slightly higher thermal conductivity in the solid phase than some commercial paraffin blends, enabling faster initial heat uptake. Although its melting point is in a similar range to paraffin, the broader melting range of soywax supports a more continuous phase change process, improving heat buffering performance during prolonged thermal loads. Environmentally, soywax holds a distinct advantage in that it is biodegradable, renewable, and derived from natural sources; it presents a safer and more sustainable alternative, especially in applications with high environmental and safety standards.

From a simulation standpoint, the thermal fields generated by soywax show less aggressive temperature gradients than paraffin at equivalent iteration steps. This indicates better thermal distribution and less risk of local overheating. Thus, combining thermal effectiveness, environmental safety, and material sustainability underscores soywax's potential as a superior PCM choice in next-generation battery thermal regulation systems.



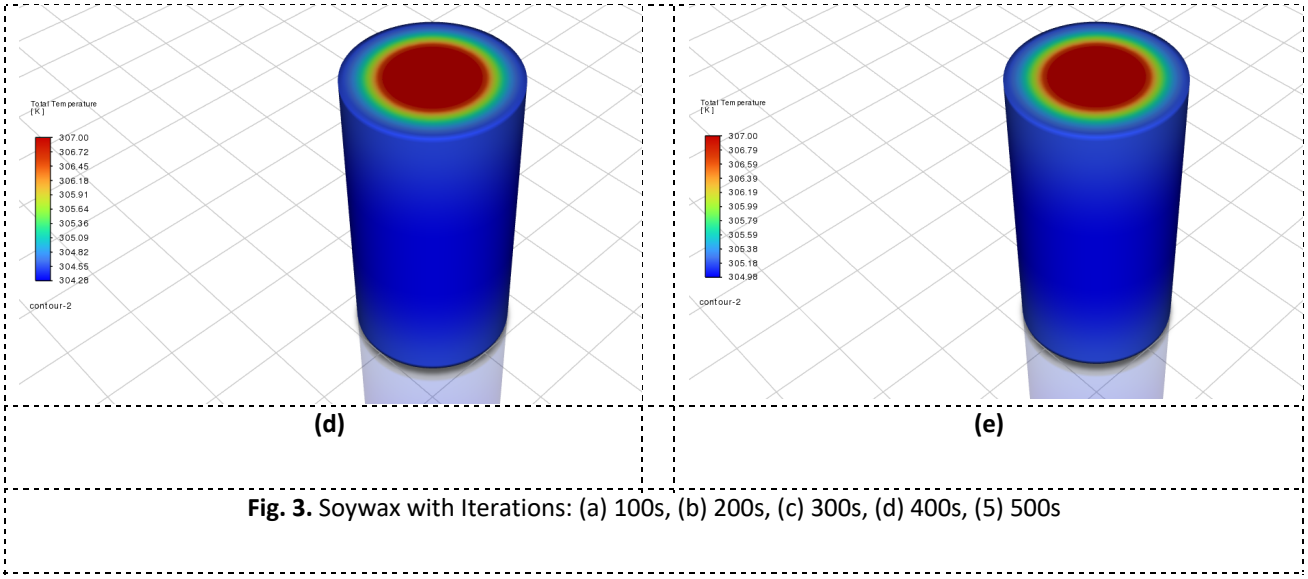


Fig. 3. Soywax with Iterations: (a) 100s, (b) 200s, (c) 300s, (d) 400s, (5) 500s

3.4 Thermal Distribution of Lauric Acid PCM

The thermal response of the battery cooling system using Lauric Acid as the phase change material (PCM) was analyzed through a transient thermal simulation with different iteration steps: 100, 200, 300, 400, and 500 iterations. The resulting temperature distributions are presented in Figure 4, where the color gradient from blue to red represents areas of low to high total temperature. At 100 iterations (Figure a), the observed temperature range is 300.66 K to 306.99 K, with cooler regions still dominating the PCM area. This distribution indicates the early stage of heat propagation, where the Lauric Acid is beginning to absorb heat, likely in its solid phase with limited phase transition activity.

