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Modeling of Flow and Thermal Energy Transport for High and Low Temperature Applications with Thermal Energy Storage

by

Ruth Herrera Reed

A dissertation submitted in partial satisfaction of the requirements for the degree of

Doctor of Philosophy

in

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in the

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of the

University of California, Berkeley

Committee in charge:

Professor Van P. Carey, Chair
Professor Ömer Savaş
Professor Per Peterson

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Modeling of Flow and Thermal Energy Transport for High and Low Temperature Applications with Thermal Energy Storage

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Ruth Herrera Reed
Abstract

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Doctor of Philosophy in Mechanical Engineering

University of California, Berkeley

Professor Van P. Carey, Chair

Maximizing the collection temperature maximizes the thermodynamic performance of subsequent energy conversion processes. A 3D model simulation using computational fluid dynamics (ANSYS) was used to assess the heat transfer from the molten glass to incoming air at ambient temperature. A system model was developed to simulate an experimental helical coil counter-flow test heat exchanger. The molten glass is also implemented as a falling thin film (< 3mm) to absorb thermal energy at a concentrating solar power plant. The phosphorous pentoxide glass flow is treated as a laminar, Newtonian and gravity-driven flow over a slightly inclined flat plate using an explicit finite difference scheme to evaluate its heat transfer performance for a concentrating solar power plant. In the cold regime (30 °C), a transient cold storage unit that uses solid-liquid phase change for thermal storage. Computational fluid dynamics (Fluent-ANSYS) was used to model the phase change behavior of lithium nitrate trihydrate (LiNO$_3$3H$_2$O) by modeling a unit cell of a thermal energy storage heat exchanger. In this analysis, the time required to input thermal energy (melt) the phase change material is calculated to assess its heat transfer performance. By modeling different unit cell domains, the overall heat transfer coefficient and mean conductance are calculated for two different heat exchanger designs.
To My Parents,

Initially they did not like the idea of my spending a long time in school, but they were always supportive at the end. Without their support, I would not have made it this far.
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Chapter 1

Introduction

1.1 Motivation of High Temperature Heat Collection and Thermal Energy Storage

Greenhouse gas emissions increments parallel with energy demand are the main driving forces to all the efforts to find various sources of renewable energy that can perform efficiently to match fossil fuel based power sources. Studies show that by 2050, energy-related emission of CO₂ will double by 2050. Finding ways to make renewable energy technologies more efficient is key to prevent major irreversible catastrophic damage to the environment. Based on the increasing demands of energy, the trends indicate that by the year of 2050, CO₂ emissions will increase by about 50% of its current amount [42].

One of the most prospective sources of energy is the conversion of solar energy to electricity, and many scientists around the world are in search of improving this technology to potentially implement it to applications that generate the highest greenhouse gases.

Another important aspect to develop and make these technologies more reliable is to develop energy storage devices. An appropriate storage system can convert the stored energy into another form, but it is still a challenge to make efficient and work in simple manner. Nevertheless, energy storage is vital to reduce the mismatch between energy demand and supply and to improve the performance and reliability of many energy systems. It allows to make the system lower in cost and reduce energy losses.

**High Temperature Collection and Storage Example Application: Concentrating Solar Power**

Among all solar power technologies, concentrating solar power (CSP) plants show promising paths to produce higher efficiency solar based electrical power. Mainly, CSP technologies are very striking in countries with long periods of sunshine and clear skies. When designed along with an appropriate storage and combustible fuel, it can supply electricity power when needed, especially at peak loads (night time). It is expected that with the improvement of
renewable energy based technologies, they could potentially match coal plants energy supply performance.

The performance of CSP is enhanced in areas with higher DNI levels. These areas are most favorable in North Africa, southern Africa, the Middle East, northwestern India, the western region of China and Australia, Chile, Mexico, Peru, and the southwestern United States.

The potentials of CSP technologies are huge and could aid in the global goal of CO$_2$ emissions reductions by 2050. For example, if CSP are fully implemented in the southwestern US states, the electricity demands would be met for the entire United States. So far, most CSP suffer their implementation due to their high cost (compared to photovoltaic solar systems), their efficiency and reliability. The reliability issue of CSP technologies is improved by implementing a thermal storage unit. Due to the high variation of sunlight (even in the sunniest areas), electrical power cannot be generated all the time to meet the demand curves. Therefore, having backup (similar to a battery system) is key to increase the implementation of CSP technologies. The system works in a simple way: throughout the day, the heated fluid is collected at a designed high temperature to generate electricity immediately and any excess of heated fluid is sent to a storage tank for later electrical power generation when electricity power is required after sunset [27].

