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# A finite element approach for phase-change analysis of paraffin

## *Parafin faz-değiştirme analizlerinde sonlu elemanlar yaklaşımı*

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# A Finite Element Approach for Phase-Change Analysis of Paraffin

## *Highlights*

- *The finite element approach allows for the time-dependent analysis of phase-changing materials with low computational costs.*
- *The thermal properties of paraffin were obtained through DSC.*
- *The time-dependent thermal analyses performed using finite element analysis are in agreement with the experimental results.*
- *The finite element approach was compared with experiments conducted at different heating rates, revealing its limitations in accurately capturing rapid phase change events.*

## *Graphical Abstract*

*This study focuses on the thermal analysis of paraffin wax using the FE method under various heating rates. The paraffin was heated up with three different heating rates with a controlled hot plate. Temperature histories during the melting process inside the paraffin were acquired with thermocouples and the data collected was used to compare finite element analyses results.*

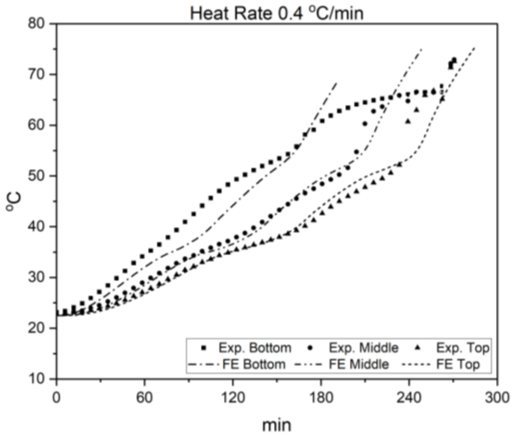

**Figure.** Temperature-time plot of the paraffin under 0.4 °c/min heating rate condition

## *Aim*

*This study utilizes finite element approach in the field of thermal analyses of phase-change materials to demonstrate its efficient in transient analyses.*

## *Design & Methodology*

*Both experimental and numerical studies were performed. Numerical studies which were finite element analyses were validated with experiments.*

## *Originality*

*This study investigated finite element approach for a phase change material and the methodology was validated under constant heating rates. Since this approach had not been examined before, it holds originality.*

## *Findings*

*Finite element heat transfer analyses can be utilized to investigate phase-change of paraffin. The method can efficiently capture phase-change phenomena, particularly if the transition is slow.*

## *Conclusion*

*The FE results demonstrated good agreement with the experimental data, particularly in terms of temperature trends over time. However, discrepancies were observed, especially during the rapid melting phase, indicating limitations in the FE model's ability to capture quick changes in phase state, particularly at the bottom of the paraffin container.*

## *Declaration of Ethical Standards*

*The author(s) of this article declare that the materials and methods used in this study do not require ethical committee permission and/or legal-special permission.*

# A Finite Element Approach for Phase-Change Analysis of Paraffin

***Araştırma Makalesi / Research Article***

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## ABSTRACT

During the design of thermal management systems involving Phase Change Materials (PCM), analysis tools are essential for determining the amount of PCM required, optimal instalment locations, and the heating-cooling transient behavior of the systems. Computational Fluid Dynamics (CFD) solvers are often employed for these tasks. However, CFD simulations can be computationally expensive, when solving transient problems. An alternative approach for PCM simulations is the Finite Element Method (FEM), which offers computationally inexpensive heat transfer analyses while providing good accuracy for thermal energy storage design. This study has focused on thermal analysis of paraffin performed by FEM. During the studies, thermal properties of the paraffin which was obtained by differential Scanning Calorimetry (DSC) analysis was adopted to the FEM model and transient analyses were performed. The results showed that the finite element results are in good agreement with the experimental data which was acquired from middle and top measurement points and less than 10% error margin was obtained. However, large discrepancies of up to 22% between the experiment and the analyses were observed. This large error margin indicated that FEM was not capable of capturing fast phase transformations. In addition to the numerical results obtained from the experiment and analyses, it was noted that the solution time was less than an hour for each case.

