Investigation of Thermofluid Processes in a PCM Based Thermal Storage Module

Luca M. Crnjac, Western University

Supervisor: Straatman, Anthony G., The University of Western Ontario
Co-Supervisor: Siddiqui, Kamran., The University of Western Ontario
A thesis submitted in partial fulfillment of the requirements for the Master of Engineering Science degree in Mechanical and Materials Engineering
© Luca M. Crnjac 2023

Follow this and additional works at: https://ir.lib.uwo.ca/etd

Part of the Energy Systems Commons

 recommended Citation
https://ir.lib.uwo.ca/etd/9878

This Dissertation/Thesis is brought to you for free and open access by Scholarship@Western. It has been accepted for inclusion in Electronic Thesis and Dissertation Repository by an authorized administrator of Scholarship@Western. For more information, please contact wlsadmin@uwo.ca.
Abstract

Latent heat thermal energy storage systems can capture and store solar thermal energy, enhancing the reliability of solar energy by facilitating a continuous and consistent energy supply. However, phase change materials used in these systems suffer from low thermal conductivities making it difficult to achieve suitable charging and discharging rates. The present research investigated this issue using computational and experimental approaches to improve the design of a thermal storage module through heat transfer enhancement. Various heat transfer enhancements including a finned honeycomb structure, and metal wool were incorporated into a thermal storage module to analyze their effect on charging and discharging rates. The findings revealed that a finned aluminum honeycomb structure was the most effective in enhancing the overall module performance as it promoted natural convection within small, localized cells which was determined to be extremely effective. The results presented in this study contribute to a deeper understanding of the optimal design for thermal storage modules.

Keywords

Phase Change Material, Thermal Energy Storage, Latent Heat, Computational Fluid Dynamics, Phase Change Modeling
Summary for Lay Audience

Global energy demand is on the rise, and currently, fossil fuels are the primary source of energy accounting for the majority of the world’s energy consumption. The burning of fossil fuels causes the release of greenhouse gases which trap heat in our atmosphere and cause an increase in global temperatures. In order to reduce the reliance on fossil fuels, there needs to be an increase in the use of renewable energy resources such as solar and wind energy. However, a major issue with these renewable energy sources is they are unreliable as a consistent source of energy due to their daytime-only availability and weather dependency. Thermal energy storage is a technology that can make renewable energy sources reliable by storing energy when it’s available so it can be supplied at any time when needed.

Some thermal energy storage systems store energy by changing the phase of the storage material from a solid to a liquid. These materials are called phase change materials (PCMs). Systems that make use of PCMs are beneficial as they can store large amounts of energy in a relatively small volume as they take advantage of the energy required to change the phase of the material from a solid to a liquid and vice versa. However, the main limitation of PCMs is that they have low thermal conductivities which means that they do not absorb or release heat quickly. This makes it difficult to design an efficient thermal energy storage system using phase change materials only.

The present research work focused on improving this type of thermal energy storage system by investigating ways to move heat into and out of the system faster. In order to accomplish this, computer simulations and physical experiments were conducted. Two different methods to improve the system performance were considered, which were the use of metal wool and metal extended surfaces or fins. The results of the study showed that a metal finned structure was the better method for improving the system compared to the metal wool.
Acknowledgments

I would like to thank my supervisors Dr. Anthony Straatman, and Dr. Kamran Siddiqui for their, expertise, and support over the past few years. Your invaluable mentorship has been instrumental in this journey, and I am grateful to have had the opportunity to work with you.

I’d also like to thank all my friends and colleagues for their technical and moral support. This journey wouldn't be the same without you.

Lastly, a special thanks to my family for their continuous support and motivation throughout my academic journey. I wouldn’t have been able to do this without you.
Table of Contents

Abstract ................................................................................................................................................. ii
Summary for Lay Audience .................................................................................................................. iii
Acknowledgments ................................................................................................................................. iv
Table of Contents ................................................................................................................................. v
List of Tables .......................................................................................................................................... viii
List of Figures ......................................................................................................................................... x
Abbreviations ......................................................................................................................................... xv
Mathematical Terms ............................................................................................................................. xv
Chapter 1 ................................................................................................................................................ 1
  1 Introduction ....................................................................................................................................... 1
    1.1 Background .................................................................................................................................. 7
      1.1.1 Thermal Energy Storage ......................................................................................................... 7
      1.1.2 Phase Change Materials ......................................................................................................... 11
    1.2 Literature Review ......................................................................................................................... 13
      1.2.1 Heat Transfer Characteristics of PCMs .................................................................................... 14
      1.2.2 Heat Transfer Enhancements in PCMs ...................................................................................... 17
      1.2.3 Computational Modeling of PCMs ............................................................................................ 22
      1.2.4 Latent Heat Thermal Storage Applications ............................................................................. 23
    1.3 Motivation and Knowledge Gaps ................................................................................................. 26
    1.4 Thesis Layout ............................................................................................................................... 28
Chapter 2 ................................................................................................................................................ 29
  2 Computational Investigation ............................................................................................................ 29
    2.1 Numerical Model Calibration ....................................................................................................... 29
      2.1.1 Numerical Formulation ........................................................................................................... 29
2.2 Calibration Procedure ....................................................................................................... 32
  2.2.1 Geometry .................................................................................................................. 33
  2.2.2 Numerical Procedure ............................................................................................... 33
  2.2.3 Material Properties of Polyfin PCM ......................................................................... 34
  2.2.4 Boundary Conditions .............................................................................................. 34
  2.2.5 Grid and Timestep Independence ............................................................................. 37
  2.2.6 Model Calibration .................................................................................................... 37

2.3 Computational Study on Module Design ....................................................................... 42
  2.3.1 Module Geometry ...................................................................................................... 42
  2.3.2 Module Configurations ............................................................................................ 43
  2.3.3 Computational Geometry ......................................................................................... 45
  2.3.4 Heat Transfer Fluid Velocity Calculation ............................................................... 46
  2.3.5 Numerical Setup ...................................................................................................... 48
  2.3.6 Results ..................................................................................................................... 49
  2.3.7 Numerical Simulation on Benchtop Design ............................................................. 60

2.4 Summary ........................................................................................................................ 67

Chapter 3 ................................................................................................................................. 69

3 Experimental Investigation .................................................................................................. 69
  3.1 Experimental Setup ........................................................................................................ 69
    3.1.1 Storage Container .................................................................................................... 69
    3.1.2 Phase Change Material ........................................................................................... 71
    3.1.3 Heating and Cooling Circuits .................................................................................. 72
    3.1.4 Temperature Measurements ..................................................................................... 74
    3.1.5 Heat Transfer Enhancement Elements ................................................................. 76
    3.1.6 Experimental Tests ................................................................................................. 80
3.2 Results......................................................................................................................... 83
   3.2.1 Overview of results................................................................................................. 83
   3.2.2 Heat Transfer Rate Analysis................................................................................ 83
   3.2.3 Characterization of the underlying physical process during melting (charging) ............................................................................................................. 86
   3.2.4 PCM Thermocouple Measurement Analysis.................................................... 89
   3.2.5 Characterization of the underlying physical process during solidification (discharging) ......................................................................................................... 93
   3.2.6 Outlet HTF Temperatures in Discharging .......................................................... 96
   3.2.7 Mass Flow Rate Analysis.................................................................................. 96
   3.2.8 Comparison of Computational and Experimental Results ...................... 102
3.3 Conclusions.................................................................................................................. 112

Chapter 4......................................................................................................................... 114
4 Conclusions and Recommendations ........................................................................ 114
   4.1 General Conclusions ............................................................................................ 114
   4.2 Contributions.......................................................................................................... 116
   4.3 Future Work............................................................................................................ 117

References.................................................................................................................... 119

Curriculum Vitae ........................................................................................................... 129
List of Tables

Table 1: Thermo-physical properties of Polyfin PCM at 25°C [23], [68]. ..........................34

Table 2: Summary of the boundary conditions imposed on the rectangular geometry with reference to Figure 10. ..........................................................35

Table 3: Results of grid independence test on rectangular cavity. .................................37

Table 4: Results of timestep independence test. ........................................................37

Table 5: Module height and tube spacing for each study. ............................................46

Table 6: Inlet tube velocity for each configuration .....................................................48

Table 7: Summary of inlet and outlet boundary conditions for the 5-pass module .........49

Table 8: Comparison of the percent increase in outlet fluent temperature after 5 module passes between a non-finned case and a finned case. .................................56

Table 9: Summary of inlet and outlet boundary conditions for the computational simulation of the benchtop module.........................................................63

Table 10: Thermo-physical properties of Polyfin at 25°C [23],[68]...............................72

Table 11: Summary of start and end conditions for each test type ...............................81

Table 12: Summary of experiments performed in this study .......................................82

Table 13: Charge and discharge times at a mass flow rate of 0.2 kg/min .................83

Table 14: Comparison of charge times using a mass flow rate of 0.1 kg/min versus 0.6 kg/min for each module type. .........................................................97

Table 15: Comparison of discharge times using a mass flow rate of 0.1 kg/min versus 0.6 kg/min for each module type. .........................................................98
Table 16: Summary of the net heat transferred into the PCM for each calculation type during melting.................................................................105

Table 17: Summary of heat transferred between the HTF and PCM for each calculation type during discharging.................................................................108
List of Figures

Figure 1: Estimation of world population [3].................................................................1

Figure 2: Global energy consumption predictions [2].....................................................2

Figure 3: Human development index (HDI) and energy use per capita, 2019 [4]..........3

Figure 4: Global primary energy consumption by source [5]........................................4

Figure 5: Predictions regarding the remaining years of fossil fuel reserves made in 2015 [8]...............................................................5

Figure 6: Example of solar energy generation and energy demand in a 24-hour period....6

Figure 7: Standard heating curve for a material that can exist in two phases..............9

Figure 8: Classification of phase change materials [11]................................................12

Figure 9: Schematic of PCM enclosure used by Jevnikar and Siddiqui [22]..............33

Figure 10: Image of rectangular geometry based on experimental study of Jevnikar and Siddiqui [22] showing boundary condition imposed in ANSYS Fluent simulations. ......35

Figure 11: Temperature vs time at various heights along the hot wall for the experiments of Jevnikar and Siddiqui [22].................................................................36

Figure 12: Image showing the impact of thermal expansion coefficient on melt progression showing a thermal expansion coefficient of 0.0005 (orange) and 0.0001 (blue)..........................................................................................................................38

Figure 13: Simulated contours of liquid fraction (bottom row) at different moments in the melting process compared to the reference physical experiment [22] (top row) showing poor agreement using a Mushy Zone Constant of $10^5$..................................................40
Figure 14: Calibrated simulated contours of liquid fraction (bottom row) at different moments in the melting process compared to the reference physical experiment [23] (top row).........................................................................................................................41

Figure 15: Melt fraction vs time comparing simulation data to reference experiment data [22].................................................................................................................................................................42

Figure 16: Image of the proposed module design showing the PCM region (gray) and the tubes (blue).................................................................................................................................................................43

Figure 17: Image of three module configurations used in this study showing the PCM (gray) and the tubes (blue)...................................................................................................................................44

Figure 18: Configuration 1 geometry used in the present study showing the wax only case (left) and the finned case (right) showing the module height ‘h’ and tube spacing ‘a’. ....46

Figure 19: Plots comparing the temperature at outlet 5 versus time for each module design........................................................................................................................................................................50

Figure 20: Overall heat transfer coefficient calculated after each pass for (i) Configuration 1, (ii) Configuration 1 fins, (iii) Configuration 2, (iv) Configuration 2 fins, (v) Configuration 3, (vi) Configuration 3 fins...................................................................................................................53

Figure 21: Plots showing the predicted temperature of outlet 5 using the overall heat transfer coefficient calculated using 1 pass versus the actual temperature at outlet 5 for (i) Configuration 1, (ii) Configuration 1 fins, (iii) Configuration 2, (iv) Configuration 2 fins, (v) Configuration 3, (vi) Configuration 3 fins. ..............................................................................................55

Figure 22: Plots showing the predicted outlet temperature after n number of modules for (i) Configuration 1, (ii) Configuration 1 fins, (iii) Configuration 2, (iv) Configuration 2 fins, (v) Configuration 3, (vi) Configuration 3 fins. ..............................................................................................58

Figure 23: Example module containing finned honeycomb structure. ..........................60
Figure 24: Image showing the cross section of the small scale benchtop prototype (outlined in red) compared to the Configuration 3 geometry. .................................................................61

Figure 25: Image showing the design of the small-scale thermal storage module indicating locations of the inlets and outlets (left), and a representation of the computational domain (right). ...........................................................................................................62

Figure 26: Plots of outlet HTF temperature versus time showing for the melting case (left) and the solidification case (right)..........................................................................................................................64

Figure 27: Simulated contours of liquid fraction about Plane 1 at different moments in time for the melting test where red represents the liquid region and blue represents the solid region.................................................................65

Figure 28: a) Simulated contours of liquid fraction about Plane 1 at different moments in time for the solidification test where red represents the liquid region and blue represents the solid region, b) Initial condition temperature contour, c) location of Plane 1 ..............66

Figure 29: Experimental Module Design in dimetric view (left), and top view (right).....70

Figure 30: Module with rubber hoses connected (left), and Module with Polystyrene Insulation (right). .................................................................................................................................71

Figure 31: Complete Experimental Setup (note some images in the figure were taken from the internet for clarity) .................................................................74

Figure 32: Schematic showing locations of thermocouples in the setup. The orange dots represent the exact thermocouple locations. ............................................................................................76

Figure 33: Image of the Reference Module containing no heat transfer enhancement elements and served as the benchmark case for comparison.........................................................77

Figure 34: Image of raw aluminum honeycomb core (left), and the aluminum honeycomb core inside the PCM module with inserted tubes (right). .................................................................78
Figure 35: Image of metal wool (left), and image of the complete module with metal wool and PCM (right) ................................................................. 79

Figure 36: Image showing the packing of the wool in the module with each layer placed perpendicular to the last for a uniform packing structure .................................................. 80

Figure 37 (a) Charge and (b) discharge rates at 0.2 kg/min where “AH” represents the aluminum honeycomb module, “AW” represents the aluminum wool module, “OW” represents the only wax module, and “SW” represents the steel wool module ............... 84

Figure 38: Images showing the melting process of the wax only module at various times during the charging processes ................................................................. 88

Figure 39: Plots of temperature at TC 15 for each module during the charging experiment at a flow rate of 0.2 kg/min where “AH” represents the aluminum honeycomb module, “AW” represents the aluminum wool module, “OW” represents the only wax module, and “SW” represents the steel wool module ............................................. 90

Figure 40: Images of solid PCM at time t=0 and t=1200s of charging experiment showing voids in PCM ................................................................. 92

Figure 41: (a) Plot of TC 15 vs time during a slow discharge process followed by a charging process showing the expected temperature profile during charging. (b) Image of the PCM at the end of the discharging process showing no voids in the PCM............. 93

Figure 42: Images showing the solidification process of the wax only module at various times during the discharging process ................................................................. 95

Figure 43: Outlet temperature versus dimensionless time comparing each module during a discharging experiment at a mass flow rate of 0.2 kg/min ............................................. 96

Figure 44: Plots of heat transfer rate vs dimensionless time showing the impact of varying the mass flow rate for a particular module in charging and discharging showing i) aluminum honeycomb charging, ii) aluminum honeycomb discharging, iii) aluminum
wool charging, iv) aluminum wool discharging, v) wax only charging, vi) wax only discharging.

Figure 45: Plots of temperature rise vs time at various flow rates for the module containing i) aluminum honeycomb core, ii) aluminum wool, and iii) only wax. 

Figure 46: Plots of temperature rise vs time comparing the outlet temperature between different modules at a flow rate of i) 0.1 kg/min, and ii) 0.6 kg/min.

Figure 47: Image showing the design of the small scale thermal storage module indicating locations of the inlets and outlets (left), and a representation of the computational domain (right).

Figure 48: Comparison between computational and experimental HTF temperature at Outlet 4 of the module.

Figure 49: Comparison of simulated and experimental melt fraction contours at various dimensionless times.

Figure 50: Plot comparing the computational to experimental temperature at (a) outlet 4, and (b) all outlets.

Figure 51: Plot of corrected numerical outlet fluid temperature to the experimental outlet fluid temperature in dimensionless time.

Figure 52: Comparison of simulated and experimental melt fraction contours at various dimensionless times.
Abbreviations

AH – Aluminum Honeycomb
ASHP – Air Source Heat Pump
AW – Aluminum Wool
CFD – Computational Fluid Dynamics
COP – Coefficient of Performance
CSP – Concentrated Solar Powerplant
GHG – Greenhouse Gas
HDI – Human Development Index
HTF – Heat Transfer Fluid
OW – Only Wax
PCM – Phase Change Material
PIV – Particle Image Velocimetry
SW – Steel Wool
TC – Thermocouple
TES – Thermal Energy Storage
UN – United Nations

Mathematical Terms

$A_{mush}$ - Mushy Zone Constant [Dimensionless]
$A_s$ – Surface Area [m$^2$]
$C$ – Heat Capacity [J/kg K]
$c_p$ – Specific heat at constant pressure [J/kg K]
$\tilde{F}$ – External Body Force [N]
\( g \) – gravity \([\text{m/s}^2]\)

\( H \) – Enthalpy \([\text{J/kg}]\)

\( h_L \) – Latent heat of fusion \([\text{kJ/kg}]\)

\( h_{\text{ref}} \) – Reference enthalpy \([\text{J/kg}]\)

\( m \) – Mass \([\text{kg}]\)

\( \dot{m} \) – Mass Flow Rate \([\text{kg/s}]\)

\( p \) – Static Pressure \([\text{Pa}]\)

\( Q_L \) – Stored Latent Heat \([\text{kJ}]\)

\( Q_s \) – Stored Sensible Heat \([\text{kJ}]\)

\( S_m \) – Momentum Source Term

\( T_f \) – Final Temperature \([\text{K}]\)

\( T_i \) – Initial Temperature \([\text{K}]\)

\( T_{\text{liquidus}} \) – Liquidus Temperature \([\text{K}]\)

\( T_{\text{solidus}} \) – Solidus Temperature \([\text{K}]\)

\( T_{\infty} \) - Ambient Temperature \([\text{K}]\)

\( t \) – Time \([\text{s}]\)

\( \overline{U} \) – Overall Heat Transfer Coefficient \([\text{W/m}^2\cdot\text{K}]\)

\( \vec{v} \) – Velocity vector \([\text{m/s}]\)

\( \alpha \) – Thermal Expansion Coefficient \([1/\text{K}]\)

\( \beta \) – Liquid Fraction \([\text{dimensionless}]\)

\( \rho \) – Density \([\text{kg/m}^3]\)

\( \tau \) – Tensor Stress \([\text{Pa}]\)

\( \tau^+ \) - Dimensionless Time \([\text{Dimensionless}]\)

\( \varphi_{\text{Wool}} \) – Porosity of Wool \([\text{Dimensionless}]\)
Chapter 1

1 Introduction

Energy plays an essential role in everyday human life. People all around the world rely on energy for powering electronics and appliances, heating and cooling homes and offices, and powering vehicles to travel. The world population is on the rise and is expected to reach 8.5 billion by 2030 and increase further to 9.7 billion by 2050 as shown in Figure 1 [1]. An increase in human population means that worldwide energy consumption will also increase, and it is predicted that the world's energy consumption will grow by nearly 50% between 2018 and 2050 as seen in Figure 2 [2].

