An Investigation into Computational Modelling of Melting and Solidification of Phase Change Materials

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A thesis submitted in partial fulfillment of the requirements for the Master of Engineering Science degree in Mechanical and Materials Engineering

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Abstract

This thesis evaluates the effectiveness of the enthalpy-porosity approach in simulating melting and solidification of phase change materials within latent heat thermal energy storage systems. It systematically investigates the sensitivity of the computational model to four adjustable parameters: mushy zone coefficient, thermal expansion coefficient, solidus/liquidus temperatures, and latent heat. The study includes individual and combined analyses of these factors in simulations of the melting process by comparing outcomes with extensive experimental data, resulting in a calibrated melting model. The calibrated model is validated across various heating conditions in the cylindrical cavity, and then in a rectangular cavity, confirming its reliability in predicting the main features of PCM melting behavior. When applied to solidification, significant discrepancies arise in terms of overall freezing time and in the temporal evolution of the interface separating the solid and liquid regions of the domain. It is thought that a key factor influencing this discrepancy is the lack of supercooling considerations in the enthalpy-porosity model that was utilized, indicating a need for improved freezing process modeling.

Keywords

Summary for Lay Audience

Given the increasing global demand for energy and the expected continued reliance on fossil fuels in the near future, discussions concerning the role of renewable energy in supporting energy security have gained prominence. A challenge currently faced by renewable energy sources is their limited capacity to generate power during specific times of the day. This obstacle can be mitigated through the implementation of energy storage systems, which can store excess energy for later use. One effective approach is to store this energy in the form of heat, using thermal storage systems. These systems are advantageous due to their affordability, long lifespan, and ease of scalability.

Phase change materials (PCMs) are unique substances capable of transitioning between a liquid and solid state at specific temperatures. This transformation is linked to the absorption or release of a significant amount of heat called latent heat. This special feature makes PCMs valuable for practical applications where effective thermal energy storage is necessary, like in solar thermal systems to provide space heating and domestic hot water. One key advantage is that during the phase change, the material remains at a nearly constant temperature, allowing for the efficient storage of a substantial amount of energy. As a result, gaining insights into how PCMs behave during the process of melting and solidifying is of utmost importance.

This research involved the application of computational models to accurately simulate the melting and solidification of PCMs. Among the various numerical methods available in this field, the enthalpy-porosity method was chosen due to its ability to simulate complex phase transitions. This study introduced and investigated four different adjustable factors inherent in this method that affect the simulation, aiming to derive a calibrated model through comparison with available experimental data. The resulting calibrated model demonstrated the capability to predict the melting process in various conditions and structures with higher accuracy than other available simulations. The research results are valuable as they can be used to develop effective energy management solutions, leading to a decrease in environmental emissions.
Acknowledgments

I would like to express my deepest gratitude to Dr. Anthony Straatman, my esteemed supervisor, for his guidance, invaluable insights, and unwavering support throughout this journey. Dr. Straatman's expertise and mentorship have been instrumental in shaping the course of my research, and I am truly fortunate to have had the opportunity to work under his tutelage.

I also extend my heartfelt thanks to all my colleagues at Western University for their collaborative spirit and camaraderie. Your diverse perspectives and collective efforts enriched this research and made the academic environment at Western an inspiring one.

Furthermore, I want to express my profound appreciation to my spouse, Emad, whose enduring support, understanding, and patience sustained me through the long hours and challenging moments. Your unflinching belief in me and our shared dreams have always been my constant motivation.
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<th>Acronym</th>
<th>Description</th>
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<tbody>
<tr>
<td>AHC</td>
<td>Apparent Heat Capacity</td>
</tr>
<tr>
<td>CFD</td>
<td>Computational Fluid Dynamics</td>
</tr>
<tr>
<td>DSC</td>
<td>Differential Scanning Calorimeter</td>
</tr>
<tr>
<td>Exp.</td>
<td>Experimental</td>
</tr>
<tr>
<td>FVM</td>
<td>Finite Volume Method</td>
</tr>
<tr>
<td>LH</td>
<td>Latent Heat</td>
</tr>
<tr>
<td>LHTES</td>
<td>Latent Heat Thermal Energy Storage</td>
</tr>
<tr>
<td>PCM</td>
<td>Phase Change Material</td>
</tr>
<tr>
<td>PIV</td>
<td>Particle Image Velocimetry</td>
</tr>
<tr>
<td>SHS</td>
<td>Sensible Heat Storage</td>
</tr>
<tr>
<td>SM</td>
<td>Solidification-Melting</td>
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List of Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
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<tbody>
<tr>
<td>$A_{mush}$</td>
<td>Mushy Zone Coefficient</td>
<td>[kg. m(^3).s(^{-1})]</td>
</tr>
<tr>
<td>$\Delta H$</td>
<td>Latent Heat Content</td>
<td>[J/kg]</td>
</tr>
<tr>
<td>$C_p$</td>
<td>Specific Heat Capacity</td>
<td>[J/kg.K]</td>
</tr>
<tr>
<td>$C_{pg}$</td>
<td>Specific Heat of Material in Gas Phase</td>
<td>[J/kg.K]</td>
</tr>
<tr>
<td>$C_{pl}$</td>
<td>Specific Heat of Material in Liquid Phase</td>
<td>[J/kg.K]</td>
</tr>
<tr>
<td>$C_{ps}$</td>
<td>Specific Heat of Material in Solid Phase</td>
<td>[J/kg.K]</td>
</tr>
<tr>
<td>$f$</td>
<td>Liquid Fraction</td>
<td>Dimensionless</td>
</tr>
<tr>
<td>$g$</td>
<td>Gravitational Acceleration</td>
<td>[m/s(^2)]</td>
</tr>
<tr>
<td>$h$</td>
<td>Sensible Enthalpy</td>
<td>[J/kg]</td>
</tr>
<tr>
<td>$H$</td>
<td>Enthalpy of Materials</td>
<td>[J/kg]</td>
</tr>
<tr>
<td>$h_f$</td>
<td>Reference Enthalpy</td>
<td>[J/kg]</td>
</tr>
<tr>
<td>$k$</td>
<td>Thermal Conductivity</td>
<td>[W/m.K]</td>
</tr>
<tr>
<td>$L$</td>
<td>Latent Heat, Solid to Liquid Phase Change</td>
<td>[J/kg]</td>
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<td>Symbol</td>
<td>Description</td>
<td>Unit</td>
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<td>--------</td>
<td>-------------------------------------------------</td>
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<tr>
<td>$L_g$</td>
<td>Latent Heat, Liquid to Gas Phase Change</td>
<td>[J/kg]</td>
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<tr>
<td>$L_p$</td>
<td>Latent Heat, Solid to Solid Phase Change</td>
<td>[J/kg]</td>
</tr>
<tr>
<td>$m$</td>
<td>Mass</td>
<td>[kg]</td>
</tr>
<tr>
<td>$m_l$</td>
<td>Liquid Mass</td>
<td>[kg]</td>
</tr>
<tr>
<td>$m_s$</td>
<td>Solid Mass</td>
<td>[kg]</td>
</tr>
<tr>
<td>$P$</td>
<td>Pressure</td>
<td>[Pa]</td>
</tr>
<tr>
<td>$Q$</td>
<td>Total Amount of Energy</td>
<td>[J]</td>
</tr>
<tr>
<td>$\dot{S}_m$</td>
<td>Momentum Source Term</td>
<td>[N/m^3]</td>
</tr>
<tr>
<td>$S_E$</td>
<td>Energy Source Term</td>
<td>[W/m^3]</td>
</tr>
<tr>
<td>$T$</td>
<td>Temperature</td>
<td>[K]</td>
</tr>
<tr>
<td>$t$</td>
<td>time</td>
<td>[s]</td>
</tr>
<tr>
<td>$t_{end}$</td>
<td>time melting ends</td>
<td>[s]</td>
</tr>
<tr>
<td>$T_f$</td>
<td>Reference Temperature</td>
<td>[K]</td>
</tr>
<tr>
<td>$T_l$</td>
<td>Liquidus Temperature</td>
<td>[K]</td>
</tr>
<tr>
<td>$T_s$</td>
<td>Solidus Temperature</td>
<td>[K]</td>
</tr>
<tr>
<td>$T_{sl}$</td>
<td>Phase Change Temperature</td>
<td>[K]</td>
</tr>
<tr>
<td>$t_{start}$</td>
<td>time melting begins</td>
<td>[s]</td>
</tr>
<tr>
<td>$\vec{V}$</td>
<td>Velocity</td>
<td>[m/s]</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>Thermal Diffusivity</td>
<td>[m^2/s]</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Thermal Expansion Coefficient</td>
<td>[1/K]</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>Small Number</td>
<td>Dimensionless</td>
</tr>
<tr>
<td>$\mu$</td>
<td>Dynamic Viscosity</td>
<td>[kg/m.s]</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Density</td>
<td>[kg/m^3]</td>
</tr>
<tr>
<td>$\rho_f$</td>
<td>Reference Density</td>
<td>[kg/m^3]</td>
</tr>
<tr>
<td>$\tau^+$</td>
<td>Scaled Time</td>
<td>Dimensionless</td>
</tr>
<tr>
<td>$\Delta$</td>
<td>Delta/ Difference</td>
<td>Dimensionless</td>
</tr>
<tr>
<td>$\nabla$</td>
<td>Gradient</td>
<td>Dimensionless</td>
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Chapter 1

1 Introduction

1.1 Background

The pre-pandemic level of carbon dioxide emissions in 2019 was exceeded by about 180 megatons in 2021 [1], worsening global warming. On the other hand, talks about the role of renewables in enhancing energy security by displacing fossil fuels have grown due to a substantial spike in energy prices in late 2021 and the Russian Federation's invasion of Ukraine in early 2022 [1]. The building sector, one of the major consumers, is responsible for almost one-third of global final energy and half of all electricity consumption [2], accounting for a sizeable portion of overall direct and indirect energy-related CO2 emissions. Almost 70% of the spent energy in the residential segment is applied for space heating and appliances in cold climates and water heating and cooking in moderate and warm temperatures [2]. Therefore, domestic hot water supply and heating of space accounted for just under a quarter of global final energy consumption in 2021, requiring the development of alternative energy solutions in this sector. However, the heat supply in buildings remains heavily dependent on fossil fuels globally, with renewable sources meeting only around 11% of global heat demand in 2020. This percentage has remained untouched over the past ten years [1].

Most household heating applications call for low temperatures, less than 100°C, which can be achieved by using readily available renewable energy technologies like solar thermal systems, taking into account their attributes of ubiquity, abundance, and sustainability. The installation of solar home hot water or space heating systems, which can replace natural gas or electric heating, has thus been the subject of extensive research over the past ten years. However, solar energy's intermittent and temporal nature is a significant drawback, causing a large variance in available solar radiation. Peak heating demand usually occurs in the late evening or early morning when solar radiation is unavailable, although peak solar radiation occurs around noon. As a result, only when an energy storage system with a fair price is accessible, the full deployment of solar energy in supplying needed heat in the building sector is conceivable. Such a mechanism stores heat during intense sunlight, known as the charging process. Then,
the surplus heat is removed as needed during the discharging process. Additionally, it is worth noting that exploring advanced thermal storage solutions, such as phase change materials (PCMs), holds promise in enhancing the energy storage capability. These materials offer latent storage, which is known to be more efficient than sensible storage methods.

This research endeavor is committed to the progress of thermal energy storage systems, focusing on understanding phase change phenomena within these systems. By investigating the complexities of melting and solidification of phase change materials, this study aims to inform the development of efficient energy management solutions, with the goal of contributing to reduced environmental emissions and a more sustainable future for the planet.

1.1.1 Thermal Energy Storage

Energy storage plays a crucial role in conserving precious fuel resources and enhancing cost-effectiveness by mitigating energy wastage. Within most systems, there exists a discrepancy between energy supply and consumption, and energy storage acts as a crucial mechanism for rectifying this imbalance, ultimately leading to savings in capital expenses. This approach is not only desirable for improved efficiency but also promotes environmentally friendly energy utilization. Various energy storage solutions are currently being implemented globally at different levels [1]. These systems serve the purpose of preserving either electrical or thermal energy, thus ensuring a dependable and continuous energy supply. Several methods of energy storage, indicated in Figure 1.1 [3], employ distinct technologies to enhance energy supply reliability.

Figure 1-1: Categorizing energy storage technologies: a comprehensive overview [3]
Mechanical options like pumped storage and flywheels store energy through the physical movement of water and rotation, respectively. Electro-chemical alternatives, such as lithium-ion and lead-acid batteries, rely on chemical reactions to store and release energy. Chemical energy storage, involving hydrogen production and utilization, offers a versatile means of energy preservation. Thermal methods, like molten salt storage and hot water tanks, store energy as heat. These energy storage solutions play vital roles in stabilizing the grid, mitigating intermittent energy generation from renewables, and facilitating the transition to cleaner, decarbonized energy systems [1].

The practice of thermal energy storage, which dates back to the earliest days of human civilization, has been a longstanding tradition. Throughout recorded history, people have diligently harvested and stored ice for future use. Today, this ancient concept has found new relevance in modern times as thermal energy storage systems are employed within solar energy systems. To establish solar energy as a prominent and reliable energy source, it is clear that the development of efficient and cost-effective solar thermal energy storage technologies and methods is essential. Figure 1.2 schematically illustrates some examples of various modern approaches of integrating thermal energy storage systems within solar-thermal systems to provide space heating and domestic hot water in the building.

![Figure 1-2: Schematic illustration of integrating thermal energy storage systems into solar-thermal systems. (a) represents simulated solar-thermal system in TRNSYS, including a flat plate solar collector with a fixed area $36m^2$ and a 150L PCM storage module [4]. (b) symbolizes advanced air source heat pump setup with two distinct PCM thermal storage, one for providing space heating and one for providing domestic hot water, along with a local solar-PV system to produce electricity [5].](image)
Basically, thermal energy can be released and absorbed in sensible, latent, or thermochemical storage systems. Sensible heat storage (SHS) involves increasing the temperature of a solid or liquid to store thermal energy. These systems rely on the heat capacity of a fluid and the change in the working medium's temperature during the thermal charging and discharging phases [6]. Thermochemical storage operates by utilizing the energy absorbed and released during the reversible chemical reaction involving the breaking and reformation of molecular bonds. It includes utilizing materials that can undergo a chemical reaction to absorb and store energy. Later, this stored energy can be released when the same chemical reaction is reversed through the reformation of molecular bonds. This allows for the stored energy to be retrieved and used at a later time. The amount of stored heat in this context depends on factors such as the quantity of storage material, the heat generated through endothermic and exothermic reactions, and the degree to which the conversion process occurs [6]. Finally, Latent heat storage utilizes the energy stored during a phase transition of a substance from one state to another.

Figure 1.3 demonstrates the rise in internal energy resulting from the introduction of heat energy into a substance [7]. This effect leads to either an increase in temperature, referred to as sensible heating, or a phase transformation, known as latent heating. Starting from an initial solid state represented by point A, the addition of heat to the substance initially leads to sensible heating of the solid, illustrated as the A–B region, followed by a solid-to-solid phase transition marked by a change in crystalline structure, depicted in the B–C region. Subsequently, there is another phase of sensible heating for the solid, seen in the C–D region, followed by a solid-to-liquid phase transition, highlighted in the D–E region. This is then succeeded by sensible heating of the liquid, shown in the E–F region, a liquid-to-gas phase change, delineated in the F–G region, and ultimately sensible heating of the gas, captured in the G–H region.
The total amount of energy stored can be expressed as [7]:

\[ Q = m \left[ \int_{T_A}^{T_D} C_{ps}(T) dT + L_P + L + \int_{T_E}^{T_F} C_{pl}(T) dT + L_g + \int_{T_G}^{T_H} C_{pg}(T) dT \right] \quad (1.1) \]

Here, \( m \ [kg] \) represents the mass of material, \( C_{ps} \ [J/kgK] \) denotes the specific heat of the material in its solid phase, \( C_{pl} \ [J/kgK] \) signifies the specific heat of the material in its liquid phase, \( C_{pg} \ [J/kgK] \) stands for the specific heat of the material in its gas phase, \( L_P \ [J/kg] \) corresponds to the latent heat involved in the solid-to-solid phase change, \( L \ [J/kg] \) represents the latent heat involved in the solid-to-liquid phase change, and \( L_g \ [J/kg] \) indicates the latent heat of the liquid-to-gas phase change. Based on Eq. (1.1), the material's ability to store energy relies on two key factors: its specific heat capacity and latent heat values. Therefore, it is advantageous for the storage medium to possess a substantial specific heat capacity and latent heat value. In simpler terms, a good energy storage material should be able to absorb a lot of heat and undergo phase changes efficiently.

Comparing different forms of thermal energy storage, latent heat thermal energy storage (LHTES) systems, which typically employ phase change materials as the medium to store and release heat, outperform both sensible heat and thermochemical alternatives for several reasons. First and foremost, latent heat storage boasts a significantly higher energy density.
compared to sensible heat storage [8]. LHTES systems predominantly store heat in the form of latent heat, which results in an energy storage density that is 5-10 times greater than that of sensible heat storage systems [6]. Consequently, latent heat storage systems are far more space-efficient, requiring less physical area for installation. This property proves highly beneficial in the design and implementation of thermal energy storage systems for practical applications, particularly when space constraints are a relevant and critical consideration. Moreover, LHTES systems are notably easier to handle in comparison to thermochemical storage solutions [8].

Additionally, the temperature of the phase change medium in latent heat thermal energy storage systems remains relatively constant during the phase change process, facilitating higher and more consistent heat transfer. This ensures that the stored energy can be efficiently retrieved when needed. Also, the choice of PCMs allows for customization of the phase change temperature to suit specific purposes. This flexibility in PCM selection enables the design of latent heat storage systems tailored to meet the precise thermal requirements of a given application, further enhancing their practicality and performance. More information about PCMs is provided in the following section.

Latent heat storage can be categorized according to the type of phase change it involves, which includes solid-to-solid, solid-to-liquid, solid-to-gas, and liquid-to-gas transitions. Solid-to-gas and liquid-to-gas transformations, despite having the highest latent heats, are typically not utilized for energy storage due to the substantial volume increase associated with gases [8]. This volumetric expansion results in system complications and impracticality due to its size. In contrast, solid-to-solid transitions involve the conversion of heat as the material changes from one crystalline structure to another. However, these transitions generally exhibit small latent heats, making them less appealing for energy storage purposes [7]. On the other hand, the latent heat storage method through solid-to-liquid phase transition is highly attractive. This technique offers a notable advantage in terms of energy storage density and has the capability to store energy as the latent heat of fusion at a constant temperature, which corresponds to the phase transition temperature.
1.1.2 Phase Change Materials

Phase change materials, known as PCMs, are substances used to store thermal energy as latent heat. They can absorb and release heat during phase transitions, making them valuable for a wide range of applications where efficient thermal energy storage is needed. Initially, solid-liquid PCMs behave much like conventional storage materials, experiencing temperature increases as they absorb heat. However, what sets them apart from traditional (sensible) storage materials is their remarkable ability to absorb and release heat at a nearly constant temperature [9].

PCM Classification

In the realm of thermal energy storage, phase change materials fall into three distinct categories based on their chemical composition: organic, inorganic, and eutectic PCMs, as illustrated in Figure 1.4 [10]. Organic PCMs are typically further divided into paraffin and non-paraffin materials, while inorganic PCMs predominantly comprise metallic and hydrated salts. Eutectic PCMs, on the other hand, are engineered by combining more than two individual PCMs, thereby enabling customization of the melting point by adjusting the component ratios [10].

Among the various PCM types, organic PCMs are the most widely utilized, which encompass a broad spectrum of PCMs, including those from the paraffin family \((C_nH_{2n+2})\) and the fatty acids family \((CH_3(CH_2)_{2n}COOH)\) [8]. One of the key advantages of organic PCMs is their
widespread availability, affordability, and ease of handling, making them a popular choice. On the other hand, one significant drawback of most organic PCMs is their notably low thermal conductivity, which hinders their efficiency. The low thermal conductivity, as seen in the case of most paraffin waxes, where it is approximately around \(0.2\) \([W/m\ K]\), affects their ability to efficiently transfer heat during the charging and discharging processes in energy storage systems [8]. This limitation can lead to slower heat transfer rates, potentially impacting the system's overall charging and discharging speed.

The inorganic group encompasses salts and salt hydrates. Salt hydrates, specifically, are combinations of various inorganic salts like oxides, carbonates, sulfates, nitrates, and halides with water molecules in specific ratios, denoted as \(\ast n\ H_2O\) [8]. These materials exhibit a broad range of melting points, spanning from 10 to 900°C. In applications where the melt temperatures align with those of paraffin’s and fatty acids, inorganic PCMs are not commonly employed. However, as the required melt temperatures increase, inorganic PCMs become the preferred choice [8]. Inorganics offer sharp transitions at their melting points, contrasting with the extended mushy phase observed in organics. They boast latent heats comparable to organic PCMs and exhibit higher thermal conductivities, although further improvements in thermal conductivity are often pursued. Inorganics also undergo smaller density changes during the phase transition from liquid to solid, reducing containment challenges. Their higher densities can be advantageous in terms of energy density, but they can also lead to increased weight, which may be detrimental in certain applications.

One notable issue with salt hydrates, a subset of inorganic PCMs, is their susceptibility to significant instabilities [11]. These hydrates tend to dehydrate during heating cycles, causing the breakdown of the material. Moreover, all salt based PCMs tend to break down and separate into their constituent parts after repeated cycling [11]. Additionally, inorganic PCMs are prone to supercooling [12], a condition which is characterized by the PCM existing in a metastable state, where it remains in a liquid form below the designated melting temperature. During this phase, only sensible heat is exchanged with the surroundings [13]. Typically, this metastable state is disrupted when the initial crystal forms, either on an impurity within the PCM or at the PCM-container interface, through a process called heterogeneous nucleation [13]. The
temperature difference between the liquidus melting point and the crystallization temperature is referred to as the degree of supercooling. When nucleation is triggered and crystals start to grow, it results in a rapid release of latent heat within the material, leading to an increase in the PCM's temperature. This undesirable instability poses challenges when attempting to solidify the melted PCM for subsequent thermal cycles. Numerous research works are accessible, providing comprehensive lists of properties for a wide array of potential organic, inorganic PCMs and various combinations of them [10-12, 14].