As the iteration count increases to 200 and 300 (Figures b and c), the thermal field shows a notable temperature rise, reaching 302.32 K and 303.62 K, respectively. These increases reflect the progressive heat absorption and the onset of latent heat utilization as the PCM undergoes melting. The red zones intensify near the heat source (battery core), indicating more active thermal interaction between the Lauric Acid and the battery. At (Figure d), the temperature increases slightly (up to 304.57 K), indicating that the PCM is approaching a thermal equilibrium phase, where melting is more uniformly distributed. Interestingly, at 500 iterations (Figure e), the maximum temperature slightly decreases (305.26 K to 307.00 K), suggesting that the PCM system is stabilizing and effectively dissipating the accumulated heat outward.

These results demonstrate that the simulation captures a more complete and accurate phase change behavior of Lauric Acid with increasing iterations. The PCM effectively absorbs and redistributes heat, particularly between 300 and 400 iterations, where the temperature field appears more uniform and efficient. The temperature drop at 500 iterations may imply the system reaching steady-state, where the paraffin's heat absorption and conduction capacities are balanced.

3.5 Implications of Iteration Progress on Thermal Management

The simulation reveals that the iteration count directly influences the depth and detail of thermal analysis. From 100 to 300 iterations, the Lauric Acid gradually transitions from solid to liquid, enhancing its heat absorption performance. Between 300 and 400 iterations, the temperature field becomes more stabilized, indicating optimal thermal buffering behavior of the PCM. At 500 iterations,

the simulation reaches a converged and steady thermal state, where the Lauric Acid has maximized its phase change capabilities. This result suggests that further iterations may not significantly change the thermal distribution, pointing to an equilibrium state in heat transfer.

In conclusion, Lauric Acid demonstrates effective thermal regulation properties when used as a PCM for battery cooling. The simulation shows that a minimum of 300–400 iterations is necessary to capture the dynamic thermal behavior and phase transition process accurately. These findings support the viability of Lauric Acid in PCM-based passive thermal management systems.