**Keywords: Phase Change Materials (PCM), Finite Element Analysis, Thermal Analysis, Differential Scanning Calorimetry (DSC).**

# Parafin Faz-Değiştirme Analizlerinde Sonlu Elemanlar Yaklaşımı

## ÖZ

Faz Değiştiren Malzemelerin (FDM) kullanıldığı termal sistemlerinin tasarımı sırasında, analiz araçlarının kullanımı önem arz eder. Nümerik analizler, FDM miktarının, optimal uygulama yerlerinin ve ısınma-soğuma sürelerinin belirlenmesi için esastır. Bu amaç doğrultusunda genellikle Hesaplamalı Akışkanlar Dinamiği (HAD) çözücüleri kullanılır. Ancak; HAD, zamana bağlı çözümlerde oldukça hesaplama maliyeti getirir. FDM simülasyonları için bir alternatif yaklaşım olarak Sonlu Elemanlar Yöntemi (SEY) tercih edilebilir. Bu çalışma, SEY ile gerçekleştirilen parafinin termal analizine odaklanmıştır. Çalışma süresince, parafinin Taramalı Diferansiyel Kalorimetre (DSC) analizleri ile elde edilen termal özellikleri sonlu elemanlar modeline adapte edilmiş ve zamana bağlı analizler gerçekleştirilmiştir. Analiz sonuçlarının, orta ve üst noktalardan alınan sıcaklık ölçümleri ile uyum içerisinde olduğu ve deney sonuçları ile nümerik hesaplamalar arasındaki hatanın %10'dan az olduğu belirlenmiştir. Ancak, ısıtıcıya en yakın bölgedeki ölçüm sonuçları ile analiz sonuçları arasında %22'ye varan hata olduğu saptanmıştır. Bu durum hızlı faz değişiminin bulunduğu bölgelerde SEY'in yetersiz kaldığını göstermektedir. Elde edilen sonuçlara ek olarak, analizleri gerçekleştirilen her bir senaryonun çözüm süresinin bir saatten daha kısa sürdüğü gözlemlenmiştir.

**Anahtar Kelimeler: Faz Değiştiren Malzemeler (FDM), Sonlu Elemanlar Analizi, Termal Analiz, Diferansiyel Taramalı Kalorimetre (DSC).**

## 1. INTRODUCTION

Phase Change Materials (PCMs) are integral components of heat storage systems because of their notable heat of fusion and constant phase-change temperatures. Their ability to store heat makes them versatile, finding use across various sectors, including electronics cooling and the thermal management of buildings and solar collectors [1-2]. According to Aravindhan et al., PCMs have demonstrated the capability to store significantly more heat per unit volume compared to traditional storage materials such as water, masonry, or rock, ranging from 5 to 14 times higher [3].

As depicted in Figure 1, PCMs absorb heat during the melting process and release it upon solidification. Given that these phase transitions occur at relatively stable temperatures, PCMs are well-suited for applications requiring specific temperature ranges. Phase Change Materials are classified into three primary categories: Organics, inorganics, and eutectics. Organic PCMs exhibit congruent melting behaviour, enabling them to undergo repeated melting and freezing cycles without experiencing phase separation or degradation of their latent heat of fusion.

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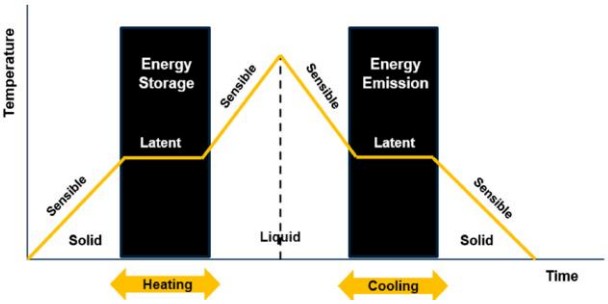

**Figure 1**. Schematic diagram of the phase change transition [4]

Additionally, they demonstrate self-nucleation properties, crystallizing with minimal or no supercooling, and are typically non-corrosive. Salt hydrates constitute the predominant type of PCM, offering advantages such as high latent heat of fusion per unit volume, relatively enhanced thermal conductivity, and negligible volume changes upon melting. Eutectic PCMs represent the minimum-melting composition of two or more components, resulting in a blend of crystallized component crystals during the crystallization process [2].