![Figure 1.1: Concentrating Solar Power Plant Schematic with Thermal Energy Storage Unit.](image)

CSP systems are mainly composed of a field of heliostats which are mirrors that reflect light rays of sun into a point known as the receiver. The receiver, located at the top of the tower, is where the heat transfer fluid runs and get heated (See Fig.1.2). The receiver is the
main entrance of the thermal energy that passes from the field collection to the thermal-electrical cycle. Some challenges of the receiver is to withstand high heat fluxes (up to 1 MW/m²) and run safely without having a limitation of the incident fluxes concentrated by the heliostat field at their maximum performance. Many factors play an important role to achieve high performance of the receiver: geometry (optimal dimensions), thermodynamic behavior (heat transfer fluid performance) and material selection of the receiver. One main challenge of designing an optimal receiver is to minimize its thermal losses. These thermal losses are due to phenomena, such as, reflection, radiation, convection and conduction. The thermal losses are mainly minimized by reducing the area of the receiver which is exposed to the incoming solar flux. In conventional receivers, the working heat transfer fluid runs through tubes from the top of a manifold and gets collected at high temperatures. Receivers could be internal (located in a cavity) and external (circumferential shape).

Along CSP technologies, other applications, such as fuels and chemicals, industrial power heating, electrical power production, concentrated solar power and thermal energy storage can improve their overall thermal efficiency if their collection temperature is higher than 850°C. For example, the maximum operational temperature reached by an eutectic carbonate mixture of molten salt is about 580°C leading to a maximum cycle efficiency (Carnot cycle) of 64.5%. However, if a heat transfer fluid can reach a maximum operational temperature of 1000°C, the maximum cycle efficiency increases to 76.2%. Reaching high temperatures (above 850°C) is very desirable since it improves the efficiency of power production system and leads to a reduction in size and cost of the thermal storage system.

Other factors limiting the maximum cycle efficiency is the gas cycle used in an electrical power plant. Current electrical power plant rely on the Rankine cycle. Steam being the main fluid that runs through the turbines that generate electricity, can safely reach a maximum temperature of 600°C. A super-critical CO₂ Brayton cycle has been looking more attractive even though is currently not in the low-cost range as compared to other power cycles. Not only in the solar industry, but also in the nuclear and geothermal sectors, sCO₂ Brayton cycles are making their way to improve high temperature power generation. In a study by Iverson at al. [21], a prototype sCO₂ power cycle under transient operating conditions similar to a solar power plant was tested. Although the operating temperature conditions and pressures are lower to the real case model or desired model for high efficiency achievement, the data collected in the prototype was used to validate large scale systems by pointing out the main areas of mechanical and thermal losses in the advancement of sCO₂ Brayton turbomachinery for solar applications. Although efficiencies of the sCO₂ were below the expected 50%, the limitations were mainly due to the scaled-down prototype power cycle.
CHAPTER 1. INTRODUCTION

Direct Absorption Receivers

In a CSP, the place where the heat transfer fluid absorbs and gains thermal energy is called receiver. There are many designs of receivers, and in the original receiver design, the heat transfer fluid is enclosed in tubes which conduct the heat transfer fluid to the top of the tower and from the top to the bottom when it is at a higher temperature and gets collected for storage or sent to a heat exchanger to produce electrical power [53]. The radiation heats up the outer walls of the tubes, and then it is transferred to the heat transfer fluid by conduction at the wall and convection into the heat transfer fluid. This design does not allow to heat up the fluid to the higher temperature since it gets through the walls of the tubes, some energy loss takes place by absorption of the incoming energy in the tube material, and in consequence, this does not allow efficient heat transfer between the incoming concentrating solar flux and the heat transfer fluid. To improve thermal efficiency, it is important to increase the source temperature encouraging the motivation to use receiver designs that can potentially reduce thermal energy losses [54].

Another concept of the concentrating solar receiver is the direct absorption receiver (DAR) [52]. In this design, the heat transfer fluid is falls over a flat surface and is directly exposed to the incoming solar flux getting maximum temperature rise as it falls. It has been demonstrated that DAR designs as concentrating solar receivers along with thermal storage can be more efficient than other conventional heat exchanger designs (e.g. water-steam heat exchanger) since it has the ability to reach higher outlet temperatures [52]. It also has higher heat losses, especially due to radiation heat transfer with the environment, but it can overcompensated by the net gain thermal energy in the power block efficiency resulting in a higher overall efficiency of the system [23].