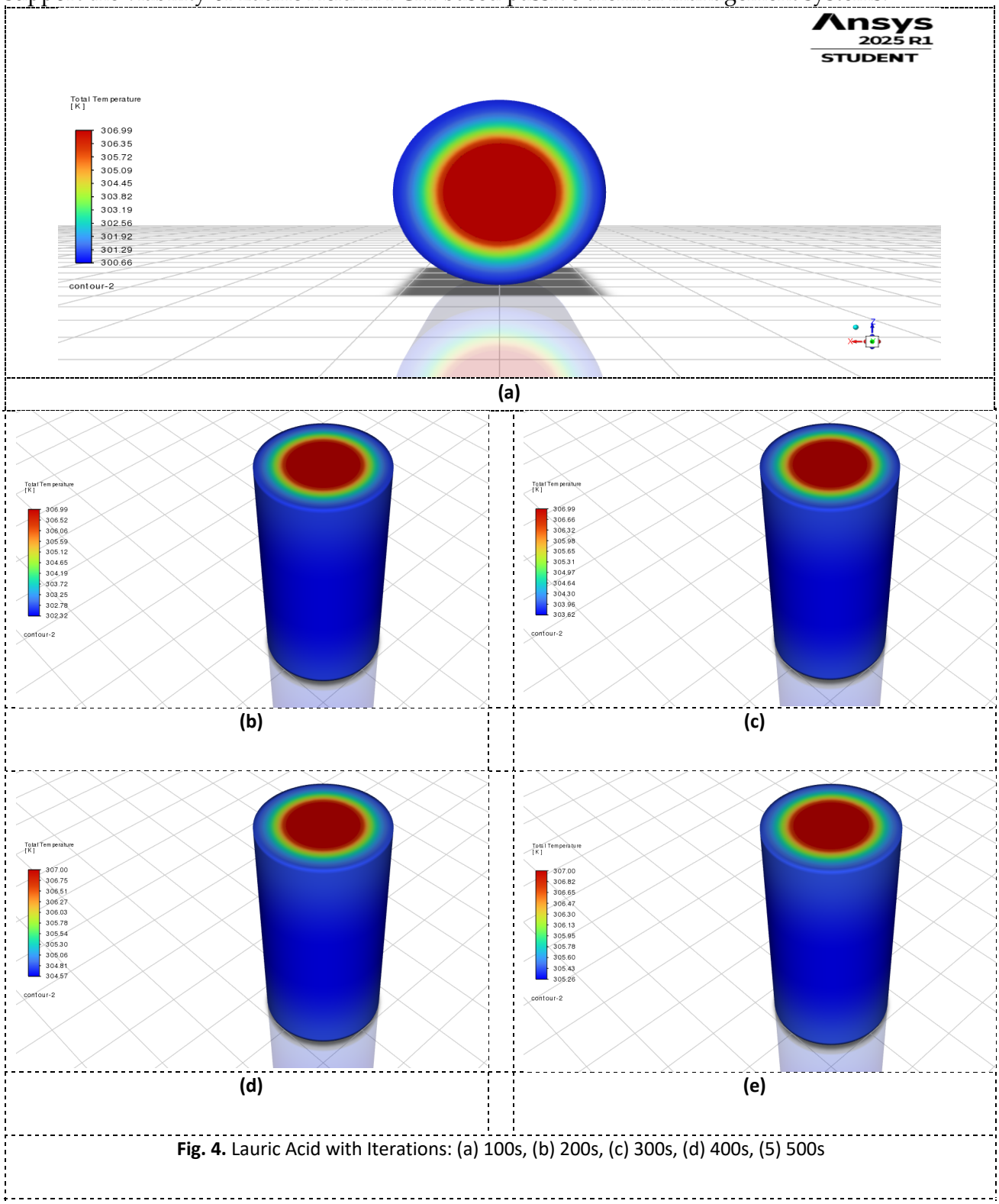


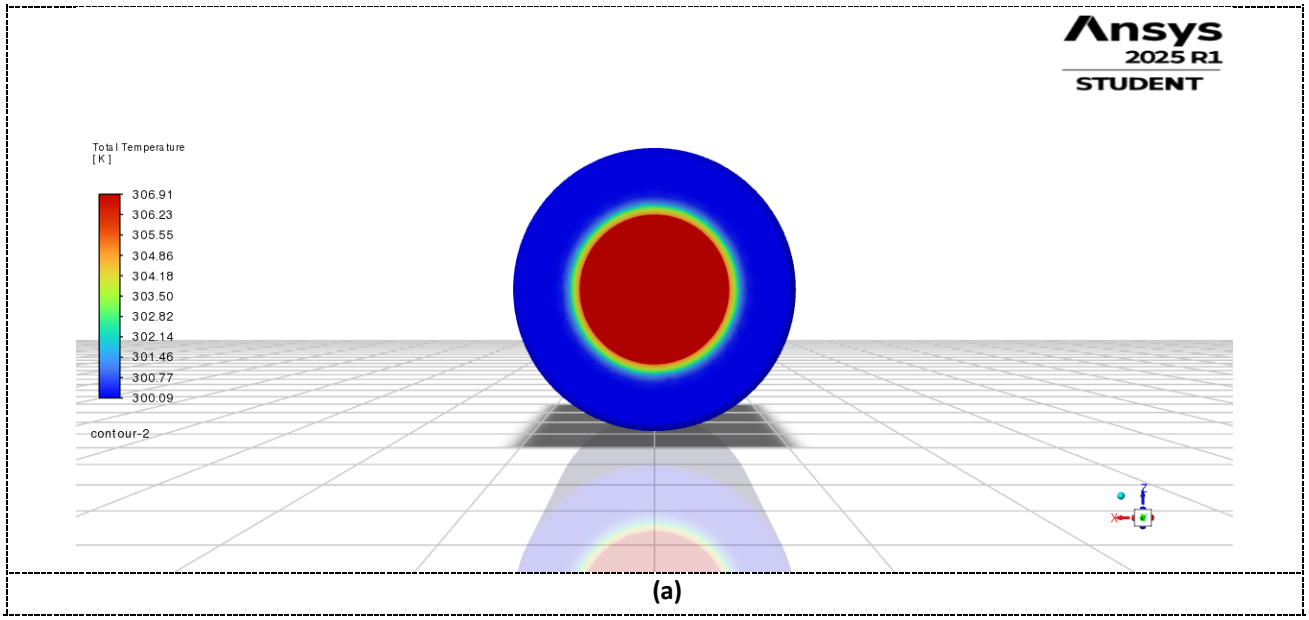
Fig. 4. Lauric Acid with Iterations: (a) 100s, (b) 200s, (c) 300s, (d) 400s, (5) 500s