PCM types falling into eutectic category can be described as blends consisting of two or more components, each of which freezes and melts congruently, leading to a mixture of their individual crystals during the crystallization process [14]. These PCMs are characterized by their high thermal conductivity and density. However, in terms of latent heat and specific heat, they typically exhibit lower values compared to salt hydrates and paraffin. Eutectic PCM mixtures are created by combining components in specific ratios, which can include organic-organic, inorganic-inorganic, or a combination of two different PCMs, tailored to meet requirements.

**PCM Selection**

PCMs come in a variety of forms, each melting with a specific heat of fusion within a desired temperature range. However, for their effective use in latent heat storage applications, these materials must possess specific thermodynamic, kinetic, and chemical properties. Additionally, economic feasibility and the accessibility of these materials must be considered in their selection [9].

The melting temperature is the foremost factor to consider when selecting a PCM for a latent heat thermal energy storage system. It is crucial that the PCM's melting point lies below the heat source's temperature and above the system's ambient conditions. Selecting a PCM with a melting point too low would result in it already being in liquid form before absorbing heat from the intended source, rendering it ineffective. Especially in systems designed for precise thermal management, the strategy is to choose a PCM with the highest feasible melting point while still staying below the desired thermal control temperature [8]. This choice offers the
advantage of a longer melting time, thus extending the effective thermal management duty cycle before the PCM is completely liquefied.

After determining a suitable melting range for the PCM, the next critical factor to consider is the material's latent heat of fusion [8]. As mentioned in the previous section, this measure quantifies the amount of energy that can be stored within a specific mass of material during melting process and released during solidification. A higher latent heat of fusion indicates greater energy efficiency for the system, allowing for the use of less material and thus reducing the system's size. Therefore, the ideal choice is a material with the highest latent heat of fusion within the predetermined melting temperature range [8].

Materials with high latent heats of fusion commonly exhibit relatively high specific heats as well. In the context of energy storage applications, a high specific heat is just as valuable as a high latent heat of fusion. This is because it enables the storage of a substantial amount of energy during both the sensible heating stage as the PCM approaches its melting point, and the latent heating phase during the melting transition [8].

In addition, high thermal conductivity is a valuable attribute when choosing the optimal PCM, as it helps prevent thermal bottlenecks at the heat source [8]. Nevertheless, it can be challenging to identify materials that possess both high latent and specific heats, along with elevated thermal conductivities. In most scenarios, the preference is to prioritize storing more energy (with high latent heat), often taking precedence over the necessity for high thermal conductivity, primarily driven by the specific demands of the applications.

There are several other important factors when selecting a PCM for latent heat thermal energy storage systems. The chosen material should demonstrate stability, both chemically and physically, even when subjected to repeated thermal cycling with consistent melting and freezing cycles [9]. Additionally, it is crucial to assess the compatibility of the selected PCM with the casing and other system materials since some PCMs may have corrosive tendencies or exhibit chemical incompatibility [8]. Lastly, it is highly preferable for the PCM to meet environmental safety standards by being nonflammable, nontoxic, and environmentally friendly, ensuring the overall safety and sustainability of the energy storage system [9].
To summarize, thermal energy storage systems are indispensable for solar domestic heating systems to fully utilize solar energy and off-peak cover periods. However, systems with sensible energy storage have considerable energy losses to the environment because they need a high storage temperature. Therefore, latent thermal energy using PCMs is the most efficient thermal energy storage due to its high storage capacity, low storage volume, and almost isothermal operation during the charging and discharging phases [15]. Between different ways of phase transition, solid-liquid technologies have been proven to be the most financially appealing method for use in thermal energy storage because melting and freezing processes can be repeated indefinitely without changing the material's physical or chemical properties [6]. This strategic combination of solar energy utilization and PCM-based latent heat energy storage not only enhances energy accessibility round the clock but also contributes to a sustainable and environmentally conscious approach to meeting the heating and hot water needs.

1.1.3 Melting and Solidification of PCMs

In the realm of PCM-based latent heat thermal energy storage systems, the processes of melting and solidification take center stage. These transformations are pivotal as they enable the efficient storage and release of thermal energy. Comprehending how PCMs behave during these transitions is of paramount importance, similar to deciphering the "language" of these materials and unlocking their full potential. The investigation of PCM behavior during melting and solidification is not merely an academic pursuit; it directly influences the optimization of PCM-based LHTES systems.

In the context of conduction heat transfer within a PCM, a remarkable dynamic unfolds as the material transforms from one phase to another. This complicated phenomenon is characterized by the presence of a continually moving interface that separates the two phases [16]. Such scenarios are commonly referred to as either moving boundary problems or free boundary problems.

One essential feature of these problems is their inherent transience, particularly during the motion of the interface. Notably, the precise motion and location of this boundary are not
known in advance and must be determined as an integral part of the solution process. A key factor to consider is that the material properties undergo changes as the phase transformation progresses [16]. Additionally, due to the abrupt change in temperature gradients occurring at the interface, each phase necessitates its unique temperature function for accurate modeling. Moreover, changes in density play a significant role in driving the motion of the liquid phase within the material. When the effect of this motion is substantial, the heat equation relating to the liquid phase must include a convective term to account for heat transport driven by the flow. However, this convective effect is often omitted or neglected for simplification in many theoretical scenarios.

A moving front which is undergoing a phase change is governed by non-linear boundary conditions. The inherent non-linearity of these conditions poses a challenge, leading to a few exact solutions for such phase change problems. However, a valuable approximation approach that facilitates the solution of a wide range of problems relies on what's known as the quasi-steady model [16]. Within this model, the Stefan number, which represents the ratio of sensible heat to latent heat, is assumed to be significantly smaller than unity. When the Stefan number is small, it implies that the contribution of sensible heat is minor compared to the latent heat. This assumption simplifies the complex non-linear equations governing phase change problems and obtains approximate solutions that are both feasible and insightful.

To grasp the significance of a small Stefan number, one must consider the hypothetical scenario of a material with zero specific heat, resulting in a Stefan number approaching zero. In this case, infinite thermal diffusivity ensues, signifying that thermal effects propagate at an infinite speed. Consequently, as the phase change interface shifts, a steady state is reached almost instantaneously, leading to an immediate uniformity in temperature distribution [16]. Conversely, a material with infinite latent heat maintains a stationary interface, requiring an immense amount of energy to initiate any interface motion. When the Stefan number is small, the phase change boundary moves slowly, resulting in temperature distributions that closely resemble a steady state at each moment [16]. This approximation simplifies the mathematical treatment of phase change problems significantly. Nonetheless, it is crucial to recognize that, in many practical scenarios where thermal properties and phase change rates vary significantly,
the quasi-steady model may not be applicable, necessitating the use of more complex models for accurate system representation.

One of the earliest studies concerning the exact solution for phase change between solid and liquid materials was conducted by J. Stefan in 1891 [16] known as Stefan Condition. This condition characterizes the speed of the interface between solid and liquid phases within the same substance. It relies on the equilibrium of heat flows from both phases and the latent energy involved in the melting or solidification process. The Stefan solution is a special case of Neumann’s problem. More details about this approach can be found in [16] as it is outside the scope of this discussion.

Only certain one-dimensional problems have been addressed through analytical solutions [16]. In practical situations, several factors come into play that make it challenging to apply analytical solutions to phase change problems. Firstly, in reality, the liquid involved is often not initially at the precise melting temperature. As the process unfolds, heat diffusion occurs not only in the solid but also within the liquid domain. Additionally, gravitational forces induce buoyancy effects, causing natural convection, which can shift the dominant mode of heat transfer from conduction to convection. This shift is further compounded as the solid-liquid interface progresses, leading to transient changes in heat transfer dynamics.

Moreover, the heat transfer in such scenarios occurs in a three-dimensional form, making it even more complicated. The shape of the solid-liquid interface becomes intricately intertwined with heat transfer patterns and fluid flow dynamics. This complexity can result in interfacial instabilities and non-equilibrium conditions, which further challenge the application of analytical solutions. Another crucial factor is the variation in material properties between phases, including density differences that impact the flow within the system due to volume changes. Consequently, the solid phase might exhibit buoyancy, causing it to rise or sink within the liquid. Furthermore, it is important to recognize that phase change doesn't occur at a single fixed temperature but over a range of temperatures. This leads to the formation of a transitional layer of partially melted material along the solid-liquid interface, known as the "mushy region."
In summary, the melting and solidification of PCMs are exceptionally complex, and while exact solutions do exist, they are currently limited to a small number of highly simplified scenarios, making them insufficient for addressing the intricacies encountered in practical applications. Therefore, to gain deeper insights into PCM behavior during phase transitions researchers turn to practical experiments, often conducted on a small scale, and leverage numerical simulations as invaluable tools. Consequently, the following section embarks on a comprehensive exploration of both experimental and numerical methods used to understand the PCM behavior.

1.2 Literature Review

1.2.1 Numerical Methods Used to Investigate Melting and Solidification

During the transition from solid to liquid, temperature-induced density changes combined with gravity lead to fluid movement. This affects heat transfer through natural convection and the progression of the solid-liquid boundary. Simulating this phenomenon and its interaction with the boundary is crucial but demanding. The challenge arises not just from simulating complex convection but also from dealing with a moving boundary whose evolution is part of the puzzle.

Various techniques exist for numerically simulating phase changes between solid and liquid states. These approaches can be generally categorized into three main groups: fixed-grid models [17], adaptive mesh models [18] and mixed Eulerian-Lagrangian methods [19]. Fixed-grid models employ a consistent mesh across the entire domain, regardless of liquid phase location. Adaptive mesh models dynamically adjust the mesh to track the liquid-solid boundary's evolution. In Eulerian-Lagrangian methods, calculations occur on a fixed grid, but an additional set of points explicitly traces the interface movement.

Among these approaches, fixed-grid enthalpy-based models are simpler both mathematically and computationally as a single set of equations are used for both the solid and liquid phases. In this method, the solution to the energy equation involves employing an enthalpy-based approach, where enthalpy and temperature are interconnected [20]. This method offers the benefit of ensuring the fulfillment of boundary conditions at the solid-liquid interface. Moreover, the enthalpy method eliminates the necessity of treating the solid and liquid
domains as distinct entities and removes the need for precise tracking of the interface boundary. Apparent heat capacity, effective heat capacity and source-base enthalpy methods are different forms of enthalpy approach [20] used in solving melting and solidification problems.

Brent et al. [21] introduced a novel formulation for the enthalpy technique by separating the enthalpy into two distinct components: latent heat and sensible heat. This approach has been integrated into the governing equations with the necessary source terms. Throughout the phase change process, the energy equation reflects the inclusion of sink or source terms corresponding to the absorption or release of latent heat. Notably, the inclusion of a source term in the momentum equation has influenced the condition of zero velocity, which is crucial for identifying the transition from liquid to solid phase. This technique is recognized as the enthalpy-porosity method, which is the main focus in this study and will be described more in the second chapter.

1.2.2 Application of CFD to Simulate Melting and Solidification of PCMs

Numerous investigations involving conjugated heat transfer phenomena have been conducted using general purpose Computational Fluid Dynamics (CFD) software to solve melting and freezing processes. In most cases, fixed-grid enthalpy-based models are implemented due to their accuracy and simplicity.

A limited number of investigations have been conducted utilizing OpenFOAM and DESIGN BUILDER [20]. OpenFOAM, denoting "Open-source Field Operation And Manipulation," serves as a C++ toolkit for customized problem-solving and the preprocessing/post-processing of fluid flow scenarios. Recently, researchers in [22] developed a computational model to simulate phase transitions, heat transfer, and fluid flow in latent heat storage systems by adopting OpenFOAM. Within this environment, they made a custom solver called porousHeatTransferFoam, built on the SIMPLE algorithm, and additional libraries. This solver allows them to model granular materials with complex enthalpy-temperature diagrams during phase transitions, significantly expanding OpenFOAM's capabilities. Notably, the solver exhibits impressive computational speed, providing results in minutes to hours. DESIGN BUILDER software also employs the apparent heat capacity method [20], allowing users to
input enthalpy-temperature data within the PCM material property section to simulate phase change materials.

COMSOL Multiphysics software is another powerful tool to simulate melting and solidification problems [20]. Arena et al. [23] utilized apparent heat capacity method in this software to develop a numerical model that simulated a finned double tube heat exchanger configuration. This system was filled with Rubitherm RT35, serving as the phase change material. Through this model, they investigated the intricate interplay of heat transfer mechanisms and phase change dynamics within the system. By manipulating factors such as temperature gradients and material properties, the authors gained insights into the system's thermal behavior and its ability to store and release energy during phase transitions. Enthalpy-porosity approach can also be used in COMSOL. Yan et al. [24] created a specialized numerical model to simulate the unconstrained melting of lauric acid as PCM confined within cylindrical containers submerged in hot water tanks. The model was based on the enthalpy-porosity method, employing the direct linear solver within the COMSOL Multiphysics software.

ANSYS FLUENT is the most common commercially available software that is mainly based on the enthalpy-porosity approach through solidification and melting model (SM), but apparent heat capacity (AHC) can also be employed. Researchers in [25] compared these two approaches for modeling phase change materials in ANSYS Fluent. They have found that while the SM model utilizes a linear liquid fraction representation between solidus and liquidus temperatures, the AHC method captures the non-linear behavior of phase transitions by incorporating a curve shape and specific heat capacity information. They evaluated these methodologies through comparisons with the analytical solution of the two-phase Stefan problem. Both models exhibited minor deviations, staying below 2%. Notably, the AHC model displayed a slightly greater divergence, which is connected to the presence of an uneven heat capacity curve leading to a non-linear phase transition. They also made a comparison involving two different PCMs, one from existing literature and another obtained through a new experiment. While both the SM and AHC models maintain their phase prediction validity even with the introduction of natural convection behavior, the SM model encounters challenges
when applied to various cases. This is primarily due to the reliance on fitting experimental data with the mushy zone coefficient. On the other hand, for the successful implementation of the AHC approach, proper incorporation of temperature-dependent material parameters is crucial. The viscosity, in particular, requires an artificially elevated value in the solid region.

The enthalpy-porosity approach used in ANSYS Fluent is still the most practical method to simulate PCM melting and freezing problems. Many researchers have adopted this approach to capture the complex behavior of phase transitions due to its suitability for analyzing heat transfer and fluid flow. Simple geometries, such as spherical capsules and cylindrical or rectangular cavities, are typically selected to be studied in melting and solidification processes because the results can be used to examine PCM-based latent heat thermal storage systems.

Tan et al. [26] applied the enthalpy-porosity approach in ANSYS Fluent to simulate the constrained melting of paraffin wax inside a spherical capsule by focusing on the significance of buoyancy-driven convection. The research findings highlighted that as the PCM melts, it tends to rise along the spherical container's walls, displacing cooler fluid and resulting in substantial thermal stratification in the upper half of the PCM sphere. Additionally, the study attributes the formation of irregularities at the solid PCM's bottom during the melting process to the presence of an unstable fluid layer, enclosed by vertical recirculation currents on all sides.

In 2019, Ghosh and Guha [27] used the same numerical approach to investigate the effect of the thermal properties of the cavity material on the melting process. A spherical cavity filled with RT27 was selected as the main numerical domain. The findings indicated that materials with greater thermal diffusivity exhibit a faster melting rate due to an amplified influence of buoyancy and convection. Moreover, it has been observed that a higher Stefan number is associated with increased natural convection effects and a peak velocity profile, which ultimately leads to an improved melting process.

The solidification process of paraffin wax was also simulated numerically by the same authors in [28]. In this research, they applied the enthalpy-porosity method in ANSYS Fluent to investigate freezing process of RT27 in both a spherical cavity and a rectangular cavity under
varying thermal boundary conditions. The study emphasized that the shape of the cavity has a significant impact on solidification time; surprisingly, despite the spherical cavity's larger size compared to the rectangular one, solidification is much quicker in the spherical cavity, underscoring the importance of cavity geometry in shaping the solidification process.

In 2021, Ismail et al. [29] evaluated the solidification behavior of three specific paraffin waxes called RT47, RT50, and RT60 enclosed within spherical capsules by simulating them in ANSYS Fluent. They extracted dimensionless equations for solidification time and the quantity of released energy through numerical analysis. These equations can be utilized in the design of packed bed latent heat thermal energy storage systems.

Both melting and solidification of the PCM were investigated in a rectangular cavity by Yang et al. [30]. They applied the enthalpy-porosity method in ANSYS Fluent to explore the melting and freezing processes in a novel way by focusing on the evolution of the mushy region. They provided a detailed explanation of how heat transfer, fluid flow, and phase change processes interact within the mushy area, revealing that the mushy region experiences significant suppression during melting and substantial expansion during solidification.

The enthalpy-porosity approach is also employed in [41-66] to simulate a wide range of PCMs in different geometries and thermal conditions. More information about these research works is provided in the following sections. Therefore, as it is clear, the enthalpy-porosity method, contained within the computational framework of ANSYS Fluent, stands as a cornerstone technique extensively utilized by researchers for the simulation of phase change materials undergoing melting and solidification processes. Its widespread adoption in scientific investigations is attributable to its capacity to simulate complex phase transitions.

1.2.3 Experimental Methods Used to Investigate PCM Behavior

The inclusion of experimental methodology is imperative as it underscores the initial calibration process required for computational models generated within ANSYS Fluent based on the enthalpy-porosity method. The experimental approaches outlined here are the most conventional and commonly employed methods for investigating phase change materials. In the majority of such experiments, the primary focus is on observing and tracking the
transformation of the solid-liquid interface. This involves a transparent wall that provides an unobstructed view to a camera, allowing for detailed observations. A secondary approach involves the installation of multiple thermocouples within the encapsulating container, with temperature readings used to estimate the position of the interface. These thermocouples are typically positioned at various heights along the vertical centerline.

In 2009, Tan et al. [26] delivered one of the pioneering and most comprehensive sets of experimental data in this field. They conducted a combined experimental/computational study to understand PCM behavior. The central element of the experiment featured a spherical glass enclosure housing paraffin wax. As indicated in Figure 1.5 (a), a total of 11 Type-K thermocouples were employed in the setup. The researchers represented the dynamic PCM behavior during constrained melting through instantaneous streamlines and temperature fields at various time points, although there is not a direct comparison between experimental and numerical results in their work. They also precisely tracked the solid-liquid interface within the spherical capsule as it evolved over time and compared liquid fraction values obtained computationally and experimentally. Other researchers [31-33] also validated their numerical results based on the experimental data provided in [26].

Another aspect of this work was the collection of detailed temperature data along the vertical centerline of the capsule during melting, allowing for a comprehensive evaluation of their computational fluid dynamics (CFD) simulations. The same methods were used in [34]. However, they did not provide any information regarding the numerical parameters’ selection, such as mushy zone coefficient or phase change temperature range, and their compatibility with experimental data.

In 2019, Ghosh and Guha [27] created an experimental setup to validate their numerical approach. As shown in Figure 1.5 (b), they immersed a spherical shell containing solid PCM into a controlled-temperature water bath. Throughout the melting process, they captured images using a high-speed digital camera at different stages. These images underwent meticulous analysis via digital image processing techniques to derive experimental melt fraction values at various time points as an indicator to validate their numerical results. Additionally, they conducted a comparison between the experimental images and density
contours. However, it is important to note that in the digital image processing technique utilized, while it accurately identified the complete liquid phase, distinguishing solid and semisolid phases proved to be a challenge. Furthermore, they did not address numerical parameter selection in their work and determined the mushy zone coefficient for their numerical simulations based on the information collected from the existing literature. Researchers in [28] employed the same validated computational model from [27] for the solidification part, indicating that they did not conduct a distinct calibration or validation specifically for the freezing process.

(a) Vertical centerline thermocouples [26].

(b) Digital image processing technique [27].

Figure 1-5: Examples of experimental methodologies used to investigate PCM behavior during the change transitions.

In 2021, Ismail et al. [29] carried out a validation set up for their numerical model, which aimed to replicate the solidification process of paraffin waxes within a spherical capsule. To achieve this, they first conducted experiments to determine the thermal properties of paraffin waxes, such as the onset and offset temperatures of PCMs and latent heat, using a Differential Scanning Calorimeter (DSC) Setaram EVO131, but other required material properties were acquired from the existing literature. RT-47 was encapsulated within a spherical capsule and placed in a water bath. Temperature measurements were taken using four thermocouples located within the PCM during the solidification process. Additionally, four K-type thermocouples were inserted from the top of the capsule, at different heights along its vertical
To validate their numerical model, the researchers compared the temperature profiles obtained from the experiments with those generated by the numerical model at the same positions as the thermocouples during solidification. They also compared the solid-liquid interface contours between the experimental and numerical results, although only at the initial and final stages of the process because visualizing the liquid-solid interface of the PCM over the internal surface was not feasible. Therefore, the total solidification time could only be determined experimentally. However, researchers in [35] expanded the dataset by capturing experimental images immediately after cutting open the shells and draining the residual liquid. Again, numerical parameters values such as mushy zone coefficient and thermal expansion coefficient are assumed based on what is suggested in the literature.

In a number of experimental studies aiming to understand how phase change materials behave, scientists have placed thermocouples in a grid inside a flat, two-dimensional container holding the material. Examples of such studies include the work by Jevnikar and Siddiqui [36], who heated a rectangular container from one edge, and the research conducted by Bashar and Siddiqui [37], where they used a U-shaped tube to heat a rectangular container. However, the results of these studies heavily rely on interpolation techniques to create temperature distribution. This is mainly because it is quite challenging to install a large number of thermocouples in this setup. Additionally, because these sensors have a finite size, they can't accurately measure temperatures very close to the container walls. Moreover, because thermocouples are intrusive devices, their presence can influence the way the material behaves during heating and cooling experiments.