There are several design of DARs. Wu et al. [53] studied three different concepts of DAR. Their first concept uses a liquid falling film (molten salt) where the receiver has a shape of a facing-down cylindrical barrel. The second and third concept use small particles instead of the liquid falling film. The second DAR concept has the face-down cylindrical barrel, whereas, the third DAR concept includes a centrifugal acceleration allowing the solid particles to rotate as they heated by the incoming solar flux. The study calculated annual performance using a software called HFLCAL. In their studies, the included convective and radiative losses. The operational temperature depended on the heat transfer medium. The range of the operational temperature for the molten salt was between $385^\circ C$ to $620^\circ C$. The solid particles reached a maximum temperature of $1000^\circ C$. From their studies, it was concluded that the liquid falling film receiver had the highest efficiency (94.5 %) compared to the solid particles falling (90 % and 83 %) respectively.

Molten glass as a Heat Transfer Fluid

A main key component to improve the overall efficiency of the system is to find the appropriate heat transfer fluid that can reach very high temperatures and remain as a liquid at atmospheric pressure. Molten salt has been investigated in multiple studies analyti-
cally and experimentally for direct absorption receivers showing promising performance over water-steam. However, it has some design limitations, such as not being able to reach temperatures higher than 900°C, corrosive behavior at this temperature and stability issues at higher low flow rates. Meanwhile, there is a strong research active area to find heat transfer fluids that solve current challenges.

A novel material to explore as a heat transfer fluid is molten glass. Glass is commonly known as one of the most abundant material on the earth's crust due to its composition, basically mixture of oxides. Oxide glasses contain certain attractive characteristics to face the challenges by current heat transfer fluids. Most glasses have a high thermal stability at high temperatures[34]and [35]. In addition, oxides have low vapor pressures which makes them appealing for designs of thermal systems and storage tanks [13].

A certain type of novel oxide glass material is chosen to be investigated to be used as a heat transfer fluid in a solar power plant. This novel material was developed at the Halotechnics facilities using their combined chemistry R&D [12]. This oxide glass material has as its base component phosphorous pentoxide (P₂O₅), and it met important criteria to become a potential heat transfer fluid and thermal energy storage material for a high collection temperature system.
1.2 Previous Studies Related to High Temperature Collection Thermal Energy

Many previous studies have been performed to assess the collection in the high temperature operational temperature range. The studies include understanding the performance of the heat transfer fluids and their highlights in their performance. In addition, I summarize the implementation of DARs. Several studies use this receiver design as their case study to collect high temperature thermal energy. Most of these studies were performed experimentally and analytically. Finally, I go through an overview of what current techniques to enhance the heat transfer fluids already in use. This literature review allowed me to foresee the route of my research in the high temperature collection section and to make my research different to what has already been investigated.

Current Heat Transfer Fluids for High Temperature Collection

As previously mentioned, the appropriate selection of a heat transfer fluid is a crucial decision when designing a high temperature application, such as, since their performance is directly linked to the collection temperature of the heat transfer fluid. The heat transfer fluid ideal material properties are to have a high thermal conductivity, high heat capacity and low viscosity. However, finding a fluid that presents all main thermal properties qualities is challenging [46]. Moreover, other important material properties are also important when the fluid operates at high temperatures, such as, their corrosion levels and low vapor pressures since they need to be compatible with the materials to encase them. At the same time, the heat transfer fluid have to be low in cost. Based on this criteria to find an appropriate heat transfer fluid, the most common heat transfer fluids that are used in solar power plants are water (in its steam phase), synthetic oils, and molten salts. These three fluids were compared in a parabolic through solar power plant[29]. Using a thermo-fluid-dynamic model, different design options were carried on to calculate the energy and exergy efficiency for each heat transfer fluid. From this study, it was found that direct steam generation systems are more efficient for parabolic through systems even though it is not the highest operational temperature fluid since the molten salt was heated up to 560 °C [40]. This was because the direct steam generation system did not require an heat exchanger device to heat another fluid like in the case of molten salts and synthetic oils. A direct steam generation solar power plant (PS10 located in Sevilla, Spain) heats steam up to 250 °C and 40 bar [1]. The plant is designed to produce above 100,000 kg/hr of saturated steam. The receiver is formed by 4 vertical panels, 5.40 m by 12.00 m making a surface area of 260 m². The receiver is located in a cavity and has a semi-cylinder shape with a 7.00 m radius. When the plant operates at full load, it receives a maximum of 55 MWt of concentrated solar radiation (yielding a peak solar flux of 650 kW/m²). The plant is also composed of a water thermal storage system with a capacity of 20 MWh. The thermal storage are loaded with part of the generated steam at the receiver. With a net production of 10 MW, its overall efficiency is rated at 9.5
CHAPTER 1. INTRODUCTION

% . Not only fluids have been investigate to transport thermal energy. For example, using solid particles like sand, bauxite and zirconia can also accomplish the same goal. These solid particles have the capability to withstand very high temperatures at atmospheric pressure (up to 1000 °C); however, they present challenges, such as, transportation from the local heat point to transfer thermal energy to another working fluid [7].