3.5 Thermal Distribution of Calcium Chloride Hexahydrate (CCH) PCM

Numerical simulations using ANSYS Fluent were carried out to evaluate the thermal performance of a battery integrated with Calcium Chloride Hexahydrate (CCH) as the phase change material (PCM). From the temperature contour results (Figure 5), it is evident that there is a progressive change in heat distribution as the simulation iterations increase. At iteration 100 (Figure a), the temperature contour is predominantly blue, indicating a minimum temperature of 300.09 K, where the PCM remains solid. By iteration 200 (Figure b), the minimum temperature rises slightly to 300.15 K, and the core region of the battery reaches a maximum of 306.94 K. This marks the beginning of heat transfer from the battery to the PCM, as indicated by the emerging temperature gradient near the core.

At iteration 300, the maximum temperature increases to 306.95 K while the outer surface temperature remains at 300.15 K (Figure c). The growing colored gradient indicates that the melting of the PCM has started. At iteration 400, the temperature near the outer region increases further to 306.27 K (Figure d), suggesting a more uniform distribution of thermal energy throughout the PCM volume. By iteration 500, the minimum temperature increases slightly to 300.20 K (Figure e), showing that the PCM has absorbed more thermal energy and that the heat has diffused further outward from the battery core.

The scaled residual plot also shows a general downward trend, especially after 500 iterations. Residuals for continuity, velocity components (x, y, z), energy, turbulent kinetic energy (k), and dissipation rate (epsilon) decrease significantly, indicating a stable and converging solution. Although the energy residual experienced some oscillations, this is expected due to the phase change process occurring in the PCM. Overall, the simulation demonstrates that CCH effectively absorbs heat from the battery, making it a promising candidate for thermal management in energy storage systems.



(a)