![Figure 1: Estimation of world population](image)

Figure 1: Estimation of world population [3].
The Human Development Index (HDI) is a composite measure of human well-being developed by the United Nations (UN) in 1990. It considers factors such as life expectancy, education, and per capita income, and provides a broader picture of human well-being and development beyond just economic factors. Each country is scored on a 0 to 1 scale reflecting low to high development. A plot of HDI compared to energy use per capita is displayed in Figure 3. From this figure, it is seen that there is a strong correlation between HDI and energy use per capita. Countries with low levels of human development (HDI < 0.5) use much less energy than countries with high HDI scores. The plot also shows that a nation can move from a low stage of human development, using 1 to 5 GJ per capita, to a medium stage of human development by increasing energy use to 10 GJ per capita. Furthermore, increasing energy use to 20 to 40 GJ per capita typically places the country in the high human development category [4]. Therefore, to increase the quality of life, especially in developing countries, more energy is required.
Fossil fuels, such as coal, oil, and natural gas, are the primary sources of energy and currently account for about 80% of global energy use (Figure 4). When burned for energy production and transportation, fossil fuels cause the release of harmful greenhouse gases (GHG) including carbon dioxide, methane, and nitrous oxide. These gases trap heat in the earth’s atmosphere leading to the greenhouse effect and ultimately contributing to global warming and climate change. The rapid accumulation of GHGs has led to international efforts to reduce emissions and transition to cleaner and more sustainable sources of energy.
The Paris Agreement is a legally binding treaty on climate change that was adopted by 196 parties in the United Nations (UN) [6]. The goal of the Paris Agreement is to limit the global average temperature increase to 1.5°C below pre-industrial levels. Should global average temperatures increase beyond 1.5°C, the world will face unavoidable consequences including extreme weather conditions (extreme heat in Earth’s mid-latitudes, and extreme cold in high latitudes), as well as more droughts and floods. Additionally, it will have a massive impact on biodiversity leading to an increased number of species extinctions, and loss of ecosystems. The UN stated that in order to reach this goal, GHG emissions must peak before 2025 and decline by 43% by 2030. However current trends project average temperatures to increase to 2°C by 2050 [7].

Another important consideration when thinking about our use of fossil fuels is that there is a limit to the fossil fuels on earth, and the supply of fossil fuels is finite. As stated previously, the global population is on the rise and there is a growing demand for energy. Since fossil fuels remain the primary source of energy consumption worldwide, the global reserves of fossil fuel resources are rapidly depleting and are expected to run out within decades [8]. Therefore, not only it is important to reduce our reliance on fossil fuels to protect the planet, but it is also essential to reduce our reliance on fossil fuels before they run out. Figure 5 displays the projected energy reserves for coal, gas, and oil. A careful
examination of the graph reveals that the global oil reserves are anticipated to be depleted by about 2065, with gas following suit by about 2067, and coal by approximately 2129.

Figure 5: Predictions regarding the remaining years of fossil fuel reserves made in 2015 [8].

In order to reduce the reliance on fossil fuels, and combat the effects of climate change, there is a need to shift towards using more renewable and sustainable energy resources. The main sources of renewable energy come from solar, hydro, and wind. Hydropower is the most popular renewable energy source making up about 7% of global energy consumption, whereas wind makes up 5.3%, and solar makes up 2.7% [9]. Although hydropower is currently the most popular source of renewable energy, it faces drawbacks which limit further expansion. Firstly, introducing hydroelectric power plants, such as dams, can disrupt the ecosystems in which they are built and harm the aquatic life. Secondly, there is a limit to hydroelectric energy since dams cannot be built anywhere, and most locations suitable for hydroelectric energy have already been built [10]. Therefore, solar and wind energy have become an attractive alternative to non-renewable resources. One of the main challenges with using solar and wind as energy sources is their time-of-day and weather dependency as the sun is not always shining, and the wind is not always blowing, therefore making them unreliable as a consistent energy source. In addition, when looking particularly at solar energy, there is a mismatch between energy demand and peak
solar power generation as seen in Figure 6. Peak solar generation often occurs in the middle of the day when energy demands are low. Lastly, a major issue with renewable energy resources is their intermittency since renewable resources cannot be increased or decreased to meet demand, unlike non-renewable resources which can be rapidly increased to change power output.

![Figure 6: Example of solar energy generation and energy demand in a 24-hour period.](image)

Energy storage is a technology that can improve the reliability of renewable energy resources, as well as improve the overall effectiveness of the energy generation and management system by storing energy when available. Energy storage can be used at the point of production by storing surplus energy when available, then supply it consistently when needed to meet energy demands. Additionally, energy storage can be implemented at the point of use by storing energy during times at which energy demand and cost is low. This benefits the end user as it decreases their monthly energy bill and benefits the energy grid by leveling out load use.

Thermal energy storage is the concept of accumulating and storing thermal energy by heating or cooling a storage medium so that the stored energy can be used later on for heating and cooling applications, and power generation [11]. In the Canadian residential
sector, space and water heating account for 80% of total energy use, and 50% of this energy comes from burning natural gas. This is due to the majority of homes using natural-gas based furnaces to provide heat [12]. Gas furnaces are relatively inexpensive to install and operate compared to using renewable energy sources. Additionally, natural gas is widely available in many areas and is considered a reliable source of energy due to the fact that it can be operated on demand. Modern gas furnaces are about 80% - 90% efficient making them a desirable option for homeowners.

In recent years, heat pumps have gained a lot of attraction as a more sustainable way to provide heat to homes. The major benefit to using heat pumps is the high efficiency they can provide compared to traditional furnaces. Air-source heat pumps typically have a coefficient of performance (COP) ranging from 2.0-5.4, meaning that for a heat pump with a COP of 3, it produces 3kWh of heat for every 1kWh of energy supplied to the heat pump. This is possible because heat pumps operate using a traditional refrigeration cycle and use the supplied electricity to move heat rather than generate heat. Heat pumps are beneficial as they can be used in any climate to provide heating and cooling to homes. However, heat pumps typically have higher upfront costs to install, and the time-of-use cost for electricity makes the use of heat pump during peak hours, economically unfeasible compared to traditional furnaces.

Thermal energy storage (TES) is a technology that helps to resolve both the solar energy reliability as well as heat pump time-of-use issues by storing thermal energy from the sun when available or from the heat pump during off-peak hours and then supplying it consistently as needed. The research work presented herein is performed with the goal of supporting the development of an efficient thermal energy storage system that will be used for HVAC applications to provide space and water heating to residential homes.

1.1 Background

1.1.1 Thermal Energy Storage

Solar energy is the most abundant and most suitable source of thermal energy. During the daytime, a massive amount of energy is being released towards the earth due to a nuclear
fusion reaction taking place in the sun. It is estimated that the potential of solar energy of the sun is about 85 times more than the world’s annual energy supplied [13]. However, energy supplied from solar, geothermal, and wind combined make up only 1.4% of energy consumption [13]. This implies that the sun possesses the capacity to meet the global energy requirements, yet it is presently being significantly underutilized.

Thermal energy storage (TES) is the concept of accumulating and storing thermal energy when available, so it can be used at any time when needed [11]. This is accomplished by supplying heat to a storage medium, and therefore increasing its thermal energy. This technology makes it possible to utilize solar energy at all times of the day even when the sun is not available, thus reducing the dependency on conventional non-renewable energy sources. When implemented in an energy system, TES has the potential of an increase in overall efficiency, better reliability, better economics, and less pollution to the environment [14].

Thermal energy storage can be subdivided into two categories, sensible heat storage, and latent heat storage. These two types of storage are associated with different parts of a standard heating curve for a generic material that can exist in multiple phases which can be found in Figure 7. With reference to Figure 7, the material begins as a solid, and as thermal energy is supplied, the energy content is stored as sensible heating which increases the temperature of the solid until the phase transition temperature is reached. At this point, the material is in the phase transition region where any increase in thermal energy content contributes to converting the solid into a liquid until the material has completely changed phase. The heat absorbed by the material during this process is referred to the latent heat of fusion. After this point, any further increase in thermal energy content contributes to sensible heating in which the temperature of the material increases.
Sensible heating involves storing thermal energy in a medium by changing its temperature but not its state, meaning the medium remains at a constant phase throughout the process. The amount of energy stored in the material is dependent on the heat capacity of the material, the mass of the material, and the difference between its initial and final temperature. This can be described using the following expression:

\[ Q_s = \int_{T_i}^{T_f} m \, C \, dt = m \, C \, (T_f - T_i) \]  

(1.1)

Where \( m \) is mass, \( C \) is heat capacity, \( T_f \) is final temperature, and \( T_i \) is initial temperature.

In general, materials typically used in sensible heating systems are low cost solid or liquid materials with high specific heat capacity. Materials with high specific heat capacities are able to store more thermal energy and are therefore better suited for sensible heat systems.
For commercial and residential applications where the amount of stored thermal energy is minimal, Water is one of the most commonly used materials as it is readily available, inexpensive, and has a high specific heat capacity [11]. In higher thermal energy applications where temperatures exceed 100°C, oils, molten salts, or liquid metals are used [11].

One of the main drawbacks of sensible heat storage is the rate of heat transfer into sensible heat systems is proportional to the temperature difference between the storage medium and heat source. As a result, as the temperature of the storage medium reaches the heat source, charging rates decrease due to the decrease in temperature difference [15]. In addition, sensible heat storage systems used in higher temperature applications often suffer from low efficiencies due to their tendency to lose heat to their surroundings, which also makes them unstable for long-term energy storage [16].

1.1.1.2 Latent Heat Storage

Latent heat refers to the energy released or absorbed during the melting–solidification cycle known as the latent heat of fusion. During this process, energy is released or absorbed during the change of state of a body due to the change in enthalpy associated with phase change. The amount of heat stored is dependent on the mass of the material, and its latent heat of fusion, and can be described using the following equation:

\[ Q_L = m h_L \]  

(1.2)

Where \( m \) is mass and \( h_L \) is the latent heat of fusion.

Latent heat storage is particularly attractive for thermal storage systems due to its high energy storage density. Latent heat systems have energy storage densities that are 50-100 times larger than sensible heat systems [13].

In addition, since the energy transfer occurs during phase transition, this process is nearly isothermal. This is beneficial as the temperature difference between the storage medium and heat source remains constant, which is an attractive property for energy storage systems that require a steady rate of heat transfer [15]. Also, the isothermal nature makes
it easier to prevent heat losses from the storage container leading to increased efficiencies and longer storage times [13].

1.1.2 Phase Change Materials

Materials used in latent heat energy storage systems are referred to as phase change materials (PCMs). There are four main types of phase transitions that PCMs can undergo: solid–liquid, solid–gas, liquid–gas, and solid–solid. Solid–gas and liquid–gas have higher latent heat of phase transition but are not commonly used due to the large volume change the material undergoes during phase transition. This volume change causes problems as it requires either a large storage container or a container that can withstand high pressures. Therefore, solid–liquid transition is more attractive due to its small volume change which makes it easier to use in a thermal energy storage system [14].

When choosing a phase change material, several properties must be taken into consideration. Thermal properties play a crucial role, and a suitable PCM should possess a phase transition temperature that is appropriate for its application, along with high latent heat of fusion and high thermal conductivity. Physical properties are also important, and a good PCM should have a high density, minimal volume change, and low vapor pressure. Moreover, the PCM should be chemically stable for an extended period, non-corrosive, and non-toxic to ensure safety. Finally, economic factors are essential, and an ideal PCM should be abundant, readily available, and cost-effective [14].

Phase change materials are classified into three main categories: Organic, Inorganic, and Eutectic. A classification diagram is presented in Figure 8 below.
Figure 8: Classification of phase change materials [11].

Organic PCMs are categorized as paraffin and non-paraffin compounds. Paraffin waxes consist of mostly straight chain \( n \)-alkenes \( CH_3-(CH_2)_n-CH_3 \), in which the crystallization of the \( CH_3 \) chain releases a large amount of latent heat [11]. In general, paraffin waxes are safe, reliable, predictable, inexpensive, noncorrosive, and have a wide variety of phase transition temperatures (5-80°C) [11].

Non-paraffin organic PCMs consist of materials such as fatty acids, alcohols, esters, and glycols. Non-paraffin organic PCMs are the most abundant PCMs and have a variety of material properties. In general, Non-paraffin PCMs have high latent heat of fusion, low thermal conductivity, low flash point, and instabilities at high temperatures.

Inorganic PCMs are typically used in higher temperature applications and are mainly categorized as salt hydrates and metallics. Salt hydrates can be regarded as inorganic salts and water forming a crystalline solid of the form \( AB \cdot n\text{H}_2\text{O} \). Salt hydrates have been extensively studied in recent years and have proven to be suitable materials for thermal storage applications. Salt hydrates typically have high latent heat of fusion, and relatively high thermal conductivity (about double compared to paraffins). However, salt hydrates typically suffer from incongruent melting, supercooling, and corrosion with certain metals.
Although several studies have shown that some additives can be combined with salt hydrates to prevent some of these disadvantages [17], [18], [14].

Metallic PCMs consist of low melting point metals and alloys (30 – 125°C) [11]. Metallics have not been extensively studied in research and are scarcely used in thermal storage applications due to their low heat of fusion per unit weight. However, metallics can be an attractive choice as they have high thermal conductivity which is not common in other types of PCMs.

Eutectic PCMs are a combination of two or more organic PCMs which melt and freeze simultaneously. The main benefit of this type of PCM is their properties can be customized by using different weight percentages of each PCM to optimize its properties [14]. The PCM can be engineered to have a defined melting temperature and latent heat of fusion.

In summary, thermal energy storage systems pose a viable and promising option for reducing our reliance on fossil fuels and increasing our use of renewable energy resources. In particular, latent heat thermal storage systems are an attractive option, when compared to sensible heat systems, due to their increased energy storage densities, and isothermal charging and discharging nature. In addition, while there are a variety of PCMs available which can be used in thermal storage systems, the ideal candidate for a PCM is one with a high thermal capacity, high thermal conductivity, and an appropriate phase transition temperature.

### 1.2 Literature Review

In general, PCMs are desirable for use in latent heat thermal storage applications due to their high latent heat of fusion, but they often suffer from low conductivity in all phases. This is an undesirable property of PCMs as this makes it difficult to achieve suitable charging and discharging rates in thermal storage systems. As such, in recent years, several studies have been conducted related to investigating methods of enhancing heat transfer to PCMs. To do this, it is important to understand the underlying physics of the phase change process that occurs in PCMs during melting and solidification. Therefore, the first part of the literature review focuses on heat transfer characteristics of phase change materials and
methods of enhancing heat transfer to PCMs. The second part of the literature review covers methods for modeling PCMs, and current applications of thermal storage systems.

1.2.1 Heat Transfer Characteristics of PCMs

Though both are phase changes, the melting and solidification processes are vastly different from each other. Thus, it is important to critically analyze the fundamental physics of the melting and solidification processes to optimize the design of large-scale thermal storage systems. Many studies have been conducted analyzing the melting and solidification of PCMs using simple geometric enclosures (rectangular, circular, cylindrical), to understand the heat transfer characteristics. It is also important to distinguish constrained and unconstrained melting processes. Constrained melting restricts the solid PCM from sinking or floating, whereas unconstrained melting allows the solid PCM to sink or float.

Wang et al [19] experimentally investigated the melting process of a rectangular enclosure heated from a single vertical wall. In this study, polyethylene glycol 900 (PEG900) was used as the PCM. A total of 5 experiments were conducted, each with a different wall heat flux condition, and temperature measurements, as well as visual measurements, were used to calculate convective heat transfer rates and determine the temporal position of the solid-to-liquid interface. From these tests, the authors identified three heat transfer regimes. The first is the conduction regime which occurs at the beginning of the melting process. This regime is characterized by a large Nusselt number which is attributed to minimal heat losses to the surroundings resulting in a rise of heat transfer absorbed by the PCM. The second regime is the transition regime in which conduction and convection contribute to the melting process. Lastly, as time progresses, the effect of conduction diminishes and leads to the last regime known as the convection regime in which natural convection dominates the melting process. The authors also identified a critical Rayleigh number in which the transition from the conduction regime to the convection regime occurs for each test.

Shokouhmand and Kamkari [20] found similar results in their study analyzing the melting of lauric acid in a rectangular enclosure heated from one wall. The authors identified the same three regimes as Wang et al (conduction dominant, transition from conduction to
convection, and convection dominant), but also identified a fourth regime in which convection vanishes. The authors noted that during the convection dominant regime, the intensity of the natural convection begins to decrease once the melt front contacts the opposite wall. This was proven by analyzing the Nusselt number which showed a decreasing trend indicating the weakening of the convective currents.

Tan [21] experimentally studied constrained and unconstrained melting of n-octadecane inside a spherical container that was heated from all sides. The heat transfer characteristics in constrained melting were similar to what was observed in the previously discussed study; initially dominated by conduction, followed by natural convection driving the melting process. However, in unconstrained melting the solid PCM sunk to the bottom of the container due to the expansion of the PCM on melting. It was observed that the continuous heat conduction at the lower part of the PCM accelerated the melting process compared to constrained melting.

Jevnikar and Siddiqui [22] experimentally investigated the melting process of rectangular enclosure heated from one side and filled with an organic PCM called ‘Polyfin’. The authors used particle image velocimetry (PIV) to measure the velocity fields in the liquid PCM, and used an array of thermocouples to measure thermal temperature fields. Using these techniques, detailed images of the velocity fields, temperature fields, and solid to liquid interface were created. The authors also investigated the impact of the heat source orientation at three tilt angles of the enclosure which were 0°, 8°, and 18°. The result of the study found that on average the melting rates for the 8 degree and 18 degree cases were about 6% and 13% higher that the 0 degree case respectively. The increase in inclination angle caused the buoyancy driven flow to advect upward, therefore enhancing mixing and increasing melting rates.

Tan and Chan [23] experimentally investigated the solidification process inside a sphere. The authors used n-hexane as the PCM and submerged a spherical container in a water bath to mimic a constant surface temperature boundary condition. Three different temperatures were considered in their study of the solidification process. The study found that conduction was the dominant mode of heat transfer throughout the entire process. Natural
convection was observed in the liquid region due to the cold wall and the liquid, however, it appeared to be weak and did not cause any significant impact on the solid–liquid interface.

Gau and Viskanta [24] conducted a study analyzing the melting and solidification of a rectangular enclosure cooled from one side. The PCM used in this experiment was gallium which is a metal that has a phase transition temperature of 29.76°C. During solidification experiments, the authors found that the solid – liquid interface shape was irregular and difficult to reproduce. It was speculated that this was due to anisotropy in the thermal conduction along with the crystallographic effects. The authors also noted that conduction played the dominant role in solidification.

Janghel et al [25] saw similar results in their study analyzing successive solidification and remelting of n-octadecane in a rectangular enclosure cooled from the bottom, left, and right wall. The authors noted a high heat transfer rate at the beginning of the solidification process due to natural convection taking place as a result of the temperature difference between the walls and the PCM. However, as solidification progresses, conduction becomes the dominant mode of heat transfer.

Teather and Siddiqui [26] experimentally conducted a detailed analysis of the phase change process within circular geometries. The authors captured detailed velocity and temperature data for the melting and solidification processes using PIV and an array of thermocouples. In addition, a non-invasive technique to capture temperature data was introduced which made use of a thermal camera. One key finding of this work included a characterization of the regions of flow that occur during the constrained melting process of the PCM. Two characteristic convection regions were observed which include two counter-rotating symmetric vortices which are formed at the sides of the solid PCM, and an unstable 3D flow structure which forms at the bottom of the cavity. The natural convection in these regions was found to dominate and accelerate the melting process.

In summary, the literature shows that natural convection is very important in the melting of PCM, whereas conduction is more important in the solidification process of the PCM.
1.2.2 Heat Transfer Enhancements in PCMs

As mentioned previously, one of the main drawbacks that most PCMs suffer is low thermal conductivity (~0.1 – 1 W/m K). This is undesirable and makes it difficult to achieve the necessary charging and discharging rates of thermal batteries required for residential space and water heating. In all thermal storage applications, it is necessary to have a high rate of heat transfer in and out of the system in order to meet energy demands. As such, extensive research has been conducted investigating methods of enhancing heat transfer to PCMs. Typical methods involve using fins, metal wools, highly conductive nanoparticles, and carbon fibers.

1.2.2.1 Fins

Fins are the most popular technique for enhancing the heat transfer rate in thermal energy storage systems [27]. Fins are effective as they substantially enhance the surface area of contact between the PCM and the heat source/sink thereby accelerating the melting and solidification processes. Various sizes, shapes, and arrangements of fins have been tested to investigate how they impact the heat transfer rates of thermal storage systems.