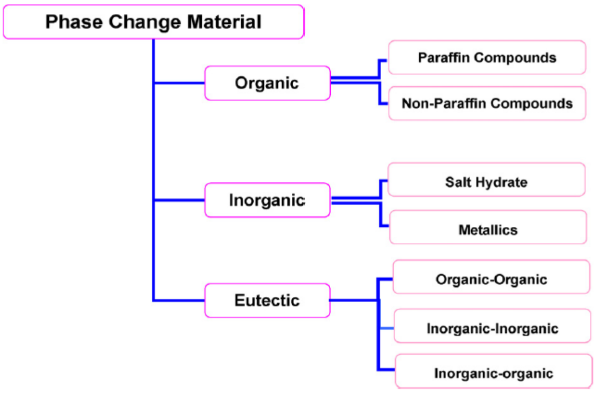

**Figure 2.** PCM classification [2]

While PCMs exhibit a high capacity for storing heat, their thermal conductivity is relatively low. Because of this reason, PCMs are frequently paired with materials that offer superior thermal conductivity, such as aluminum, nickel, or copper. Therefore, paraffin impregnated open cell foam materials are investigated both experimentally and numerically by various authors [5-8]. Marri and Balaji conducted research to found out effect of porosity and pore density on PCM-metal foam composite heat sinks. They pointed out that porosity had major effect on effective thermal conductivity [9]Additionally, there have been experimental investigations aimed at enhancing thermal conductivity through the incorporation of nanoparticles into paraffin [10-11]. Furthermore, analysis techniques have been developed with PCM-foam and PCM-nanoparticle composites. Zhu et al. conducted research on the influence of pore density on thermal conductivity using a numerical approach. They found that the effective thermal conductivity of PCM increases with higher pore density. [12]. Another study concentrated on the numerical analysis of a PCM integrated finned heat sink. The authors noted that natural convection intensifies as the liquid fraction inside the melted PCM increases [13]. Yand and Wang carried out three-dimensional numerical simulations of a portable electronic device integrated with a PCM. They analysed different power rates, charge and discharge modes and orientations [14]. In addition to the numerical approaches, various theoretical methods were employed in order to calculate effective thermal conductivity of PCM-Metal foam composites [15-19].

Finite element (FE) is one of the analysis methods used to perform in heat transfer simulations of PCMs. Because of their stability and computationally efficient, FE analyses of PCMs are frequently preferred especially in transient thermal simulations. Gong and Mujumbar utilized FE method to investigate cyclic heat transfer in a PCM integrated shell-and-tube heat exchanger [20]. Additionally, Zhou et al utilized an explicit FE approach to evaluate the impact of PCM in buildings [21].

This study focuses on the thermal analysis of paraffin wax using the FE method under various heating rates. Paraffin’s thermal properties were obtained from Differential Scanning Calorimetry (DSC) analysis. The paraffin was heated up with three different heating rates with a controlled hot plate. Temperature histories during the melting process inside the paraffin were acquired with thermocouples and the data collected was used to compare finite element analyses results.

## 2. METHODOLOGY

During the study, both experimental and numerical investigations were conducted. Experimental activities were undertaken to validate the numerical analyses. Following the experimental studies, finite element (FE) analyses were performed using ANSYS APDL.