In a recent series of experimental works conducted by Teather and Siddiqui [38], they represented a landmark in PCM research, particularly focusing on PCM encapsulations with circular cross-sections, such as horizontal cylinders and spheres. The researchers developed two innovative, non-invasive experimental techniques. The first technique involves utilizing single-exposure images of particles, similar to those obtained in Particle Image Velocimetry
(PIV), to digitally construct instantaneous streak visualizations. The second technique employs thermal cameras to remotely measure and predict the internal temperature of the PCM.

These cutting-edge techniques were complemented by high-resolution grids of thermocouples and PIV. Together, they enabled the researchers to capture transient velocity and temperature fields during the constrained melting and solidification processes within circular PCM enclosures [38]. The experiments were conducted across varying levels of applied heating for melting and cooling for freezing, thus providing a comprehensive understanding of the dynamic behavior of PCMs in circular geometries.

As previously discussed, the enthalpy-porosity method in ANSYS Fluent is widely recognized as the predominant approach for simulating melting and solidification within phase change materials, offering significant advantages. However, it's crucial to emphasize that precise calibration of the computational model is essential, given the significant impact of various parameters on numerical results. To achieve accurate calibration, an extensive experimental dataset is required. Existing literature primarily relies on data limited to tracking the solid-liquid interface and temperature readings from thermocouples. For a more comprehensive understanding and effective calibration of numerical parameters, additional detailed data, such as flow patterns and velocities, are essential. In this regard, the research conducted by Teather and Siddiqui [38] provides the best available data, serving as a crucial resource for calibration and validation in the present study.

1.2.4 Manipulation of the Enthalpy-Porosity Model

As mentioned in the previous section, ANSYS Fluent software heavily relies on a model known as the enthalpy-porosity, which was first introduced by Voller et al. [17, 21, 39]. What makes this method interesting is a unique factor it incorporates; a certain parameter that plays a crucial role in how it handles movement. This parameter ensures that when dealing with solid objects the speed of movement is zero. To achieve this, a special value comes into play, referred to as the mushy zone coefficient [21]. This constant \( A_{mush} \) appears in an added source term in the momentum equations, which is defined by Eq. (1.2):
\[ \dot{s}_m = \frac{(1-f)^2}{f^3 + \varepsilon} A_{mush}(\bar{V}) \]  

\( A_{mush} \) is the mushy zone coefficient \((kg \ m^{-3} \ s^{-1})\), \( f \) is the liquid fraction, \( \varepsilon \) is a very small number to avoid division by zero and \( \bar{V} \) is velocity \((m/s)\). A full description of the governing equations and effective parameters are provided in Chapter 2. The intriguing aspect is that \( A_{mush} \) can vary significantly, ranging from quite small to extremely large values, anywhere from \(10^3\) to \(10^{11}\), as discussed in [40].

Another distinctive feature of the enthalpy-porosity model is its incorporation of a temperature range associated with changes in phases. This temperature range is linked with a specific heat value. Typically, scientists determine these physical characteristics using a method known as thermal analysis, with the most common technique being differential scanning calorimetry (DSC) [40]. However, achieving precise measurements for these characteristics presents challenges. Uncertainties arise due to various factors, including how the tests are conducted, such as the amount of material used or the rate at which it is heated. The nature of the material being tested can also introduce complexities, especially when dealing with impurities or mixtures.

Interestingly, there is still a limited amount of research dedicated to investigating how these diverse factors collectively influence the outcomes of computer simulations. Table 1.1 shows the value of these parameters in a number of numerical research works employed the enthalpy-porosity method in ANSYS Fluent to simulate melting and solidification of a PCM in the last 10 years. Phase change temperature, latent heat, and thermal expansion coefficient are typically reported in material properties, while mushy zone coefficient should be selected in each work. In cases where experimental data from an actual storage system was available, researchers commonly opted to select the mushy zone coefficient in a straightforward manner, aiming to align their calculations with the experimental results [50-51]. In some cases, the value of mushy zone coefficient was drawn from earlier research endeavors [27, 28, 29, 41, 48, 52, 54, 56], while in different cases, they simply employed a specific value without providing any detailed explanation or justification for its selection [42-47, 49, 53, 55].
A number of studies showed the impact of mushy zone coefficient in numerical modelling of melting or solidification. In 2016, Hameter and Walter [57] conducted a comprehensive comparison of simulation outcomes by varying this parameter within the range of $10^5$ to $10^8$ in a 3D numerical model of melting and solidification behavior of $NaNO_3$ in ANSYS Fluent. However, they did not validate their computational model. The numerical analysis highlighted that higher mushy zone coefficients correspond to extended times for both charging and discharging processes. Importantly, the inclination of the phase front becomes more horizontal with increasing mushy zone coefficient values. This phenomenon stems from the larger damping term introduced by higher mushy zone coefficients, which leads to quicker

<table>
<thead>
<tr>
<th>PCM Type</th>
<th>Mushy Constant $[kg \cdot m^{-3} \cdot s^{-1}]$</th>
<th>Phase Change Temp $[K]$</th>
<th>Thermal Expansion $[1/K]$</th>
<th>Latent Heat $[kJ/kg]$</th>
<th>Process</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Paraffin wax</td>
<td>$1 \times 10^5$</td>
<td>350.15-358.15</td>
<td>0.001</td>
<td>176</td>
<td>Solidification</td>
<td>[41]</td>
</tr>
<tr>
<td>Paraffin wax</td>
<td>$1 \times 10^5$</td>
<td>301.15-303.15</td>
<td>0.0009</td>
<td>179</td>
<td>Melting</td>
<td>[42]</td>
</tr>
<tr>
<td>Paraffin wax</td>
<td>$1 \times 10^5$</td>
<td>331-333</td>
<td>Not mentioned</td>
<td>213</td>
<td>Both</td>
<td>[43]</td>
</tr>
<tr>
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<td>$1 \times 10^5$</td>
<td>302.93</td>
<td>0.00012</td>
<td>80.16</td>
<td>Melting</td>
<td>[44]</td>
</tr>
<tr>
<td>Lauric acid</td>
<td>$1 \times 10^5$</td>
<td>317.37</td>
<td>0.000615</td>
<td>173.8</td>
<td>Melting</td>
<td>[45]</td>
</tr>
<tr>
<td>Paraffin wax</td>
<td>$1 \times 10^8$</td>
<td>319.15-321.15</td>
<td>Not mentioned</td>
<td>173.4</td>
<td>Melting</td>
<td>[46]</td>
</tr>
<tr>
<td>RT82</td>
<td>$1 \times 10^5$</td>
<td>350.15-358.15</td>
<td>0.001</td>
<td>176</td>
<td>Solidification</td>
<td>[47]</td>
</tr>
<tr>
<td>Paraffin wax</td>
<td>$1 \times 10^8$</td>
<td>319.15-321.15</td>
<td>0.001</td>
<td>173.4</td>
<td>Melting</td>
<td>[48]</td>
</tr>
<tr>
<td>RT42</td>
<td>$1 \times 10^5$</td>
<td>311.15-315.15</td>
<td>0.0001</td>
<td>165</td>
<td>Melting</td>
<td>[49]</td>
</tr>
<tr>
<td>RT27</td>
<td>$1 \times 10^5$</td>
<td>301-303</td>
<td>Not mentioned</td>
<td>179</td>
<td>Melting</td>
<td>[27]</td>
</tr>
<tr>
<td>RT27</td>
<td>$1 \times 10^5$</td>
<td>301-303</td>
<td>Not mentioned</td>
<td>179</td>
<td>Solidification</td>
<td>[28]</td>
</tr>
<tr>
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<td>$1 \times 10^6$</td>
<td>350.15-358.15</td>
<td>0.001</td>
<td>176</td>
<td>Melting</td>
<td>[50]</td>
</tr>
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<td>317.45-324.25</td>
<td>0.0006</td>
<td>173.6</td>
<td>Solidification</td>
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</tr>
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<td>317.65-321.45</td>
<td>0.0006</td>
<td>178.78</td>
<td>Melting</td>
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<td>Not mentioned</td>
<td>173.4</td>
<td>Melting</td>
<td>[53]</td>
</tr>
<tr>
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<td>$1 \times 10^5$</td>
<td>354</td>
<td>Not mentioned</td>
<td>176</td>
<td>Solidification</td>
<td>[54]</td>
</tr>
<tr>
<td>Lauric acid</td>
<td>$1 \times 10^6$</td>
<td>315-317</td>
<td>0.00011</td>
<td>178.7</td>
<td>Both</td>
<td>[55]</td>
</tr>
<tr>
<td>RT42</td>
<td>$1 \times 10^5$</td>
<td>311-315</td>
<td>0.0001</td>
<td>165</td>
<td>Melting</td>
<td>[56]</td>
</tr>
</tbody>
</table>
suppression of buoyancy-driven currents within the mushy zone, ultimately decreasing the overall heat transfer rate.

The same range of mushy zone coefficient is explored in a research work done by Kumar and Krishna in 2017 [58]. The focus of their study revolved around investigating the impact of this parameter on the melting behavior of gallium as a PCM, through 2-D transient numerical simulations within a rectangular enclosure using ANSYS Fluent. To be able to use their computational model, they validated it by comparing simulated melting fraction interface with the equivalent experimental results in the literature. It was noted that there is a clear connection between the mushy zone coefficient and the behavior of the phase change process; with an increase in mushy zone coefficient value a decrease in size of the wake was observed. Also, as mushy zone coefficient increased, the strength of convection decreased, subsequently leading to a reduction in the overall heat transfer rate.

Fadl and Eames in [59] also showed that utilizing the smallest values of the mushy zone coefficient ($< 10^5$) led to inaccurate projections of the development of the melting front. Conversely, employing higher values of this parameter led to a delay in predicting the onset of melting within the PCM. They explored a range of values for the mushy zone coefficient and systematically compared their computational predictions of solid-liquid interface with available experimental data. Their analysis led to a notable conclusion: when employing a higher value of the mushy zone coefficient, the curvature along the melt interface became significantly sharper. Specifically, for $A_{mush} = 5 \times 10^5$, the computational model closely mirrored the curvature observed in the experimental results. This finding highlights the pivotal role of the mushy zone parameter in influencing the accuracy of their predictions.

In 2022, Soliman et al. [60] revealed that the appropriate mushy zone coefficient varies across different storage configurations. They investigated how the value of mushy zone parameter influenced the melting process of the paraffin wax within circular, vertical oval, and horizontal oval storage capsules. To validate their computational model, they generated an experimental setup by employing image processing on photos of the liquid fraction. The numerical results for the PCM temperature and liquid fraction were compared with experimental data to determine the optimal value for each capsule shape, leading to $2 \times 10^6$ for circular, $1 \times 10^5$
for vertical oval, and $1 \times 10^6$ for horizontal oval capsules. Again, higher mushy zone coefficient values resulted in decreased heat transfer rates, convection, and fluid velocity. Other researchers who examined the effects of the mushy zone coefficient arrived at identical findings [61-62].

In a few studies, researchers analyzed mushy zone coefficient impact along with lower or hyper-gravity conditions. In 2019, Hong et al. [63] performed a numerical study to address the effect of mushy parameter ($1 \times 10^4 < A_{mush} < 1 \times 10^8 \text{ kg m}^{-3}\text{ s}^{-1}$) and gravitational acceleration ($1 \cdot 635 < g < 9 \cdot 81 \text{ m s}^{-2}$) for both melting and freezing processes of paraffin wax in a rectangular cavity. They conducted a comparison of their findings with a previously validated numerical model [46] to validate their own research. It was demonstrated that melting characteristics of the PCM are notably affected by both the mushy zone coefficient and the force of gravity, leading to substantial differences in liquid fraction, reaching up to 88%. The tendencies of thermal storage performance are found to strengthen as the mushy zone coefficient decreases and gravitational acceleration increases. On the other hand, the impact on the freezing process was minimal, resulting in a maximum difference in liquid fraction of only 2%.

The same geometry, PCM and range of mushy parameter was investigated in [64] but under hyper gravity conditions ($1g < \text{gravity} < 20g$). Simulated Solid- liquid interface was compared with existing experimental results in the literature. They concluded that when gravitational acceleration increases, the PCM's melting rate improves across various mushy zone coefficient values. Nevertheless, the manner of increase varies with $A_{mush}$. At $A_{mush} = 10^4$, a nearly linear relationship emerges under hyper-gravity conditions of $5g$, $10g$, and $20g$. Conversely, for higher mushy values, the rate initially rises and then declines due to liquid region dynamics. Notably, the melting rate's increase is more substantial at lower gravitational levels compared to higher ones, stemming from limitations in the liquid region's vertical expansion due to cavity dimensions.

In 2020, Yang et al. carried out a work in [65], studying the impacts of both the isothermal assumption in non-isothermal phase transitions and the mushy zone coefficient on the anticipated heat storage performance. Predicted melt fraction and temperature contours were
compared with available experimental results to validate the numerical model. Similar to [57-59, 65], they concluded that mushy zone coefficient significantly impacts phase change behavior by regulating the depth to which convective flow can penetrate the mushy zone. This effect remains remarkable even during solidification, where conductive heat transfer dominates, owing to the role played by convection within the expanded mushy zone. Additionally, they found that the assumption of isothermal conditions can lead to inaccurate predictions of mushy zone phase change behaviors. Hence, as the temperature range is inherent to phase change materials, special attention should be given to this property, especially when modifying PCMs for enhanced performance attributes like higher thermal conductivity and latent heat.

In a series of research works done by Beust et al. [40, 66], they explored the impact of both mushy zone coefficient and temperature range wherein phase change occurs. These factors were examined for their effects on the temperature and melting time of the phase change material (PCM) within a laboratory-scale shell-and-tube latent heat storage system equipped with external circular fins in [66]. The comparison between numerical and experimental tests regarding PCM temperature and melting fraction revealed a strong agreement. They found that while these parameters did influence local aspects of the simulation, they did not significantly impact the overall performance of the storage module because natural convection was not the dominant mode of heat transfer in their setup. They concluded that when significant formation of natural convection rolls is permitted, these two factors have a more significant impact. Consequently, the effect of the mushy zone, along with the associated model parameters, can exhibit considerable variation based on the geometry being studied.

In the other research work conducted by the same authors. [40], they expanded and deepened the investigation into how the mushy zone coefficient and phase change parameters mutually influence simulation outcomes. As with many other research endeavors, a comparison was made between the position of the liquid-solid interface and previously established experimental findings to validate the numerical model. They showed that the mushy zone coefficient, as a penalization term, can either compete with or obscure the effects of temperature transition range. Based on their results, if there is awareness of inaccuracies in thermo-physical
characterizations or uncertainty in determining the temperature range, it is possible to rectify the physical behavior by raising the value of mushy zone coefficient. This adjustment effectively intensifies the damping of velocity within the melting zone. However, this presents a dilemma as it can either help correct or hide inconsistencies in characterization. The study also suggested that relying solely on temperature comparisons is insufficient for validating simulations against experiments.

1.2.5 Identifying Research Gaps in the Literature

In summarizing the findings from the literature survey, it becomes evident that the primary parameter explored in existing research is the mushy zone coefficient. However, it is essential to note that there are several other crucial adjustable parameters, including thermal expansion, latent heat, and solidus-liquidus temperatures, which can significantly influence numerical results. Current studies often do not raise critical questions regarding the values assigned to material properties. These properties are typically derived directly from experimental measurements, such as DSC curves, or borrowed from prior research, sometimes relying on handbook values or default parameters recommended in user guides. This practice can be concerning, given that experimental methods for measuring material properties inherently carry uncertainties. Consequently, the reliability of numerical simulations heavily depends on the accuracy of these material property values, making it necessary to calibrate computational models. However, surprisingly, there is a notable absence of studies that investigate the combined impact of these tuning factors.

Furthermore, in many situations, research merely presents patterns and trends emerging from the variation of these parameters, without conducting a thorough comparison with experimental data. Thus, a noticeable gap exists in the literature, as we could not identify any work where a computational model was rigorously calibrated by simultaneously adjusting these parameters and then validated against experimental datasets. This underscores the need for further research in this direction to enhance the accuracy and reliability of the enthalpy-porosity method in ANSYS Fluent in the context of phase change materials.
1.3 Motivation and Objectives

The review of the literature in the field of phase change research reveals a common thread of challenges that persist across various approaches—be it analytical, numerical, or experimental. While exact solutions do exist, they are often confined to highly simplified scenarios, neglecting critical aspects of the physics involved, thus falling short of faithfully representing real-world processes.

Among the numerical methods employed in this domain, the enthalpy-porosity model implemented in ANSYS Fluent stands out as the dominant approach for simulating the melting and solidification processes within phase change materials. Its prominence is underscored by its ability to offer advantages in terms of computational efficiency and accuracy. However, despite its widespread adoption, the calibration of the computational model is essential due to the presence of parameters that have significant influence over numerical results. In this regard, summarizing the findings from the literature survey, it becomes apparent that the primary parameter under scrutiny in existing research is the mushy zone coefficient. However, several other equally crucial adjustable parameters, including thermal expansion, latent heat, and solidus-liquidus temperatures, hold the potential to exert a profound influence on numerical results.

On the other hand, existing experimental data used to validate numerical simulations typically focus on tracking the solid-liquid interface and acquiring temperature readings through thermocouples. While these data sources are invaluable, they form only part of the larger picture. To attain a more profound understanding of how various numerical parameters impact the simulation results and to calibrate them effectively, a more detailed dataset is required. This dataset should encompass not only the critical metrics of solid-liquid interface behavior and temperature profiles but also the intricate details of flow patterns and velocities within the phase change materials.

Therefore, it is imperative to conduct a thorough investigation of how various tuning parameters in the enthalpy porosity model interact, demanding a meticulous calibration process that encompasses the adjustment of these parameters and their validation against experimental
datasets. This endeavor is essential to enhance our understanding of computational model utilization to design more efficient PCM-based latent heat thermal energy storage systems.

The objectives of this research work are as follow:

1- To elucidate the enthalpy-porosity approach and describe adjustable parameters used in simulating melting and solidification of phase change materials.

2- To develop a calibrated model for constrained melting in a cylindrical cavity using the enthalpy-porosity approach through systematic investigation of the sensitivity of adjustable parameters and their combined influence within this framework. An important part of this objective is to determine whether the calibrated model commutes across different heating conditions within the same geometric model, and to different geometric models.

3- To analyze the PCM solidification process in a cylindrical cavity and assess the feasibility of extending the calibrated model established for the melting phase to accurately represent the freezing process.

1.4 Thesis Outline

This section serves to outline the structure of the thesis document, providing the reader with a clear understanding of the logical flow of information within it.

Chapter 1 establishes the context for the subsequent chapters by presenting an in-depth overview of the current state-of-the-art in the field, identifying key knowledge gaps, and outlining the overall research objectives.

Chapter 2 involves an exploration of the enthalpy-porosity approach with a detailed examination of the governing equations for mass, momentum, and energy during melting and solidification of phase change materials. Additionally, the chapter introduces the most critical adjustable parameters utilized for precision control and calibration of numerical simulations related to both melting and freezing processes. Among the principal parameters of focus in this study are the thermal expansion coefficient, mushy zone coefficient, solidus and liquidus temperatures, and the latent heat. The functions of these parameters within the primary
governing equations are elucidated. Lastly, the numerical procedures employed for solving governing equations are described, offering insight into the computational methods and algorithms employed in this research.

Chapter 3 focuses on the practical implementation of the enthalpy-porosity approach, with an emphasis on the melting process within a cylindrical cavity. The examination is followed by an analysis of the individual impacts exerted by adjustable parameters. The accuracy and reliability of the model are ensured through comparisons with a dataset of existing experimental data. The combined effects of all tuning parameters are then systematically explored, culminating in the development of a precisely calibrated model. This model is subsequently tested under various heating conditions in the same geometry and compared with equivalent experimental data to be validated. The chapter also addresses the effects of changing geometry by applying the validated calibrated melting model to simulate the melting process of the same PCM in a rectangular cavity.

Chapter 4 encompasses an investigation of the enthalpy-porosity approach as applied to the solidification process. The previously validated calibrated model for melting process is extended to freezing, with results compared to existing experimental data. The chapter also evaluates the influence of factors such as the mushy zone coefficient, thermal expansion coefficient, and supercooling phenomenon on the solidification process, contributing to a comprehensive understanding of this phase transition.

Chapter 5 concludes the thesis by summarizing research findings and providing recommendations for future work in the field.
Chapter 2

2 General CFD Model

As mentioned in section 1.2.2, various numerical techniques can be employed to solve dynamic boundary problems like moving interfaces within phase change materials, where phase transitions take place. Fixed-grid enthalpy methods have gained widespread usage due to their relatively simpler mathematical and computational characteristics. In this method, it is not necessary to fulfill heat conditions at the phase transition boundary, although the condition of zero velocity during the transition from liquid to solid must still be taken into consideration [39]. Researchers in [17, 21] developed a general enthalpy method called enthalpy-porosity that is able to solve both mushy and single point phase change problems well. This technique finds application within ANSYS Fluent software to simulate the processes of melting and solidification. In this chapter, a full description of the enthalpy-porosity approach is provided along with introducing the most significant adjustable parameters used in this method to control and calibrate the numerical simulation of melting and freezing.

2.1 Enthalpy-Porosity Model Description

The enthalpy techniques incorporate latent heat into the energy equation by allocating a latent heat value to each computational cell based on its temperature. When a phase change occurs, the cell's latent heat content is modified to accommodate the absorption or release of latent heat. This modification is then represented in the energy equation as either a heat source or a heat sink. Details will be shown in the governing equation section. As mentioned earlier, one notable benefit of this approach is that there is no requirement to explicitly track energy conservation conditions at the interface between solid and liquid phases [21].

At the same time, computational cells experiencing a phase transition are characterized as a pseudo-porous medium in the enthalpy-porosity approach. This is done to address the issue of zero solid velocity in fixed-grid solutions [21]. Porosity is a function of latent heat and ranging between 1 and 0 for fully liquid and solid cells, respectively. These concepts are usually expressed as “liquid fraction” and “mushy zone” in the enthalpy-porosity approach. The liquid fraction denotes the proportion of the cell volume occupied by liquid and is calculated during
each iteration using an enthalpy balance. The mushy zone refers to an area where the liquid fraction ranges from 0 to 1. Once a cell is entirely solidified, its porosity diminishes to zero, resulting in zero velocities as well [67]. The reduced porosity in the mushy zone appears as sink terms in momentum equations that will be discussed in the next sections.