Kalbasi and Salimpour [28] numerically investigated horizontal fins for improving the performance of phase change materials in rectangular enclosures. Various parameters such as aspect ratio, number of fins, and fin length were studied to determine their effect on melting times. The authors found that for each case there is an optimum number of fins which results in the minimum melting times and adding more fins than the optimal number decreases convection inside the enclosure leading to increased melting times.

Similar results were found by Choi and Kim [29] who experimentally investigated the effects of adding horizontal fins to the outer surface of a vertical tube. The tube passed through a cylindrical vessel constructed of Pyrex glass which contained magnesium chloride hexahydrate PCM. Heat transfer fluid passed through the inner part of the tube, and horizontal fins were welded to the outer surface of the tube to increase heat transfer to the PCM. Three cases were considered consisting of an un-finned tube, a 5-finned tube, and a 10-finned tube. The authors concluded that the 5-finned tube decreased melting times
by 25% compared to the unfinned case. However, the 10-finned case showed negligible improvements when compared to the 5-finned case.

Boulaktout et al [30] numerically investigated the thermal behavior of a horizontal annular container consisting of longitudinal fins. Heat transfer fluid flowed through the center of the cylinder, and n-eicosane PCM filled the annular space. Three geometries were analyzed. Geometry 1 consisted of no fins, geometry 2 had two fins aligned horizontally, and geometry 3 consisted of two fins aligned vertically. The study concluded that both fin geometries melted quicker than the case without fins. However, the vertical alignment of the fins melted 2.5 times faster than the horizontally aligned fins. This shows that vertical fins promote natural convection and therefore accelerate melting, whereas horizontal fins dampen natural convection thereby increasing melting time.

Shademan and Nezhad [31] numerically investigated the melting process in vertical finned tubes and shell containers. Water was used as the heat transfer fluid (HTF) which flowed through the center of the cylinder. An organic paraffin PCM (RT50) filled the annular region of the container. The authors analyzed the impact of adding 4, 8, 16, and 32 fins into the container. The study concluded that the charging time decreased by 73% when the number of fins was increased from 0 to 32.

Jmal and Baccar [32] numerically studied PCM solidification in a horizontal finned tube thermal storage. In this study, a PCM-air heat exchanger was studied containing three coaxial cylinders. The inner and outer cylinder contained air which was used as the heat transfer fluid. Air was passed vertically upwards through the inner cylinder, then redirected downwards through the outer cylinder. The middle cylinder contained a paraffin PCM, and aluminum fins extending inside the inner cylinder were used to enhance the heat transfer rate between the air and the PCM. Four configurations were analyzed, Case 1 consisted of no fins, and Case 2 through 4 consisted of three, five, and nine fins respectively. The study found that although natural convection is not the dominant mode of heat transfer in the solidification of PCMs, it should be taken into consideration when conducting numerical models as there was a significant difference in exit air temperature (~3 degrees) between cases considering and not considering natural convection. The study found that including
fins led to a maximum of 20% reduction in discharging times when compared to the no-fin case. However, the study also showed that there was an insignificant improvement in the heat transfer rate between the 5 fin and 9 fin case indicating that there exists a critical number of fins in which the maximum heat transfer rate occurs.

A similar study was conducted by Nóbrega et al. [33] who investigated the effects of adding vertical fins longitudinally along tubes and observed how it impacts the solidification of the PCM. A numerical and experimental approach was used in which an experimental study on one fin case was run and used to validate the numerical model. The numerical model was then used to conduct the parametric study on the number of fins. This study used water as the PCM for cold storage applications. The authors concluded that increasing the number of fins and the fin width led to a reduction in solidification times.

### 1.2.2.2 Metal Wools

Another method of increasing heat transfer to PCMs involves using porous media or metal wools. Using metal wools has not been studied as extensively as fins. However, metal wools are an economical and easy to implement alternative that warrants consideration.

Prieto et al. [34] experimentally and numerically investigated the influence of using stainless steel wool to increase the effective conductivity of pure sodium nitrate PCM. This PCM is an inorganic material used in high temperature applications having a melting temperature of 307°C. A large rectangular enclosure was constructed with a 24mm diameter steel tube fixed in the center. Metal wool was packed into the enclosure resulting in a porosity of 90%. The result of the study found that the use of metal wool increased the effective thermal conductivity of the PCM by 300%. The study also found that when compared to using a finned structure of equal volume, the use of steel wool has significantly improved heat transfer characteristics.

Gasia et al. [35] conducted a similar study experimentally comparing the use of fins to metal wool as a heat transfer enhancement technique in a latent heat thermal energy storage system. A multi-pass shell and tube heat exchanger was filled with n-octadecane as the PCM. Four configurations were analyzed which included a reference case with no
enhancements, a case that included aluminum fins, a case evenly packed with steel wool throughout the enclosure, and a case with steel wool compacted in fin shapes. The study found that using fins was the most effective method of increasing heat transfer rates and achieved a maximum increase of 51.1% compared to the reference case. The metal wool was found to increase the heat transfer rate in charging by about 14% and showed negligible improvements in discharging. Overall, this study found that the metal wool cannot compete with the aluminum fins. However, it should be noted that the material used for the metal wool was a low-grade carbon steel which has a conductivity about 4 times less than that of the aluminum fins. This decrease in conductivity could be one of the reasons for the decreased performance.

One of the first studies conducted on increasing heat transfer to phase change materials was conducted by Bentilla et al. in 1966 [36]. Part of their study investigated using a variety of materials as heat transfer enhancements in the PCM. This included using aluminum fins, aluminum wool, aluminum foam, copper foam, and aluminum honeycomb. The study analyzed various porosities of aluminum wool including 10% wool and 18% wool. The study found that regardless of the porosity, marginal improvements were seen when comparing aluminum wool to the reference case in both charging and discharging. This marginal improvement was likely due to the long heat path in the wool, and the thermal contact resistance between the fibers. The result of the study found that using an aluminum honeycomb was the most effective method of increasing heat transfer to the PCM in both charging and discharging since it provided a larger heat transfer surface area compared to the metal wools and foam.

1.2.2.3 Nanoparticles

The use of highly conductive nanoparticles is another commonly investigated method for increasing the effective thermal conductivity of PCMs. The use of nanoparticles offers advantages over using methods such as fins or metal wools. Firstly, while most techniques employed to improve the thermal conductivity of PCMs increase the system's weight and volume, the utilization of nanoparticles does not [37]. Secondly, most heat transfer enhancement techniques often dampen or block natural convection in the system, however, while the addition of nanoparticles increases the dynamic viscosity of the PCM, the strong
natural convective currents are not affected or restricted [38]. Lastly, engineering various types of nanoparticles has become less expensive due to recent advancements in nanotechnology [39].

Nitsas and Koronaki [40] experimentally investigated heat transfer improvements when adding two types of nanoparticles to an organic paraffin wax called RT50 [41]. The authors investigated the use of copper nanoparticles, as well as aluminum oxide nanoparticles, and analyzed how they impacted melting and solidification times. Notably, both nanoparticles were effective at reducing melting times, however, the use of copper nanoparticles was found to be the most effective reducing the thermal charge duration by 25.3%, compared to aluminum oxide which reduces the duration by 10.8%.

Bashar and Siddiqui [42] experimentally investigated the transient melting and heat transfer behavior of nanoparticle-PCM mixtures in a rectangular enclosure. Four different types of nanoparticles were considered: silver, copper oxide, aluminum oxide, and multi-walled carbon nanotubes. The PCM used was a commercially available paraffin wax called Polyfin. A dispersant was added to the PCM-nanoparticle mixture to reduce particle settlement and improve particle dispersion in the PCM. The result of the study showed improved thermal performance in all cases including nanoparticles. The authors also noted that the dispersant counteracted the viscosity rise due to the nanoparticles and saw no significant reduction of natural convection in the presence of nanoparticles. The study concluded that the best thermal performance was found when using copper oxide nanoparticles achieving a melting rate and heat flux about 25% higher than that of plain PCM.

1.2.2.4 Carbon Fiber

Other methods of improving heat transfer to PCMs include using carbon fiber for enhanced thermal conductivity. Carbon fiber offers some benefits over metallic alternatives including high thermal conductivity (175 – 200 W/m.K). In addition, many inorganic PCMs have compatibility issues with metals, often causing corrosion. Carbon fibers are strongly resistant to corrosion making them a viable option for use with inorganic materials.
Fruteri et al [43] experimentally investigated the use of randomly distributed carbon fibers in PCM to observe its impact on thermal conductivity. An inorganic salt hydrate called PCM44 was used as the PCM and formed into brick shapes. Three different fiber lengths were used: microfibers (0.2mm length), fibers 3mm in length, and fibers 6mm in length, and their thermal conductivity was measured. The result of the study found that the use of microfibers was the most effective in increasing thermal conductivity. The authors also noted that the system containing microfibers remained homogeneous throughout multiple charging and discharging cycles.

1.2.3 Computational Modeling of PCMs

In recent years, many algorithms and methods have been developed for conducting melting and solidification problems, and the most popular software’s used to conduct computational fluid dynamics (CFD) studies include COMSOL, MATLAB, and ANSYS Fluent [44].

COMSOL is a commercial CFD software which employs the apparent heat capacity method for solving melting and solidification problems. This method effectively captures the phase change interphase by addressing it implicitly. This is accomplished by solving the heat transfer equation with effective material properties for both phases. The latent heat capacity is taken into account by modifying the materials heat capacity [45]. COMSOL has been used by many researchers in recent years to study both 2D and 3D phase change studies in a variety of geometries [46], [47], [48], [49], [50], [51].

Some studies analyze solidification and melting problems by developing numerical solvers in MATLAB. For example, in 2015, Raj et al [52] developed a numerical model based on the enthalpy method in order to investigate the performance of cylindrical PCM storage system. The model was validated using experimental results which showed good agreement.

ANSYS Fluent is the most popular method for numerically analyzing melting and solidification problems [44]. ANSYS Fluent utilizes the enthalpy-porosity method which is a method in which the solid-liquid interface is not explicitly tracked, but rather the mushy
zone is treated as a “pseudo” porous medium. Many studies have been conducted using this method and show good agreement with experimental results [53], [54], [55], [56], [57], [58], [59]. ANSYS Fluent was used in the present research work, and a more detailed explanation of the enthalpy-porosity model is presented in Section 2.1.1.

1.2.4 Latent Heat Thermal Storage Applications

Many studies have been conducted investigating the practical application of using PCMs in latent heat thermal storage systems. Extensive reviews have been conducted analyzing current systems that implement latent heat thermal storage [13], [14], [16], [60]. These reviews generally divide thermal storage systems into two categories. High temperature thermal storage, which is often used at a grid scale in electrical generation, and low temperature applications, which are often used in residential applications.

Concentrated solar power plants (CSP) are a method of generating electricity using sunlight and a large array of mirrors. In these plants, sunlight is reflected off the mirrors and concentrated onto a specific point to heat a working fluid and create steam which drives a steam turbine to generate electricity. To generate electricity at all times of the day, even when the sun is not shining, thermal storage is used to store the energy when available to provide a consistent supply of energy on demand when needed.

A study was conducted by Denholm and Mehos [61] who investigated the benefits of load shifting using CSP with thermal storage. The authors noted there are two main benefits to implementing CSP / TES plants. Firstly, thermal storage allows for the efficient shift in solar resources from peak solar outputs when energy demand is low, to reduced solar output periods when energy demand is high, thereby increasing the use of solar resources. Secondly, given the large thermal capacity of CSP / TES systems, they have the potential to replace conventional coal power plants and provide a more sustainable electrical generation mix.

PCMs are also used in building applications and are classified as either passive or active systems. Passive systems collect, store, and supply thermal energy naturally whereas active systems rely on fans and pumps to supply heat.
Many studies have been conducted investigating the use of PCM in building materials to help passively maintain the desired temperature of a room thus improving the room's thermal performance. This is commonly accomplished by carefully selecting materials with a high heat capacity as building materials which will by nature passively store and release thermal energy to maintain a comfortable room temperature. Common materials used in the past include concrete and brick, however, recent studies have been conducted that use PCMs in the walls of buildings due to their increased heat capacities. In fact, a study conducted during the summer in Germany found that incorporating PCMs into the walls of building structures can save the user up to 30% in energy costs [62].

Active residential systems use pumps to circulate a heat transfer fluid during the charging and discharging processes [13]. These systems are typically used as a sustainable alternative to providing space and water heating in domestic applications over traditional natural gas furnaces.

Lu et al [63] conducted a performance study on a novel latent heat thermal storage for use with an air source heat pump (ASHP). The thermal storage design consisted of a rectangular multi-pass shell and tube enclosure filled with a composite PCM with a melting temperature of 45.26°C. A numerical approach was used to conduct a parametric study on the design investigating parameters such as pipe diameter, tube pitch, and fin arrangement. The optimal design was built and experimentally tested using an ASHP as the heat source. The results of the ASHP coupled with thermal storage were compared to a control case consisting solely of the ASHP to investigate the benefits of incorporating thermal storage into the system. The result of the study found that the ASHP coupled with thermal storage reached a 89.7% effective heat storage efficiency and a 92.5% heat release efficiency. The study also concluded that the annual operation costs of the combined system save 32.9% compared to using an ASHP on its own.

A similar study conducted by Zou et al [64] investigated the performance of an ASHP coupled with a PCM water storage tank. This proposed system has increased benefits over a traditional system as the water tank is enclosed in a steel casing with PCM filled in the annular cavity between the water tank and casing. A condenser coil is wrapped around the
outside of the water tank which is in contact with the PCM. Fins are also welded to the outer wall of the water tank for increased heat transfer. Charging and discharging experiments found that heat storage was increased by 14% over a traditional water storage tank, and the discharge efficiency of the PCM reached 83.9%.

Another interesting group of proposed thermal storage systems make use of cascading PCMs with different melting temperatures in order to maintain a more constant heat flux [16]. This is because the PCMs are typically arranged in order of decreasing melting temperatures, and a nearly constant temperature difference between the HTF and PCM melting temperature can be achieved even though the HTF temperature decreases in the flow direction [65].

Mao and Chen [66] numerically investigated the design of a single tank. The cylindrical tank had a HTF tube placed in the center, and two cascade geometries were analyzed. The first design featured a radial cascade arrangement in which the PCM varied radially away from the HTF tube. The second design featured an axial cascade arrangement in which the PCM varied axially along the tube. When analyzing the discharging process, both cascade arrangements resulted in a higher total energy release capacity when compared to a single PCM system. However, when comparing the arrangements to each other, the radial design was the favored system as it decreased discharge times by 2.09% compared to the axial design which decreased discharge time by 1.89%.

Elbahjaoui and Hanchi [67] numerically investigated the design of a solar domestic water heating system incorporation a cascading PCM thermal storage tank. The three PCMs used in the study are RT44HC, RT 54HC and RT62HC which are all organic paraffin PCMs with melting temperatures of 43°C, 54°C, and 63°C respectively. A performance study was conducted on the proposed design over a 9 hour charging period for a typical summer day in Morrocco. The study determined that the optimal design had an increased collection efficiency of 3.47% when compared to a single PCM tank. This increased efficiency led to higher heat transfer rates throughout the day.
1.3 Motivation and Knowledge Gaps

In efforts to reduce global carbon emissions, and limit dependency on fossil fuels for energy, many research efforts have been conducted investigating latent heat thermal energy storage systems. Considering the large-scale use of natural gas in residential applications in Canada, there is an urgency to switch to an alternate heating option. A TES system is a crucial component to make intermittent solar energy a reliable alternative and to make heat pumps an economically feasible option. Although there has been significant research conducted on improving heat transfer to PCMs and PCM-based TES systems, very few commercially available products exist and are implemented in the energy grid. In addition, current and proposed systems are not modular which limits their storage capacity and functionality. Thermal storage systems could benefit from a modular design as it would be easy to scale up or down the system based on energy demands. In addition, a modular design allows for a cascading PCM system which has shown to increase efficiency.

The literature review has shown that extensive research has been conducted on using fins to increase heat transfer rates into PCMs, However, most studies only study the use of a few fins, and there is a lack of research conducted on finned structures such as a honeycomb core. These finned structures would provide a much larger surface area of contact between the PCM and fins, however, would impede natural convection which could negatively impact module performance.

In addition, using metal wool as a heat transfer method is less expensive and easier to implement than using fins, but not much research has been done analyzing the effectiveness of different types of metal wools. The use of metal wool could increase the effective thermal conductivity of the PCM, similar to that of highly conductive nanoparticles, but would not have issues with particle settlement. In addition, there is a lack of research directly comparing the use of fins and metal wools to each other (i.e., same quantity, and same material).

The present research aims to address some of these knowledge gaps by investigating a modular thermal energy storage system both computationally and experimentally. Various heat transfer enhancements to increase heat transfer rates to PCMs are considered including
the use of a finned aluminum honeycomb core as well as aluminum and stainless steel wool.

The objectives of this thesis are as follows.

- Develop and calibrate a numerical model, conduct a parametric study, and create a design for a small-scale benchtop thermal storage module.

- Experimentally investigate and compare the impact of various heat enhancement techniques on the heat transfer rates of a small-scale benchtop module.

Computational simulations will be conducted using ANSYS Fluent. Experimental studies will be conducted to analyze the thermal behavior of the module concepts using high-resolution thermocouple temperature measurements.
1.4 Thesis Layout

Chapter 1 provides comprehensive information regarding the current issues surrounding global warming and the use of fossil fuels. The concept of thermal energy storage was introduced, and details were provided regarding how thermal energy storage can be used to increase the reliability and consistency of renewable energy resources. The literature review provided information surrounding the current state of knowledge of increasing heat transfer rates to PCMs, as well as some current and proposed systems making use of PCMs and thermal energy storage.

Chapter 2 contains a numerical study of various thermal storage module concepts. This begins with a description of the numerical model and governing equations, and a calibration of the numerical model. The calibrated numerical model was then used to study three performances of three thermal storage module concepts, each with and without the use of fins. The results of this study were used to design a small-scale thermal storage module for benchtop testing.

Chapter 3 presents the experimental investigation on the performance of using various heat transfer enhancement techniques in a small scale thermal storage module. This includes a detailed explanation of the experimental setup, as well as a detailed comparison of the various tested methods.

Chapter 4 Summarizes the results and findings from this research work and provides recommendations for future work.
Chapter 2

2 Computational Investigation

The goal of this chapter is to present the results of a numerical investigation of a thermal storage module. ANSYS Fluent [68] was used to conduct melting and solidification simulations to analyze the transient performance of the thermal storage modules. The first part of this chapter presents the numerical formulation including a description of the governing equations used to conduct melting and solidification simulations using the enthalpy-porosity method. Calibration of the numerical model was performed by numerically replicating the results of a physical experiment that had been conducted. The second part of this chapter uses the calibrated numerical model to analyze the design and performance of a multi-pass thermal storage module.

2.1 Numerical Model Calibration

This section presents the governing equations solved by ANSYS Fluent when conducting melting and solidification simulations. The numerical setup, geometry, boundary conditions, and grid and timestep independence tests are then presented. This section concludes with a description of the calibrated numerical model that is used in Section 2.3.

2.1.1 Numerical Formulation

The flow during the melting and solidification of PCMs is characterized as laminar, incompressible, and Newtonian [14]. The governing equations that need to be solved for melting and solidification problems include the conservation of mass, conservation of momentum, and conservation of energy.

Conservation of Mass

The mass equation is expressed as: [69]

$$\frac{d\rho}{dt} + \nabla \cdot (\rho \vec{v}) = 0$$

(2.1)

where $\rho$ is the density, $t$ is time, and $\vec{v}$ is the velocity vector.
Conservation of Momentum

The momentum equation is expressed as:[69]

\[
\frac{d}{dt}(\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot \tau + \rho \vec{g} + \vec{F} + S_m
\]  

(2.2)

where \( p \) is the static pressure, \( \tau \) is the tensor stress, and \( \rho \vec{g} \) and \( \vec{F} \) are the gravitational body force and external body forces, respectively. \( S_m \) represents a source term that characterizes the momentum damping due to the mushy zone region between the solid and fluid phases during the melt.