### 2.1. Experiment

An experimental setup was constructed, as depicted in Figure 3. The setup included a heater controlled by a PID temperature controller. A ZELIO RTC48 temperature controller from Schneider Electric was employed in conjunction with a thermocouple-type temperature sensor for feedback. This configuration allowed the heater to maintain either a constant temperature or a constant heating rate across its surface. Furthermore, a GRAPHTEC data logger was utilized to capture the temperature history inside the paraffin. The acquired data was stored on an SD card for analysis.

K type thermocouples were used to acquire temperature data. The thermocouples were installed 3 mm, 22mm and 45mm above from the bottom of the container. Moreover, an extra thermocouple was placed on the heater in order to provide temperature feedback for the controller. Experiments were conducted using constant heating rates of 0.4°C/min, 0.8°C/min, and 1.6°C/min. The purpose of varying the heating rates was to investigate transient effects by applying different heat inputs.

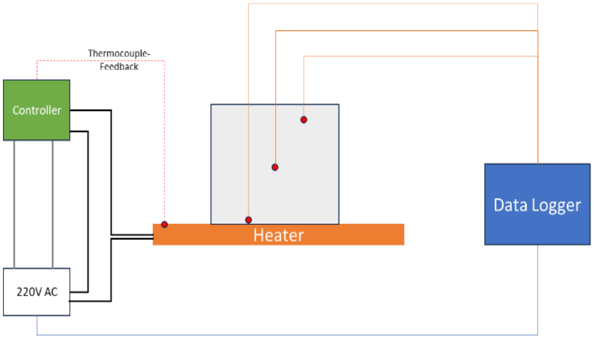

**Figure 3.** Schematic experiment setup

### 2.2. Measurement Uncertainty

The uncertainty of temperature measurement depended on the uncertainty of the thermocouples ($U_{thermocouple}$) which are ±2.2°C. The uncertainty of the heater was a combination of the controller's uncertainty and the uncertainty of the feedback controller. Thus, heater's uncertainty ($U_{heater}$) was expressed as:

$$U_{heater} = \sqrt{U_{controller}^2 + U_{thermocouple}^2} \tag{1}$$

According to the specification given for the ZELIO RTC48 controller, the uncertainty of the temperature control was ±0.1°C, and uncertainty of the K type thermocouple was ±2.2°C.

$$U_{total} = \sqrt{0.1^2 + 2.2^2} = 2.2023 \tag{2}$$

Therefore, $U_{heater}$ was accepted as equal to $U_{thermocouple}$ which is ±2.2°C.

### 2.3. Finite Element Analysis

The heat transfer problem was numerically implemented using the finite element method. Equation (3) expresses the typical finite element heat transfer formulation:

$$[C]\{\dot{T}\} + [K]\{T\} = \{Q\} + \{q\} \tag{3}$$

In this equation, {T} represents the temperature vector, [C] stands for the capacitance, [K] denotes the element conductivity, {Q} represents the internal heat generation, and {q} includes boundary flux terms. These matrices and vectors are defined using Galerkin's method as follows [22]:

$$[K] = k \iiint_V \left[ \frac{\partial [N]^T}{\partial x}\frac{\partial [N]}{\partial x} + \frac{\partial [N]^T}{\partial y}\frac{\partial [N]}{\partial y} + \frac{\partial [N]^T}{\partial z}\frac{\partial [N]}{\partial z} \right] dV \tag{4}$$

$$[C] = \rho c \iiint_V [N][N]^T dV \tag{5}$$

$$\{Q\} = \iiint_V Q[N]^T dV \tag{6}$$

$$\{q\} = -\iint_A k \left[ \frac{\partial T}{\partial x} n_x + \frac{\partial T}{\partial y} n_y + \frac{\partial T}{\partial z} n_z \right] [N][N]^T dA \tag{7}$$

In this equation, [N] represents the shape function, $n_x$, $n_y$, $n_z$ denote the unit surface normal in the global x, y, z directions, and $Q$ represents the magnitude of internal heat generation.