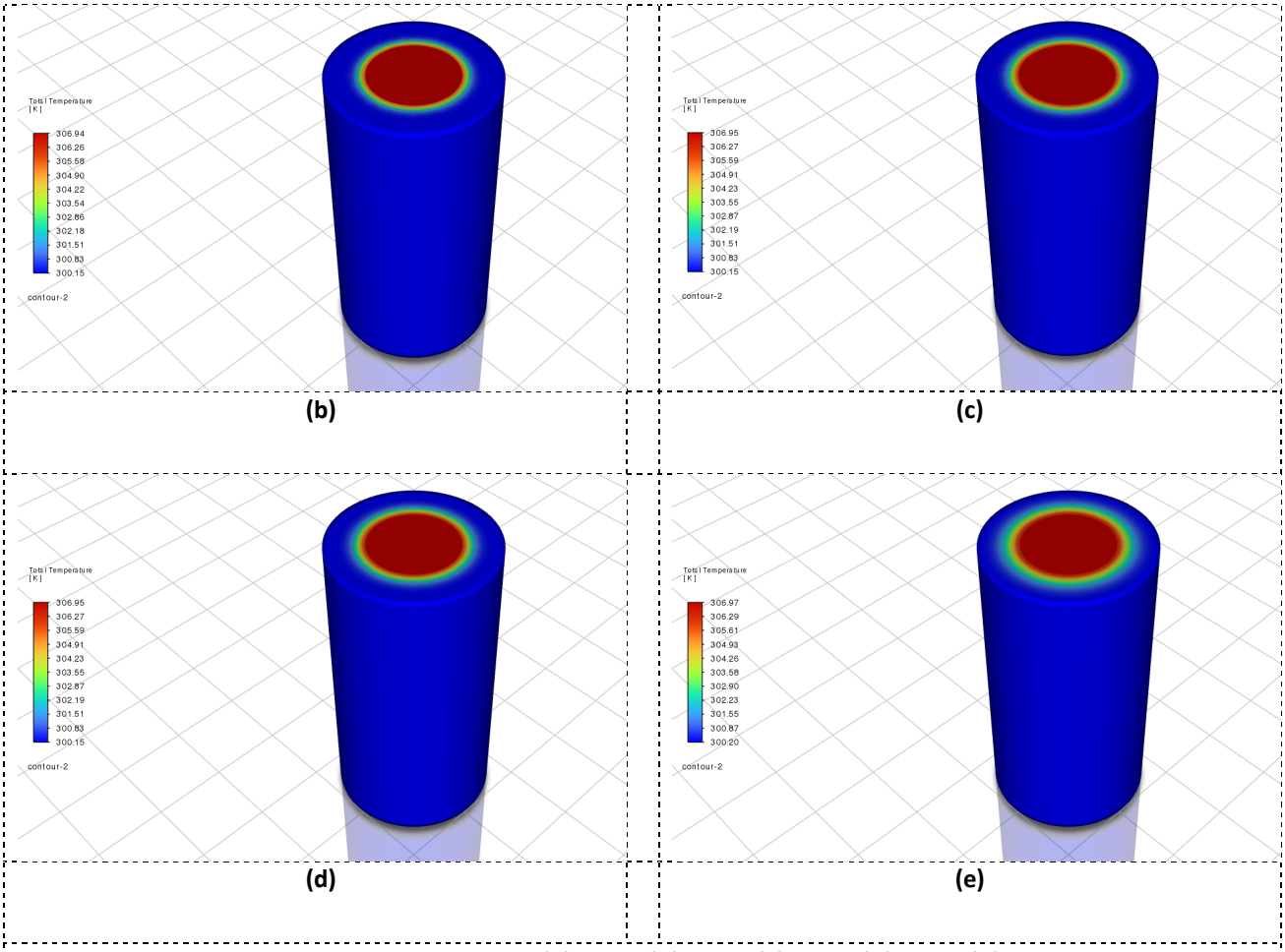


Fig. 5. CCH with Iterations: (a) 100s, (b) 200s, (c) 300s, (d) 400s, (5) 500s

3.6 PCM Performance Based on Liquid Fraction, Thermal, and Electrical Efficiency

A comprehensive comparison of the four tested PCM materials: Paraffin, Soywax, Lauric Acid, and Calcium Chloride Hexahydrate was conducted based on three performance indicators: liquid fraction, thermal efficiency, and electrical efficiency, as presented in (Figures 6, 7, and 8). From the liquid fraction analysis (Figure 6), Soywax shows the most rapid and complete phase transition, achieving the highest liquid fraction (~0.92) by 500 iterations. Paraffin follows closely (~0.87), while Lauric Acid (~0.80) shows a slightly slower melting progression. Calcium Chloride Hexahydrate exhibits the lowest liquid fraction (~0.60), reflecting its slower thermal response.