Melting and Solidification Model

Melting and solidification problems deal with the change of state of materials and are classified as moving boundary problems. In these problems, the position of the solid and liquid interface constantly changes with time, and it is critical to accurately track this interface. The simulations were conducted herein using ANSYS Fluent which utilizes an enthalpy–porosity formulation that eliminates the need to track the liquid–solid interface explicitly. Rather, each cell is characterized by a liquid fraction which is calculated using an enthalpy balance. The enthalpy is computed as the sum of the sensible enthalpy \( h \) and the latent heat \( \Delta H \): [69]

\[
H = h + \Delta H
\]  

(2.3)

where,

\[
h = h_{ref} + \int_{T_{ref}}^{T} c_p dT
\]  

(2.4)

where \( h_{ref} \) is the reference enthalpy, \( T_{ref} \) is the reference temperature, and \( c_p \) is the specific heat at constant pressure.

The liquid fraction \( \beta \) is defined as: [69]

\[
\beta = 0 \; \text{for} \; T < T_{solidus}
\]  

(2.5)
\[ \beta = 1 \quad \text{for } T > T_{\text{liquidus}} \]  
\[ \beta = \frac{T - T_{\text{solidus}}}{T_{\text{liquidus}} - T_{\text{solidus}}} \quad \text{for } T_{\text{solidus}} < T < T_{\text{liquidus}} \]  

Regions where the liquid fraction is between 0 and 1 are referred to as “mushy regions” or mushy zones. These regions arise in cells where phase change is occurring, and a cell contains both liquid and solid phases due to the transfer of latent heat within the material. Throughout the phase change process, the material remains at its phase transition temperature, as any heat entering or leaving the system is utilized solely for the change in state rather than affecting the temperature. Using the liquid fraction, the latent heat content is calculated using the following equation: [69]

\[ \Delta H = \beta L \]  

where \( \Delta H \) represents the latent heat content, and \( L \) represents the latent heat of the material.

Within the enthalpy-porosity approach, the mushy region is also treated as a porous region that acts as a momentum sink wherein the porosity in each cell is equal to the liquid fraction calculated for that cell. In fully solidified regions where the liquid fraction equals 0, all velocities are set to zero. In a physical scenario, this momentum sink occurs when liquid comes into contact with the solid-liquid interface and slows down. The source term in the momentum equation due to the momentum sink takes the following form: [69]

\[ S_m = \frac{(1-\beta)^2}{(\beta^3+\epsilon)} A_{\text{mush}} (\mathbf{\bar{v}} - \mathbf{\bar{v}}_p) \]  

where \( \beta \) is the liquid fraction, \( \epsilon \) is a small number (0.001) used to prevent division by zero, \( A_{\text{mush}} \) is the mushy zone constant, and \( \mathbf{\bar{v}}_p \) is the pull velocity vector.

The mushy zone constant is a parameter that characterizes the magnitude of the damping of the velocities. Typical values range from \( 10^4 \) to \( 10^8 \) [70], and the larger the number, the more quickly the velocities are forced to zero as the material solidifies. The mushy zone constant is a case-specific property that has a large influence on the solid-liquid interface profile throughout the melt, as well as the intensity of the natural convection within the
PCM. This constant is not typically listed in literature and is, therefore, important to calibrate using experimental data.

**Buoyancy Modeling**

The Boussinesq approximation was used in this study to account for the influence of density variations in the buoyancy terms. This allows for density to be treated as a constant everywhere except in the momentum equation. By neglecting the density variations in all equations except the buoyancy term, the Boussinesq approximation greatly simplifies the governing equations. When the Boussinesq approximation is applied, buoyancy is modeled using a thermal expansion coefficient, which is a material property that quantifies the change in volume of a material with respect to temperature variations. The Boussinesq approximation is represented as: [69]

\[
(\rho - \rho_0) g \approx \rho_0 \alpha (T - T_0) g
\]

where \( \rho_0 \) is the constant density, \( T_0 \) is the operating temperature, and \( \alpha \) is the thermal expansion coefficient. Similar to the Mushy Zone constant, the thermal expansion coefficient is typically not published in literature or listed on material data sheets, and, therefore, is another parameter that needs to be calibrated using experimental data. By the calibration approach described below, the coefficient is considered not just as thermal expansion coefficient but rather as a coefficient that characterizes the aggregate effect of all properties changing through the melting process to yield the correct intensity of convection.

### 2.2 Calibration Procedure

To accurately simulate charging and discharging on the prototype module, the numerical model first needed to be calibrated; more specifically, the mushy zone constant and thermal expansion coefficient. The experimental study conducted by Jevnikar and Siddiqui [22], which considers a simple rectangular geometric model, was utilized for calibration. An iterative approach was taken in which the thermal expansion coefficient and mushy zone constant were varied, and the results were compared to those presented by Jevnikar and Siddiqui [22] until similar results were obtained.
2.2.1 Geometry

A schematic of the experiment conducted by Siddiqui and Jevnikar is shown in Figure 9. In this study, a thin rectangular acrylic enclosure was filled with Polyfin PCM to investigate two-dimensional melting. A heating circuit was used which passed water at 80°C through a machined aluminum manifold. One side of the aluminum manifold was in direct contact with the PCM and acted as the heat source. The top of the chamber was left open to the atmosphere to allow for expansion of the liquid PCM during melting. The entire enclosure was insulated using polystyrene sheets (k=0.028 [W/m K]) to minimize heat losses.

![Figure 9: Schematic of PCM enclosure used by Jevnikar and Siddiqui [22].](image)

2.2.2 Numerical Procedure

The pressure-based solver in ANSYS Fluent was used as this must be enabled when conducting melting and solidification simulations. Transient calculations were conducted to study the melting and solidification process of the PCM. Gravity was enabled to allow for buoyancy driven natural convection to occur in the PCM. The SIMPLE algorithm was used for pressure–velocity coupling. The PRESTO! algorithm was used for the pressure discretization as it is recommended for natural convection. Higher order schemes were
used wherever possible except for the momentum discretization as higher order schemes caused instabilities and inaccurate results.

2.2.3 Material Properties of Polyfin PCM

The phase change material used in this experiment was Polyfin. Polyfin is an organic PCM containing a mixture of paraffin wax and copolymer alloys. The material properties of Polyfin are listed in Table 1.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting temp [°C]</td>
<td>55</td>
</tr>
<tr>
<td>Density [kg/m³]</td>
<td>920</td>
</tr>
<tr>
<td>Specific Heat [kJ/kg K]</td>
<td>2.89</td>
</tr>
<tr>
<td>Thermal Conductivity [W/m K]</td>
<td>0.18</td>
</tr>
<tr>
<td>Dynamic Viscosity [kg/m s]</td>
<td>0.00506</td>
</tr>
<tr>
<td>Latent Heat of Fusion [kJ/kg]</td>
<td>180</td>
</tr>
</tbody>
</table>

The initial value for the mushy zone constant was selected to be $10^5$, as this is the default value used in ANSYS Fluent. The thermal expansion coefficient for Polyfin was not listed on the material data sheet, or found in literature, and therefore an initial value of 0.0007 was used as it falls within the range of typical thermal expansion coefficients for paraffin waxes, which range from 0.00011 to 0.0008 based on available literature [22], [39], [71].

2.2.4 Boundary Conditions

The boundary conditions for the domain are described in Table 2 and Figure 10.
Table 2: Summary of the boundary conditions imposed on the rectangular geometry with reference to Figure 10.

<table>
<thead>
<tr>
<th>Location and Type</th>
<th>Boundary Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hot Wall</td>
<td>- Constant temperature condition described by a polynomial (Equation 2.11)</td>
</tr>
</tbody>
</table>
| Free Slip Wall    | - Convective thermal condition  
|                   | - Zero shear, free slip wall condition |
| No Slip Wall      | - Convective thermal condition  
|                   | - No slip condition |
| Symmetry Wall     | - symmetry |

Figure 10: Image of rectangular geometry based on experimental study of Jevnikar and Siddiqui [22] showing boundary condition imposed in ANSYS Fluent simulations.
A constant temperature thermal condition was used at the hot wall. In the experiment, thermocouples were fixed to the hot wall at various heights, and when analyzing the data, it was observed that the wall temperature varied with height. Figure 11 shows the temperature data for all the thermocouples measuring the wall's temperature. When looking at the data, it is seen that from \( t > 2000 \)s to the end of the experiment, the temperatures remained relatively constant at all heights. Therefore, the average temperature at each height between \( t=2000 \)s and \( t=43000 \)s was used to define a polynomial for temperature as a function of the height of the hot wall. The polynomial takes the form:

\[
T = 9523.1y^3 + 2299.2y^2 + 200.73y + 344.12
\]

(2.11)

where \( T \) is the temperature of the wall in units of kelvin and \( y \) represents the vertical location of the wall relative to the lower left corner in units of meters.

For the free slip wall and no slip wall boundary conditions, a small convective loss was needed since the acrylic container in the physical experiment was not perfectly insulated, and therefore a convective thermal condition was used with a heat transfer coefficient, \( h \), set to 2 [W/m K].

Figure 11: Temperature vs time at various heights along the hot wall for the experiments of Jevnikar and Siddiqui [22].
2.2.5 Grid and Timestep Independence

When conducting CFD studies, it is important to ensure that the results are independent of mesh size and timestep size. In the present study, the ANSYS Meshing tool was used to create the meshes. An initial mesh of 181500 elements was used with a timestep of 1s. The domain was initialized at a temperature of 293.15K and the simulation was run until the liquid melt fraction exceeded 90%. The mesh was refined to 366860 elements keeping the timestep at 1s which produced a percent difference of 0.58% for the time to achieve 90% liquid melt fraction. As such, a mesh of 181500 was considered to produce grid-independent results. Table 3 summarizes the results of the grid independence test.

Table 3: Results of grid independence test on rectangular cavity.

<table>
<thead>
<tr>
<th>Mesh Number</th>
<th>Mesh Size</th>
<th>Melt Time (s)</th>
<th>Percent Difference (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>181500</td>
<td>11958</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>366860</td>
<td>12028</td>
<td>0.58</td>
</tr>
</tbody>
</table>

Table 4 shows the result of the timestep independence test. The percent difference between using a timestep of 1s versus using a timestep of 0.5s for achieving 90% liquid fraction was 0.067%. Therefore, it was concluded that a mesh of 181500 elements and a timestep of 1s produced grid and timestep independent results.

Table 4: Results of timestep independence test.

<table>
<thead>
<tr>
<th>Mesh Number</th>
<th>Time Step (s)</th>
<th>Melt Time (s)</th>
<th>Percent Difference (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>11958</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>0.5</td>
<td>11966</td>
<td>0.067</td>
</tr>
</tbody>
</table>

2.2.6 Model Calibration

The two key parameters that require calibration are the mushy zone constant and the thermal expansion coefficient. An iterative approach was taken to calibrate these parameters, and the results were compared to a physical experiment to establish calibrated
values. In the present study, the solidus and liquidus temperatures were assumed to have the same value of 328.15K.

**Thermal Expansion Coefficient**

As stated before, the Boussinesq approximation was used to account for changes in density related to buoyancy. When using the enthalpy-porosity approach, the thermal expansion coefficient is considered an aggregate coefficient that characterizes the intensity of the convection process that occurs in melting and has a large effect on the melt time of the simulation. The thermal expansion coefficient was found to be inversely proportional to melt times since larger values produce stronger convective currents which decrease melt times. In the present study, values considered for the thermal expansion coefficient ranged from 0.0001 to 0.0008 which were found to be typical values for paraffin waxes based on literature. Figure 12 shows the impact that the thermal expansion coefficient has on the melt progression. It is seen that when the thermal expansion coefficient is too low (TE=0.0001), the PCM takes longer to melt. However, when the thermal expansion coefficient is too high (TE=0.0005), the PCM melts too quickly.

![Figure 12: Image showing the impact of thermal expansion coefficient on melt progression showing a thermal expansion coefficient of 0.0005 (orange) and 0.0001 (blue)](image-url)
The final selected value was chosen to be 0.0004 since it had the best agreement with the experimental data for total melting time. This result is presented in Figure 15.

**Mushy Zone Constant**

The mushy zone constant is not a thermophysical property, but rather a constant that is used to characterize the impact that the interface region has on momentum in the simulations. As such, it is not listed on material data sheets, and is not often found in literature. This value is material- and case-specific and therefore requires calibration.

The mushy zone constant was found to have a large impact on the shape of the solid-liquid interface profile throughout the melt. Higher values led to steeper damping curves and fluid velocities dropping to zero much more quickly when contacting the solid-liquid interface. Additionally, the mushy zone constant was found to be proportional to melt times as higher values were found to weaken natural convection leading to increased melt times. However, the mushy zone constant did not impact melt times as much as the thermal expansion coefficient.

Typical values for mushy zone constant range from $10^4$ to $10^7$, however in the present study, values ranging from $10^5$ to $4 \times 10^5$ were considered. Figure 13 shows simulated contours of the liquid fraction compared to the reference physical experiment. In this case, the mushy zone constant was set to $10^5$ which was the lowest value tested in this study. As seen in the plots, the simulated contours show poor agreement with the reference experiment. In this experiment, the PCM is heated from the left wall causing the liquid PCM in contact with the wall to heat up and rise due to a decrease in density. When the PCM reaches the upper surface, the flow is diverted towards the solid-liquid interface. When the liquid PCM contacts the solid-liquid interface, the velocities in the horizontal direction drop to zero, and heat is transferred from the liquid PCM to the solid PCM causing the liquid PCM to descend as a result of its increased density. In this case, the mushy zone constant was too low which prolonged the time in which the horizontal velocity of the liquid PCM to drop to zero when contacting the solid-liquid interface. This allowed more time for heat to transfer between the liquid and solid PCM causing the upper region of liquid PCM to melt prematurely.
Figure 13: Simulated contours of liquid fraction (bottom row) at different moments in the melting process compared to the reference physical experiment [22] (top row) showing poor agreement using a Mushy Zone Constant of $10^5$.

The final calibrated value for the mushy zone constant was selected to be $3\times10^5$ as it had the best agreement with the experimental data.

**Final Calibrated Results**

Figure 14 shows the calibrated transient melt fraction profiles at various times. Comparing the results of the numerical study to the results from Jevnikar and Siddiqui, it is seen that the simulated results of the melt fractions show relatively good agreement compared to the experimental profiles. The shape of the solid-liquid interface is governed by the flow patterns that occur in the liquid domain inside the module due to natural convection. Therefore, since the computed interface profiles are similar to the experimental profiles, it provides a good indication that the fluid velocity and flow patterns are being correctly modeled.
Additionally, Figure 15 shows a plot of melt fraction versus time comparing the calibrated numerical results to results presented by Jevnikar and Siddiqui. Once again, it is seen that the results are in relatively good agreement, and the RMS error between the computed and experimental melt fraction was calculated to be 0.03.

Figure 14: Calibrated simulated contours of liquid fraction (bottom row) at different moments in the melting process compared to the reference physical experiment [23] (top row)
2.3 Computational Study on Module Design

The calibrated computational model was used to conduct a study to analyze the design of a thermal storage module and investigate the benefits that adding fins has on the thermal storage system. In addition, a strategy is presented for estimating the performance of multiple thermal storage modules by numerically analyzing a single pass of heat transfer fluid.

2.3.1 Module Geometry

The ultimate goal for this project is to contribute to the design a highly effective thermal storage system capable of fulfilling a home's space and water heating needs throughout an entire day. In this case, effectiveness is judged on the basis of how quickly heat energy can be added and removed from a module such that the module can be fully charged and discharged at the timescales of heat availability and usage requirement, respectively. In Ontario, the average household consumed 95 gigajoules of energy annually in 2019, with space and water heating accounting for 80% of that usage [72]. To meet these requirements, a complete thermal storage system must have the capacity to store approximately 208 megajoules per day. If this energy were to solely be stored as latent heat, it would require about 1150kg of Polyfin PCM. Within the scope of the broader thermal storage project

Figure 15: Melt fraction vs time comparing simulation data to reference experiment data [22].
being undertaken within the research group, a modular design has been proposed wherein the complete thermal storage unit will be comprised of several individual modules which operate independently, but combine to provide the full storage capacity. It was decided that 10kg of PCM per module would serve a manageable module size, and that each module would be a rectangular prism of approximately 20 cm x 20 cm x 30 cm such that the modules could be tightly packed to reduce the total volume of the thermal storage unit. Figure 16 shows a sketch of a module consisting of a rectangular volume of PCM (gray) with tubes containing heat transfer fluid (blue) running through the module.

![Module Sketch](image)

Figure 16: Image of the proposed module design showing the PCM region (gray) and the tubes (blue).

### 2.3.2 Module Configurations

The general design for the modules consisted of a rectangular shaped container with tubes containing heat transfer fluid passing through the module. While this system closely resembles a shell and tube heat exchanger which are typically cylindrical in shape, the rectangular design leads to better packing of the modules and increased space utilization. Rectangular modules allow for efficient utilization of space when arranged side by side. This compact arrangement is particularly crucial in residential applications where space is limited.
The number of tubes in the module plays a huge role in the charging and discharging performance, as more tubes lead to a higher surface area of contact between the HTF and PCM. However, from an economic and practical perspective, more tubes require more materials which means the cost to make the module is increased. Additionally, more tubes lead to heavy modules which is not desirable.

Three different tube configurations were analyzed. For all studies, a constant module cross section of 20.32 cm × 20.32 cm (8in × 8in), a PCM mass of 10 kg, and a mass flow rate of 0.5 [kg/min] through the module was used. The number of tubes per module, and spacing between tubes were varied, and the three configurations can be seen in Figure 17. Configuration 1 consists of 36 tubes with a tube spacing of 3.175 cm (1.25 in) apart. Configuration 2 consists of 25 tubes with a tube spacing of 4.064 cm (1.6 in), and Configuration 3 consists of 16 tubes with a tube spacing of 5.08 cm (2 in).

![Figure 17: Image of three module configurations used in this study showing the PCM (gray) and the tubes (blue).](image)

The primary objective of this study was to assess whether the proposed module designs could effectively heat water to meet the standards for residential hot water supply. In the broader context of the project, groundwater enters the thermal storage system at approximately 10°C. As the water passes through the system, it must heat up significantly to meet the hot water demands of a typical household. The primary hot water uses in domestic settings, such as showers and washing machines, require water temperatures
ranging from 40°C to 55°C. Consequently, the thermal storage system needs to increase the water temperature to about 45°C as it passes through the system.

Given the modular nature of the design, additional modules can be incorporated in series if one module does not adequately heat the fluid. Moreover, modules can be added in parallel to enhance the mass flow through the thermal storage system. However, a constraint was set for this study that the temperature of the HTF should be sufficiently heated after it passes through 5 modules in series.

2.3.3 Computational Geometry

This study aimed to analyze the change in outlet HTF temperature after passing through a given module five times, considering configurations with and without the use of fins. Due to the computational intensity of melting and solidification simulations, simplifications were made to the geometry to reduce the computational domain's size.

The geometry for each configuration included five tubes arranged in a row, aligning with the spacing in each configuration. It's worth noting that in Configurations 1 and 3, achieving a strict alignment of five HTF passes in a row was not possible, potentially introducing inaccuracies. However, the goal of this study was to investigate the change in HTF temperature after making 5 passes through each configuration. Since the tube spacing in this geometry matched the tube spacing in each configuration, the arrangement of the tube passes was not expected to significantly impact the results.

The geometry used in this CFD study can be seen in Figure 18. Symmetry was taken advantage of to further reduce the size of the computations. It is important to note that this assumption would also lead to some inaccuracies since there would be some heat losses at the walls, and the wall effects are not analyzed. However, given the study's purpose of estimating the proposed module design's performance and predicting outlet fluid temperatures during discharging, this assumption was deemed valid as it did not drastically affect the results.
Figure 18: Configuration 1 geometry used in the present study showing the wax only case (left) and the finned case (right) showing the module height ‘h’ and tube spacing ‘a’.