2.1.1 Governing Equations

The liquid phase of PCMs is usually considered as an incompressible Newtonian fluid due to the uniform density and viscosity properties maintained during these transitions [57-62]. Also, the liquid PCM is categorized as laminar flow justified by the typically low velocities and gradual fluid movement characteristic of the process, leading to orderly and smooth flow patterns rather than turbulent motion [57-62]. Considering these assumptions, the governing equations for thermal behavior and phase change of a PCM including mass, momentum and energy conservation are written as equations (2.1) – (2.15) [67]:

**Continuity Equation,**

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{V}) = 0
\]  

(2.1)

where \( \rho \) represents the density of the fluid (\( kg/m^3 \)), \( t \) is time (s) and \( \vec{V} \) indicates the vector of velocity (\( m/s \)).

**Momentum Equation,**

\[
\frac{\partial}{\partial t} (\rho \vec{V}) + \nabla \cdot (\rho \vec{V} \vec{V}) = -\nabla P + \nabla \cdot (\mu \nabla \vec{V}) + \rho \vec{g} + \vec{S}_m
\]  

(2.2)

where \( \mu \) signifies the dynamic viscosity (\( kg/m \cdot s \)), \( \vec{V} \) is velocity vector (\( m/s \)), \( P \) stands for the static pressure (\( Pa \)), \( \vec{g} \) describes the acceleration of gravity vector (\( m/s^2 \)) and \( \vec{S}_m \) corresponds to the heat source. As reported in [68], it is very common to consider constant density for PCMs to avoid modeling a container that accommodates volumetric expansion. However, an alternative approach, like Boussinesq approximation, must be utilized to account for the impacts of buoyancy-driven natural convection during the melting and freezing.
Density is expressed as the sum of a reference density \( (\rho_{\text{ref}}) \) and a fluctuation \( \Delta \rho \):

\[
\rho = \rho_{\text{ref}} + \Delta \rho \tag{2.3}
\]

Based on the Boussinesq approximation, density variations due to temperature changes are negligible in comparison to the reference density. This allows simplification of momentum equations by treating the fluid as incompressible and maintaining a constant density in all terms, except for the buoyancy. This approximation is standard in scenarios such as melting and solidification processes where natural convection plays a substantial role and temperature variations remain minor. Considering a constant value for density in temporal and convection terms in Eq. (2.2):

\[
\rho \frac{d\vec{V}}{dt} + \rho \nabla \cdot (\vec{V} \vec{V}) = -\nabla P + \nabla \cdot (\mu \nabla \vec{V}) + (\rho_{\text{ref}} + \Delta \rho) \vec{g} + \dot{s}_m \tag{2.4}
\]

At constant pressure, any increase in temperature most often leads to a decrease in density. In this regard, the coefficient of thermal expansion is defined as:

\[
\alpha = -\frac{1}{\rho_{\text{ref}}} \frac{\partial \rho}{\partial T} = -\frac{1}{\rho_{\text{ref}}} \frac{\rho - \rho_{\text{ref}}}{T - T_{\text{ref}}} \tag{2.5}
\]

\[
\Delta \rho = -\alpha \rho_{\text{ref}} (T - T_{\text{ref}})
\]

It leads to the simplified form of momentum equation as Eq. (2.6):

\[
\rho \left( \frac{d\vec{V}}{dt} + \nabla \cdot (\vec{V} \vec{V}) \right) = -\nabla P + \nabla \cdot (\mu \nabla \vec{V}) - \rho \dot{\alpha} \beta (T - T_{\text{ref}}) + \dot{s}_m \tag{2.6}
\]

where \( T \) represents the temperature \( (K) \), \( T_{\text{ref}} \) indicates the reference temperature \( (K) \) that is the melting temperature of the PCM, \( \alpha \) defines volumetric thermal expansion coefficient \( (1/K) \), and \( \dot{s}_m \) is the heat source due to phase change effects on convective heat transfer, described by Eq. (2.7):

\[
\dot{s}_m = \lambda(\vec{V}) = \frac{(1 - f)^2}{f^3 + \varepsilon} A_{\text{mush}}(\vec{V}) \tag{2.7}
\]
$A_{mush}$ is the mushy zone coefficient ($kg \cdot m^{-3} \cdot s^{-1}$), which will be discussed in more detail in the following sections. $f$ is the liquid fraction, and $\varepsilon$ is a very small number to avoid division by zero (0.001 in ANSYS Fluent).

**Energy Equation**

There are two common ways to formulate energy equation within the enthalpy-porosity method. The first one is written based on the enthalpy of the material,

$$\frac{\partial}{\partial t}(\rho H) + \nabla \cdot (\rho \vec{V} H) = \nabla \cdot (k \nabla T) \quad (2.8)$$

here, $k$ is thermal conductivity ($W/m \cdot K$). The sum of the sensible enthalpy ($h [J/kg]$) and the latent heat content ($\Delta H [J/kg]$) is used to compute the enthalpy of the materials during the phase change process, Eq. (2.9):

$$H = h + \Delta H \quad (2.9)$$

$$h = h_{ref} + \int_{T_{ref}}^{T} C_p \, dT \quad (2.10)$$

$$\Delta H = fL \quad (2.11)$$

Where $h_{ref}$ is the reference enthalpy ($J/kg$), $C_p$ ($J/kg \cdot K$) is specific heat at constant pressure and $L$ stands for latent heat ($J/kg$). Equations (2.12) and (2-13) are used to define liquid fraction $f$ as a function of mass and temperature of liquid and solid phases for constant and variable phase-change temperature cases, respectively [31].

$$f(m) = \begin{cases} 
0 & T < T_{sl} \\
1 & T > T_{sl} \\
\frac{m_l}{m_l + m_s} & T = T_{sl} 
\end{cases} \quad (2.12)$$

$$f(T) = \begin{cases} 
0 & T < T_s \\
1 & T > T_l \\
\frac{T - T_s}{T_l - T_s} & T_s < T < T_l 
\end{cases} \quad (2.13)$$
Here, $m_l$, $m_s$, $T_{el}$, $T_s$ and $T_l$ are liquid mass, solid mass, phase-change temperature, solidus temperature and liquidus temperature, respectively. The functional relationship between $f$ and $T$ in Eq. (2.13) leads to a linear relation between enthalpy and PCM temperature during the phase change. However, it is important to note that this is merely an approximation, as the actual curves tend to exhibit nonlinearity, a characteristic influenced by the material properties.

Another way to write the energy equation is isolating latent heat effects in the source term by using sensible enthalpy in convection and diffusion terms [39] as shown in Eq. (2.14).

$$\frac{\partial}{\partial t} (\rho h) + \nabla \cdot (\rho \vec{V} h) = \nabla \cdot (a \nabla h) + S_E$$

(2.14)

Where $a$ is thermal diffusivity ($m^2/s$) and $S_E$ is a source term to apply the impact of solid form and latent heat evolution into the energy equation defined by Eq. (2.15) [21].

$$S_E = \frac{\partial}{\partial t} (\rho \Delta H) + \text{div} (\rho \vec{V} \Delta H)$$

(2.15)

In isothermal phase changes, the term $\text{div} (\rho \vec{V} \Delta H)$ disappears [21].

### 2.2 Adjustable Parameters

As discussed in the previous part, in the enthalpy-porosity method, equations (2.1), (2.6) and (2.14) are utilized for mass, momentum and energy equations, respectively. Buoyancy and source terms ($\vec{S}_m$) in the momentum equation and the latent heat source term ($S_E$) in the energy equation contain parameters that can be used to control and calibrate the numerical simulation. The main four tunable parameters investigated in this study are thermal expansion coefficient ($\beta$), mushy zone coefficient ($A_{mush}$), solidus ($T_s$) and liquidus ($T_l$) temperatures and the latent heat ($L$). It is necessary to say that material properties such as density, specific heat capacity, and thermal conductivity are considered to be constant.
**Thermal Expansion Coefficient**

Thermal expansion coefficient effectively controls the density variations that drive buoyancy forces in Eq. (2.6). This, in turn, determines the intensity of natural convection currents.

When thermal expansion coefficient is higher, PCM expands more with increasing temperature. This expansion leads to a decrease in density, making the fluid or material lighter in the heated region. As a result, buoyant forces are stronger, causing the fluid to rise and creating convective currents. This accelerates the mixing of the melted and solid portions of the material, reducing the time taken for complete melting. Conversely, a lower thermal expansion coefficient results in less volumetric expansion with temperature increase. The material remains denser, inhibiting the buoyant forces and natural convection. This leads to slower mixing and a prolonged melting time.

As a critical factor influencing the rate, uniformity, and overall behavior of melting and solidification, the choice of the thermal expansion coefficient holds substantial significance. However, its numerical value is often omitted from PCM material data sheets and is rarely discussed in literature. In addition, it plays a key role in characterizing the aggregate influence of property variations, thereby regulating the intensity of the convection process. Therefore, in this study, it is not merely regarded as a material property, but rather as a crucial tuning parameter that exerts control over the scale and dynamics of the convection process.

**Mushy Zone Coefficient**

The source term introduced in Eq. (2.6) is for satisfying the conditions that all velocities in solid regions are zero. This objective is fulfilled by assuming that elements behave comparably to porous materials. Then, the source term in the momentum equations is defined as

\[ \tilde{S}_m = \lambda \langle \vec{V} \rangle = \frac{(1-f)^2}{f^3 + \varepsilon} A_{mush} \langle \vec{V} \rangle \]

that replicates the principles of the Carman-Kozeny equations, which describe fluid flow in porous materials [21].

In fully liquid cells, the source term \( \tilde{S}_m \) has no influence because \( \lambda = 0 \) as \( f = 1 \). However, in areas undergoing a phase transition, the value of \( \lambda = \frac{(1-f)^2}{f^3 + \varepsilon} A_{mush} \) becomes the dominant
factor compared to the transient, convective, and diffusion-related components of the momentum equations. In fully-solid cells, the considerably high value of $\lambda$ supersedes all other terms in the governing equations, effectively driving all velocity predictions to nearly zero. Therefore, controlling the value of $\lambda$, which is a combination of liquid fraction and mushy zone coefficient, can considerably affect the fluid behavior in the mushy zone.

$A_{mush}$ in Eq. (2.7) determines how fast the material's velocity decreases as it solidifies, with a higher value causing a more rapid transition to zero velocity [67]. The mushy zone coefficient can also have a substantial impact on mushy region morphology and plays a key role in determining how deeply the convection field penetrates the mushy area [21]. It is necessary to say that, in scenarios involving an isothermal phase transition, the fluid movement within computational cells undergoing melting or freezing does not adhere to the governing principles of flow within a porous medium [21]. In such cases, the transition boundary is a precisely defined line without the presence of a band or width. So, it is expected that mushy zone coefficient does not impact the morphology of the phase change front as it does in the context of a phase change within a mushy region. However, it should be big enough to make velocities in solid areas become zero.

Hence, it is important to be cautious when assigning a specific value to mushy zone coefficient. Despite its importance, it is not typically documented in existing literature. Therefore, it is considered as another adjustable parameter in this investigation.

**Solidus-liquidus Temperatures**

The solidus temperature is the temperature at which a material begins to transition from a fully solid state to a mixture of solid and liquid phases. It represents the lowest temperature at which the material's solid phase coexists with its liquid phase. At temperatures below the solidus, the material remains predominantly solid. The liquidus temperature is the temperature at which a material is fully transformed from a solid state to a fully liquid state. It signifies the upper limit of temperature at which the material is completely in the liquid phase. Above the liquidus temperature, the material exists primarily as a liquid. Then, these parameters help define the
temperature range within which the material undergoes melting or solidification and determine the size of the mushy zone.

Based on Eq. (2.13), solidus and liquidus temperatures are directly used to formulate the liquid fraction in variable phase-change temperature cases. At the same time, considering equations (2.7) and (2.15), liquid fraction is a significant factor in defining source terms $S_m$ and $S_e$ in both momentum and energy equations, respectively. Hence, these parameters play an important role in controlling the value of source terms. The influence of mushy zone coefficient is also under the impact of solidus and liquidus temperatures; In isothermal cases where $T_s = T_l$, the conventional form of mushy zone, which typically encompasses regions with $0 < f < 1$ across multiple cells, does not exist. Instead, the mushy region is confined to a single control volume that separates pure fluid from pure solid. In this scenario, only a very small number of cells have values of $0 < f < 1$, indicating the presence of this limited mushy zone. As a result, the influence of the mushy zone coefficient on shaping the solid-liquid interface may be relatively minor in such cases. Therefore, an accurate consideration for solidus and liquidus temperatures is vital for simulating and analyzing phase change behavior, which is investigated in this research work.

**Latent Heat**

The last adjustable parameter used in this study is latent heat. It is important to acknowledge the persistent uncertainty in the reported data on various material properties. Considering this, an approximation strategy was employed, which can be deemed reasonably rational. This involved transitioning from the value of reported heat storage capacity in the PCM datasheet and segregating it into distinct components: one representing the sensible heat and the other being the latent heat. This division was determined through an approximation process based on the provided temperature range in the datasheet.

The estimated value for the latent heat plays a significant role in either transient and convection terms in Eq. (2.8) or the source term in Eq. (2.14). In this way, the temporal aspect of the melting or solidification processes can be controlled effectively.
2.3 Numerical Procedure

The computational fluid dynamics (CFD) software ANSYS FLUENT 2022 R1 is employed to solve the governing equations in this study. The approach involves utilizing the finite volume method (FVM), which encompasses dividing the domain into discrete control volumes through a computational grid. Subsequently, the mass, momentum, and energy equations are integrated across these individual control volumes to establish algebraic equations governing discrete velocity and temperature. In this section, general characteristics of the developed numerical model are provided, but more details are discussed in chapters 3 and 4.

**Solver:** PCMs used in this problem are considered to be incompressible. Therefore, pressure-based solver is applied. In terms of velocity formulation, absolute velocity formulation is used because domain boundaries are not moving. Moreover, gravitational acceleration is considered in the Y-direction because the motion of the liquid phase in PCMs is under the impact of gravitational force. Also, transient for time is assumed to simulate the whole melting or solidification process in different conditions as this is the fundamental purpose of this study.

**Solution Method:** In transient problems, segregated methods are more appropriate as they are faster per iteration [67]. In addition, because of applying the melting and solidification model, increasing the pressure-correction under-relaxation to 1.0 can lead to instability due to high mesh skewness. For such cases, it is necessary to use one or more skewness correction schemes, or use a slightly more conservative under-relaxation value (up to 0.7), or use the SIMPLE algorithm. Therefore, SIMPLE scheme is used in this problem for pressure-velocity coupling in which pressure and velocity are updated sequentially.

**Spatial Discretization:** The gradient of a given variable is used to discretize the convection and diffusion terms in the flow conservation equations. The accuracy of the least-squares gradient method is comparable to that of the node-based gradient (and both are much more superior compared to the cell-based gradient). However, it is less expensive to compute the least-squares gradient than the node-based gradient [67]. Therefore, it has been selected as the default gradient method in the ANSYS Fluent solver. For the pressure, the **PRESTO!** scheme is
more comprehensive than the other schemes. Therefore, it is designated instead of the second order method.

In addition, the second-order upwind scheme is used for convection terms in the energy equation, but the First-order upwind scheme is more appropriate for modeling momentum equations in such simulations. The reason is that there is a probability of instability because of the Boussinesq approximation, and the first-order discretization method generally yields better convergence than the second-order scheme. Also, second-order implicit is selected to model transient formulation.

**Solution Control:** Because of the nonlinearity of the equation set being solved by ANSYS Fluent, it is necessary to control the change of parameters. This is typically achieved by under-relaxing variables, reducing the change of variables produced during each iteration. In this work, under-relaxation factors of pressure, velocity, energy, and liquid fraction are 0.3, 0.7, 1, 0.9, respectively, to achieve a converged solution.

The described method is used in the following chapters to conduct sensitivity study of melting and solidification of phase change materials.
Chapter 3

3 A Systematic Sensitivity Analysis of Constrained Melting Process

The intricate phenomenon of melting holds a pivotal role in the realm of latent heat thermal energy storage systems. This chapter is dedicated to the implementation of the model introduced in Chapter 2, with a primary focus on investigating the melting process within the context of these systems. Utilizing the enthalpy-porosity approach as its foundational framework, this research endeavors to provide a calibrated model capable of accurately representing this complex thermal phenomenon. What sets this work apart is the systematic approach to calibration, which aims to not only assess the sensitivity of the parameters but also evaluate the inherent capability of the enthalpy-porosity model itself. The significance of this research lies in its potential to revolutionize latent heat thermal energy storage, offering precise control and predictability of the melting process within confined spaces.

The investigation begins with the examination of melting within a cylindrical cavity, followed by an exploration of the influence of adjustable parameters. To ensure the model's accuracy and reliability, it undergoes comparison with a set of existing experimental data, marking the first instance where all different tuning parameters are considered together. This approach not only enhances the robustness of the model but also presents a comprehensive understanding of the interplay between these parameters in the context of melting within confined spaces. The calibration approach results in the development of a refined tool, which is subsequently subjected to testing under various heating conditions. Additionally, the chapter delves into the impacts of changing geometry within the melting process, contributing to a deeper understanding of the enthalpy porosity method’s effectiveness.

3.1 Cylindrical Cavity Model

In this section, attention is directed toward the investigation of the melting process within a cylindrical cavity. This specific choice of geometry has been made purposefully, driven by the availability of ample and well-documented experimental data in [38].
3.1.1 Geometry and Material Description

The same circular PCM cavity employed in the physical experiment conducted by Teather and Siddiqui [38] has been selected as the primary domain for simulating the melting process. Figure 3.1 (a) shows a schematic depiction of the physical reference experiment, wherein a clear acrylic tube forms an outline of the domain. The tube is securely attached to rectangular acrylic plates, each measuring 146 mm by 199 mm and having a thickness of 6 mm. The secure attachment is achieved by employing square acrylic bars that seal the periphery of these plates effectively. This configuration results in the creation of two distinct sealed volumes: the central circular PCM cavity and an encompassing larger region encircling the PCM cavity's perimeter. The outer region serves as a water jacket for regulating heating and cooling processes.

In this numerical study, the primary emphasis centers on simulating the behavior of the phase change material within the central cylindrical cavity. As depicted in Figure 3.1 (b), this configuration comprises a quasi-two-dimensional cylindrical cavity with an internal diameter of 70 mm (2.75 inches), a depth of 12.7 mm (0.5 inches), and a wall thickness measuring 6.35 mm (0.25 inches). Heat is introduced into the cavity through the radial wall, which is in direct contact with the constant temperature water jacket. To maintain quasi two-dimensional conditions, insulation is applied to both the front and back facets of the cavity, minimizing heat transfer through these surfaces.

The internal volume of the cylindrical cavity is filled with the PCM. A slight airspace is intentionally left at the upper region of the cavity to accommodate thermal expansion of the PCM. During the volumetric expansion of the PCM, any excess air is permitted to escape through a small hole drilled at the top of the cylinder's wall [38]. The initial location of the PCM-air interface, specifically when the PCM is in its initial solid state, is approximately 24 mm (0.95 inches) above the center point of the cavity [68]. Experimental data are collected on the vertical mid-plane, positioned approximately 12.35 mm (0.5 inches) inward from each end of the cylindrical cavity.
Rubitherm RT26, a commercially available paraffin-based phase change material, was chosen for use in both the physical reference experiment and the present computational study. Paraffin-based PCMs, such as Rubitherm RT26, are widely favored in practical applications due to their non-toxic, inert, cost-effective, and readily obtainable characteristics. Furthermore, Rubitherm RT26 is notable for its high latent heat of fusion, a fundamental property essential for effective energy storage and release during phase transitions. The material properties of acrylic walls and RT26 are summarized in Table 3.1 and Table 3.2, respectively.

Table 3-1: Characteristics of acrylic material [67]

<table>
<thead>
<tr>
<th>Property</th>
<th>Typical Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specific Heat Capacity</td>
<td>1470</td>
<td>[J/kg K]</td>
</tr>
<tr>
<td>Thermal Conductivity</td>
<td>0.2</td>
<td>[W/m.K]</td>
</tr>
<tr>
<td>Density</td>
<td>1190</td>
<td>[Kg/m³]</td>
</tr>
</tbody>
</table>
Table 3-2: Material properties of Rubitherm RT26 [69]

<table>
<thead>
<tr>
<th>Property</th>
<th>Typical Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting Temperature</td>
<td>298 – 299</td>
<td>[K]</td>
</tr>
<tr>
<td>Congealing Temperature</td>
<td>299 – 298</td>
<td>[K]</td>
</tr>
<tr>
<td>Heat Storage Capacity ± 7.5%</td>
<td>180</td>
<td>[kJ/kg]</td>
</tr>
<tr>
<td>Combination of latent and sensible heat in a temperature range of 19°C to 34°C</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Specific Heat Capacity</td>
<td>2000</td>
<td>[J/kg K]</td>
</tr>
<tr>
<td>Density Solid</td>
<td>880</td>
<td>[Kg/m³]</td>
</tr>
<tr>
<td>Density Liquid</td>
<td>750</td>
<td>[Kg/m³]</td>
</tr>
<tr>
<td>Heat Conductivity</td>
<td>0.2</td>
<td>[W/m.K]</td>
</tr>
<tr>
<td>Volume Expansion</td>
<td>12.5</td>
<td>%</td>
</tr>
</tbody>
</table>

3.1.2 Mesh Generation

The core of numerical simulations relies on the creation of a well-suited computational mesh, a fundamental process defining the accuracy and reliability of the entire simulation. In this study, the adoption of a structured mesh characterized by a high degree of uniformity is necessary due to the dynamic presence of a progressing front within the computational domain. This front exhibits a uniform motion across the whole of the domain, demanding a mesh that maintains this consistency throughout.