Transient thermal analyses were performed with ANSYS APDL software. Paraffin and stainless-steel container were discretized with linear hexahedral elements defined as SOLID278. As seen in **Hata! Başvuru kaynağı bulunamadı.**, due to the symmetry conditions, only a quarter part of the container and paraffin wax were modelled. SURF152 3D thermal surface effect elements were applied on the outer surfaces of the container. Natural convection was assumed on outer surfaces of the container. Also, reference temperature for the convection was applied as 22.5 °C which measured room temperature during the experiments.

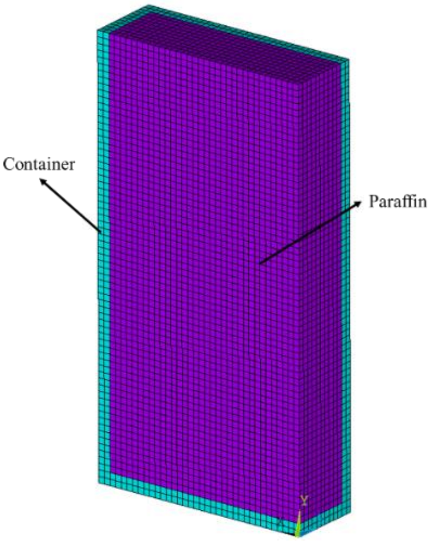

**Figure 4.** Finite element model

The container's material was stainless-steel and thermal properties used in the analyses were given in Table 1.

**Table 1.** Thermal properties of the container

| | |
|---|---|
| Density | 7800 kg/m$^3$ |
| Thermal Conductivity | 15 W/mK |
| Specific Heat | 480 J/kgK |

The density and thermal conductivity of the paraffin was also given in Table 2. Specific heat and latent heat of the paraffin was taken from the DSC analysis.

**Table 2.** Thermal properties of the paraffin

| | |
|---|---|
| Density | 790 kg/m$^3$ |
| Thermal Conductivity | 0.2 W/mK |

### 2.4. Differential Scanning Calorimetry Analysis

Paraffin was selected as PCM material due to its high latent heat and low melting point. Thermal properties of the paraffin were determined by Differential Scanning Calorimetry (DSC) which is an analysis technique that looks at how specific heat capacity (Cp) is changed by temperature. 4.1 mg paraffin wax was analyzed by DSC. Differential scanning calorimetry curve of the paraffin is shown in Figure 5. As stated in the DSC curve, latent heat of fusion of the PCM is 228 J/kg. Melting onset is 50 °C and melting finishes at 59 °C.

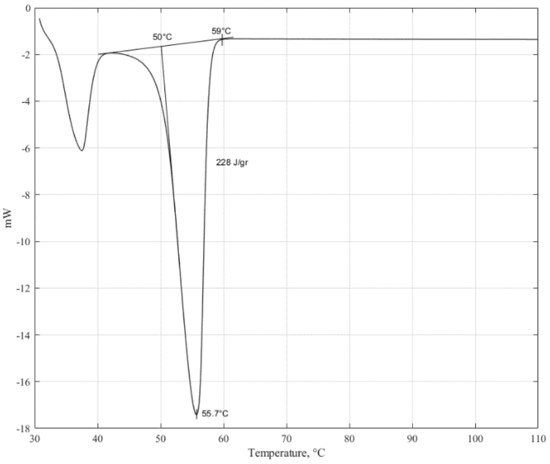

**Figure 5.** DSC curve

Although DSC curve presents heat capacity change, enthalpy-temperature relation is required to perform heat transfer FE analysis. Therefore, enthalpy-temperature curve was calculated by integrated DSC curve with respect to time. Figure 6 displays the enthalpy change of the PCM. The zone defined between 50-59°C has highest gradient and this region is called as mushy zone where melting occurs.