In addition, as mentioned earlier, each module contained 10kg of PCM with a constant cross-section. To maintain this requirement for each configuration, module heights were slightly adjusted to compensate for space occupied by tubes and fins. Table 5 provides the model heights and tube spacing for reference.

<table>
<thead>
<tr>
<th>Configuration Number</th>
<th>Wax only module height (m)</th>
<th>Finned module height (m)</th>
<th>Tube Spacing (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.270</td>
<td>0.274</td>
<td>3.175</td>
</tr>
<tr>
<td>2</td>
<td>0.268</td>
<td>0.271</td>
<td>4.064</td>
</tr>
<tr>
<td>3</td>
<td>0.266</td>
<td>0.269</td>
<td>5.080</td>
</tr>
</tbody>
</table>

2.3.4 Heat Transfer Fluid Velocity Calculation

To ensure a fair comparison between each configuration, a consistent mass flow rate into the module was maintained. As a result, module configurations with more tubes
experienced a reduced fluid velocity in each tube since the mass flow was distributed among a greater number of tubes.

As mentioned before, each module consists of HTF passing through 5 tubes before exiting the module. This section of 5 tube passes will be herein referred to as a cycle. Establishing the number of cycles in each configuration was critical for determining the fluid velocity in each tube. The number of cycles per module was calculated using the following equation:

\[ n_{cycles} = \frac{n_{tubes}}{n_{passes}} \]  \hspace{1cm} (2.12)

where \( n_{cycles} \) is the number of cycles in the configuration, \( n_{tubes} \) is the number of tubes in the Configuration, and \( n_{passes} \) is the number of HTF tube passes before exiting the module. For example, Configuration 2 has 25 tubes, and therefore using this equation results in a total of 5 cycles.

Configuration 1 and Configuration 3 have a number of tubes that is not divisible by 5 and therefore the number of cycles per module was approximated resulting in Configurations 1 and 3 having a non discrete number of cycles. While this is not physically possible in the real world, the computational simulations only studied one cycle, and this approximation was only used to calculate the velocity of the HTF in the tube in order to ensure that the theoretical mass flow rate into the module was kept constant across all configurations. The mass flow rate in a tube was then calculated using the following equation:

\[ \dot{m}_{tube} = \frac{\dot{m}_{module}}{n_{inlets}} \]  \hspace{1cm} (2.13)

where \( \dot{m}_{tube} \) is the tube mass flow rate and \( \dot{m}_{module} \) is the total flow into the module.

Lastly, the velocity in the tube for each configuration was calculated using the following equation:

\[ v_{tube} = \frac{\dot{m}_{tube}}{\rho A} \]  \hspace{1cm} (2.14)
where \( v_{\text{tube}} \) is the tube velocity, \( \rho \) is the fluid density, and \( A \) is the tube cross-sectional area.

Using this equation, for a total mass flow into the module of 0.5 [kg/min], the tube flow velocity for each Configuration is as follows:

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Tube Flow Velocity (m/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.0433</td>
</tr>
<tr>
<td>2</td>
<td>0.0623</td>
</tr>
<tr>
<td>3</td>
<td>0.0974</td>
</tr>
</tbody>
</table>

### 2.3.5 Numerical Setup

The computational setup from the calibration process was used in the present study. In addition, grid density and timestep size used in the calibration study were used here to ensure results were spatially and temporarily independent.

A summary of the boundary conditions used in this study is presented in Table 7. All fluid outlets used the zero-pressure outlet boundary condition as it was assumed the outlet pressure would equal the atmospheric pressure. Inlet 1 used an inlet condition in which the temperature was set to 283.15 K (10\(^\circ\)C), and the velocity was set with reference to Table 6. Inlets 2 – 5 had their temperature set to equal the mass-weighted average of the temperature at outlets 1 – 4, respectively, to ensure that the inlet of the current pass was equal to the outlet of the previous pass. This technique may introduce inaccuracies since it necessitates the redevelopment of the thermal boundary layer in each tube. However, in the physical system, the 180-degree tube bend between each tube pass induces mixing of HTF thereby disrupting the thermal boundary layer. Therefore, this approach was not expected to have a significant impact on the results.
All surrounding vertical walls (y-x and y-z planes in Figure 18) used a symmetry boundary condition since it was assumed that symmetry occurred about these faces. The top PCM faces used a free slip adiabatic wall boundary condition as there would be a small air gap at the top of the module to allow for the expansion of the PCM as it changes phase, and it was assumed that this surface would be perfectly insulated.

Table 7: Summary of inlet and outlet boundary conditions for the 5-pass module

<table>
<thead>
<tr>
<th>Boundary Name</th>
<th>Boundary Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet 1</td>
<td>Temperature: 283.15K</td>
</tr>
<tr>
<td></td>
<td>Velocity: refer to Table 6</td>
</tr>
<tr>
<td>Outlet 1</td>
<td>Zero pressure outlet</td>
</tr>
<tr>
<td>Inlet 2</td>
<td>Temperature: Equal temperature at Outlet 1</td>
</tr>
<tr>
<td></td>
<td>Velocity: Equal to the velocity at Outlet 1</td>
</tr>
<tr>
<td>Outlet 2</td>
<td>Zero pressure outlet</td>
</tr>
<tr>
<td>Inlet 3</td>
<td>Temperature: Equal temperature at Outlet 2</td>
</tr>
<tr>
<td></td>
<td>Velocity: Equal to the velocity at Outlet 2</td>
</tr>
<tr>
<td>Outlet 3</td>
<td>Zero pressure outlet</td>
</tr>
<tr>
<td>Inlet 4</td>
<td>Temperature: Equal temperature at Outlet 3</td>
</tr>
<tr>
<td></td>
<td>Velocity: Equal to the velocity at Outlet 3</td>
</tr>
<tr>
<td>Outlet 4</td>
<td>Zero pressure outlet</td>
</tr>
<tr>
<td>Inlet 5</td>
<td>Temperature: Equal temperature at Outlet 4</td>
</tr>
<tr>
<td></td>
<td>Velocity: Equal to the velocity at Outlet 4</td>
</tr>
<tr>
<td>Outlet 5</td>
<td>Zero pressure outlet</td>
</tr>
</tbody>
</table>

In each test, the domain was initialized at 335.15K which is seven degrees above the phase transition temperature. This meant that the PCM in each test was initially in its liquid phase. The test concluded once the melt fraction of the PCM reached 0.05 as this meant that the majority of the PCM had been solidified, and the latent heat had been discharged from the PCM.

2.3.6 Results

Figure 19 shows a plot of the exit fluid temperature at outlet 5 for all three Configurations. In all cases, it is seen that the highest outlet temperature occurs at the beginning of the
discharging process, and as time progresses, the outlet fluid temperature decreases. This result is expected since the discharging process transfers stored thermal energy from the PCM to the HTF. As time progresses, the thermal energy content (including the sensible and latent heat) in the PCM begins to decrease. Since part of the energy is stored as sensible heat, a decrease in thermal content translates to a decrease in average PCM temperature thus reducing the temperature difference between the HTF and the PCM causing a decrease in outlet HTF temperatures.

In addition, comparing the modules with only wax, it is seen that Configuration 1 showed the best results with an average temperature increase of about 9.4 degrees. Configuration 2 had an average temperature increase of about 6.0 degrees, and Configuration 3 had an average temperature increase of 3.5 degrees. Looking at the finned cases, it is seen that Configuration 1 had the highest average temperature increase of about 19.0 degrees, whereas Configuration 2 and Configuration 3 had average outlet temperature increases of about 13.7 degrees, and 8.9 degrees respectively. This result is expected since Configuration 1 has the greatest number of tubes and therefore the highest surface area between the HTF and the PCM.

Figure 19: Plots comparing the temperature at outlet 5 versus time for each module design.
2.3.6.1 Predicting Outlet Fluid Temperatures

**Calculating Overall Average Heat Transfer Coefficient**

Melting and solidification simulations are very computationally expensive, and it is not feasible to simulate multiple modules in a single simulation. This section will outline how the correlation for the log mean temperature difference can be used to predict the outlet fluid temperature of multiple modules.

It follows that the log mean temperature difference correlation to describe internal flow in a tube with a constant free stream external fluid temperature is [73]:

$$\Delta T_o = \frac{T_{\infty} - T_{m,o}}{T_{\infty} - T_{m,i}} = \exp \left( - \frac{\overline{U} A_s}{mc_p} \right)$$  \hspace{1cm} (2.15)

Where $T_{\infty}$ is the constant temperature of the free stream external fluid, $T_{m,o}$ is the outlet fluid temperature, $T_{m,i}$ is the inlet fluid temperature, $\overline{U}$ is the overall heat transfer coefficient, $A_s$ is the tube surface area, $m$ is the mass flow rate of the fluid, and $c_p$ is the specific heat of the fluid.

In the following study, it was assumed that the bulk free stream temperature was equal to the phase transition temperature of the PCM (55°C), and the results from the CFD simulations were used to determine $T_{m,o}$ rearranging Equation (2.15) for $\overline{U}$ takes the following form:

$$\overline{U} = \left( -mc_p \ln \left( \frac{T_{\infty} - T_{m,o}}{T_{\infty} - T_{m,i}} \right) \right) / A_s$$  \hspace{1cm} (2.16)

This equation was used to calculate the overall heat transfer coefficient between the HTF and the PCM. Figure 20 shows plots for the overall heat transfer coefficient versus time for each module type. In each plot, the overall heat transfer coefficient was calculated for each pass of HTF fluid to determine if the heat transfer coefficient remains constant as the fluid passes through the module. For example, for the line showing 1 pass, $T_{m,o}$ equals the fluid outlet temperature at outlet 1, and $A_s$ is equal to the surface area of 1 tube. Moreover, the line labeled 5 pass uses outlet 5 temperature as $T_{m,o}$, and $A_s$ is the surface area of 5 tubes.
Looking at the plot, it is seen that in the non-finned cases, the overall heat transfer coefficient is relatively the same no matter how many fluid passes are used in the calculation. From this result, it is concluded that the overall heat transfer coefficient is independent of the number of passes, and could be used to estimate the outlet fluid temperature of \( n \) number of passes.

In the finned case, the overall heat transfer coefficient shows good agreement between the fluid passes, however, it is seen that the overall heat transfer coefficient slightly increases with an increase in fluid passes. The largest difference between the overall heat transfer coefficient occurs in plot (ii) which is the Configuration 1 finned case. The maximum percent difference between any two heat transfer coefficients is about 16%. Although this shows that there is some dependency between the number of fluid passes and the overall heat transfer coefficient, the plots show relatively good agreement with each other.
Figure 20: Overall heat transfer coefficient calculated after each pass for (i) Configuration 1, (ii) Configuration 1 fins, (iii) Configuration 2, (iv) Configuration 2 fins, (v) Configuration 3, (vi) Configuration 3 fins.
Comparing Predicted to Actual Fluid Outlet Temperature

The average heat transfer coefficient calculated using a single pass of heat transfer fluid was used to predict the outlet fluid temperature after 5 passes. Figure 21 shows plots of the predicted vs actual temperature at outlet 5 where the actual temperature of outlet 5 was determined using the results of the CFD study.

The x axis in each plot uses a dimensionless time scale $\tau^+$ which was presented in the works of Teather and Siddiqui [26]. The calculation for $\tau^+$ takes the following form.

$$\tau^+ = \frac{t - t_{\text{start}}}{t_{\text{end}} - t_{\text{start}}}$$  \hspace{1cm} (2.17)

Where $t$ represents the time, $t_{\text{start}}$ is the time when melting / solidification begins, and $t_{\text{end}}$ is the time that the test ends. However in the work of Teather and Siddiqui [26], an acrylic enclosure was submerged in a water bath, and therefore there was a time delay in which thermal energy conducted through the acrylic wall and into the PCM ($t_{\text{start}}$). In the present study, thin stainless steel tubes are used which conduct heat and the onset of melting and solidification happens immediately, and therefore $t_{\text{start}}$ was not relevant. Hereinafter the non-dimensional time ($\tau^+$) will be referred to as the time fraction which takes the following form:

$$\tau^+ = \frac{t}{t_{\text{end}}}$$  \hspace{1cm} (2.18)

When analyzing the plots in Figure 1, it is seen that the predicted and actual temperatures show good agreement with each other. The highest deviation between the predicted and actual temperatures occurred when analyzing Configuration 1 with fins which had a maximum percent difference of 13.1% between the two temperatures. In all cases, the predicted temperatures were underestimated compared to the actual temperatures meaning that the predicted results can be interpreted as a conservative estimate of the outlet fluid temperature.
Figure 21: Plots showing the predicted temperature of outlet 5 using the overall heat transfer coefficient calculated using 1 pass versus the actual temperature at outlet 5 for (i) Configuration 1, (ii) Configuration 1 fins, (iii) Configuration 2, (iv) Configuration 2 fins, (v) Configuration 3, (vi) Configuration 3 fins.
Predicting Outlet Temperatures of Multiple Modules in Series

Using log-mean temperature difference approximation allows for a relatively accurate estimation of the outlet fluid temperature after $n$ number of passes using the overall heat transfer coefficient calculated for 1 pass. This is beneficial as CFD simulations can be done on a single pass of HTF, rather than multiple passes, in order to estimate the overall heat transfer coefficient for the proposed module design. Melting and solidification simulations are very computationally expensive, and transient simulations can be quite time consuming. Reducing the computation to a single pass of HTF, and using the result to calculate the overall heat transfer coefficient can be a good method to approximate the performance of a thermal storage system.

In the present study, in each case, the outlet fluid temperature was predicted for 2, 3, 4, and 5 modules arranged in series, and the results are presented in Figure 22. Analyzing the plot, it is seen that the highest outlet fluid temperatures are seen in plot (ii) which shows the results for the Configuration 1 finned case which had an average outlet fluid temperature of 49.0°C after 5 module passes. This result is not surprising since this geometry uses the highest number of tubes, and therefore has the highest surface area of HTF in contact with the PCM. However, analyzing the results for Configuration 2 and Configuration 3, it is seen that the use of fins led to adequate outlet fluid temperatures when 5 modules were used. The average outlet fluid temperature of the Configuration 2 finned case after 5 module passes was 44.7°C, and the average outlet fluid temperature after 5 module passes for Configuration 3 was 37.8°C. Table 8 summarizes the outlet fluid temperature after 5 module passes for each configuration, and shows the percent increase in outlet fluid temperature when fins were employed.

Table 8: Comparison of the percent increase in outlet fluent temperature after 5 module passes between a non-finned case and a finned case.

<table>
<thead>
<tr>
<th>Configuration Number</th>
<th>Temperature No Fins (°C)</th>
<th>Temperature Fins (°C)</th>
<th>Percent increase (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>39.5</td>
<td>49.1</td>
<td>24.3</td>
</tr>
<tr>
<td>2</td>
<td>32.1</td>
<td>44.7</td>
<td>39.0</td>
</tr>
<tr>
<td>3</td>
<td>24.6</td>
<td>37.8</td>
<td>53.9</td>
</tr>
</tbody>
</table>
Recall that the goal of this study was to achieve an outlet fluid temperature of at least 45°C with a restriction of 5 modules. From Table 8 can be seen that Configurations 1 and 2 were able to achieve this goal with the use of fins. Although Configuration 3 did not achieve this goal, it is important to note that this configuration saw the highest percent increase in outlet fluid temperature when the use of a couple fins were employed. It is predicted that the use of more fins could be used to further increase the performance of this configuration.
Figure 22: Plots showing the predicted outlet temperature after n number of modules for (i) Configuration 1, (ii) Configuration 1 fins, (iii) Configuration 2, (iv) Configuration 2 fins, (v) Configuration 3, (vi) Configuration 3 fins.
2.3.6.2 Impact of Fins

In the present study, numerical solidification studies on various tube arrangements with and without the use of fins. As established in the literature review, the main mode of heat transfer in solidification is conduction, and the main mode of heat transfer in melting is convection. The previous section showed that the use of fins had a positive impact on improving the performance of the modules in discharging since the fins provided a larger surface area for the heat to transfer between the HTF and the PCM. However, it is important to note that the heat transfer enhancement techniques must benefit the module's performance in solidification and melting. Adding fins in the module will undoubtedly restrict the convective currents that occur inside the module which would could negatively impact the performance of the module in melting. Literature has shown that using longitudinal fins leads to decreased melting times, however, these studies only use a few fins which do not significantly impact the convective currents inside the system. There is a lack of research conducted using a large array of fins, such as a honeycomb structure, especially in tall geometries to enhance the conductivity of the PCM such as in Figure 23. Using a finned structure like this would prohibit the formation of large convective currents to occur inside the module, but would allow for small localized natural convection to occur inside each pore. Analyzing a geometry like this using software would be extremely computationally expensive as producing an adequate mesh for this large array of thin fins would result in a massive mesh size. Therefore, this phenomenon will be experimentally tested in the next chapter.
2.3.7 Numerical Simulation on Benchtop Design

In the present study, three Configurations of tube arrangements were presented, and the performance of each Configuration was tested with and without the use of fins. This study found that Configuration 1 performed the best in terms of increasing outlet fluid temperatures in discharging, however, it was also determined that Configuration 3 saw the highest percent increase in outlet fluid temperatures between the non finned and finned cases. From an economic perspective, the use of fewer tubes provides value as it involves fewer parts per module resulting in cheaper module cost. In addition, using fewer tubes decreases the mass of the modules which would be beneficial as it would be easier for users to install the modules.

In the next chapter, a small scale benchtop module will be experimentally tested to compare various methods of heat transfer enhancements in a single module with a fixed number of tubes. Rather than choosing the more densely packed tube arrangements, Configuration 3 was chosen since this study found that the use of heat transfer enhancements can significantly improve the performance of the module. The benchtop module will be a scaled down version of the module presented in which 4 tubes will be analyzed rather than
16 tubes. The cross section of the benchtop module will be the same as a quarter section of Configuration 3 which is outlined in red in Figure 24.

![Diagram showing cross section](image_url)

Figure 24: Image showing the cross section of the small scale benchtop prototype (outlined in red) compared to the Configuration 3 geometry.

Due to limitations with Lab equipment, the experimental studies on the small scale module will hold 1.25kg of PCM. Figure 25 shows a representation of the small scale module in which the fluid passes through the module 4 times before exiting the module. In addition, the computational domain is presented in this figure showing the PCM, HTF, and tube domains.
2.3.7.1 Numerical Setup

The computational setup from the calibration process was used in this study. In addition, the grid density and timestep size used in the calibration study were used here to ensure results were spatially and temporally independent.

The purpose of this study was to get an estimate of how the benchmark small scale module will perform during experimental testing without any heat enhancements. This study was also compared to the results of the experimental test presented in the next chapter as a basis for further validating the numerical model and allowed for the opportunity to identify the strengths of the calibrated enthalpy porosity model. Two sets of tests will be conducted in order to analyze the melting and solidification process inside the module.

In the first test, the melting of the module was studied in which the domain was initialized at room temperature (23°C), and water at 80°C flowed through the module in order to melt the PCM. The test concluded once the temperature at Location 1 reached 60°C. Location 1 was located at the bottom corner of the module nearest the fourth and final tube pass. This
was the location inside the module that melted last and therefore was used to determine when all the PCM in the module was melted.

The second test studied the discharging of the module. In this case, the initial condition was set equal to the ending condition of the melting study. This was done to overcome the practical challenges of using an isothermal start condition in the physical experiments. Therefore, this initial condition is used in order to allow for direct comparison between the computational results and the experimental results.