Simulations indicated that deviating from a structured mesh and filling the geometry with tetrahedral cells results in divergence. Therefore, as indicated in Figure 3.2, an O-Grid technique in ICEM CFD is utilized to generate a relatively uniform structured mesh. More details associated with this technique are provided in Appendix A. Also, Figure 3.3 demonstrates the final generated mesh using the described method.
As shown in Figure 3.3, the mesh quality is high. Detailed quality metrics are available in Appendix A. Using a high-quality mesh accelerates result generation compared to a low-quality mesh, offering substantial time savings in computational processes.

3.1.3 Boundary Conditions

In this section, a detailed description of the boundary conditions utilized to recreate the conditions observed in the physical experiment is provided.

Front Face: The insulation on the front wall of the PCM cavity remained intact except during image capture intervals, with insulation removal lasting a total of 2.5 minutes for each measurement [38]. Given the negligible temperature differential between the PCM melting temperature and room temperature, any heat loss to the surroundings is anticipated to be
minimal. Therefore, it is considered that the front face of the domain is subjected to an adiabatic thermal condition, Heat Flux \( [W/m^2] = 0 \), as it is effectively insulated to minimize heat dissipation during experiments. Additionally, a no-slip condition is imposed because this surface directly interfaces with the liquid phase of the PCM during the melting process.

**Rear Face:** Similar conditions are applied to the rear face as well. The rear face remains insulated throughout the experiment, using a fixed 25mm thick layer of expanding foam [38], effectively impeding heat transfer and warranting an adiabatic condition. Furthermore, no-slip boundary conditions are imposed on this surface in line with the approach applied to the front face.

**Outer Walls:** The boundary conditions for the outer wall involve the application of a constant temperature setting to the external surface of the acrylic shell. This specific condition is introduced to mimic the role of the water jacket, which was employed in the physical experiment to sustain a stable and uniform temperature environment. Additionally, a no-slip boundary condition is enforced on the outer wall, ensuring that there is no relative motion between the fluid and the wall's surface. As described in Appendix A, the shell conduction option in ANSYS Fluent is utilized to simulate the acrylic wall.

**Air Boundary:** The PCM-to-air interface, referred to as the air boundary, is configured with a convection thermal condition to emulate the heat exchange observed between the PCM and the adjacent air pocket, mirroring the physical experiment's conditions. For precise determination of the heat transfer coefficient at the air boundary, a separate simulation of the air gap is conducted for each heating scenario in alignment with the conditions observed in the physical experiment [38]. More details related to air gap simulation are provided in Appendix B. Furthermore, a zero-shear, slip condition is imposed to replicate a free-surface condition at this boundary.

A summary of all described boundary conditions can be found in Table 3.3. Furthermore, Table 3.4 displays the values assigned for initial conditions and thermal boundary conditions in various scenarios, aligning them with the corresponding experimental tests (H1-H3) [38].
Table 3-3: An overview of boundary conditions for melting and solidification simulations in cylindrical cavity.

<table>
<thead>
<tr>
<th>Surface</th>
<th>Boundary Condition</th>
<th>Momentum</th>
<th>Thermal</th>
</tr>
</thead>
<tbody>
<tr>
<td>Front Face</td>
<td>No Slip Condition</td>
<td>Adiabatic</td>
<td></td>
</tr>
<tr>
<td>Rear Face</td>
<td>No Slip Condition</td>
<td>Adiabatic</td>
<td></td>
</tr>
<tr>
<td>Outer Walls</td>
<td>No Slip Condition</td>
<td>Constant Temperature</td>
<td></td>
</tr>
<tr>
<td>Air Boundary</td>
<td>Zero-shear, slip condition</td>
<td>Convection Thermal Condition</td>
<td></td>
</tr>
</tbody>
</table>

Table 3-4: Assigned values for initial and thermal conditions in various scenarios of melting process.

<table>
<thead>
<tr>
<th>Surface</th>
<th>Thermal Condition Type</th>
<th>Assigned Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Outer Walls</td>
<td>Temperature [K]</td>
<td>306.05 310.25 314.05</td>
</tr>
<tr>
<td>Air Boundary</td>
<td>Heat Transfer Coefficient [W/ m².K]</td>
<td>6.2 7.6 9</td>
</tr>
<tr>
<td>Initial Conditions</td>
<td>Temperature [K]</td>
<td>292.45 292.45 292.45</td>
</tr>
</tbody>
</table>

3.1.4 Convergence Criteria

In the realm of computational simulations, one widely adopted strategy to enhance efficiency is the adjustment of convergence criteria, a practice extensively explored in the literature [70]. Particularly, when dealing with the numerical simulation of 3D and real-scale latent heat thermal energy storage units, the choice of convergence criteria plays a pivotal role. Different residual values can strike a balance between computational accuracy and efficiency. Lower residual values may yield more accurate results but require longer computation times. Higher residual values provide quicker results but may sacrifice accuracy. Hence, it is crucial to grasp how various convergence criteria influence the outcomes. In this section, different values of residuals are investigated to evaluate how much the simulation reacts to changes in these criteria.

As depicted in Figure 3.4, the impact of different residual values, ranging from $10^{-3}$ to $10^{-6}$, is explored across the mass, momentum, and energy equations. The examination focuses on the liquid fraction during the initial 10,000 seconds of the melting process, as illustrated in
Figure 3.4 (a), and encompasses the calculation of relative differences throughout the entire duration, as presented in Figure 3.4 (b).

The maximum relative difference emerges during the early stages of the melting process, diminishing steadily after the first hour. While transitioning from a convergence criterion of $10^{-3}$ to $10^{-4}$ results in a maximum relative difference of approximately 3% for the entire process, further reducing the residuals to $10^{-5}$ paradoxically leads to an increase in the difference. This observation underscores the fact that the simulation outcomes remain sensitive to the choice of convergence criteria. Thus, a lower threshold was tested. As visible from Figure 3.4 (b), the transition from $10^{-5}$ to $10^{-6}$ yields a relative difference close to zero, signifying that $10^{-5}$ suffices for the residuals. By opting for a smaller value, the divergence in results does not significantly diminish, yet it escalates computational costs. Therefore, the final, optimal choice for the residuals governing the continuity, momentum, and energy equations in this study is $10^{-5}$, achieving a balance between result accuracy and computational efficiency.

![Figure 3-4: Impact of residual values on liquid fraction variation during the first 10000s of melting process simulation of RT26 inside a cylindrical cavity.](image)
3.1.5 Grid and Time Independence Tests

To validate the reliability of the numerical simulations and ensure their accuracy, a comprehensive grid- and time-independence analysis has been undertaken. This testing assesses whether the simulation outcomes remain consistent and robust by varying both spatial and temporal discretization factors. The key parameters under scrutiny during this process are the melting time and liquid fraction.

To conduct the grid-independence tests, simulations were executed using different grid resolutions, shown in Figure 3.5, while keeping the initial time step size fixed at 1 second. For each resolution, the simulations were allowed to run for up to 100 iterations at each time step, or until the residual values reached the specified convergence criteria of $10^{-5}$, as discussed in detail in the previous section.

![Image of grid resolutions](image)

(a) Coarse Mesh: 29040 Cells  
(b) Medium Mesh: 58870 Cells  
(c) Fine Mesh: 122740 Cells

Figure 3-5: Various mesh sizes used to investigate grid-independence test.

In Table 3.5, the total melting time is compared using different grid sizes. Sensible heating takes place during the initial phases of the simulation until the PCM reaches its melting temperature, triggering the onset of the melting process. It is important to note that the duration of sensible heating is incorporated within the total melting time reported for each case. As demonstrated, the percentage difference when transitioning from coarse to medium mesh is merely 0.759%, and from medium to fine mesh, it is just 0.339%. These minimal differences affirm that the melting time results remain consistent and unaffected by variations in grid size.
Table 3-5: Grid size impact on the total melting time in cylindrical cavity.

<table>
<thead>
<tr>
<th>Mesh Size</th>
<th>Coarse (29040 Cells)</th>
<th>Medium (58870 Cells)</th>
<th>Fine (122740 Cells)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting Time (s)</td>
<td>18445</td>
<td>18585</td>
<td>18648</td>
</tr>
<tr>
<td>Difference (%)</td>
<td>-</td>
<td>0.759%</td>
<td>0.339%</td>
</tr>
</tbody>
</table>

Figure 3.6 (a)-(b) shows the results of the detailed analysis of liquid fraction variation and relative difference for different mesh sizes.

(a) Mesh size influence on liquid fraction variation.

(b) Comparative analysis of relative differences in liquid fraction measurements across different mesh sizes over time.

Figure 3-6: Grid-independence test for the melting process: liquid fraction variation and relative difference analysis. total number of cells for coarse, medium, and fine meshes are 29040, 58870, 122740, respectively.
Initially, variations in the results are influenced by the difference in the start times of the melting process. However, as the process progresses, the disparities in melting fraction become small. Specifically, the average differences are 0.314% when transitioning from a coarse to medium mesh and 0.201% when shifting from a medium to fine mesh. The low variance in both melting time and liquid fraction demonstrates that a medium mesh resolution suffices to yield grid-independent results. As such, the medium mesh resolution is adopted for all subsequent simulations in this study, ensuring computational efficiency and reliable outcomes.

To investigate time-independence test, three distinct time step sizes $\Delta t = 0.5s$, $\Delta t = 1s$ and $\Delta t = 2s$ were employed in the tests while maintaining a medium grid resolution. These assessments systematically altered the time step sizes to assess their influence on both melting time and liquid fraction, thus offering valuable insights into the temporal stability and accuracy of the simulations.

Table 3.6 and Figure 3.7 demonstrate how different time step sizes impact total melting time and liquid fraction variation, revealing near-identical results across three time step sizes with minimal differences. In this study, the final choice of a 1s time step size over 2s is motivated by efficiency considerations. With a 1s time step, approximately half the number of iterations, typically ranging from 20 to 30, suffices to achieve a convergence level of $10^{-5}$ per time step. In contrast, when using a 2s time step, a notably higher average of 60 to 70 iterations per time step is required to attain a similar level of convergence. This efficiency advantage makes the 1s time step a more practical choice for the simulation, reducing computational time requirements.

Table 3-6: Time step size impact on the total melting time in cylindrical cavity.

<table>
<thead>
<tr>
<th>Time Step Size</th>
<th>$\Delta t = 0.5s$</th>
<th>$\Delta t = 1s$</th>
<th>$\Delta t = 2s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting Time (s)</td>
<td>18584</td>
<td>18585</td>
<td>18586</td>
</tr>
<tr>
<td>Difference (%)</td>
<td>-</td>
<td>0.0054%</td>
<td>0.0.0054%</td>
</tr>
</tbody>
</table>
Investigating the Individual Impact of Adjustable Parameters on the Melting Process

As described in the second chapter, the adjustable parameters play key roles in shaping the behavior of PCMs during the melting process. To investigate their impacts, it is crucial to comprehend their individual contributions before addressing their collective influence. This approach serves a dual purpose. Firstly, it enables the unique influence of each adjustable parameter to be discerned, offering valuable insights into their independent effects. Secondly, this understanding leads to a more focused range of parameters for consideration in the subsequent section, where the computational model will be calibrated by incorporating the combined impact of these factors.

Four distinct tuning parameters are examined individually in different levels: the mushy zone coefficient, $A_{mush}$ [kg m$^{-3}$s$^{-1}$], across four levels ($10^4$, $10^5$, $10^6$, $10^7$), the thermal expansion coefficient, $\beta$ [1/K], spanning four levels (0.00005, 0.0001, 0.0005, 0.001), solidus temperatures, $T_s$ [K], at four levels (296, 297, 298, 299), and latent heat, LH [KJ/kg], at two levels (150 and 180). Liquidus temperature, $T_l = 299$ [K], is kept constant in all simulations. The initial selection of these levels was based on values reported in existing literature or provided material.
properties for Rubitherm RT26. As mentioned, one objective of this section is to limit the range of each factor to more practical values, as simulating all possible combinations \((4 \times 4 \times 4 \times 2 = 128)\) would not be computationally feasible, given that running each simulation requires a minimum of 15 days of wall-clock time.

Several approaches are commonly employed in such situations to minimize the number of levels within each factor, such as the orthogonal method detailed in [71]. Nonetheless, the number of cases recommended by these methods remains considerable, rendering them impractical and computationally unfeasible to run, considering the time required for each simulation. Therefore, a more refined approach is deemed necessary. In this study, the reduction of levels for each factor is undertaken through individual assessments of adjustable parameters, accompanied by comparisons with experimental data to confirm the reduction.

**Mushy Zone Coefficient**

In section 2-2, the pivotal role played by the mushy zone coefficient in determining the velocity damping amplitude within the semi-porous mushy region of the PCM was described. In this section, an investigation is undertaken to assess the influence of the mushy zone coefficient on the melting process within a cylindrical cavity, with comparisons made to the data presented in [38]. The analysis begins with the adoption of a thermal expansion coefficient value, \(\beta = 0.0005 \left[\frac{1}{K}\right]\), as provided by Rubitherm company for RT26. Additionally, the latent heat value of 180 \([kJ/kg]\) is obtained from the RT26 datasheet [69]. The initial solidus temperature reference point, \(T_s = 296 [K]\), is based on the estimated interface temperature outlined in [38]. Also, a constant liquidus temperature of \(T_l = 299 [K]\) is maintained throughout all simulations.

As demonstrated in Figure 3.8 (a), during the initial stages of the melting process, the impact of the mushy zone coefficient on liquid fraction variation is relatively minor. This is primarily attributed to the prevalence of sensible heat transfer, which plays a significant role in this phase. However, as the process advances, after approximately 2000 seconds in this case, a divergence in results becomes evident. Higher mushy zone coefficients begin to manifest a substantial influence by causing a reduction in the liquid fraction at specific instants in time. Notably, the rate of change in the liquid fraction curve becomes steeper for lower mushy zone
coefficients. This observation underscores the inverse correlation between the mushy zone coefficient and the extent of convection that transpires during the melting process. Higher values of the mushy zone coefficient effectively suppress convective phenomena, resulting in an extended duration of the melting process due to the decreased convective heat transfer. This phenomenon becomes more evident when observing Figure 3.8 (b): as the mushy zone coefficient is increased, there is a decrease in the total heat transfer rate during the phase transition, resulting in a prolonged melting process.

Figure 3-8: The influence of mushy zone coefficient on the melting process within the cylindrical cavity, considering $\beta = 0.0005 \frac{1}{K}$, $T_s = 296 [K]$, $T_t = 299 [K]$. Latent Heat $= 180 \frac{kJ}{kg}$. 

(a) The influence of mushy zone coefficient on the liquid fraction variations.

(b) The influence of mushy zone coefficient on total heat transfer rate (W).
To achieve an understanding of the impact of mushy zone coefficient on the melting process, consideration must also be given to the behavior of the PCM itself. In this context, the flow patterns are compared with experimental data across various mushy zone coefficient scenarios, as illustrated in Figure 3.9. Furthermore, transient, dimensionless temperature fields of the PCM, obtained from thermal imaging data outlined in [38], are utilized as representations of liquid-solid interface shapes. These representations are then compared with the simulated liquid fraction contours, as depicted in Figure 3.10. Dimensionless time, $\tau^+$, introduced in the figures hereinafter is defined as Eq. (3.1).

$$\tau^+ = \frac{t - t_{\text{start}}}{t_{\text{end}} - t_{\text{start}}}$$  \hspace{1cm} (3.1)

where $t$ is the time, $t_{\text{start}}$ is the time at which melting begins, and $t_{\text{end}}$ is the time at which melting ends. It is important to note that the primary focus in the figures depicting flow patterns is directed towards illustrating the structural aspects of the phenomena and visualizing convective structures, as demonstrated in experimental work [38]. To achieve this objective, a localized color scale is employed to capture the entire spectrum of motions in each scenario. The rationale for employing a localized scale is rooted in the potential of a global scale to obscure specific motion-related information in certain cases. Also, it is worth highlighting that the interpretation of colors may differ between images due to the utilization of the localized scale. The shift toward the red end of the spectrum signifies increased speeds, while movement toward the blue spectrum indicates reduced speeds.
Figure 3-9: Exploring the influence of mushy zone coefficient on simulated liquid flow dynamics during melting inside a cylindrical cavity: a comparative analysis of experimental streak visualizations compiled from the PIV data at various times during melting and numerical insights. Utilizing a localized color scale in numerical results to illuminate the full spectrum of motions and highlight convective structures to be able to compare with equivalent experimental results.
Based on Figure 3.9, in cases with lower mushy zone coefficients, the presence of a sloped region along the sides of the PCM is less pronounced. This discrepancy is attributed to observations in experimental tests, where as the melting process progresses, two robust, symmetric, counter-rotating vortices form along the cavity’s sides. However, with lower mushy zone coefficients, several vortices emerge on both sides of the solid PCM.

To elucidate this phenomenon, it is essential to delve into the dynamics of the process. As the material undergoes melting, the fluid gains the freedom to rise along the boundary due to buoyancy-driven forces. However, this ascending motion encounters resistance precisely at the interface where the solid meets the liquid phase, effectively decelerating the fluid’s upward movement, resulting in vortex formation.

The formed vortices are subject to the influence of two opposing forces: buoyancy, which promotes fluid motion, and the mushy zone coefficient, which hinders it. The importance of $A_{mush}$ becomes evident as it directly relates to the source term in the momentum equation. A higher $A_{mush}$ corresponds to a more substantial source term and then weaker convection, creating a pronounced challenge for fluid mobility at the solid-liquid interface. Consequently, when the mushy zone coefficient is elevated, it significantly amplifies the resistance of fluid motion in the regions proximate to the solid-liquid interface. This results in the confinement of vortices predominantly to the upper portion of the geometry. Conversely, when the mushy zone coefficient is lower, additional fluid motions manifest, including rolling motions at the upper boundary. In such instants, convection patterns tend to exhibit greater strength, often leading to the disruption of organized convective motions.

Furthermore, in line with observations from experimental tests, the combination of the heating wall at the cavity’s bottom and the layer of cold PCM above it induces a thermal instability characterized by unstable stratification. This instability manifests as a distinct area of 3D convection, and its presence becomes more pronounced in cases with higher mushy zone coefficients. In addition, as shown in Figure 3.10, a visible distinction between the outcomes emerges when considering a higher mushy zone coefficient; it results in a more uniform melting of the PCM, extending from the outer hot walls toward the center, resembling observations in experimental tests.
Figure 3-10: Evaluating the influence of mushy zone coefficient on simulated liquid-solid interface morphology during melting: Experimental data in the first row are transient, dimensionless temperature fields of the PCM, obtained from thermal imaging data outlined in [38], utilized as representations of liquid-solid interface shapes. Numerical results are simulated liquid fraction contours. Omitting Scales as the focus is on the front shape progression.

In summary, a lower mushy zone coefficient yields PCM behavior that deviates from experimental results, while higher coefficients bring the PCM behavior closer to experimental
observations, though not achieving a perfect match. This underscores that while the mushy zone coefficient is a significant parameter, it alone does not suffice for effective model calibration. Additionally, the computational aspect must be considered; larger mushy zone coefficients necessitate a higher number of iterations (70-80) per time step, making them computationally unfeasible. Consequently, the initial range's lower and higher values are excluded, and the appropriate range for the mushy zone coefficient is confined to $10^5 - 10^6$.

**Solidus Liquidus Temperature**

As discussed in the second chapter, it is imperative to address the close relationship between the solidus-liquidus temperature range and the mushy zone coefficient. This connection arises from the fact that the temperature range specified essentially determines the band over which the mushy zone coefficient exerts its influence. In other words, the extent of the temperature band directly impacts the number of computational cells where the mushy zone coefficient becomes active. When the liquidus temperature equals the PCM melting temperature, a lower solidus temperature intensifies the impact of the mushy zone coefficient. For investigation purposes, a uniform temperature, $T_s = T_l = 299 [K]$, was maintained. Figure 3.11 illustrates that the effect of varying mushy zone coefficients on the liquid fraction is quite uniform in this case, except for the later stages of the melting process, where a higher mushy zone coefficient prolongs the melting process.

The observed behavior is a consequence of scenarios featuring similar solidus and liquidus temperatures. In such instances, only one computational cell contains the transition boundary between solid and liquid phases, regardless of the grid resolution employed. This solitary cell functions as a partition, featuring a distinct line that separates the solid and liquid phases within it. In contrast, in cases with differing temperatures, whole cells have the capacity to accommodate a mixture of both solid and liquid phases rather than exclusively one or the other. This behavior emerges from the interplay between the gradients of the solidus and liquidus temperatures, permitting the coexistence of both phases within individual cells. These findings underscore the significance of considering the mushy zone coefficient in conjunction with the solidus-liquidus temperature range when simulating phase change materials.
Figure 3-11: The influence of mushy zone coefficient on the melting process within the cylindrical cavity, considering constant temperature phase transition with $\beta = 0.0005 \, \left( \frac{L}{K} \right)$, $T_s = 299 \, [K]$, $T_i = 299 \, [K]$, Latent Heat = $180 \, \left( \frac{k}{kg} \right)$.