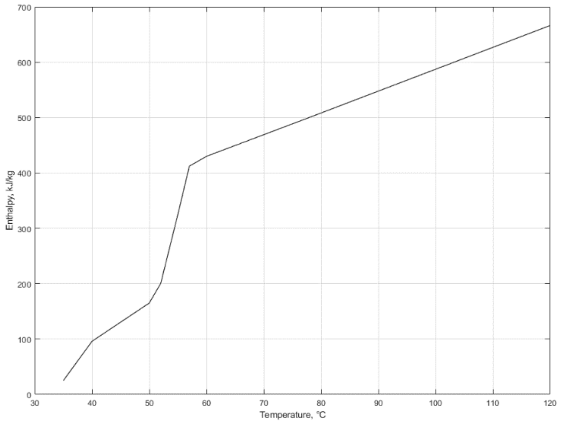

**Figure 6.** Enthalpy change

## 3. RESULTS AND DISCUSSION,

Finite element transient thermal analyses were conducted at three different heating rates and temperature history of the paraffin was given in this section. The temperature tracking points were names as bottom, middle and top corresponding to the locations of 3 mm, 22 mm and 45 mm above from the PCM container bottom.

Figure 7 shows heating condition of the paraffin under the lowest heating rate which was 0.4 °C/min. Analysis results showed good agreement with the experiment. However, it was observed that FE solutions diverged from the experiment after the melting was concluded.

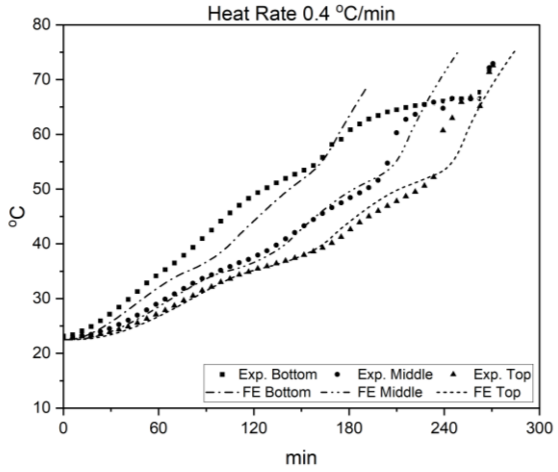

**Figure 7.** Temperature-time plot of the paraffin under 0.4 °C/min heating rate condition

Figure 8 illustrates the experimental and numerical temperature histories of the paraffin when the heating rate was 0.8 °C/min. As seen in the figure, analysis results are in good agreement with the experiment except the bottom location. It is understood that FE approach is not fully capable of capturing quick melting process occurred at the bottom location.

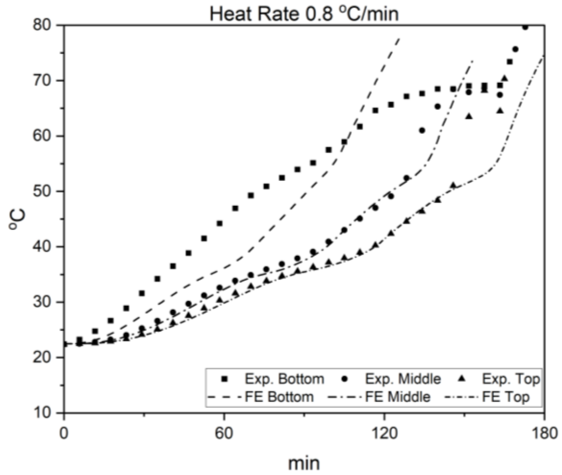

**Figure 8.** Temperature-time plot of the paraffin under 0.8 °C/min heating rate condition

The last investigated heating rate was 1.6°C/min. Similar characteristics observed in previous results can be identified for the highest heating rate condition. As shown in Figure 9, the middle and top measurement locations closely align with the experimental findings until the melting process is completed. Additionally, the correlation at the bottom point improves for the highest heating rate condition. This is attributed to the rapid completion of the mush zone, leading to a decrease in the difference between experimental and analysis results at the bottom. This phenomenon highlights a limitation of the finite element approach in accurately representing the mush zone.