A summary of the boundary conditions used in this study is presented in Table 9. All fluid outlets used the zero-pressure outlet boundary condition as it was assumed the outlet pressure would equal the atmospheric pressure. Inlet 1 used an inlet condition in which the temperature was set to 353.15K (80°C) for the melting test and 283.15 K (10°C) for the discharging test. For each test, a mass flow rate of 0.2 kg/min through the tube was used, and this translated to an inlet velocity of 0.125 m/s. Inlets 2 – 4 had their temperature set to equal the mass-weighted average of the temperature at outlets 1 – 3, respectively, to ensure that the inlet of the current pass was equal to the outlet of the previous pass. All surrounding vertical walls (y-x and y-z planes in Figure 25) used an adiabatic boundary condition since it was assumed that there would be minimal heat losses. The top PCM faces used a free slip adiabatic wall boundary condition as there would be an air gap at the top of the module to allow for the expansion of the PCM as it changes phase, and it was assumed that this surface would be perfectly insulated.

Table 9: Summary of inlet and outlet boundary conditions for the computational simulation of the benchtop module

<table>
<thead>
<tr>
<th>Boundary Name</th>
<th>Boundary Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet 1</td>
<td>Temperature (Melting): 353.15K</td>
</tr>
<tr>
<td></td>
<td>Temperature (Discharging): 283.15K</td>
</tr>
<tr>
<td></td>
<td>Velocity: 0.125 m/s</td>
</tr>
<tr>
<td>Outlet 1</td>
<td>Zero pressure outlet</td>
</tr>
<tr>
<td>Inlet 2</td>
<td>Temperature: Equal temperature at Outlet 1</td>
</tr>
<tr>
<td></td>
<td>Velocity: Equal to the velocity at Outlet 1</td>
</tr>
<tr>
<td>Outlet 2</td>
<td>Zero pressure outlet</td>
</tr>
</tbody>
</table>
### 2.3.7.2 Results

Figure 26 shows the results of the outlet fluid temperatures after each pass versus time. In the melting case, it is seen that the average HTF temperature at the outlet will be about 78.6°C, whereas in the solidification case, it is seen that the average HTF temperature at the outlet will be about 11.3°C with no heat transfer enhancements. In addition, it is seen that the melting case will take approximately 24000s (6.7h) to complete, and the solidification case will take approximately 20000s (5.5h) to complete.

![Figure 26: Plots of outlet HTF temperature versus time showing for the melting case (left) and the solidification case (right).](image)

Figure 27 shows plots of the simulated liquid fractions about Plane 1 for the melting case. It is seen that the progression of the melt shows similar trends to that of the simple rectangular geometry in which the PCM was heated from a vertical wall. This result makes sense because in both cases the PCM is being heated from a vertical heat source. At time t
= 0 min, the PCM begins as a solid, and conduction is the dominant mode of heat transfer between the steel tubes and the solid PCM. At time $t = 30$ min, a small liquid region forms between the HTF tubes and the solid PCM which convection starts to become the dominant mode of heat transfer. After time $t = 90$ min, a large liquid region forms at the top of the domain as a result of the natural convective currents. After this time, the convective currents drive the melt from the top to the bottom of the domain.

Figure 27: Simulated contours of liquid fraction about Plane 1 at different moments in time for the melting test where red represents the liquid region and blue represents the solid region.
Figure 28 shows simulated contours of the liquid fraction about Plane 1 for the solidification test. As mentioned before, the initial condition for the solidification test was equal to the ending condition for the melting test. Thus, a temperature gradient is present inside the module in which the top of the PCM is hotter than the bottom (Figure 28 (b)). Due to this temperature gradient, solidification begins more quickly at the bottom of the enclosure since less sensible heat is required before phase change. Since conduction is the dominant mode of heat transfer in solidification, the solid region grows relatively uniformly as time progresses.

Figure 28: a) Simulated contours of liquid fraction about Plane 1 at different moments in time for the solidification test where red represents the liquid region and blue represents the solid region, b) Initial condition temperature contour, c) location of Plane 1
In the next chapter, these studies will be replicated experimentally and the computational results will be compared to the experimental results to further validate the numerical model, as well as identify the strengths of the calibrated enthalpy porosity model.

### 2.4 Summary

In summary, this chapter outlined a method used to conduct computational solidification and melting experiments on a multipass thermal storage module and predict the outlet HTF temperature after \( n \) number of modules.

First, calibration of the mushy zone constant and thermal expansion coefficient was performed by analyzing a simple rectangular geometry of PCM and comparing it to experimental data. The result of that study found that using a mushy zone constant of \( 3 \times 10^5 \) and a thermal expansion coefficient of 0.004 were the best tuning parameters for Polyfin PCM as it showed good agreement with the experimental data.

Next, the calibrated numerical model was used to study three different tube arrangements for a module, and the performance of the module was studied with and without the use of fins. The results found that Configuration 1 with fins produced the highest outlet fluid temperature when only analyzing a single module. In addition, the overall heat transfer coefficient was calculated for each geometry, and it was determined that the overall heat transfer coefficient was independent of the number of fluid passes. The overall heat transfer coefficient was then used to predict the outlet HTF temperature after 5 passes, and compared to the actual temperature, and it was determined that there was good agreement between the predicted and expected outlet fluid temperature.

The performance of multiple modules arranged in series was investigated. It was determined that the use of fins resulted in Configurations 1 and 2 being able to produce an outlet HTF temperature of over 45°C when 5 modules were arranged in series. However, the introduction of fins into the module had a higher percent increase in outlet fluid temperatures in Configuration 3.

Lastly, a small scale thermal storage module was introduced based on the design of Configuration 3. The benchmark case with no heat enhancements was numerically
investigated in order to estimate the performance of the module. In the next chapter, the small-scale module will be constructed and experimentally tested. The analysis in this chapter aims to explore the effectiveness of longitudinal fins and compare them with the use of metal wool as a heat transfer enhancement method.
Chapter 3

3 Experimental Investigation

The present chapter focuses on the experimental investigation of the heat transfer processes during melting (charging) and freezing (discharging) of a small-scale thermal storage module.

As discussed previously in Chapter 1, the literature shows that natural convection is the dominant mode of heat transfer in melting, and conduction is the dominant mode of heat transfer in solidification. In addition, it is well known that PCMs used in thermal storage systems often suffer from low thermal conductivities making it difficult to achieve suitable charging and discharging rates, and therefore the use of heat transfer enhancement techniques is often desirable.

The addition of any heat enhancement element inside the thermal storage system influences how the heat is transferred between the PCM and the heat source. In the case of melting, it has been demonstrated that natural convection plays a dominant role in driving and accelerating the melting process [19], [20], [21]. However, the use of heat transfer enhancing elements may disrupt these convective currents, and consequently could negatively impact the heat transfer rates.

In the present study, two heat enhancement elements, a finned honeycomb structure, and the metal wool are considered to investigate their effectiveness in increasing the heat transfer rates in the thermal storage module.

3.1 Experimental Setup

3.1.1 Storage Container

A schematic of the experimental module used in this study is provided in Figure 29. The module has an internal height of 203.2 mm (8 in) and an internal cross-section of 101.6 mm × 101.6 mm (4 in × 4 in). The enclosure was constructed from 12.7 mm (0.5 in) thick acrylic sheets and featured a removable lid secured with 4 fasteners. Acrylic was chosen
for the construction of the box due to its low cost and ease of manufacturing. Additionally, acrylic has low thermal conductivity \((k \approx 0.2 \text{ W/m K})\) and would, therefore, provide insulation to prevent heat loss in the system. Acrylic is also highly resistant to heat degradation and is impermeable to solid and liquid PCM. The acrylic sheets were bonded together using acrylic solvent glue.

Four stainless steel tubes passed through the module, each with an outer diameter of 6.35 mm (0.25 in) and a wall thickness of 0.254 mm (0.01 in). The tubes were arranged in a square grid with a spacing of 50.8 mm (2 in) between each other (see Figure 29). The stainless steel tubes were press-fit into the bottom face of the module and sealed with superglue. This design ensured a watertight seal that remained intact during the melting and freezing of the PCM.

![Experimental Module Design](image)

Figure 29: Experimental Module Design in dimetric view (left), and top view (right)

To achieve four passes of HTF through the module, pieces of hose made of Buna-N Rubber were used to connect pairs of stainless steel tubes, creating a continuous path for the HTF to flow through the module. The entire enclosure was further insulated using 25 mm thick polystyrene boards \((k \approx 0.028 \text{ [W/m K]})\), as illustrated in Figure 30. These polystyrene sheets had an R-value of 5.
In all experiments, the module was filled with 1.25 kg of PCM, leaving approximately 50 mm of space between the top of the PCM and the module container's top face. This space was incorporated into the design for two main reasons. The first reason was to ensure sufficient room in the module to accommodate the volume change of the PCM due to thermal expansion. The second reason was to provide adequate space in the module to accommodate any volume changes related to the addition of heat transfer enhancing elements.

### 3.1.2 Phase Change Material

The PCM used in this study was Polyfin. Polyfin is a commercially available mixture of paraffin wax and copolymer alloys, and its thermophysical properties are presented in Table 10.
Table 10: Thermo-physical properties of Polyfin at 25°C [22],[39].

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting temp [℃]</td>
<td>55</td>
</tr>
<tr>
<td>Density [kg/m³]</td>
<td>920</td>
</tr>
<tr>
<td>Specific Heat [kJ/kg K]</td>
<td>2.89</td>
</tr>
<tr>
<td>Thermal Conductivity [W/m K]</td>
<td>0.18</td>
</tr>
<tr>
<td>Dynamic Viscosity [kg/m s]</td>
<td>0.00506</td>
</tr>
<tr>
<td>Latent Heat of Fusion [kJ/kg]</td>
<td>180</td>
</tr>
</tbody>
</table>

### 3.1.3 Heating and Cooling Circuits

Figure 31 shows a representation of the complete experimental setup including all the components used to provide heating and cooling to the module for PCM melting and freezing, respectively. Water was used as the working fluid. The hot water circuit consisted of a 10-gallon steel drum with a 3000W electrical resistive heater submerged in the tank. In order to maintain the hot water at a constant temperature, a Zesta Engineering ZCPS13 equipped with a ZEL 9100 proportional-integral-derivative (PID) controller was used with a K-type thermocouple for feedback. Furthermore, a mixing impeller was employed to ensure the water bath remained consistent and under near-isothermal conditions. During heating (PCM melting) experiments, the heating circuit was controlled such that the water temperature at the inlet of the module was maintained at a constant value of 80°C ±1°C.

The cold-water circuit made use of two Coleman ice coolers. One cooler held an ice-water mixture (~0°C) as a cold source, and the other cooler (referred to as the supply cooler) kept water at 10°C, which supplied water to the module during the freezing experiments. An Arduino controller was used to maintain the temperature of the supply cooler and consisted of a K-type thermocouple (as feedback) along with an L289N motor controller and an impeller pump. The Arduino controller would read the temperature of the water in the supply cooler, and if the temperature was greater than 10°C it would activate the cold
source circuit where the ice water is pumped through a closed circuit copper coil to regulate the temperature of the supply cooler (see Figure 31). In addition, a mixing impeller was used in the supply cooler to maintain near-isothermal conditions. For each freezing experiment, the temperature of water at the inlet of the module was maintained at a constant value of 10°C ±1°C.

Multiple shut-off valves were incorporated into the water circuit to switch from heating to cooling of the module. The maximum flow rate of the impeller pump used in the water circuit was about 0.8 kg/min, and a flow adjustment valve was used to throttle down the flow to the required flow rate. An Omega Engineering FL-2023 flow meter was used to monitor the flow rate of water during each test. The flow rate was also measured at the beginning and end of each test using a beaker and stopwatch to confirm the flow rate consistency during the test.
3.1.4 Temperature Measurements

A total of 16 thermocouples were used to measure temperature at various locations during each test. The thermocouples used were Neoflon-PFA insulated T-type thermocouples.

Figure 31: Complete Experimental Setup (note some images in the figure were taken from the internet for clarity)
made by Omega Engineering (hereinafter referred to as TC). A wire gauge of 36AGW was selected to minimize the interference of the thermocouples with the PCM and HTF. The position and locations of thermocouples inside the module are illustrated in Figure 32. These thermocouples were rated for special limits of error (SLE) which have a high degree of accuracy and have an uncertainty of ±0.5°C. All thermocouples were calibrated by submerging the ends in a well insulated hot water bath. Temperature data were recorded using data acquisition cards (NI-9211) and controlled using a LabVIEW program recording data at a rate of 1Hz. A high accuracy mercury thermometer with graduations of 0.2°C was used as the reference temperature. The calibration process spanned temperatures from 0°C to 80°C, with 2°C intervals. During each interval, 30 seconds of data was recorded and then time-averaged for each thermocouple. Afterward, a calibration curve was generated for each thermocouple, indicating a consistent linear trend across all calibration equations.

The description of 16 thermocouples that were used to record and monitor temperatures inside the module for each experimental test is provided as follows (also see Figure 32). Thermocouples 0 through 7 were used to measure fluid inlet and outlet temperatures inside each tube. These data were used to calculate the rate of heat transfer into the PCM after each tube pass. Thermocouples 8 through 11 were used to measure the surface temperatures of each tube. These thermocouples were attached to the tubes using Kapton tape which is often used for mounting surface thermocouples as it is able to sustain high operating temperatures and has excellent solvent resistance. Thermocouples 12 and 13 were attached to the inside and outside of the acrylic wall respectively. These thermocouples were used to estimate heat loss out of the module. Thermocouple 14 was attached to the bottom corner of the module closest to the outlet tube. This thermocouple was used to monitor the time at which melting was complete. This location in the module takes the longest time to melt, and so once this thermocouple reads 55 degrees or higher (the melting temperature of the PCM), it was concluded that all the PCM in the module has melted. Lastly, Thermocouple 15 was used to measure the temperature at the center of the module.
3.1.5 Heat Transfer Enhancement Elements

Four modules were constructed, each using a different method of heat transfer enhancement. The first module had no heat transfer enhancement elements and served as a benchmark for comparing and analyzing the impact of different heat transfer enhancers. This module (hereinafter referred to as the only wax or OW Module) can be seen in Figure 33 below.
The second module contained an aluminum honeycomb core. Literature has shown that the use of vertical longitudinal fins has a positive impact on increasing heat transfer rates into and out of the PCM; however, there is a lack of research investigating finned structures. In this module (herein after referred to as the Aluminum Honeycomb or AH Module), the aluminum honeycomb structure served to investigate how a densely packed structure of fins would impact the heat transfer performance. The aluminum honeycomb core was purchased from Plascore (model number: PACL-XR1-5.7-3/16-20-P-5052). This honeycomb core was constructed from aerospace-grade 5052 aluminum and had a cell size of 3/16”. The core was cut to have a cross-section of 101.6 mm x 101.6 mm with a height of 203.2 mm to fit into the module. Since the cell size was smaller than the HTF tube diameter, some modifications had to be made to allow the tubes to pass through the module. A 0.25-inch diameter steel dowel was used to punch holes into the honeycomb core, slightly increasing the cell size at the location of the tubes. This method was effective as it allowed for a tight fit and good thermal contact between the aluminum honeycomb core and the stainless-steel tubes. Images of the raw aluminum honeycomb core and the complete module are shown in Figure 34.
The third and fourth modules utilized metal wool as heat transfer enhancement elements. It was hypothesized that the metal wool would enhance the effective conductivity of the PCM allowing for higher thermal performance in a fashion similar to that of adding highly conductive nanoparticles to the PCM [39], [74]. The literature review discussed that nanoparticles were an effective method of improving heat transfer rates in PCMs, but suffered from decreased performance over multiple heating cycles due to particle settlement [39]. The reason for selecting metal wool in the present study was that it would maintain a consistent structure, unlike nanoparticles, while still increasing the effective conductivity of the PCM. Two types of metal wools were considered, aluminum wool and stainless steel wool. The module with the aluminum wool (hereinafter referred to as the Aluminum Wool or AW Module) allowed the direct comparison with the aluminum honeycomb case to assess the difference between the shape of heat transfer enhancers (fins versus porous media). The other material used was stainless steel wool, selected for its better compatibility with inorganic hydrated salt phase change materials (PCMs), such as sodium acetate trihydrate (SAT), hereinafter referred to as the Stainless Steel Wool or SW Module. These materials are commonly studied in conjunction with organic paraffin wax for thermal energy storage. However, SAT is known to react with and corrode aluminum.
Therefore, despite stainless steel having significantly lower conductivity than aluminum (around 20 W/m.K for stainless steel compared to approximately 200 [W/m K] for aluminum), both metals still exhibit significantly higher thermal conductivities than Polyfin PCM (0.2 [W/m K]). Therefore, this study aimed to explore whether metal wools with varying conductivity could still provide benefits in charging and discharging processes. An image of the stainless steel metal wool as well as a completed module with metal wool can be seen in Figure 35.

For packaging in the module assembly, the wool was cut into 101.6mm pieces and arranged in layers inside the module. In each layer, the wool was positioned perpendicular to the last layer, ensuring a uniform wool structure throughout the module, as illustrated in Figure 36.

Figure 35: Image of metal wool (left), and image of the complete module with metal wool and PCM (right).
Figure 36: Image showing the packing of the wool in the module with each layer placed perpendicular to the last for a uniform packing structure.

As seen above, three of the four modules built for testing used different heat transfer enhancement elements. In order to ensure that the results from each module could be compared to each other and with the OW Module, the same volume of heat transfer enhancement element was kept in each case. Since the aluminum honeycomb structure was a pre-made structure, its volume was used as the reference volume for all other heat transfer enhancement elements. The volume of the aluminum honeycomb core was 52.61 cm\(^3\), and therefore the equivalent volumes of aluminum wool and steel wool were used in their respective modules.

### 3.1.6 Experimental Tests

Experimental tests were conducted on the four modules which include the module with only wax (OW module), an aluminum honeycomb core (AH module), stainless steel wool (SW module), and aluminum wool (AW module). For each module type, experiments were conducted for both charging and discharging. It was important to establish consistent start conditions for all experimental tests to ensure that the results across each module type could be compared to each other. Ideally, an isothermal start condition (i.e. the uniform temperature of the PCM) would be used for each experiment, however, an isothermal start condition posed many practical challenges, and was difficult to achieve a perfectly isothermal start condition. Although the modules were insulated, the heat losses in the system prevented a perfect isothermal start condition. Therefore, a different approach was taken.
The phase transition temperature of the PCM used in this study was 55°C, and therefore the start and end conditions were decided to be 5°C above and below this temperature. In all cases, the testing began when the modules were at the room temperature. The hot water circuit was turned on, which supplied water at 80°C into the modules at a specified flow rate until thermocouple TC 14 reached 60°C. TC 14 was located at the bottom corner nearest to the 4th pass tube and was the location which melted last in the module, and therefore all the PCM in the module was melted at this time.

Once TC 14 reached 60°C, the “Discharging” experiment began in which the cold-water circuit was immediately turned on which pumped water at 10°C through the system. The discharging experiments ended once TC 15, located at the center of the module, reached 50°C. This temperature was chosen since it is 5°C lower than the phase transition temperature. Therefore, once the TC 15 reached 50°C, it was determined that the entire PCM in the module was solid and thus fully discharged.

The end of the discharging experiments also posed as the beginning of the “Charging” experiments. Once TC 15 reached 50°C, the hot water circuit was turned on. The test ended once TC 14 reached 60°C, indicating all the PCM had melted, and thus the module was fully charged. A summary of the start and end conditions for the discharging and charging experiments can be seen in Table 11.

Table 11: Summary of start and end conditions for each test type

<table>
<thead>
<tr>
<th>Test Type</th>
<th>Start Condition</th>
<th>End Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Discharging</td>
<td>TC 14 = 60°C</td>
<td>TC 15 = 50°C</td>
</tr>
<tr>
<td>Charging</td>
<td>TC 15 = 50°C</td>
<td>TC 14 = 60°C</td>
</tr>
</tbody>
</table>

Since each module contained a different heat transfer enhancement element, the melting and solidification processes differed between modules, as expected, resulting in slightly different temperature gradients inside each module type at the start of the charging and discharging experiments. However, these thermal gradients would exist in any real world application of the thermal battery and would impact the charging and discharging. Therefore, since the locations of TC14 and TC15 were kept constant across all modules,
these thermocouple readings were used to determine the start and end of the charging and discharging processes.