However, the influence of solidus-liquidus temperature range extends beyond mushy zone coefficient impacts, affecting the configuration of the solid-liquid interface, particularly during the final stages of the melting process, as evident from Figures 3.12 and 3.13. Throughout most of the melting process, variations in the solidus-liquidus temperature range do not yield significant differences in convective structures. Nevertheless, towards the end of the melting phase, distinctions emerge. In instants where the solidus-liquidus temperature range is lower, there is a more pronounced penetration of side vortexes into the lower regions, thereby altering the shape of the three-dimensional rolls at the bottom of the system. This effect is also pronounced in the solid-liquid interface shapes observed in the last column of Figure 3.13.
Figure 3-12: The influence of solidus-liquidus temperature ranges on the convective structures during the melting process within the cylindrical cavity, considering $\beta = 0.0001 \ \frac{1}{K}$, $A_{mush} = 10^6$, $Latent \ Heat = 180 \ \frac{kJ}{kg}$. Utilizing a localized color scale in numerical results to illustrate the full spectrum of motions and emphasize convective structures.
Figure 3-13: The influence of solidus-liquidus temperature ranges on solid-liquid interface shapes during the melting process within the cylindrical cavity, considering $\beta = 0.0001 \left[ \frac{1}{K} \right]$, $A_{mush} = 10^6$, $Latent\ Heat = 180 \left[ \frac{kJ}{kg} \right]$. Experimental data: transient, dimensionless PCM temperature fields from thermal imaging [38], representing liquid-solid interface shapes. Numerical results: simulated liquid fraction contours.
Based on the provided results, it is evident that using identical solidus and liquidus temperatures in the simulation restricts the influence of the mushy zone coefficient. Consequently, the higher value of \( T_s = 299 \) [K] is omitted from the reasonable range. Additionally, when comparing with experimental results, it becomes apparent that the closest resemblance to the experimental outcomes is achieved with a mere 1°C difference in the solidus-liquidus temperature range, with \( T_s = 298 \) [K] emerging as the top-performing case, followed by \( T_s = 296 \) [K] as the second-best option. Hence, the range of solidus temperature under investigation in the subsequent section is limited to \( T_s = 296 \) [K] and \( T_s = 298 \) [K].

**Thermal Expansion Coefficient**

In the second chapter, the role of thermal expansion coefficient in numerical simulations of phase change materials was discussed. Traditionally perceived as a material-specific property, it is transcended by this characterization and instead serves as a comprehensive parameter that represents the cumulative influence of various material properties, including density and viscosity, as they respond to temperature changes during the melting process. Consequently, the thermal expansion coefficient is better understood as a parameter that defines the entire convective process, rather than solely being an inherent material property. In practical terms, it functions as a tuning parameter that directly impacts the dynamics of the melting process within simulations, underscoring its significance as a process-related parameter in the realm of computational analysis. Therefore, its precise selection holds critical importance in calibrating the degree of convection accompanying melting in simulations.

The analysis starts by using a widely accepted value for the mushy zone coefficient, which is commonly found in the literature, set at \( 10^5 \). Other parameters include a latent heat value of 180 [kJ/kg], a solidus temperature of \( T_s = 296 \) [K], and a constant liquidus temperature of \( T_l = 299 \) [K] maintained across all simulations.

Figure 3.14 illustrates how variations in the thermal expansion coefficient impact the liquid fraction during the melting process. This aligns with the predictions made in Chapter 2, where it was anticipated that higher thermal expansion coefficient values would lead to more
pronounced convection in the fluid phase, resulting in a higher liquid fraction at a specific time and consequently reducing the overall melting duration.

![Graph showing the influence of thermal expansion coefficient on the melting process](image)

Figure 3-14: The influence of thermal expansion coefficient on the melting process within the cylindrical cavity, considering $A_{mush} = 10^5$, $T_s = 296$ [K], $T_i = 299$ [K], Latent Heat=180 [kJ/kg].

To further support this observation, Figures 3.15 and 3.16 offer insights into the fluid pattern and the solid-liquid interface for different thermal expansion coefficient values. At the initial stages of the melting process, the flow patterns appear similar across various thermal expansion coefficient values. However, as the melting process advances, distinct vortex structures emerge at the upper portion of the cylindrical cavity in cases with higher thermal expansion coefficients. It is attributed to the intensified convection within the fluid regions, leading to the disruption of organized convective structures.
Figure 3-15: Evaluating the influence of thermal expansion coefficient on simulated liquid flow dynamics during melting: a comparative study with experimental observations. Consistent with prior figures, numerical results employ a localized color scale to represent the complete range of motions and highlight convective structures.
Figure 3-16: Examining thermal expansion coefficient impact on simulated liquid-solid interface morphology during melting: a comparative study with experimental observations. Experimental data features transient, dimensionless PCM temperature fields from thermal imaging [38], representing liquid-solid interface shapes. Numerical results show simulated liquid fraction contours, both emphasizing front shape progression without scales.
Upon comparing the simulated results with the experimental data, it becomes evident that none of the cases exhibit strong agreement. This emphasizes the conclusion that while thermal expansion plays a significant role, it is not the sole determining factor of system behavior. However, it is worth noting that employing lower thermal expansion coefficients results in a closer resemblance in behavior. Then, the higher value ($\beta =0.001$) is excluded from the range. Conversely, the lower value of $\beta =0.00005$, even though it aligns more closely with experimental results, deviates from any reported values in the literature, suggesting an unrealistic limitation on the influence of convection components. Hence, the reasonable levels for the thermal expansion coefficient are determined to be $\beta = 0.0001$ and $\beta = 0.0005$.

**Latent heat**

In Chapter 2, the latent heat value's potential impact on the melting process was discussed. An estimated latent heat value of 150 [kJ/kg] was calculated based on the temperature range provided in RT26 datasheet [69] and subsequently incorporated into the model to assess its effects. Various combinations of other adjustable parameters have been employed to elucidate the model's variations when latent heat is set at 150 [kJ/kg] as opposed to 180 [kJ/kg].

Estimated Sensible Heat = $c_p \Delta T = 2 \times (34 - 19) = 30 [\frac{kJ}{kg}]$

Estimated Latent Heat = 180 - 30 = 150 [kJ/kg]

As an illustration of the obtained results, Figure 3.17 demonstrates that the primary impact of changing latent heat value is the adjustment in the time required for complete melting. In this figure, 't' represents real-time. What is noteworthy is that, apart from its effects on time, there is no significant change in the overall melting process as the PCM exhibits the same behavior when examined on a scaled time basis. This implies that when there are errors or uncertainties regarding the reported latent heat value, it doesn't fundamentally change the nature of the melting process itself; rather, it influences the rate at which the process occurs.

This outcome can be attributed to the model's nature, which simplifies many complex factors into a few adjustable parameters. In essence, it underscores how various aspects of the melting process are interconnected and how altering one parameter, such as latent heat, can specifically
impact the time factor without causing a radical transformation in the entire process. Hence, in
the subsequent section where the cumulative impact of various adjustable parameters is
assessed, this specific parameter is maintained at a single level, LH=150 [KJ/kg].

\[ \beta = 0.0001 \left(\frac{1}{K}\right), A_{mush} = 10^6, T_s = 298 [K], T_l = 299 [K] \]

$t = 7800s$  $t = 11700s$  $t = 18000s$

$t = 9000s$  $t = 13800s$  $t = 21000s$

$t = 5100s$  $t = 8100s$  $t = 12300s$

$t = 6300s$  $t = 9000s$  $t = 14400s$

Figure 3-17: The impact of latent heat value on the solid-liquid interface evolution over both scaled
time ($\tau^+$) and real-time ($t$) in two different combinations of adjustable parameters. Experimental data
includes transient, dimensionless PCM temperature fields [38]. Numerical results display simulated
liquid fraction contours, both emphasizing front shape progression without scales.
3.1.7 Calibration Study (H1 scenario)

In the previous section, an investigation was conducted to evaluate the individual impacts of various adjustable parameters on the simulation. The first crucial insight from the investigation was that focusing on a single factor is insufficient in achieving a calibrated model that faithfully replicates experimental data. To attain such a model, it is imperative to consider the combined influence of all tuning parameters concurrently.

Secondly, it was found that higher mushy zone coefficients affect model's accuracy by controlling convective structures, whereas lower thermal expansion coefficients help by reducing convective intensity. Also, maintaining uniform solidus-liquidus temperatures results in inaccuracies due to constraints in computational cells within the mushy zone. Additionally, latent heat values, despite not impacting flow patterns or material behavior, are involved in regulating the melting time. These findings emphasize the intricate nature of model calibration, highlighting the need for developing an evaluation matrix encompassing four distinct factors at different levels.

As running all possible combinations is not computationally feasible, reasonable values obtained from individual investigations, as summarized in Table 3.7, are employed in the establishment of an evaluation matrix. Within this matrix, consisting of 8 unique combinations ($2^4 = 8$) of the four factors at varying levels, insights from individual investigations are systematically synthesized, enabling a thorough examination of diverse scenarios through different parameter configurations.

| Table 3-7: Summary of reasonable values obtained from individual investigation of four tuning parameters. |
|---|---|---|---|---|
| **Adjustable Parameter** | $A_{mush} \ [	ext{kg m}^{-3}\text{s}^{-1}]$ | $\beta \ [\frac{1}{K}]$ | $T_s \ [K] - T_l \ [K]$ | $LH \ [\frac{kJ}{kg}]$ |
| **Reasonable Values** | $10^5$ | 0.0001 | 296-299 | 150 |
| | $10^6$ | 0.0005 | 298-299 |

Figure 3.18 exhibits eight distinct parameter arrangements within the evaluation matrix. In each case, numerical results were compared with experimental data, assessing factors including
melting time, liquid fraction variation, PCM temperature, the morphology of the solid-liquid interface, flow characteristics and velocities within the PCM. For simplicity, only two important factors, including melting time and solid-liquid interface at a specific instant, are shown in this figure to illustrate how the calibration process has been carried out.

<table>
<thead>
<tr>
<th>$A_{mush}$</th>
<th>$\beta$</th>
<th>$T_s$</th>
<th>Front Shape</th>
<th>Melting Time (s)</th>
<th>$A_{mush}$</th>
<th>$\beta$</th>
<th>$T_s$</th>
<th>Front Shape</th>
<th>Melting Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^5$</td>
<td>0.0001</td>
<td>296</td>
<td><img src="image1" alt="Image" /></td>
<td>17859</td>
<td>$10^6$</td>
<td>0.0001</td>
<td>296</td>
<td><img src="image2" alt="Image" /></td>
<td>20436</td>
</tr>
<tr>
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<td>0.0001</td>
<td>298</td>
<td><img src="image3" alt="Image" /></td>
<td>20355</td>
<td>$10^6$</td>
<td>0.0001</td>
<td>298</td>
<td><img src="image4" alt="Image" /></td>
<td>23437</td>
</tr>
<tr>
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<td>0.0005</td>
<td>296</td>
<td><img src="image5" alt="Image" /></td>
<td>15887</td>
<td>$10^6$</td>
<td>0.0005</td>
<td>296</td>
<td><img src="image6" alt="Image" /></td>
<td>17053</td>
</tr>
<tr>
<td>$10^5$</td>
<td>0.0005</td>
<td>298</td>
<td><img src="image7" alt="Image" /></td>
<td>17301</td>
<td>$10^6$</td>
<td>0.0005</td>
<td>298</td>
<td><img src="image8" alt="Image" /></td>
<td>19635</td>
</tr>
</tbody>
</table>

Latent Heat = 150 [kJ/kg]

Experimental [38]

![Image](image9)

Latent Heat = 150 [kJ/kg]

Experimental [38]

![Image](image10)

Figure 3-18: Comparative analysis of total melting time and simulated solid-liquid interface at $\tau^+ = 0.57$ against experimental results for eight distinct parameter configurations in the evaluation matrix.

When examining each factor individually, multiple scenarios exhibit similarities to experimental data. For instance, as shown in Figure 3.18, both parameter sets ($10^6$, 0.0001, 296, 150) and ($10^6$, 0.0001, 298, 150) align with the experimental melting front shape. However, only the latter satisfies the criteria for total melting time. This approach is systematically applied to all other factors to find the calibrated model. Following a thorough
analysis, the optimal combination of tuning parameters has been identified and is presented in Table 3.8.

<table>
<thead>
<tr>
<th>Adjustable Parameter</th>
<th>( \lambda_{\text{mush}} \text{ [kg m}^{-3}\text{s}^{-1}] )</th>
<th>( \beta \text{ [1/K]} )</th>
<th>( T_s \text{ [K]} - T_i \text{ [K]} )</th>
<th>( LH \text{ [kJ/kg]} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Utilized Value in Calibrated Model</td>
<td>10^6</td>
<td>0.0001</td>
<td>298 – 299</td>
<td>150</td>
</tr>
</tbody>
</table>

The subsequent section will present a detailed comparison between the model simulated using these parameters and experimental data, providing an assessment of the calibrated model. The lowest heating condition (Case H1 in Table 3.4) from [38] is utilized due to its extended melting duration and the superior temporal resolution of infrared temperature measurements.

The initial assessment of the calibrated model focused on the total melting time. Experimental tests indicated a melting time of approximately 22,741 seconds, while the numerical simulation yielded a value of 23,436 seconds. This discrepancy represents a minor error of approximately 3%, suggesting a favorable level of agreement between the two sets of results.

As experimental results are presented in scaled time, the corresponding numerical results are also provided in scaled time, defined in Eq. (3.1), in the subsequent figures. Figure 3.19 presents a comparison between the numerical results derived from the calibrated model and experimental data, focusing on both the average PCM temperature and liquid fraction, both of which are computed using volume averages.

As illustrated in Figure 3.19(a), the simulated overall average PCM temperature exhibits a sharp initial increase followed by a consistent upward trend. The initial rise underscores the heightened thermal gradients during the early stages, mirroring observations made in the experimental tests. Furthermore, as depicted in Figure 3.19(b), it becomes evident that the rate of melting experiences a slight increase during the initial stages of the melting process, followed by a steady progression for the majority of the melting duration, and ultimately a decrease towards the process ending. The accelerated initial melting rate can be attributed to the presence of elevated temperature gradients. Subsequently, melting progresses steadily due to the dominance of natural convection driven by vortices, governing heat transport. In the
final stages of melting, natural convection weakens, and heat transport shifts towards conduction.

Figure 3.19: PCM temperature and liquid fraction evolution in scaled time for calibrated model during the melting process ($A_{mes} = 10^6 \ [kg \ m^{-3} \ s^{-1}]$, $\beta = 0.0001 \ \left[\frac{1}{K}\right]$, $T_s = 298 \ [K]$, latent heat = 150 [kJ/kg]) vs. experimental data.

As demonstrated, there is a close alignment between the numerical and experimental findings. The minor differences are related to the water temperature in experimental tests, where the boundary conditions should remain constant throughout the experiment. However, a practical challenge emerged due to the relatively large volume and a low flow rate of approximately two gallons per hour. This limited flow rate causes heat to be introduced into the water bath at a slow pace, resulting in a gradual warm-up period at the beginning, a phenomenon not considered in the simulated average PCM temperature.

Figure 3.20 presents a comparison between the convective structures and flow patterns observed in experimental tests and those obtained from the calibrated model.
Figure 3-20 : Analyzing calibrated model predictions and experimental liquid flow patterns in the melting process: Expanding on prior figures, the numerical results employ a refined localized color scale to illustrate the entire range of motions, with a specific focus on highlighting convective structures. Key among these structures are symmetric vortices and intricate 3D recirculation patterns beneath the solid PCM observed consistently in both experimental and numerical analyses.

As the melting process progresses, a pair of strong symmetric counter-rotating vortices emerges along the cavity's walls. These vortices result from the combined effects of two
phenomena driving convective motion. The fluid near the heated wall rises because of buoyancy, gaining heat and accelerating as it moves upward. Meanwhile, along the solid-liquid interface, the fluid cools as it transfers heat to the cooler solid. These opposing buoyant forces work together to create vortices on both sides of the solid mass. This process improves heat transfer from the heating wall to the PCM and shapes the solid-liquid interface.

Another significant observation pertains to the three-dimensional convection pattern located at the base of the cavity. Within this area, thermal instability arises due to the unstable stratification induced by the heating wall and the cooler PCM layer above it. Notably, the calibrated model effectively captures this dynamic 3D region, marking a notable achievement. To the best of the author's knowledge, previous numerical studies have struggled to accurately predict the behavior of this 3D region.

Figure 3.21 compares the velocity vectors obtained from the calibrated model with those from the experimental dataset. The experimental results do not include the representation of the 3D region, but it is depicted in the simulated model. Also, in Figure 3.22, the simulated evolution of the solid-liquid interface during the melting process is compared with corresponding experimental data at the same scaled time.
Figure 3-21: Comparing experimental and simulated velocity vector fields using the calibrated model to examine flow patterns throughout melting process. It's important to highlight that the scale of the velocity vector field is modified for each time segment, providing a more precise depiction of the flow velocity patterns.
Figure 3-22: Analyzing simulated liquid-solid interface shapes during the melting process and comparing them with experimental findings. The transient, dimensionless temperature fields described in [38] serve as representations of the liquid-solid interface in the experimental components. The numerical results show simulated liquid fraction contours, both emphasizing the progression of front shape without specific scales.
As demonstrated in Figure 3.21, the flow patterns observed in Figure 3.19 are reinforced by the velocity fields. Furthermore, the increasing magnitude of velocity within the side vortices is illustrated as the fluid moves up the heated wall and descends along the interface. As the fluid travels along the hot wall within these vortices, it accumulates velocity and temperature. The maximum velocity and temperature are reached when the fluid reaches the top surface, at which point it changes direction due to momentum and interfaces with the solid PCM. This fluid, possessing the highest temperature and velocity, imparts the most heat to the solid PCM at this juncture. Subsequently, as the fluid descends along the solid-liquid interface, it continues to cool, leading to an increase in density that supports the downward motion of the liquid PCM.

The results indicated in Figure 3.22 emphasize observations from Figures 3.20 and 3.21. As the melting progresses, the solid PCM is shaped into an almost elliptical form, driven by the accelerated melting near the free surface due to the side vortices and the accelerated melting near the bottom caused by the 3D region. This elliptical configuration of the solid-liquid interface persists until the melting process ends. With an increasing liquid fraction, the velocities gradually decrease, eventually reaching a near-stagnant state at the end of melting, resulting in the formation of slow-moving, symmetric D-shaped vortices.

Significantly, the behavior observed in the simulated model closely aligns with the experimental results, confirming the calibrated model's ability to accurately predict flow patterns. This underscores the notion that relying solely on a single tuning factor does not yield optimal simulations, highlighting the necessity of considering all adjustable parameters collectively. This emphasizes the importance of conducting a systematic sensitivity study.

3.1.8 Model Validation (H2 and H3 scenarios)

In the previous section, the calibrated model was attained by applying the best combination of different tuning parameters, and the results were compared with the experiments. In this section, the calibrated model is validated by simulating higher heating conditions (H2 and H3) as specified in Table 3.4, using the same combinations of adjustable parameters. The results for H2 and H3 scenarios are also compared with available experimental data.
Figure 3.23 illustrates the average PCM temperature over the dimensionless time for all three cases (H1, H2, and H3) in contrast to corresponding experimental data. In each case, the overall average PCM temperature exhibits an initial sharp increase followed by a gradual rise, with the rate of increase being more pronounced as the applied heating intensifies, mirroring observations made in experiments.

![Figure 3-23: Comparative analysis of simulated and experimental average PCM temperature profiles across different heating conditions.](image-url)

The disparity between the experimental and numerical results becomes more pronounced under higher heating conditions, primarily due to uncertainties associated with maintaining constant boundary conditions in the laboratory tests. In fact, small temperature changes can significantly affect PCM melting behavior, especially in higher heating conditions. This sensitivity is due to potential inaccuracies in temperature measurement devices like thermocouples. Even a slight calibration error in these devices can result in significant discrepancies in the outcomes.

In order to assess velocity contours, flow patterns, and the liquid-solid interface under three distinct heating conditions, each category is examined at a specific scaled time as a representative snapshot of the entire melting process. Additionally, where applicable, these results are compared with available experimental data to validate the calibrated model.
Figure 3.24 provides a comparison of resultant velocity patterns at scaled time = 0.28 across various levels of applied heating. Within each row, the velocity scale remains consistent for H1, H2, and H3. However, there is a difference in the velocity scales between the numerical and experimental data. This adjustment is essential to ensure clarity in visualization, as the experimental velocity range encapsulates the entire process, and thus, it surpasses the numerical velocity range at shown scaled time. Also, the 3D region at the bottom of the cavity, while included in the numerical simulations, is not accounted for in the experimental results.

<table>
<thead>
<tr>
<th></th>
<th>H1</th>
<th>H2</th>
<th>H3</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \tau^+ = 0.28 )</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Figure 3-24: Comparative analysis of resultant velocity patterns at scaled time = 0.28 under varied heating conditions: refining visualization with consistent scales for the numerical results and acknowledging disparities between numerical and experimental scales, a deliberate adjustment ensuring clarity.

The primary objective of this comparison is to demonstrate that the velocity contours exhibit similar flow structures across various heating conditions, with the overall flow becoming more vigorous as the applied heating intensifies. This trend aligns with experimental findings, where an approximately 150% increase in velocity between H1 and H3 has been reported [38].
Comparing the solid-liquid interface shape at scaled time 0.40 in Figure 3.25, there is a favorable agreement between experimental and numerical simulations. It becomes evident that under higher heating conditions, there is an accelerated melting process observed in the upper regions of the cavity. This acceleration is attributed to the slightly more advanced natural convection within the side vortices as the applied heat increases. Furthermore, it is apparent that the slope of the phase interface becomes somewhat steeper with increased heating. Similarly, it is possible that the melting process across the top of the solid PCM, resulting in the formation of the near-elliptical shape, progresses more rapidly under higher heating conditions, suggesting that the stably stratified layer forms more quickly in such scenarios.

Figure 3-25: Examining solid-liquid interface configurations at scaled time 0.40: Predictions of the calibrated model versus experimental data under diverse heating conditions. The experimental data incorporates dynamic, dimensionless PCM temperature fields obtained through thermal imaging [38], serving as representations of liquid-solid interface shapes. Numerical results present simulated liquid fraction contours, both highlighting the evolution of front shapes without specific scales.

Figure 3.26 illustrates the flow patterns and convective structures across various scenarios at dimensionless time 0.65. Notably, side vortices and the 3D region at the cavity's bottom are
discernible in all cases. As heating conditions intensify, there is a tendency for the side vortices and the 3D region at the cavity's bottom to merge. Nevertheless, a consistent self-similarity persists among the different cases.

Figure 3-26: Flow patterns and convective structures at dimensionless time 0.65 across varied heating conditions. The interpretation of colors may vary across images because of the application of the localized scale. Movement towards the red end of the spectrum denotes heightened speeds, while progression towards the blue spectrum signifies diminished speeds.