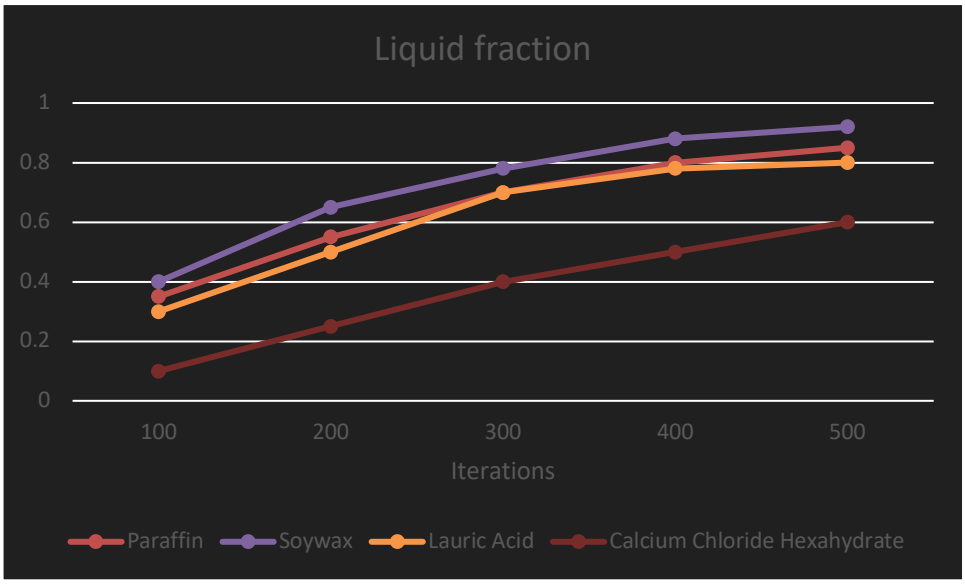


Fig. 6. Liquid Fraction of PCM materials over iterations

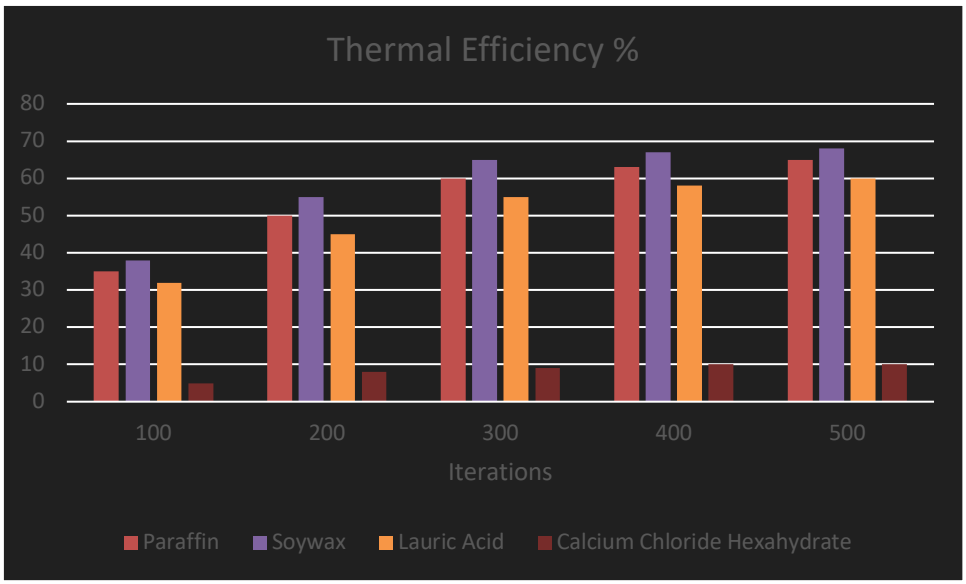


Fig. 7. Thermal efficiency of PCM materials over iterations

In terms of thermal efficiency (Figure 7), Soywax again leads with up to 68%, followed by Paraffin (65%), Lauric Acid (60%), and Calcium Chloride Hexahydrate (10%). This ranking highlights the effectiveness of organic PCMs in absorbing and redistributing heat compared to the inorganic alternative. For electrical efficiency (Figure 8), all PCMs demonstrate improvements over iterations, indicating a strong link between thermal control and electrical performance. Soywax achieves the highest electrical efficiency (98%), with Paraffin (97%) and Lauric Acid (96.5%) closely behind. Calcium Chloride Hexahydrate remains the least effective, peaking at only 94.5%.