For three of the modules, charging and discharging experiments were performed at 4 different flow rates: 0.1 [kg/min], 0.2 [kg/min], 0.4 [kg/min], and 0.6 [kg/min]. The SW module was only tested at a flow rate of 0.2 [kg/min], and was not tested at other flow rates due to the poor performance of this module. This will be further discussed in the results section. A summary of the tests performed in this study is presented in Table 12.

Table 12: Summary of experiments performed in this study.
3.2 Results

3.2.1 Overview of results

Table 13 presents the charge and discharge times for each module at a mass flow rate of 0.2 kg/min. The module using only wax, serving as the benchmark for comparison, showed a charge time of 18152 s and a discharge time of 9584 s. The top-performing module was the one featuring the aluminum honeycomb core, which significantly outperformed the benchmark by reducing the charge time by a factor of about three and the discharge time by a factor of about four. The module with Aluminum wool also performed well, decreasing the charge time by a factor of about 1.6 and the discharge time by a factor of about 2.3 compared to the reference case. However, the module with steel wool performed the poorest, increasing the charge time by a factor of about 1.6 and reducing the discharge time by a factor of about 1.3 compared to the reference case. Subsequent sections will offer a detailed analysis of each module and provide plausible explanations for their respective performances.

<table>
<thead>
<tr>
<th>Module Type</th>
<th>Charge Time (s)</th>
<th>Charge Time (h)</th>
<th>Discharge Time (s)</th>
<th>Discharge Time (h)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Only Wax (OW) (Benchmark)</td>
<td>18152</td>
<td>5.0</td>
<td>9584</td>
<td>2.7</td>
</tr>
<tr>
<td>Aluminum Honeycomb Core (AH)</td>
<td>5838</td>
<td>1.6</td>
<td>2469</td>
<td>0.7</td>
</tr>
<tr>
<td>Aluminum Wool (AW)</td>
<td>11206</td>
<td>3.1</td>
<td>4117</td>
<td>1.1</td>
</tr>
<tr>
<td>Steel Wool (SW)</td>
<td>29726</td>
<td>8.3</td>
<td>7511</td>
<td>2.1</td>
</tr>
</tbody>
</table>

3.2.2 Heat Transfer Rate Analysis

Charge and discharge times are directly related to the heat transfer rate to and from the PCM inside the module. Each module had the same mass of PCM, and therefore module types with the higher heat transfer rates had the quickest charging and discharging times.
Heat transfer rates of the module were calculated by analyzing the temperature change of the HTF at the inlet and outlet of the module using the following equation:

\[
\dot{q} = \dot{m} c_p (T_{inlet} - T_{outlet})
\]

where \(\dot{q}\) is the heat transfer rate in kW, \(\dot{m}\) is the mass flow rate of the HTF in kg/s, \(c_p\) is the specific heat capacity of the HTF measured in kJ/kg.K, \(T_{inlet}\) is the HTF temperature at the inlet of the module (in this case it is the temperature measured by TC 0), and \(T_{outlet}\) is the HTF temperature at the outlet of the module (in this case it is the temperature measured by TC 7). Figure 37 shows the heat transfer rates during charging and discharging for each module at a mass flow rate of 0.2 kg/min. Note that a positive heat flux indicates heat being transferred into the PCM, and a negative heat flux indicates heat transferred out of the PCM.

As seen in the plots in Figure 37 (a), the heat transfer rate during charging decreases with time. As time progresses, the module becomes more charged resulting in an increase in thermal energy. Some of this energy is stored as sensible heat which results in an increase in the average PCM temperature. Since the PCM temperature increases, the temperature difference between the PCM and HTF decreases resulting in a reduced heat transfer rate. A similar behaviour is observed in discharging (Figure 37 (b)).

![Figure 37 (a) Charge and (b) discharge rates at 0.2 kg/min where “AH” represents the aluminum honeycomb module, “AW” represents the aluminum wool module, “OW” represents the only wax module, and “SW” represents the steel wool module.](image-url)
The heat transfer rates during charging and discharging were compared for OW, AH and AW modules. The results show that on average, the aluminum honeycomb core increased the heat transfer rate by about 2.6 times during charging and 4.9 times during discharging compared to the benchmark (OW module). Whereas the aluminum wool increased the average heat transfer rate by about 1.4 times during charging and 3 times during discharging compared to the benchmark case. Both these modules used the same material (aluminum), and the same volume of the material for their heat transfer enhancement elements, however, there is a significant difference between the performance of a finned honeycomb structure as compared to the metal wool.

The difference in performance between the metal wool and the finned honeycomb structure can be attributed to the specific ways in which these elements increase heat transfer rates. The finned honeycomb structure functioned as an extension to the HTF tubes, creating additional surface area between the heat source and the PCM. Despite not being physically attached to the tubes, the close fit between the stainless-steel HTF tubes and the finned aluminum structure resulted in minimal thermal resistance. In contrast, the metal wool was utilized to enhance the effective thermal conductivity of the PCM. This approach aimed to improve overall heat conduction through the module, enhancing heat transfer between the PCM and the HTF. The present study suggests that it is more effective to improve the surface area between the heat source and the PCM rather than improving the thermal conductivity of the PCM at large.

The other reason for the difference in performance between the use of metal wool and a finned aluminum structure is their impact on natural convection especially in the melting process. In the finned aluminum case, the honeycomb pores were vertically aligned, thus, favoring the formation and growth of convective cells along the pore wall, hence contributing to the enhancement of natural convection. One limitation, however, was the small pore size, which restricted the lateral extent of the convective cells. In the case of metal wool, convection is partially obstructed in all directions, which suppressed the formation and growth of convective cells. This suggests that it is more important to allow the formation and growth of convective cells using a finned surface that aligns with gravity.
Comparing the performance of the steel wool module to the benchmark wax-only module is another indicator of the importance of allowing natural convection to occur during melting. Comparison of the results show that the heat transfer rate in the steel wool module is slightly lower than the benchmark case during charging and slightly higher during discharging. The conductivity of stainless steel is about 16.5 [W/m K], knowing the porosity of the wool (about 2% of the volume inside the module), the effective conductivity of the PCM can be estimated using the following equation.

\[
k_{eff} = (k_{PCM} \times \varphi_{wool}) + (k_{wool} \times (1 - \varphi_{wool}))
\]

Where \(k_{eff}\) is the effective thermal conductivity of the PCM, \(\varphi_{wool}\) is the porosity of the wool, and \(k_{wool}\) is the conductivity of the wool.

The results show that in the presence of the steel wool, the effective thermal conductivity of the PCM increased to 0.5 [W/m K], which is an increase in thermal conductivity by a factor of about 2.8 compared to the original value. However, this effective thermal conductivity increase is still quite low. It is likely that this increase in effective thermal conductivity was not enough to compensate for the suppression of convective motion caused by the wool during charging. However, during discharging where conduction is dominant, the increase in effective thermal conductivity due to the steel wool resulted in an increase in the heat transfer rate compared to the benchmark.

### 3.2.3 Characterization of the underlying physical process during melting (charging)

In order to understand how these heat transfer enhancements affect convection in the module during charging, it is important to understand the melting process without any heat enhancement element. Figure 38 shows images of the melting process at various stages during the melting process inside the benchmark wax only module.

The images show trends similar to that of the melting process in small rectangular geometries in which the PCM is heated from a vertical surface as reported in previous studies [22].
The melting process begins with heat transfer through conduction between the hot tubes and the solid PCM. The PCM quickly begins to melt at the tube walls causing a small liquid region to form. As this liquid region grows, natural convection begins due to the vertical alignment of the heat source i.e. the liquid PCM in contact with the tubes begins to rise due to a decrease in density caused by an increase in temperature, whereas the liquid PCM in contact with the solid PCM on the other side, begins to fall due to an increase in density caused by a decrease in temperature. As the buoyancy driven flow rises along the hot tubes and reaches the upper surface, the flow is diverted away from the tubes and towards the solid PCM region, hence establishing convective cells. The hot liquid travels horizontally until it reaches the solid PCM region in which heat is transferred from the hot liquid PCM to the cold solid PCM. This accelerates the melting process at the top of the enclosure, and with the progression of time (around 1 hr, see Figure 38), the increased buoyancy forces, driven by the natural convective flow, forms a liquid recirculation region at the top of the PCM. As time further progresses, this recirculation region grows vertically which accelerates the melting process from the top to the bottom of the enclosure.
Figure 38: Images showing the melting process of the wax only module at various times during the charging processes.
The concept of how the melt progresses in the module without any enhancements can be related to the performance of each heat transfer enhancement technique. The total thermal resistance between the HTF and PCM consists of a convective resistance between the HTF and the inner surface metal tube, a conductive resistance through the metal tube, a conductive resistance of the enhancement element, and a convective resistance from the enhancement element to the PCM. There is a convective resistance from the metal tube to the PCM but considering that the enhancement element is distributed throughout the module, the tube to PCM convective resistance is expected to be insignificant compared to the convective resistance between the enhancement element and the PCM. In the case of the aluminum honeycomb module, the honeycomb structure divides the PCM into numerous thin and tall vertically aligned cells, each region surrounded by an aluminum wall. During melting, the high conductivity of the aluminum allows heat to effectively conduct through the structure and acts as a heat source, heating each of these cells from all vertical walls. The presence of the convective motion within each cell of the honeycomb reduces the convective resistance within the PCM which was effective in improving the heat transfer rate compared to the benchmark case. In addition, the vertical arrangement of the cells augments natural convection within each cell which accelerates the melting process within these localized regions.

However, in the case of the modules with metal wool, the addition of metal wool obstructs the formation of convective cells within the liquid PCM thus dampening the effect of natural convection resulting in a reduced heat transfer rate in the presence of the aluminum wool module compared to the aluminum honeycomb. This also explains the poor performance of the stainless-steel wool during charging which was a result of dampened natural convection.

3.2.4 PCM Thermocouple Measurement Analysis

Figure 39 shows the time history of the PCM temperature at TC 15 located in the top middle of the module during a charging experiment for all modules at the mass flow rate of 0.2 kg/min. All modules show relatively similar trends in terms of how the temperature at this location changes with respect to time.
As mentioned earlier, each charging experiment started immediately after the corresponding discharging experiment ended. Recall that during the discharging experiments, water entered through the inlet of the module at a temperature of 10°C, and the experiment ended when TC 15 reached 50°C. Since TC 15 was located along the center axis of the module, when the discharging experiments ended, there existed a thermal gradient in which the temperature at the tube walls was colder than the temperature at the center of the module. Thus, when the charging experiment began, it took some time for the heat to diffuse through the PCM and reach the center of the module, and therefore heat continued to transfer between the colder part of the PCM (closer to the tube walls) and the warmer part of the PCM (center of the module) resulting in an initial decrease in temperature at TC 15. After some time, the diffused heat reached the center of the module resulting in a relatively constant increase in the temperature. Once the solid-liquid interface reached TC 15, the PCM transitioned from solid to liquid, and the natural convection inside the module caused the temperature of TC 15 to rapidly rise. The slope of the temperature profile then began to decrease as it approached the temperature of the heat source (80°C).

Figure 39: Plots of temperature at TC 15 for each module during the charging experiment at a flow rate of 0.2 kg/min where “AH” represents the aluminum honeycomb module, “AW” represents the aluminum wool module, “OW” represents the only wax module, and “SW” represents the steel wool module.
The analysis of the results in the above Figure 39 depicts another indicator of the impact of the metal wool on the magnitude of convection. A comparison of the wax only module to the metal wool cases shows that the PCM transitions from solid to liquid more quickly in the only wax module compared to the modules with metal wool. As explained before, convection plays an important part in driving the melting process in the wax only module. It is reasonable to assume that the reduced flow velocities of the liquid PCM, caused by the interference of metal wool, weakened the effects of natural convection, prolonging the time needed for the PCM at TC 15 to melt.

The plot also shows that the temperature for the wax only module has a slightly different profile in the beginning compared to the other cases. After the slight decrease in temperature at the beginning of the experiment, the temperature rapidly increases, then decreases, then rapidly increases again. When observing the experiment, it was found that the phase transition occurs at the second rise of the temperature (~t = 5000s), and therefore the first rapid temperature rise was unexpected.

Additional tests were conducted to investigate this unexpected behavior observed during the charging experiments. Upon closer inspection, it was observed that voids were formed in the PCM near the center of the module (around TC 15) after the discharging process. When the charging process began, liquid PCM filled these voids, thus pre-maturely increasing the temperature of the PCM near TC 15 leading to a sudden increase in temperature. This phenomenon explains the initial rapid temperature rise observed in TC 15 during charging.
Figure 40: Images of solid PCM at time t=0 and t=1200s of charging experiment showing voids in PCM.

This hypothesis was confirmed by allowing the PCM to slowly solidify to avoid void formation by letting it sit and cool for about 12.5 hours, keeping it insulated, and allowing heat losses to cool the PCM. Figure 41 (a) shows a plot of the PCM temperature at TC 15 versus time which illustrates that the slow discharge of the module (blue) followed by the normal charging of the module (orange) eliminated that sharp temperature rise, thus confirming that the rapid temperature rise observed earlier is associated with the formation of voids during freezing. Figure 41 (b) shows an image of the PCM at the end of the slow discharge process, and it is seen that the surface is much more uniform with no voids.
3.2.5 Characterization of the underlying physical process during solidification (discharging)

The discharging process inside the wax only module is visually illustrated in Figure 42. It is important to note that these images were taken during the discharging experiment in which the starting condition of the PCM was not isothermal. Rather, a temperature gradient of about 10-15 degrees was present where the top of the domain was hotter than the bottom of the domain. The analysis of the image sequence shows that at the 10 minute mark, the solidification begins at the tube surface where solidification progresses slightly faster at the bottom of the tubes than at the top. This is likely a result of the initial thermal gradient inside the domain as mentioned above. Since the bottom of the domain is slightly cooler than the top, less sensible heating is required before a change in phase, thus accelerating the solidification in this region. As time progresses, the solidified region grows relatively uniformly, and after about 110 min, the PCM is fully solidified.

During discharging, the total thermal resistance between the HTF and the PCM consists of a convective resistance between the HTF and the inner surface metal tube, a conductive resistance through the metal tube, a conductive resistance associated with the enhancement
element, and a conductive resistance through the solid PCM. Relating the discharging process to the performance of the heat transfer enhancement elements, in the case of the aluminum honeycomb, the aluminum structure once again effectively conducted the heat from the PCM to the tubes. The large uniform surface (finned) area of the aluminum structure reduced the conductive resistance within the PCM compared to the benchmark case. In addition, solidification first begins at the surface of the heat sink, and the large uniform surface area of the honeycomb allowed the PCM to solidify at the fin surface. Since the honeycomb cells were small, it did not take a long time for the PCM in each cell to solidify.

For the metal wool module, while the solidification process is conduction dominant, the aluminum wool exhibited reduced heat transfer rates approximately 1.5 times lower than that of the aluminum honeycomb. This is likely a result of the aluminum honeycomb having a larger, more uniform surface, interacting with the PCM thus accelerating the solidification process as compared to the aluminum wool.
Figure 42: Images showing the solidification process of the wax only module at various times during the discharging process.
3.2.6 Outlet HTF Temperatures in Discharging

Figure 43 illustrates the time history of the outlet fluid temperature during discharging for all four module cases at a flow rate of 0.2 kg/min. The data show that the aluminum honeycomb module caused the highest temperature rise of water, with an average increase of about 10 degrees. Following closely is the aluminum wool module, which raised the water temperature by an average of approximately 6 degrees. The steel wool proved to be the least effective, increasing the outlet temperature by about 3 degrees, only slightly higher than the wax-only module, where the water temperature increased by about 2 degrees. These findings are consistent with the results observed in discharge time and heat transfer rate, providing a coherent pattern of performance across the different enhancement elements (refer to Table 13, and Figure 37).

![Outlet temperature versus dimensionless time comparing each module during a discharging experiment at a mass flow rate of 0.2 kg/min.](image)

3.2.7 Mass Flow Rate Analysis

The aluminum honeycomb, aluminum wool, and wax only modules were tested at three other mass flow rates to study the impact of mass flow rate on the module performance. Figure 44 presents the heat transfer rate versus dimensionless time at various flow rates for the three module designs. Each plot represents the heat transfer rate for a given module.
during either charging or discharging, where a positive heat rate represents heat transferred from the HTF to the PCM (charging), and a negative heat rate represents heat transferred from the PCM to the HTF (discharging).

Analysis of the results show that, in general, the mass flow rate is directly proportional to the heat transfer rate, as higher flow rates lead to a higher heat transfer rate. This result is expected because a higher mass flow rate implies the HTF has less time to heat up as it passes through the module, resulting in a hotter heat source and an increase in temperature difference between the PCM and the HTF. However, upon further analysis of the results, it is evident that the mass flow rate did not drastically change the heat transfer rates. On average, there was about a 20% increase in heat transfer rate when increasing the mass flow rate from 0.1 kg/min to 0.6 kg/min, which is not significant, considering the mass flow rate increases by a factor of six.

Heat transfer rates are inversely proportional to charge and discharge times, as higher rates lead to shorter times. Table 14 and Table 15 display the percent decrease in charge and discharge times, respectively, for each module type at the two extreme mass flow rates considered in this study i.e. the mass flow rates of 0.1 kg/min and 0.6 kg/min. From the results, it is evident that the mass flow rate does not significantly impact the charge and discharge times, as the maximum percent decrease in charge and discharge times was 22%.

Table 14: Comparison of charge times using a mass flow rate of 0.1 kg/min versus 0.6 kg/min for each module type.

<table>
<thead>
<tr>
<th>Module Type</th>
<th>Charge Time 0.1 kg/min (s)</th>
<th>Charge Time 0.6 kg/min (s)</th>
<th>Percent decrease (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aluminum Honeycomb (AH)</td>
<td>6664</td>
<td>5162</td>
<td>22</td>
</tr>
<tr>
<td>Aluminum Wool (AW)</td>
<td>12653</td>
<td>10231</td>
<td>19</td>
</tr>
<tr>
<td>Only Wax (OW)</td>
<td>19541</td>
<td>16125</td>
<td>17</td>
</tr>
</tbody>
</table>
Table 15: Comparison of discharge times using a mass flow rate of 0.1 kg/min versus 0.6 kg/min for each module type.

<table>
<thead>
<tr>
<th>Module Type</th>
<th>Discharge Time 0.1 kg/min (s)</th>
<th>Discharge Time 0.6 kg/min (s)</th>
<th>Percent decrease (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aluminum Honeycomb Core (AH)</td>
<td>2748</td>
<td>2193</td>
<td>20</td>
</tr>
<tr>
<td>Aluminum Wool (AW)</td>
<td>4432</td>
<td>3697</td>
<td>16</td>
</tr>
<tr>
<td>Only Wax (OW)</td>
<td>9858</td>
<td>9053</td>
<td>8</td>
</tr>
</tbody>
</table>
Figure 44: Plots of heat transfer rate vs dimensionless time showing the impact of varying the mass flow rate for a particular module in charging and discharging showing i) aluminum honeycomb charging, ii) aluminum honeycomb discharging, iii) aluminum wool charging, iv) aluminum wool discharging, v) wax only charging, vi) wax only discharging.
3.2.7.1 Impact of Mass Flow on Outlet Fluid Temperature

Another important parameter to consider, especially during discharging, is the outlet fluid temperature of the module. As stated in the previous chapter, as water flows through the thermal storage system, its temperature should be sufficiently heated in order to meet the hot water demands in a domestic residential unit dwelling. In this current study, a single small scale module is being analyzed, so it is not expected that this will be able to provide all the heating requirements. However, analyzing the relationship between the outlet fluid temperature and the mass flow rate can be beneficial in implementing this concept to a larger scale application.