The experimental findings consistently demonstrate a robust self-similarity within the melting process across different heating conditions. This self-similarity is reaffirmed when employing the calibrated model to simulate H2 and H3 scenarios.

In summary, obtained results collectively underscore the validity and reliability of the calibrated model. Its ability to accurately predict the intricate melting dynamics within the cylindrical cavity across diverse heating conditions establishes its efficacy as a dependable tool for forecasting and understanding the melting process under varying circumstances. In addition, the impressive agreement between experimental and numerical results highlights the intrinsic capability of the enthalpy-porosity method, the foundation of the calibrated model, in accurately simulating the melting process of paraffin-based PCM.

3.1.9 Quantitative Analysis

As discussed, the numerical results presented in scaled time demonstrate a strong accordance with experimental findings, confirming the effectiveness of the enthalpy porosity approach in simulating the melting process. In this section, the aggregate results are presented and
consolidated, allowing for the reconciliation of the actual quantitative disparities between computational and experimental outcomes in different scenarios.

Table 3-9 presents a comparison between the computational and experimental total melting times under varying heating conditions, encompassing both sensible and latent heat transfer. As previously elucidated, the calibrated model was derived based on the H1 scenario, resulting in minimal disparities between the numerical and experimental total melting times (R=1.03 in Table 3-9). However, as heating conditions escalate, disparities emerge and intensify (R=1.419 and R=1.52 for H2 and H3, respectively).

<table>
<thead>
<tr>
<th>Total Melting Time (s)</th>
<th>H1</th>
<th>H2</th>
<th>H3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experimental [38]</td>
<td>22741</td>
<td>10591</td>
<td>7531</td>
</tr>
<tr>
<td>Numerical</td>
<td>23437</td>
<td>15029</td>
<td>11450</td>
</tr>
<tr>
<td>R=Numerical/Experimental</td>
<td>1.03</td>
<td>1.419</td>
<td>1.52</td>
</tr>
</tbody>
</table>

The initial observation indicates that, despite using a calibrated model, the predicted melting times tend to be overestimated under higher heating conditions. This discrepancy arises because the computational simulation exhibits a prolonged melting process duration compared to the experimental observations, mainly attributable to a lower heat transfer rate during the simulation. To align the computational results with the experimental data, it is necessary to adjust the total heat transfer rate by applying a scaling factor signified as R in Table 3-9.

Figure 3-27 illustrates the normalized total heat transfer rate over scaled time for various heating conditions. The term 'normalized' denotes that the actual numerical values for the total heat transfer rate in real-time have been adjusted by the R-values from Table 3-9 in each scenario. This adjustment is necessary because the x-axis represents scaled time, and to ensure a meaningful comparison, the y-axis has been scaled by a factor of R. Given the satisfactory alignment between experimental and numerical results shown in Figure 3-27, this adjustment reaffirms that the enthalpy porosity model still effectively captures the fundamental features of the melting process, although it does so within a longer real-time framework.
Disparities in the results presented in Figure 3-27 under conditions of elevated heating can be attributed to unaccounted heat losses occurring in the experimental setup. These heat losses, which stem from heat dissipation within the experimental apparatus, are not considered in the computational simulations due to the imposition of adiabatic boundary conditions. Therefore, the omission leads to progressively higher normalized total heat transfer rates in the computational results for scenarios characterized by higher heating rates, where the impact of heat losses becomes increasingly pronounced.

An additional approach to demonstrate the efficacy of the enthalpy porosity model in capturing the primary characteristics of the melting process involves eliminating the scaled time parameter and presenting the total normalized heat transfer rate as a function of liquid fraction. Data of this nature holds practical utility, particularly in applications such as packed beds where heat transfer rate analysis within small-scale domains is significant. Such results for the H1-H3 scenarios are presented in Figure 3-28. Notably, the displayed outcomes exhibit a high degree of consistency in this context, although disparities emerge under conditions of elevated heating. These disparities can once again be attributed to unaccounted heat losses within the numerical simulations.
In summary, the findings from this section highlight the enthalpy porosity capability to represent fundamental melting process features, albeit within varying temporal contexts, thus supporting its utility in assessing the melting process.

3.2 Melting of RT26 in a Rectangular Enclosure

To further evaluate the efficacy of the enthalpy-porosity model and the calibration approach, this section delves into the influence of changing geometric parameters. The calibrated model originally developed for the melting behavior of RT26 within a cylindrical cavity, with adjustable parameters provided in Table 3.8, is applied to simulate the melting process of the same PCM within a rectangular cavity. The geometric features of the new cavity are detailed in Appendix C. The primary aim is to evaluate the suitability of the previously validated calibrated model for modeling the PCM's behavior within an altered geometry under comparable thermal conditions.

The total melting time obtained from computational simulations is compared to the experimental data in Table 3-10, revealing an overestimation of the actual melting time by approximately 18% within the simulated model. However, it is important to note that this disparity, as observed in the previous section, does not necessarily imply a fundamental
inaccuracy in the computational model's ability to predict the essential aspects of the melting process. More analysis is required, as elaborated in the following figures.

Table 3-10: Comparison of total melting time of RT26 in the rectangular cavity: computational simulation vs. experimental data.

<table>
<thead>
<tr>
<th></th>
<th>Total Melting Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experimental</td>
<td>46850</td>
</tr>
<tr>
<td>Numerical</td>
<td>55447</td>
</tr>
<tr>
<td>R=Numerical/Experimental</td>
<td>1.183</td>
</tr>
</tbody>
</table>

Figure 3-29 presents a comparative analysis of the simulated liquid fraction variations for RT26 within a rectangular cavity and the corresponding experimental data. The observed pattern closely resembles the one discussed in Figure 3-19(b) for the same PCM within a cylindrical cavity. In both cases, the melting process rate exhibits a small increase during its initial stages, followed by a sustained and relatively uniform progression throughout the majority of the melting duration, ending with a decline as the process nears completion. As shown in Figure 3-29, numerical simulation captures the same fundamental pattern as observed in the experimental results, although with a slight underestimation of the melting fraction during the intermediate stage of the process, where convection heat transfer is dominant.

Figure 3-29: Comparison of liquid fraction variations during the melting process of RT26 in a rectangular cavity: computational vs. experimental data in scaled time.
Figure 3-30 presents a comparative analysis of the solid-liquid interface development during the melting process of RT26 within a rectangular cavity, using both computational and experimental data. It is necessary to mention that the irregular, concave shapes observed in time intervals $0.19 < \tau^+ < 0.23$, particularly near the upper region, are due to the interference between thermocouples and the convective flow field in the experimental tests. Disregarding these unusual shapes, the comparison reveals close agreement with the experimental results.

A slight delay in convective heat transfer along the phase interface is evident in the numerical outcomes, resulting in a slower progression of the inclined region near the upper part during the intermediate stages of the melting process. This delay is reminiscent of what was observed in Figure 3-29. However, by the end of the melting process, the numerical simulation aligns well with the experimental data. This is attributed to the fact that, in this specific geometric configuration, as time elapses, fluid velocities decrease, and conduction becomes the dominant mode of heat transfer. Therefore, it appears that during phases of the melting process when convection prevails, the numerical simulations slightly underestimate the melting fraction, while they match well when conduction dominates. Nevertheless, this effect seems to be relatively minor. These findings indicate that applying the calibrated model for RT26, serving as an organic phase change material, in a distinct geometric configuration, yields accurate predictions of PCM behavior. This suggests that while the timeline may differ slightly, the flow pattern and melting behavior are accurately forecasted.

In summary, the findings of this chapter highlight the effectiveness of employing the calibrated melting model under varying thermal conditions and within different structural configurations for an organic phase change material. The model accurately predicts PCM behavior when considering scaled time, with disparities primarily emerging in predicting the actual melting duration. This demonstrates the model's capability to commute across different heating conditions and geometries, reinforcing the efficacy of the enthalpy-porosity approach in representing the fundamental characteristics of the melting process for an organic PCM.
Figure 3-30: Comparison of solid-liquid interface progression in RT26 melting process within a rectangular cavity: computational vs. experimental data in scaled time.
Chapter 4

4 Analysis of PCM Solidification Process in a Cylindrical Cavity

Solidification plays a central role in PCM-based latent heat thermal energy storage systems, where thermal energy is efficiently stored through phase transitions. An in-depth understanding of the solidification process is imperative for optimizing the design of these systems as the final purpose of such systems is efficient heat transfer during the discharging process.

The primary objective of this chapter is to assess whether the previously validated calibrated model, established for the melting phase in Chapter 3, can be extended to precisely represent the solidification process. To ensure the model's accuracy, a comprehensive comparison is conducted with an existing experimental dataset for the freezing process within the cylindrical cavity [38], mirroring the methodology employed in Chapter 3 to validate the model's performance during the melting process. This chapter is also concerned with evaluating the influence of different factors, such as adjustable parameters introduced in Chapter 2, on the solidification process, drawing parallels with observations made during the melting phase.

4.1 CFD Setup for Solidification Process in a Cylindrical Cavity

The primary domain for simulating the solidification process consists of a circular PCM cavity, which is identical in geometry to the one utilized in the physical experiment conducted in [38]. The parameters and settings, such as PCM material properties, final generated mesh, types of boundary conditions, convergence criteria, grid- and time- independence tests remain consistent with those outlined in Chapter 3 and are not reiterated here. The only distinction is in the initial and thermal conditions, as detailed in Table 4.1 for the solidification process. These conditions are derived from the experimental conditions employed in scenario C1 [38], specifically in the freezing process.
Table 4-1: Assigned values for initial and thermal conditions in solidification process.

<table>
<thead>
<tr>
<th>Surface</th>
<th>Thermal Condition Type</th>
<th>Assigned Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Outer Walls</td>
<td>Temperature [K]</td>
<td>291.85</td>
</tr>
<tr>
<td>Air Boundary</td>
<td>Heat Transfer Coefficient [W/ m².K]</td>
<td>8</td>
</tr>
<tr>
<td>Initial Conditions</td>
<td>Temperature [K]</td>
<td>306.05</td>
</tr>
</tbody>
</table>

As shown in Table 4.1, the numerical simulation endeavors to replicate the experimental laboratory conditions, wherein the PCM was initially in a completely melted state at a temperature surpassing its melting point. Following this, the temperature surrounding the PCM cavity's outer wall was lowered below the melting temperature through the utilization of a water jacket. Testing continued until the PCM underwent full solidification. To approximate adiabatic conditions, effective insulation of both the front and rear surfaces of the cavity was employed.

4.2 Utilizing the Calibrated Model for the Solidification Process in a Cylindrical Cavity

As previously indicated, the primary objective of this chapter is to assess the applicability of the validated calibrated model developed in Chapter 3 for the melting process to the solidification process. To address this, identical adjustable parameters, as outlined in Table 3.8, were employed to conduct simulations for the C1 scenario and then compared with experimental results.

The initial assessment emphasizes the total time required for solidification. Experimental tests showed a freezing time of around 10,900 seconds, while numerical simulation yielded a duration of 55,695 seconds. This substantial discrepancy, which is five times greater than expected, highlights the need for further investigation to uncover the underlying causes.

Figure 4.1 depicts the outcomes of solidification process in terms of average PCM temperature and liquid fraction variation. The results in Figure 4.1(a) reveal that the trend observed for the average PCM temperature closely aligns with the experimental findings. Initially, the average PCM temperature exhibited a rapid decline, followed by a sudden reduction in the rate of
temperature decrease. Then, this reduced rate gradually increased towards the end of the solidification process, although remaining lower than the initial rate.

Figure 4.1(b) presents a distinct pattern in the simulated change of liquid fraction over the scaled time. It indicates that while the temperature follows a pattern analogous to the experimental data, the PCM's solidification behavior in the simulations does not align with the observed outcomes in laboratory tests. Hence, it is essential to scrutinize the simulated flow pattern and conduct a comparative analysis with experimental data to unveil the reasons behind these disparities.

![Diagram](image)

(a) Average PCM temperature  
(b) Liquid fraction

Figure 4-1: PCM temperature and liquid fraction evolution in scaled time for calibrated model during the solidification process ($A_{mush} = 10^6 \ [kg \ m^{-3}s^{-1}], \beta = 0.0001 \ [\frac{1}{K}], \ T_s = 298 \ [K], \ \text{latent heat} = 150 \ [kJ/kg]$) vs. experimental data.

In experimental tests, the examination of velocity behavior is carried out through the utilization of PIV measurements during the initial stages of solidification when dendrite growth is limited [38]. However, as the solidification process progresses, the intricacies associated with dendrite growth pose challenges in attaining dependable velocity data. Therefore, only the initial stages are subjected to a comparison with experimental data, as illustrated in Figure 4.2.
Figure 4-2: Comparing numerical and experimental data [38]: liquid flow patterns during solidification process, applying calibrated model ($A_{mush} = 10^6 \ [kg \ m^{-3} s^{-1}], \beta = 0.0001 \ [\frac{1}{K}], T_s = 298 \ [K]$, latent heat = 150 [kJ/kg]). Numerical results employ a localized color scale to depict the complete range of motions and highlight convective structures.

Similar to Chapter 3, comparisons were conducted based on scaled time as defined by Eq. (3.1). As indicated in Figure 4.2, in the early stages of the solidification process, the simulated flow behavior aligns well with the experimental data. During this phase, the flow pattern within
the cavity consists of a single, counterclockwise rotating vortex that spans the entire height of the cavity on each side. This vortex exhibits a robust recirculation effect in the upper half of the cavity and remains relatively stagnant in the middle section of the lower half. Later, as the stably stratified layer begins to form at $\tau^+ = 0.03$, the flow gradually separates from the cavity wall. However, beyond the point represented by $\tau^+ = 0.06$, a clockwise-rotating vortex becomes apparent at the bottom of the cavity in laboratory experiments, while such a vortex is not observed in the numerical model. The difference amplifies as time progresses because, in the experimental tests, the clockwise-rotating vortex increases in height over time, ultimately leading to the presence of two vortices: a clockwise-rotating vortex along the vertical centerline, adjacent to the counterclockwise-rotating vortex on the left side. However, as evident in Figure 4.2, the formation of the second vortex in the simulated model starts from the top and occurs at a later scaled time, specifically around $\tau^+ = 0.35$, which is not depicted in the figure.

The solid-liquid interface is employed for comparing the PCM behavior throughout the remaining scaled times. Transient temperature fields, extracted from experimental data [38], are used as representatives of the front shape, compared with the simulated solid-liquid interface throughout the solidification process, as illustrated in Figure 4.3.

As depicted in the experimental results, the initial configuration of the solid-liquid interface exhibits an approximate concentric alignment with the cold circumferential wall, and uniform thermal gradients across various angular positions. Then, the interface undergoes concentric progression toward the center of the cavity until the solidification process is completed. However, the simulated PCM behavior differs considerably. It does not maintain a concentric arrangement and instead exhibits an inclination towards the upper portion of the cavity, remaining closely associated with the upper boundary throughout the entire process. This observation suggests that in the experimental tests, heat transfer predominantly occurs via conduction, whereas in the numerical model, convection exerts a more substantial influence.
Figure 4-3: Comparing solid-liquid interface during solidification process, utilizing calibrated model. Experimental data includes transient PCM temperature fields obtained through thermal imaging [38], depicting shapes of the liquid-solid interface. Numerical results display simulated contours of liquid fraction, both highlighting the progression of the front shape without specific scales.

Referring to Figures 4.1-4.3, it becomes apparent that there is a significant difference between the experimental and numerical findings when employing the calibrated model designed for the melting process in the context of the solidification process. Based on these observations, the primary source of differentiation exists in the magnitudes of the convective terms. The strength of these convection components is directly governed by the values of the mushy zone
coefficient and thermal expansion coefficient. Therefore, the initial conclusion drawn is that
the solidification process necessitates a separate combination of these coefficients, as the same
adjustable parameters utilized for the melting process do not yield accurate results for the
freezing process. Additionally, it is essential to consider the possibility of other contributing
factors to these disparities, which will be explored further in the following sections.

4.3 The Impact of Various Factors on the Simulation of
Solidification Process

The primary aim of this section is to explore the influence of various factors that can contribute
to the differences between numerical and experimental outcomes for the solidification process.

Grid and Time Step Size

As an initial step, it is essential to ensure that the results remain unaffected by variations in
grid and time step sizes by transition from melting to freezing. Therefore, a series of tests are
carried out for the solidification process, as demonstrated in Figure 4.4. It is notable that the
identical number of cells and time step size employed in the melting process can also be applied
for the freezing process. This means that the dissimilarities between numerical and experimental results are not attributable to variations in grid configurations and time step sizes.

![Graphs showing impact of grid size and time step size on liquid fraction during solidification process.](image)

**Figure 4-4:** The impact of (a) changing grid size and (b) time step size on the liquid fraction during the solidification process using the calibrated model.
A significant observation emerged when considering equal solidus and liquidus temperatures: the time independence test results failed to converge into a time step size, despite the use of extremely small $\Delta t$ as shown in Figure 4.5. This issue likely stems from the method used to calculate the liquid fraction in the enthalpy-porosity method when the solidus temperature equals the liquidus temperature. It appears that a specific error accumulates during the solidification process, and as time progresses, these errors compound. Therefore, to achieve time-independent outcomes for the solidification process, it is essential to maintain a distinction between the solidus and liquidus temperatures.

Figure 4-5: Diverged time independence test results with equal solidus and liquidus temperatures during the solidification process ($A_{mush} = 10^6 \ [kg \ m^{-3} \ s^{-1}], \beta = 0.0001 [1/K], T_s = T_l = 299 [K], \text{latent heat} = 150 [kJ/kg])

**Mushy Zone Coefficient**

To examine whether the difference between experimental and numerical results can be attributed to the mushy zone coefficient, investigations were conducted by changing the value of this parameter during the solidification process while keeping all other factors constant. The results for liquid fraction variation and front shape at specific instant are illustrated in Figures 4.6 and 4.7 (left column), respectively.
As observed, a reduction in the mushy zone coefficient yields stronger convective effects, resulting in outcomes that significantly deviate from the experimental data. However, the influence of increasing the mushy zone coefficient weakens after reaching a value of $10^7$. Beyond this point, enhancing the mushy zone coefficient does not produce substantial changes in the results, meaning that modifying this parameter cannot be used as an effective means of model calibration.
Figure 4-7: The impact of mushy zone coefficient and thermal expansion coefficient on solid-liquid interface patterns at $\tau^+ = 0.57$, during the solidification process. The values of other tuning parameters on the left column: $\beta = 0.0005 \left[ \frac{1}{K} \right]$, $T_s = 298 [K]$, latent heat $= 150 [kJ/kg]$ and on the right column: $A_{\text{mush}} = 10^5 \left[ kg \ m^{-3} \ s^{-1} \right]$, $T_s = 298 [K]$, latent heat $= 150 [kJ/kg]$. As usual, experimental data comprises transient PCM temperature fields depicting the forms of the liquid-solid interface. Numerical outcomes show simulated liquid fraction contours, both emphasizing the advancement of the front shape without designated scales.
Thermal Expansion Coefficient

Similar investigations were undertaken, this time changing thermal expansion coefficient while keeping all other parameters constant. The evolution of liquid fraction throughout the freezing process is depicted in Figure 4.8, while the solid-liquid interface at $\tau^+ = 0.57$ is displayed in Figure 4.7 (right column) and compared with experimental data.

![Graph showing liquid fraction variation during solidification process.](image)

Figure 4-8: The impact of thermal expansion coefficient on liquid fraction variation during the solidification process, considering $A_{mush} = 10^5 \ [kg \ m^{-3} s^{-1}]$, $T_s = 298 \ [K]$, latent heat = 150 [kJ/kg].

The results reveal that the application of higher values for the thermal expansion coefficient is impractical, as it significantly amplifies the convective effects. Also, adjustments to lower values do not exert a substantial impact on the ultimate outcomes. Therefore, mirroring the conclusion reached during the examination of the mushy zone coefficient, it is apparent that the thermal expansion coefficient does not serve as a suitable tuning parameter to control the PCM behavior during the solidification process.

The findings in this section revealed that various factors, including grid and time step sizes, mushy zone coefficient, and thermal expansion coefficient, had minimal impact on PCM behavior during freezing. Therefore, it is likely that another factor with a more significant influence on PCM behavior, such as supercooling, plays a crucial role. Supercooling, along
with any solid growth resulting from interface destabilization, strongly affects convective flow patterns within the geometry. Consequently, it is probable that this factor serves as the primary reason for the lack of agreement between the simulated model and experimental results, as the calibrated model does not consider the influence of supercooling. This aspect will be further explored in the following section.

4.3.1 Supercooling Impact

Supercooling, a pivotal phenomenon in the context of solidification, is characterized by the phase change material remaining in a metastable liquid state below the liquidus temperature of melting [13]. During this phase, heat exchange with the environment is purely sensible. This metastable state undergoes a transition via heterogeneous nucleation, often initiated by the appearance of a crystal on an impurity within the PCM or at the interface between the PCM and its container [13]. The temperature difference between the liquidus temperature of melting and the crystallization temperature is known as the degree of supercooling. As nucleation takes place and crystals grow, there is a rapid release of latent heat within the material, leading to a temperature rise in the PCM, a phenomenon referred to as recalescence [13]. The extent of temperature elevation during recalescence depends on the PCM's characteristics and its thermal interactions with the surrounding environment. Subsequently, the remaining liquid fraction solidifies as the PCM temperature decreases further, culminating in the complete release of the remaining latent heat content as the PCM reaches a fully solid state.

Supercooling can be attributed to two primary causes [38]. Under dynamic equilibrium conditions, molecules adhere and detach from the solid-liquid interface at an equivalent rate. However, when the interface temperature drops below the melting temperature, molecules form stronger bonds with the interface, leading to reduced detachment rates and an acceleration of the interface speed [38]. As the interface temperature decreases further, molecules may become less responsive, resulting in diminished attachment rates. This effect, which lowers the temperature of the solid-liquid interface below the melting temperature and is closely linked to the interface speed, is known as kinetic supercooling. Another factor contributing to supercooling is the presence of impurities within the solidifying material. Variations in solubility between the solid and liquid phases create concentration gradients within the liquid,
causing a reduction in the melting temperature, a phenomenon referred to as constitutional supercooling [38].