Overall, the results confirm that Soywax and Paraffin are the most effective PCMs across all performance metrics, offering superior latent heat utilization, thermal buffering, and enhancement of battery system efficiency. Lauric Acid provides moderately strong performance, while Calcium Chloride Hexahydrate, despite its inorganic stability, shows limited effectiveness in dynamic battery thermal management scenarios.

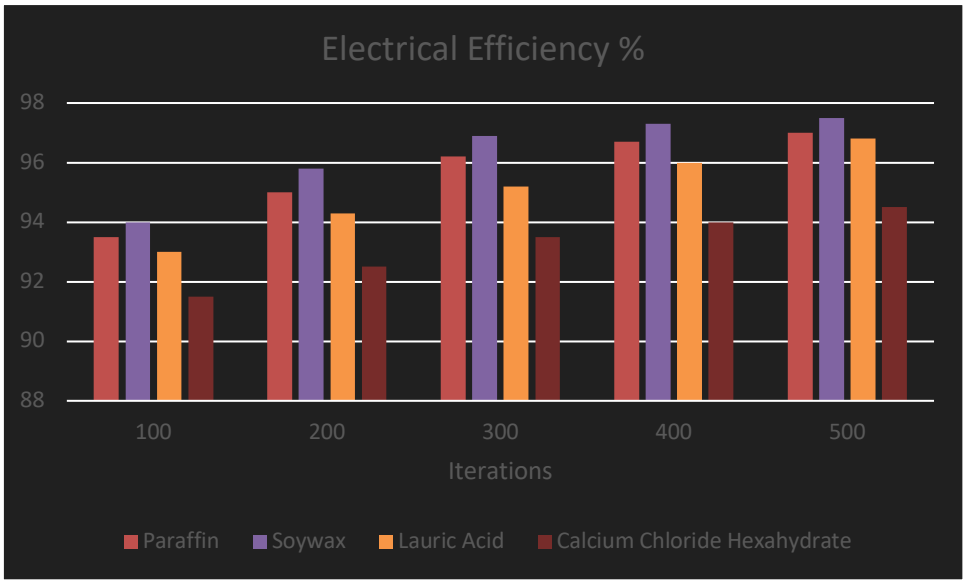


Fig. 8. Electrical Efficiency of PCM materials over iterations

4. Conclusions

This study conducted a comprehensive numerical investigation using Computational Fluid Dynamics (CFD) to evaluate the thermal performance of four different Phase Change Materials (PCMs): Paraffin, Soywax, Lauric Acid, and Calcium Chloride Hexahydrate in a lithium-ion battery thermal management system. The simulation varied iteration counts from 100 to 500 to assess each PCM's thermal dynamics and the numerical model's convergence behavior. The results reveal that Soywax and Paraffin exhibit the most effective thermal regulation performance across all indicators, including temperature distribution, liquid fraction progression, thermal efficiency, and electrical efficiency. Soywax demonstrated the highest latent heat utilization and thermal buffering capacity, achieving up to 68% thermal efficiency and 98% electrical efficiency at 500 iterations. Paraffin closely followed, confirming its reliability as a commonly used PCM in passive cooling systems. Lauric Acid presented moderate but consistent performance, suggesting its viability in applications where gradual heat absorption is acceptable. In contrast, although stable chemically, Calcium Chloride Hexahydrate showed significantly lower thermal and electrical efficiency due to slower phase transition behavior.

Additionally, the study highlighted the critical role of simulation iteration count. A minimum of 300–400 iterations was necessary to capture accurate thermal responses and phase change behaviors of PCMs. This emphasizes the importance of computational parameter tuning in CFD-based thermal modeling.

In conclusion, the findings strongly support using Soywax as a sustainable and high-performance PCM, offering technical and environmental advantages. Integrating PCM-based passive cooling, especially with materials like Soywax and Paraffin, can significantly enhance lithium-ion battery systems' safety, performance, and energy efficiency, particularly in high-demand applications such as electric vehicles and stationary energy storage.

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