Figure 45 shows the fluid temperature rise versus time for each module at each flow rate. The temperature increase was calculated as the difference between the outlet fluid temperature (TC7) and the inlet fluid temperature (TC0). Each plot represents the flow rates for a given module design. Analysis of the plots shows that in all cases the HTF temperature rise decreases with time. This is an expected behavior because as time progresses, the module is being discharged of its thermal energy and heat is being transferred from the PCM to the HTF. As the PCM loses its thermal energy, part of the energy lost is sensible heat resulting in a decrease in average PCM temperature, and thus, a decrease in heat transfer between the PCM and HTF.

In all plots, it is also seen that a lower mass flow rate leads to a larger HTF temperature rise. This result is expected since a lower mass flow rate means the fluid has more time to heat up as it passes through the module. On average, it is seen that decreasing the mass flow rate from 0.6 kg/min to 0.1 kg/min increases the outlet fluid temperatures by about a factor of 5 in all modules.
Figure 45: Plots of temperature rise vs time at various flow rates for the module containing i) aluminum honeycomb core, ii) aluminum wool, and iii) only wax.

Figure 46 shows plots of the temperature rise comparing each module type at a mass flow rate of 0.1 kg/min, and 0.6 kg/min. Across these flow rates, the temperature rise in the AH module was about 4 times higher than the benchmark case, and the temperature rise in the AW module was about 3 times higher than the benchmark case. Similar findings were observed at flow rates of 0.2 kg/min and 0.4 kg/min.
Figure 46: Plots of temperature rise vs time comparing the outlet temperature between different modules at a flow rate of i) 0.1 kg/min, and ii) 0.6 kg/min.

In summary, it is seen that the mass flow rate through the module does not significantly impact heat transfer rates and charging and discharging times, however, it plays a crucial role in controlling the outlet fluid temperature from the module.

3.2.8 Comparison of Computational and Experimental Results

In Chapter 2, numerical simulations were conducted on various module designs to estimate the performance of the thermal storage module without any heat transfer enhancements. The following section is included to compare the computational results to the experimental results to identify features that the enthalpy porosity predicts well, as well as its limitations. Figure 47 shows the computational domain with the labeled inlets and outlets as presented in Section 2.3.7.

Two tests will be compared. The first test will compare a melting case in which the domain is initialized at room temperature (23°C), and fluid passes through the module at 80°C until the temperature at TC 15 equals 60°C. The second test compares the discharging case which has the same start and end conditions as the discharging cases described in this chapter (see Table 11).
Figure 47: Image showing the design of the small scale thermal storage module indicating locations of the inlets and outlets (left), and a representation of the computational domain (right).

**Melting**

Figure 48 displays the computational and experimental HTF temperature at outlet 4 of the module. Analyzing the plot shows that there is good agreement between the computational and experimental melt times as there was a 5% difference between these two results. In addition, it is seen that the computational simulation shows good agreement with the outlet fluid temperature in the initial stages of the melting process, however, towards the end of the melting process it underpredicts the temperature drop. This difference in outlet fluid temperature towards the end of the melting process is likely due to heat losses from the thermal storage module in the experimental case. Heat losses from the external walls result in more energy needed to overcome heat losses and melt the PCM and, therefore, it is plausible that this could result in higher outlet fluid temperatures. The computational simulation set all external walls to have an adiabatic condition, and it is predicted that the outlet fluid temperatures at the end of the melting process would more closely resemble the experimental results if heat losses were accounted for.

The heat transfer into the PCM from the HTF was calculated using the following equation:

\[
Q_{in} = \int m \ c_p (T_{out} - T_{in}) \ dt
\]  

(3.3)
where $\dot{m}$ is the mass flow rate of the HTF, $c_p$ is the specific heat of the HTF, $T_{out}$ is the temperature at the outlet of the module, and $T_{in}$ is the temperature at the inlet of the module.

In the experimental study, heat losses were estimated using the temperature data collected from TC 12 and TC 13 (see Figure 32) which were placed on the inside and outside of the acrylic enclosure. Therefore, heat losses were estimated using the conduction equation across the acrylic wall as follows:

$$Q_{out} = \int \frac{k A (T_{TC12} - T_{TC13})}{L} \, dt$$ \hspace{1cm} (3.4)

where $k$ is the thermal conductivity of the acrylic, $A$ is the surface area of the module enclosure, $T_{TC12}$ and $T_{TC13}$ are the temperatures at locations TC12 and TC13 respectively with reference to Figure 32. The net heat transfer into the PCM can be calculated using the following equation:

$$Q_{net} = Q_{in} - Q_{out}$$ \hspace{1cm} (3.5)

Table 16 shows a summary of the net heat transfer into the PCM in which a theoretical, computational, and numerical approach was used for the calculation. The theoretical net heat transfer was calculated using the total energy (sensible + latent) required to heat the mass of PCM from 23°C to ~70°C, the computational result was calculated using Equation 3.3, and the experimental value was calculated using Equation 3.5. Comparing the net heat transfer into the PCM using Equations 3.4 and 3.5, it is seen that there is good agreement between the theoretical and computational results with a difference of 5%. It is also seen that there is a 26% difference between the theoretical and experimental calculations. One reason for this difference could be that the heat losses were approximated using the temperature difference at one point of the acrylic enclosure. This singular temperature difference was considered to represent the average temperature difference and used to approximate conduction losses through the entire acrylic box.
Table 16: Summary of the net heat transferred into the PCM for each calculation type during melting.

<table>
<thead>
<tr>
<th>Type</th>
<th>Net Heat Transfer into PCM (kJ)</th>
<th>Percent difference from theoretical (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>422</td>
<td>-</td>
</tr>
<tr>
<td>Computational</td>
<td>442</td>
<td>5</td>
</tr>
<tr>
<td>Experimental</td>
<td>550</td>
<td>26</td>
</tr>
</tbody>
</table>

Figure 48: Comparison between computational and experimental HTF temperature at Outlet 4 of the module.

Figure 49 compares simulated melt fraction contours to experimental images of the melt fraction at various dimensionless times. Analysis of the figure shows that there is good agreement between the simulated and experimental melt fractions at each dimensionless time.
Figure 49: Comparison of simulated and experimental melt fraction contours at various dimensionless times.

Overall, it is seen that the enthalpy porosity model performed relatively well at simulating the melting process inside the thermal storage module. Although there is a discrepancy in the outlet fluid temperature, it is predicted that the computational simulation could more closely resemble the experimental results if heat losses were considered.
**Solidification**

Figure 50 shows a plot comparing the outlet fluid temperature of the module between the experimental and computational studies. Analyzing the plot shows that there is a large discrepancy between the computed and experimental discharge times. Outlet fluid temperatures in the experimental runs were higher than the predicted computational fluid temperatures, and experimental discharge times were shorter than the predicted computational discharge time. Table 17 shows a summary of the theoretical, computational, and experimental net heat transfer in the PCM. The net heat transfer for the computational and experimental cases were determined to be 353kJ and 286kJ, respectively. This means that there is a 21% difference between the experimental and computational energy transfer. It was estimated that it should (theoretically) take about 335kJ to discharge the PCM, which is 5% less than the computational energy transfer, and 16% more than the experimentally determined energy transfer. The same material properties were used in the computational and theoretical calculation, so it makes sense that these results have good agreement. One reason for the discrepancy with the experimental case could be due to the way that heat losses were approximated (similar to the melting case). In addition, the material properties for the Polyfin PCM are not well documented, and it is possible that there was a discrepancy between the value used for the latent heat of fusion. Looking at material properties for a similar well documented PCM called RT55 [75], which is a paraffin wax with a phase transition temperature of 55°C, it does not explicitly state the latent heat of fusion but rather specifies a value called heat storage capacity. This heat storage capacity is defined as a combination of sensible and latent heat in a temperature range of 48°C to 63°C, and it has a value of 170 [kJ/kg], meaning the latent heat of fusion is ~150 kJ/kg. Therefore, it is possible that the latent heat for Polyfin could be lower than the value 180 [kJ/kg] thus contributing to a difference in total energy transferred between the PCM and HTF.
Table 17: Summary of heat transferred between the HTF and PCM for each calculation type during discharging.

<table>
<thead>
<tr>
<th>Type</th>
<th>Total Heat Transfer (kJ)</th>
<th>Percent difference from theoretical (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>335</td>
<td>-</td>
</tr>
<tr>
<td>Computational</td>
<td>353</td>
<td>5</td>
</tr>
<tr>
<td>Experimental</td>
<td>286</td>
<td>16</td>
</tr>
</tbody>
</table>

Figure 50: Plot comparing the computational to experimental temperature at (a) outlet 4, and (b) all outlets.
Figure 51 shows a plot of the outlet fluid temperature versus dimensionless time. Since time is scaled, a correction factor is also applied to the heat transfer rate to preserve the total energy being absorbed by the PCM. This correction factor is simply the ratio of the simulated and actual discharge times and takes the following form:

$$ C_f = \frac{t_{CFD}}{t_{Exp}} $$  

(3.6)

where $C_f$ is the correction factor, $t_{CFD}$ is the computational discharge time, and $t_{Exp}$ is the actual discharge time recorded during the experimental test. This correction factor was multiplied by the heat transfer rate as follows.

$$ \dot{Q} = \dot{m} c_p (T_{outlet} - T_{inlet}) $$  

(3.7)

$$ \dot{Q}_c = C_f \dot{Q} $$  

(3.8)

where $\dot{Q}$ is the computational heat transfer rate, $\dot{m}$ is the mass flow rate, $c_p$ is the specific heat capacity, $T_{outlet}$ is the outlet fluid temperature, $T_{inlet}$ is the inlet fluid temperature, and $\dot{Q}_c$ is defined as the corrected heat transfer rate.

The corrected heat transfer rate was then used to determine the corrected computational outlet fluid temperature using the following equation:

$$ T_{o,c} = \frac{\dot{Q}_c}{\dot{m} c_p} + T_i $$  

(3.9)

where $T_{o,c}$ is the corrected computational outlet fluid temperature.

Figure 51 shows a plot of the corrected computational outlet fluid temperature, and experimental outlet fluid temperature versus dimensionless time. Analysis of the plot shows that there is good agreement between these temperatures.
Figure 51: Plot of corrected numerical outlet fluid temperature to the experimental outlet fluid temperature in dimensionless time.

Figure 52 compares simulated melt fraction contours to experimental images of the melt fraction at various dimensionless times. Analysis of the figure shows that there is good agreement between the simulated and experimental melt fraction at each time.
In summary, it is seen that when looking at absolute values of the simulation results for discharging, the results do not show good agreement with experimental data. However, contour plots show reasonable agreement in terms of the melt shape; and heat flux predictions scaled by the ratio of computed to experimental freezing time yield good predictions of the outlet temperature. This implies that the enthalpy porosity model is capable of predicting important features of the freezing process.
3.3 Conclusions

The present study investigated four small-scale Phase Change Material (PCM) based thermal energy storage modules to investigate the impact of different heat transfer enhancement elements. Three types of elements including an aluminum honeycomb structure, aluminum wool, and stainless steel wool were considered. Each module had equal PCM mass and equal volume of heat transfer enhancement elements, ensuring a fair comparison between the designs. An experimental setup was constructed to study and analyze each module during the charging and discharging processes. In charging experiments, water at 80°C was supplied through the module in four passes to melt the PCM, increasing its temperature from ~50°C to ~60°C. During discharging experiments, water at 10°C was provided to the module to freeze the PCM, decreasing its temperature from ~60°C to ~50°C.

The study analyzed various parameters such as heat transfer rate, charging/discharging time, and outlet fluid temperature. When comparing the heat transfer enhancement elements, the aluminum honeycomb module consistently outperformed the other modules, followed by the aluminum wool module and then the stainless steel wool module.

This study highlighted the importance of natural convection in the melting process of the PCM. The introduction of metal wool into the module caused suppression of natural convection which impacted the module performance when both stainless steel wool and aluminum wool were implemented. The main reason for the superior performance of the aluminum honeycomb was due to its ability to facilitate natural convection in small localized cells despite dividing the module into numerous small but tall cells. The honeycomb structure offered uniform vertical surfaces, enabling the melting process to commence, and allowing natural convection to occur in each individual cell thereby accelerating the melting process. This approach was proven effective based on the observed heat transfer rates, charge times, and outlet HTF temperatures.
In addition, a comparison between the computational and numerical results determined that the calibrated numerical model was good at simulating the physical process of the melting and solidification simulations. However, for the discharging process, to get a better representation of parameters such as heat transfer rate, and outlet fluid temperatures, scaling needed to be done.
Chapter 4

4 Conclusions and Recommendations

4.1 General Conclusions

Thermal energy storage is a promising technology that will play an important role in the world’s transition to a sustainable future and reduce our reliance on fossil fuels. Thermal storage systems offer the ability to make use of solar and wind energy at all times of the day, thus making it a reliable and consistent source of energy. Latent heat thermal storage systems offer advantages over traditional sensible heat systems as they can have high energy storage densities by taking advantage of the latent heat of fusion associated with phase change. However, the main issue with phase change materials (PCMs) used in latent heat thermal storage systems is they often suffer from low thermal conductivities making it difficult to achieve suitable charging and discharging rates.

The present research work focused on investigation of a modular thermal energy storage system in which modules could be combined to meet the thermal storage capacity needs of its application. To accomplish this, a numerical and computational approach was taken.

To accurately simulate the phase change process, calibration of two key parameters was performed. These parameters included the Mushy Zone Constant and the Thermal Expansion Coefficient. These parameters were important in characterizing the interaction between the solid and liquid regions of the PCM, as well as characterizing the combined effect of all properties changing through the melting process to yield the correct intensity of convection. Calibration of these parameters consisted of an iterative approach in which various numerical values were tested, and the results were compared to a physical reference experiment in order to determine the validity of the results. The outcome of this section resulted in a calibrated numerical model that had good agreement with the reference experiment.

The calibrated numerical model was used to analyze various concepts of thermal storage modules. Each concept had a fixed mass of PCM, as well as a fixed cross-sectional area,
and the number of tubes and spacing between tubes were varied to determine their impact on outlet fluid temperatures during discharging of the module. In addition, each tube configuration was tested with and without the use of fins to compare how fins can be used to further increase outlet fluid temperatures. Throughout all cases, simulations were performed on a single section of one module, however, a method was introduced in which the computational results were used to estimate the outlet fluid temperature after multiple modules. This approach involved using the overall heat transfer coefficient derived from simulations combined with log mean temperature correlation to describe internal pipe flow with a constant surface temperature. Using this approach, it was determined that the overall heat transfer coefficient was independent of the number of fluid passes, and could therefore be used to predict the outlet fluid temperature after $n$ fluid passes, or more specifically, $n$ modules. The outcome of this section resulted in a successful study of the various thermal storage module concepts, and the results were used to design a small-scale benchtop module for experimental testing.

Experimental studies were carried out on the small-scale benchtop thermal storage module. This study focused on experimentally investigating various heat transfer enhancement techniques, and how they affect charging and discharging rates of the thermal storage module. Four modules were constructed, each with 1.25kg of PCM. Three of the modules included heat enhancement techniques, which included a finned aluminum honeycomb structure, aluminum wool, and stainless-steel wool. Each module was outfitted with 16 thermocouples to capture transient temperature data for analysis of module performance. Comparisons were made by analyzing parameters such as charge/discharge time, charge/discharge rate, and outlet working fluid temperature. Analysis of all results showed that the module with the finned honeycomb structure performed best followed by the aluminum wool, then the stainless-steel wool.

The experimental study highlighted the importance of allowing convection to occur inside the thermal storage module. The increased performance of the finned honeycomb structure in charging was a result of the formation of natural convection within small localized regions thus accelerating the melting process. In the present study, only one honeycomb structure was investigated which had a relatively small cell size of 4.76mm (3/16”). Due
to this small cell size, the structure greatly restricts the lateral extend of the convective motion induced by natural convection. Given the importance of natural convection in the melting process, it is speculated that increasing the cell size might promote the formation of stronger convective currents which could improve heat transfer (i.e. charging) rates. However, increasing the cell size reduces the finned surface area that conducts the heat between the PCM and the heat source, which could decrease the performance of the module. This indicates that there might be a tradeoff between the cell size and the charging/discharging rate. Therefore, this aspect requires a more in depth investigation in order to determine the impact of cell size on charge and discharge rates.

Finally, it was seen that in the two modules containing metal wool, the addition of metal wool obstructed the growth of convective motions within the liquid PCM resulting in reduced heat transfer rates during charging. In addition, although discharging is dominated by conduction heat transfer, the aluminum wool module had heat transfer rates about 1.5 times less than the aluminum honeycomb, and this was likely a result of the honeycomb providing a much larger and more uniform surface area in contact with the PCM thus accelerating the discharging process.

4.2 Contributions

1) The experimental study showed that the introduction of a densely packed finned structure channels heat into the PCM from the water tubes, but greatly restricts the motion of melted PCM in one or all directions. This study found that while an aluminum honeycomb structure restricts convection in the lateral direction, it allows for natural convection in the vertical direction within small, localized cells which proved to be extremely effective in enhancing heat transfer during charging and discharging.

2) Comparison of the honeycomb structure with an equivalent volume of steel wool or aluminum wool showed that the honeycomb structure was superior in terms of heat transfer enhancement. The main difference is that the metal wools restrict convective motions in both the lateral and vertical directions, which results in significant suppression of convection. This study found that the suppression of natural convection due to the metal
wool resulted in a decreased performance when compared to the aluminum honeycomb module.

3) This study also showed that a calibrated enthalpy-porosity model was capable of predicting the main features of both melting and freezing of polyfin in a bench scale thermal storage module. The present experimental research provided an opportunity to test this approach and identified the strengths and limitations of the calibrated enthalpy porosity model.

4.3 Future Work

The present study determined that a finned honeycomb structure was the best method for improving heat transfer rates than metal wool in a small-scale thermal storage module. There are many aspects related to this that could be further explored to optimize the design of a thermal storage module.

1) Analyze different cell sizes in the honeycomb structure and other vertical finned structures.

In the present study, a cell size of 4.76mm (3/16”) was used. Due to the restricted natural convection in the lateral direction, it may be possible that there exists an optimal cell size in which the maximum performance occurs. A detailed investigation of cell size would be beneficial in determining the optimal design for the thermal storage module. In addition, vertically finned tubes are a commercially available product that could enhance the performance of the thermal storage module similar to the aluminum honeycomb core. Therefore, it is recommended that these also be explored in future work.

2) Investigate different tube diameters.

In the present study, a tube diameter of 6.35mm (0.25”) was studied in both the computational work and the experimental work. A detailed investigation into the tube diameter could help further optimize the design.
3) Analyze different PCMs.

In the present study a PCM called Polyfin was used for analysis. This PCM is a paraffin wax with a phase transition temperature of 55°C. This study could be further continued to study various paraffin waxes with different melting temperatures. Additionally, different types of PCMs, such as salt hydrates, could also be analyzed. Lastly, a cascading system could be analyzed in which modules are arranged in series, each with a PCM with a different phase transition temperature. This method would maintain a constant temperature difference between the HTF and the phase transition temperature of the PCM. This approach could improve the efficiency of the system.
References


[71] B. Buonomo, D. Ercole, O. Manca, and S. Nardini, “Numerical investigation on thermal behaviors of two-dimensional latent thermal energy storage with PCM and


Curriculum Vitae

Name: Luca Matthew Crnjac

Post-secondary

MESc Mechanical Engineering – Thermofluids
Education and Degrees: University of Western Ontario

BESc Mechanical Engineering
University of Western Ontario

Honours and Awards:
Ontario Graduate Scholarship (2023-2024)
Ontario Graduate Scholarship (2022-2023)
Dean’s Honor List (2021-2022)
Dean’s Honor List (2019-2020)
Dean’s Honor List (2018-2019)
The Western Scholarship of Excellence (2017)

Related Work Experience
Teaching Assistant – Fluid Mechanics II (MME 3303)
The University of Western Ontario. Fall 2023

Teaching Assistant – Engineering Experimentation (MME 2285)
The University of Western Ontario. Winter 2023

Teaching Assistant – Thermodynamics I (MME 2204)
The University of Western Ontario. Fall 2022