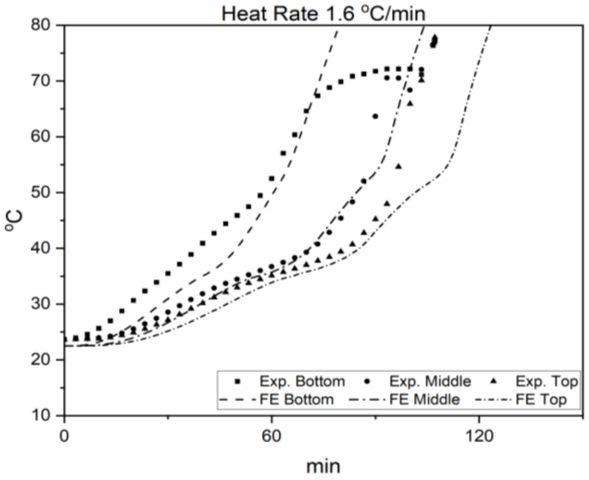

**Figure 9.** Temperature-time plot of the paraffin under 1.6 °C/min heating rate condition

In conclusion, this study has investigated the thermal behavior of paraffin wax using both experimental and numerical approaches. Since PCMs have high latent heat, they play a vital role in energy storage systems. The experimental setup involved controlled heating rates applied to paraffin samples, with temperature measurements taken at various locations. Finite Element analyses were conducted to simulate the transient thermal behavior of the paraffin under different heating rates. The FE results demonstrated good agreement with the experimental data, particularly in terms of temperature trends over time. Error margin was less than 10% when the analysis results were compared with the data acquired from middle and top measurement points for each heating case. However, discrepancies were observed, especially during the rapid melting phase, indicating limitations in the FE model's ability to capture quick changes in phase state. These discrepancies were particularly notable at the bottom of the paraffin container, where differences of up to 22% were observed. These discrepancies can be attributed to the thermal conductivity change with temperature. Therefore, implementing temperature-dependent thermal conductivity of the paraffin can increase the accuracy of the FE analyses. Overall, the combined experimental and numerical approach provides valuable insights into the thermal characteristics of paraffin wax, contributing to the understanding and optimization of PCM-based energy storage systems.

## 4. CONCLUSION

In conclusion, this study has investigated the thermal behavior of paraffin wax using both experimental and numerical approaches. Since PCMs have high latent heat, they play a vital role in energy storage systems. The experimental setup involved controlled heating rates applied to paraffin samples, with temperature measurements taken at various locations. Finite Element analyses were conducted to simulate the transient thermal behaviour of the paraffin under different heating rates. The FE results demonstrated good agreement with the experimental data, particularly in terms of temperature trends over time. Error margin was less than 10% when the analysis results were compared with the data acquired from middle and top measurement points for each heating case. However, discrepancies were observed, especially during the rapid melting phase, indicating limitations in the FE model's ability to capture quick changes in phase state. These discrepancies were particularly notable at the bottom of the paraffin container, where differences of up to 22% were observed. These discrepancies can be attributed to the thermal conductivity change with temperature. Therefore, implementing temperature-dependent thermal conductivity of the paraffin can increase the accuracy of the FE analyses. Overall, the combined experimental and numerical approach provides valuable insights into the thermal characteristics of paraffin wax, contributing to the understanding and optimization of PCM-based energy storage systems.

## ACKNOWLEDGEMENT

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## DECLARATION OF ETHICAL STANDARDS

The authors of this article declare that the materials and methods used in this study do not require ethical committee permission and/or legal-special permission.

## AUTHORS' CONTRIBUTIONS

**Mustafa OZCATALBAS:** Literature review, finite element analyses, experimental studies, interpretation of the results.

**Adnan SOZEN:** Interpretation of the results, final proofreading.

## CONFLICT OF INTEREST

There is no conflict of interest in this study.

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