Inorganic PCMs, especially salt hydrates, commonly exhibit supercooling during cooling [13], a phenomenon now incorporated into numerical models by some researchers [72]. However, when it comes to organic PCMs, like paraffin-based materials, numerical simulations of solidification, conducted by various researchers [54, 73-74], often did not consider supercooling. Investigators in these studies typically validated their models by comparing simulated PCM temperature or liquid fraction with experimental data but overlooked the analysis of flow patterns. However, a comparison of PCM behavior during solidification with experimental findings in the current study, as discussed in section 4.2, highlights that supercooling also affects pure organic PCMs like RT26.

As reported in [38], experimental tests revealed the presence of supercooling during the freezing process of RT26. In the initial stages of solidification, dendrite growth is relatively weak (Figure 4.9a), resulting in a higher level of agreement between numerical and experimental data (Figure 4.2). However, as time progresses, dendrite growth intensifies (Figure 4.9b), leading to spontaneous dendrite nucleation within the liquid region, independent of their attachment to the solid-liquid interface (Figure 4.9c). This phenomenon leads to an increased disparity between the experimental and numerical results, as shown in Figure 4.2.

The primary reason behind this phenomenon is that, although laboratory tests maintain well-insulated conditions for the front and rear faces, there are instances of heat loss through these faces. Additionally, there are short periods during which insulation is temporarily removed to facilitate optical measurements. Although these effects have minimal influence on the phase change process [38], they appear to slightly enhance dendrite progression near the front wall during solidification. However, in the simulated model, these surfaces are considered to be entirely insulated and adiabatic.
Figure 4-9: Microscopic views of the mushy zone during (a) initial, (b) intermediate, and (c) advanced solidification stages, illustrating dendritic growth and microstructural transformation at the solid-liquid interface [38].

In summary, the calibrated model designed for the melting process is not transferrable to the solidification process. To accurately replicate PCM behavior during the freezing, it is crucial to establish distinct adjustable parameters and incorporate the effect of supercooling into the enthalpy-porosity model to have precise simulation results. This adaptation is paramount, given that supercooling has a more significant impact on solidification than tuning parameters.
Chapter 5

5 Summary and Conclusions

The utilization of phase change materials within domestic solar thermal systems for latent heat thermal energy storage presents notable advantages, including high storage capacity, spatial efficiency, and consistent performance during charging and discharging cycles. Solid-liquid PCMs, among the spectrum of PCM technologies, stand out due to their cost-effectiveness and their capability to undergo repeated phase transitions without compromising material properties. However, the complexities inherent in PCM melting and solidification processes necessitate the employment of numerical simulations, as exact solutions are predominantly confined to simplified scenarios. Among the available numerical methods, the widely accepted enthalpy-porosity method plays a pivotal role in simulating these phase transitions. To ensure precision in results, precise calibration of computational models becomes paramount, given the notable influence of various adjustable parameters, including the mushy zone coefficient, thermal expansion coefficient, solidus-liquidus temperatures, and latent heat. However, there has been a noticeable gap in the literature due to a lack of comprehensive studies investigating the collective impact of all these tuning parameters, with many studies failing to rigorously compare numerical outcomes against experimental data.

To enhance the understanding of PCM behavior, this research embarked on three primary objectives: to elucidate the enthalpy-porosity approach and introduce its adjustable parameters, to develop a calibrated model for constrained melting through conducting a systematic sensitivity study, and to scrutinize PCM solidification, while also exploring the potential for extending the calibrated model's capability to represent freezing processes.

Chapter 2 delved into the enthalpy-porosity approach. In this method, latent heat was integrated into the energy equation by assigning specific latent heat values to computational cells based on their respective temperatures. Additionally, computational cells undergoing phase transitions were treated as pseudo-porous mediums. The governing equations for mass, momentum, and energy conservation were formulated, with the Boussinesq approximation being used to consider the effects of buoyancy-driven natural convection during melting and
freezing. Additional source terms were incorporated into both momentum and energy equations, featuring parameters for control and calibration of numerical simulations. Four key tunable parameters, including thermal expansion coefficient, mushy zone coefficient, solidus and liquidus temperatures, as well as the latent heat, were introduced, elucidating their influence on the governing equations and PCM behavior. The chapter was completed by describing the numerical procedure, which employed ANSYS FLUENT 2022 R1 with a pressure-based solver, utilized the SIMPLE scheme for pressure-velocity coupling, PRESTO! scheme for pressure, the second-order upwind scheme for the energy equation, and a first-order upwind scheme for the momentum equations.

Chapter 3 focused on the development of a calibrated model for simulating the melting process of RT26, an organic phase change material, within a cylindrical cavity. The model faithfully replicated the conditions and boundary parameters of existing physical experiments. Investigating four critical tuning parameters, including mushy zone coefficient in four levels, thermal expansion coefficient in four levels, solidus-liquidus temperatures in four levels, and latent heat in two levels, unveiled essential insights: Achieving a calibrated model required considering all tuning parameters collectively, rather than individually. Also, it was found that higher mushy zone coefficients and lower thermal expansion coefficients diminished convective intensity and maintaining uniform solidus-liquidus temperatures resulted in inaccuracies due to constraints in computational cells within the mushy zone. Additionally, latent heat values, while not impacting flow patterns or material behavior, played a role in regulating the melting time.

With each tuning parameter restricted to a reasonable range, an evaluation matrix was created, featuring eight distinct combinations of adjustable parameters. In each case, numerical results were compared with experimental data across various aspects to find the best case. The optimal parameter combination was determined, resulting in a model closely aligning with experimental observations, particularly with respect to two noteworthy behaviors: the emergence of symmetric counter-rotating vortices along the cavity walls and a previously challenging-to-predict three-dimensional convection pattern at the cavity base. Further validation under higher heating conditions demonstrated self-similarity and close agreement
with experimental data, affirming the enthalpy-porosity method's inherent capability and the calibrated model's reliability in accurately simulating the melting process.

Assessing the calibrated model in different thermal conditions and within a rectangular cavity validated its capability to accurately predict the behavior of the PCM when time is scaled. The main differences primarily arose in predicting the actual melting time. This illustrates the model's ability to commute across various heating conditions and geometric configurations, supporting the effectiveness of the enthalpy-porosity approach in representing the fundamental characteristics of the melting process for organic phase change materials.

Chapter 4 involved the application of the previously validated calibrated model, designed for the melting process of RT26, to investigate its suitability for the solidification process. A comparative analysis between simulated and experimental results unveiled a significant disparity in the actual freezing time. While there was an initial agreement during the early stages of solidification, discrepancies gradually emerged and continued to diverge over time. Investigations into factors such as grid and time step size, mushy zone coefficient, and thermal expansion coefficient aimed to uncover the reasons behind these discrepancies. It was found that the same grid and time step size as employed in the melting process yielded grid and time independent results for solidification, provided dissimilar solidus and liquidus temperatures were considered. Also, altering the mushy zone coefficient or thermal expansion coefficient had relatively limited impact on PCM behavior. Notably, the absence of supercooling consideration in the enthalpy-porosity model emerged as the primary cause of differences between experimental and numerical results. Finally, it was concluded that the calibrated model, originally designed for melting, is not directly transferrable to solidification, necessitating the incorporation of distinct adjustable parameters and supercooling effects into the enthalpy-porosity model for accurate results.

5.1 Recommendations for Future Work

- **Incorporating Supercooling Effects:** To bridge the gap between experimental and numerical results during the solidification process, incorporating supercooling effects within the enthalpy-porosity model is essential. Supercooling, where a substance
remains liquid below its nominal freezing point, is common in both organic and inorganic PCMs. This adjustment captures the actual initiation temperature of solidification, improving the accuracy of solidification predictions and overall model reliability.

- **Extending Calibrated Model to Inorganic PCMs:** Extending the calibrated model approach to inorganic PCMs, like Sodium Acetate Trihydrate (SAT), broadens the model's applicability. Inorganic PCMs possess unique material properties, including higher thermal conductivity and latent heat, which have the potential to significantly enhance the efficiency of PCM-based latent heat thermal energy storage systems. Exploring this research offers valuable insights into the variations in phase change phenomena across different categories of phase change materials.

- **Leveraging Detailed Simulations for Thermal Storage Advancements:** The insights gained from these detailed simulations have the potential to directly inform the development of full-scale thermal storage systems and enhance the precision of lower-order models, including the Porous Continuum Model. Additionally, they address the need for a better understanding of heat transfer in small-scale phase change encapsulated systems.
References


behaviour,” presented at the 72nd Conference of the Italian Thermal Machines Engineering Association, pp. 517–524.


[34] W. Li, Y.-H. Wang, and C.-C. Kong, “Experimental study on melting/solidification and


Appendices
Appendix A

A. Mesh generation Approach

This section delves into the principles, methodologies, and considerations that guide the mesh generation process, specifically tailored for accurate spatial discretization of a domain mirroring the physical experiment detailed in section 3.1.1 for a cylindrical cavity.

ANSYS ICEM CFD, purpose-built for engineering applications such as computational fluid dynamics (CFD) and structural analysis, is employed in this study to provide 3D geometry, mesh generation, mesh diagnostic, and repair tools. This software stands out for its ability to maintain a symbiotic relationship with geometry throughout the mesh generation process, ensuring the mesh accurately represents the complexities of the original geometry [67].

After creating the geometry in ICEM CFD, Figure A.1 (a), the blocking feature is utilized to generate a structured mesh, offering precise control over mesh parameters such as size, growth ratio, and edge biasing. As indicated in Figure A.1 (b)-(c), this technique involves creating a blocking and fitting it into the geometry by dividing the assumed 3D domain into multiple 6-sided blocks, each of which are further partitioned into hexahedral-shaped cells. The blocking feature provides a projection-based mesh-generation environment, particularly beneficial when building a structured hexa-mesh in one or more parts.

![Geometry](d) ![Initial Block](e) ![O-Grid Technique](f)

Figure A-1: Geometry and mesh preparation in ICEM CFD.
Referring to Figure A.1 (c), an O-Grid technique is the approach used to split the initial block in cylindrical cavity, which act as topological bridges between dissimilar geometries, ensuring excellent element quality. These O-Grids facilitate seamless transitions and help maintain precision in mesh alignment with geometry. Also, Other methods such as deleting, associating, and moving edges and vertices of the blocks are employed to fine-tune the blocking structure.

After block creation, a pre-mesh is generated within the blocked regions, followed by refinement on a block-by-block basis. This pre-mesh data is then converted into structured mesh data ready for integration with other simulation data or transmission to ANSYS Fluent, which is the solver in the current study. This process ensures the creation of high-quality meshes precisely tailored to the simulation's intricacies, such as the melting process within a cylindrical cavity.

To ensure the accuracy of the discretized domain, an assessment of the mesh quality is conducted. Within ANSYS Fluent solver, the focus shifts to two crucial parameters: the minimum orthogonal quality and the maximum aspect ratio. Figure A.2 provides a visual representation of these parameters for the final generated mesh. The X-axis illustrates the quality range specific to each parameter, while the Y-axis represents the number of elements falling within each corresponding histogram bar. This evaluation aids in verifying the suitability of the mesh for simulation purposes.

For hexahedral elements, the aspect ratio is defined as the ratio between the length of the minimum element edge and the length of the maximum element edge. These values are scaled, typically ranging from 1 to 20, where an aspect ratio of 1 signifies a regular high-quality element. In general, it is advisable to avoid aspect ratios exceeding 5:1 within the bulk flow region, away from the walls [67]. As depicted in Figure A.2 (a), the final mesh exhibits a maximum aspect ratio of 4.8, well within the acceptable range, considering that this value is found in less than 500 elements of the mesh.
The second parameter used to assess mesh quality is the orthogonality of individual cells. This quality metric is determined by calculating the vectors from the centroid of each cell to its respective faces, the face area vector, and the vector from the centroid of the cell to the centroid of adjacent cells [67]. Cells with optimal orthogonality have values closer to 1, while poorly oriented cells approach a value near 0. The minimum orthogonal quality for all cell types should exceed 0.01, with a higher average value greater than 0.2 [67]. As demonstrated in Figure A.2 (b), the minimum orthogonal quality in the final produced mesh registers at a highly acceptable 0.702, affirming the high quality of the generated mesh.

**Acrylic Wall Simulation**

To simulate the acrylic wall of the cylindrical cavity efficiently, the shell conduction option available in ANSYS Fluent is used. This choice is made due to the wall's small thickness and the 3D nature of the domain. Rather than modeling and generating mesh for the wall's thickness, which would be challenging, the shell conduction approach proves highly effective. By default, ANSYS Fluent treats walls as zero-thickness surfaces with no thermal resistance to heat transfer across them. However, in cases where conduction in the planar directions of the wall is significant, the shell conduction option is employed. Shell conduction allows...
modeling one or more layers of wall cells without the need to mesh the wall thickness in a preprocessor. This approach provides the capability to easily enable or disable conjugated heat transfer on any wall. If a shell is created, ANSYS Fluent will automatically grow the specified layers of cells. The cells that expand will be either prism cells or hex cells, depending on the type of face mesh used, with no visibility of cells in the displayed mesh [67].
Appendix B

B. Air Gap Simulation

As discussed in Section 3.1.1, a small airspace is left at the upper part of the cylindrical cavity to allow for thermal expansion of the PCM. Additionally, to mimic the presence of air at the top, a convective thermal condition is applied to the air boundary within the domain. Consequently, it becomes imperative to calculate the heat transfer coefficient in various scenarios. To address this requirement, a separate simulation was conducted for the crescent-shaped region at the top, as depicted in Figure B.1.

![Unstructured mesh for the air gap on top of the cylindrical cavity.](image)

The air properties are summarized in Table B.1. Due to the presence of laminar airflow, an unstructured mesh was employed to fill the geometry, with a finer mesh resolution near the boundaries. Furthermore, the boundary conditions outlined in Tables B.2 and B.3 were applied to replicate the physical experimental conditions within the domain.

<table>
<thead>
<tr>
<th>Property</th>
<th>Typical Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specific Heat Capacity</td>
<td>1006.43</td>
<td>[J/kg K]</td>
</tr>
<tr>
<td>Thermal Conductivity</td>
<td>0.0242</td>
<td>[W/m.K]</td>
</tr>
<tr>
<td>Density</td>
<td>1.225</td>
<td>[Kg/m³]</td>
</tr>
<tr>
<td>Viscosity</td>
<td>0.000017894</td>
<td>[Kg/m.s]</td>
</tr>
</tbody>
</table>
Table B-2: An overview of boundary conditions for simulated air gap on top of the cylindrical cavity.

<table>
<thead>
<tr>
<th>Surface</th>
<th>Boundary Condition</th>
<th>Momentum Condition</th>
<th>Thermal Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Front Face</td>
<td>No Slip Condition</td>
<td>Adiabatic</td>
<td></td>
</tr>
<tr>
<td>Rear Face</td>
<td>No Slip Condition</td>
<td>Adiabatic</td>
<td></td>
</tr>
<tr>
<td>Crescent Wall</td>
<td>No Slip Condition</td>
<td>Constant Temperature</td>
<td></td>
</tr>
<tr>
<td>Bottom Face</td>
<td>No Slip Condition</td>
<td>Constant Temperature</td>
<td></td>
</tr>
</tbody>
</table>

Table B-3: Assigned values for initial and thermal conditions in simulated air gap in various scenarios of melting process.

<table>
<thead>
<tr>
<th>Surface</th>
<th>Thermal Condition Type</th>
<th>Assigned Values</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>H1</td>
</tr>
<tr>
<td>Crescent Wall</td>
<td>Temperature [K]</td>
<td>306.05</td>
</tr>
<tr>
<td>Bottom Face</td>
<td>Temperature [K]</td>
<td>292.45</td>
</tr>
</tbody>
</table>

To attain the heat transfer coefficient provided in Table 3.4, the transient problem within the air gap was solved using the SIMPLE scheme. Once steady conditions were achieved, which took 1000 seconds, an average heat transfer coefficient value was computed and employed as the convective thermal conditions within the primary domain.
Appendix C

C. Rectangular Cavity Modelling

In this section, the utilization of a rectangular cavity as an alternative geometric configuration is explored. This discussion includes an examination of the cavity's geometrical characteristics, mesh structure, material properties, and assessments of grid and time independence tests. The findings are used in the simulation discussed in section 3.2.

C.1 Geometry and Material Description

The same rectangular PCM enclosure used in the physical experiment conducted by Jevnikar and Siddiqui [36], indicated in Figure C-1, has been selected as the alternative geometry to further investigate the melting process of RT26. The internal dimensions of the PCM chamber measured 125 mm in height (H), 75 mm in width (W), and 12 mm in depth (D). The enclosure featured clear cast acrylic sheets for its front, back, bottom, and right walls, with material properties provided in Table 3-1. The front and back panels were 6 mm thick, while the bottom and right face had thicknesses of 25.4 mm and 50.8 mm, respectively. The top of the chamber remained open to accommodate the expansion of liquid PCM during the melting process.

![Figure C-1: Rectangular PCM enclosure with water flowing across the aluminum block as the heat source: insulated (right) and non-insulated configurations (left) [36].]
As shown in Figure C-1 (left column), the left wall of the enclosure was constructed from machined aluminum, with material properties defined in Table C-1. This aluminum bar served as the primary heat source for the PCM. A 38 mm square section of aluminum extended from the acrylic enclosure. Within this region, a lengthwise bore allowed hot water to flow throughout the entire height of the bar, serving as the primary heat source.

### Table C-1: Characteristics of aluminum material [67]

<table>
<thead>
<tr>
<th>Property</th>
<th>Typical Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specific Heat Capacity</td>
<td>871</td>
<td>[J/kg K]</td>
</tr>
<tr>
<td>Thermal Conductivity</td>
<td>202.4</td>
<td>[W/m.K]</td>
</tr>
<tr>
<td>Density</td>
<td>2719</td>
<td>[Kg/m³]</td>
</tr>
</tbody>
</table>

To enhance thermal insulation, the entire PCM enclosure, including the aluminum block, was enveloped with polystyrene boards (Figure C-1, right column), characterized by a thermal conductivity of approximately 0.028 [W/m·K].

### C.2 Mesh Generation

As described in section 3.1.2, the use of a structured mesh with a high degree of uniformity is essential due to the dynamic progression of the front PCM within the computational domain. Hence, the same methodology described in Appendix A is applied to create a structured mesh for the rectangular cavity. Furthermore, due to the PCM's sensitivity to the temperature of the left wall, the aluminum block has also been modeled to accurately replicate the corresponding physical conditions. The final generated mesh is shown in Figure C-2.
C.3 Boundary Conditions

As depicted in Figure C-1, the entire domain, including both the PCM enclosure and the aluminum heater, is enveloped by polystyrene boards. As described in [36], to enable optical access to the enclosed PCM during imaging, a section of the insulation was selectively removed for brief periods, revealing a semi-transparent cross-hatched area in Figure C-1. Furthermore, a 4 mm thick fiberglass sheet was introduced to this sectioned cutout to mitigate convective heat loss [36].

In efforts to replicate the well-insulated conditions of the physical experiments, adiabatic conditions for all the walls are assumed in the numerical simulations. Additionally, the bored hole inside the aluminum block is maintained at a constant temperature, mirroring the conditions in the laboratory experiments where hot water consistently flows through the aluminum block as the heat source. The summarized initial and boundary conditions for the rectangular cavity are listed in Table C-2.
Table C-2: Applied initial and boundary conditions in the rectangular cavity to simulate the melting process.

<table>
<thead>
<tr>
<th>Surface</th>
<th>Boundary Condition</th>
<th>Momentum</th>
<th>Thermal</th>
</tr>
</thead>
<tbody>
<tr>
<td>Front Panel</td>
<td>No Slip Condition</td>
<td>Adiabatic</td>
<td></td>
</tr>
<tr>
<td>Back Panel</td>
<td>No Slip Condition</td>
<td>Adiabatic</td>
<td></td>
</tr>
<tr>
<td>Right PCM Wall</td>
<td>No Slip Condition</td>
<td>Adiabatic</td>
<td></td>
</tr>
<tr>
<td>Left PCM Wall</td>
<td>No Slip Condition</td>
<td>Coupled</td>
<td></td>
</tr>
<tr>
<td>Bottom PCM Wall</td>
<td>No Slip Condition</td>
<td>Adiabatic</td>
<td></td>
</tr>
<tr>
<td>Top PCM Wall</td>
<td>No Slip Condition</td>
<td>Adiabatic</td>
<td></td>
</tr>
<tr>
<td>Aluminum Block</td>
<td>-</td>
<td>Adiabatic</td>
<td></td>
</tr>
<tr>
<td>Bored Hole</td>
<td>-</td>
<td>Constant Temperature (306.05 [K])</td>
<td></td>
</tr>
</tbody>
</table>

Initial Temperature 295.15 [K]

C.4 Grid and Time Independence Tests

Similar to the approach taken for the cylindrical cavity, an analysis of grid and time independence has also been conducted for the rectangular cavity to confirm the reliability and precision of the numerical simulations.

As demonstrated in section 4.3, it has been established that the identical number of cells and time step size can be applied for both the melting and freezing processes. Hence, the solidification process is employed for the grid and time independence tests in the rectangular cavity. This choice is based on the extended computational run time needed for each melting process simulation, lasting at least one month, whereas the freezing process can be completed in approximately one week. The insights obtained from the grid and time independence tests during solidification are then utilized in simulating the melting process.

The influence of mesh size and time step size on the variation of liquid fraction during the initial 10,000 seconds of the solidification process of RT26 within the rectangular cavity is presented in Figure C-3 (a) and (b), respectively. As illustrated, employing a medium-sized mesh with a total of 191,070 cells and a time step of 1 second is sufficient to yield grid and
time-independent results. This conclusion is supported by the observation that there is minimal disparity in the liquid fraction, even when considering finer mesh or smaller time step sizes.

Figure C-3: Grid (a) and time (b) independence analysis for liquid fraction solidification of RT26 in the rectangular cavity.
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