A very well studied and known heat transfer fluid is an eutectic carbonate molten salt. This eutectic carbonate molten salt is known to reach temperatures up to 900 °C at atmospheric pressure [8]. However, it decomposes and becomes corrosive once it reaches 900 °C [22] making the fluid not very compatible with common surface materials making it challenging to find suitable construction materials. Due to its capability to reach high temperatures, this molten salt is currently very attractive for its implementation in various solar power plants. Initially, it was used a thermal energy storage fluid (it would be heated by another fluid), but then, its application as a heat transfer fluid has been implemented and widely studied. Experimentally, a prototype concentration solar power plant with a DAR was built and tested by West [52]. The DAR had a 5° titled angle and a total surface area of 103.7 m². The main goal of the experimental test was to observe the flow and heat transfer characteristics of the molten salt. An important key aspect during the experiments was to find and appropriate film thickness since it directly affects the heat transfer between the absorber plate and the fluid.

These current heat transfer fluids show good heat transfer properties and behaviors, but they present challenges in their implementations, some by having that limitation to reach higher temperature (limiting their thermal efficiencies) and/or being not compatible with materials to encase and non-environmentally friendly when operating at very high temperatures. Therefore, the need a fluid that can overcomes many of these challenges is still there. In addition, all the current fluid heat transfer assessments are representative of Prandtl number fluids below 12. It could be said that the performance of any heat transfer fluid can be predicted based on previous findings and results, but that would not necessarily apply if the prediction of the heat transfer performance of this phosphorous molten glass is needed since this molten glass Prandtl number values ranges from 6000 to 1300. Although, the heat transfer coefficient of high Prandtl numbers fluids were explored by Bays and McAdams [5]. They used constant properties and measured heat transfer coefficients using an isothermal wall. They stated that the viscosity was a major factor in the deviations between their experimental values to the Nusselt theoretical values. To fix this discrepancy, they calculated and added a correction factor in their analytical results by comparing to their experimental values of heat transfer coefficient [15]. In the case of this molten glass, a constant viscosity value cannot be used since it varies significantly with temperature (53.8 Pa.s at 400°C to 0.011 Pa.s at 1180°C) especially when the goal is to operate the molten glass from 400°C to almost 1200°C. Therefore, including a temperature-dependent viscosity is another important aspect that I investigated to collect high temperature thermal energy from the molten glass.
Previous Studies Using Molten Salt as a Heat Transfer Fluid

Many studies have been performed using molten salts in a solar power plants as currently one of the most prominent heat transfer fluids to reach high temperatures. Bohn [8] experimentally tested the eutectic carbonate molten salt in DAR concept to obtain data of the heat transfer and stability of the film [8]. Therefore, a well-fabricated small-scale absorber was tested by flowing a thin film of molten salt (between 1 and 2 mm). The DAR was then exposed to solar flux and installed in a cavity. The heat transfer coefficient between the salt and absorber was determined by measuring the absorber plate temperature, the local salt temperature and the local flux. The results were displayed using dimensionless parameters (Re, and Dimensionless heat transfer transfer coefficients). Moreover, Bohn and Wang [8] experimentally and numerically studied the flow and heat transfer performance of an eutectic carbonate molten salt in a DAR. Assuming that the fluid does not absorb thermal energy in the visible wavelength range, Bohn et al. calculated heat transfer coefficients for a range of Prandtl numbers from 5.4 to 14. The experimental and numerical data using dimensionless parameter that they calculated for the molten salt’s heat transfer performance is used in my study to compare my mathematical approach and to verify that it predicts heat transfer coefficients correctly.

Another experimental study performed by Bohn and Green was to test nitrate salt. Using a small-scaled down absorber surface and radiant energy supplied by an array of 42 quartz halogen lamps, the nitrate salt was heated, and its temperature was measured using thermocouples located along the absorber surface. The measured heat transfer coefficient between the falling salt and surface show good agreement with the turbulent correlations, and therefore, the maximum temperature of the absorber was 585 °C for an inlet temperature of 270 °C and outlet of 570 °C temperature of the nitrate salt. Being in the turbulent region, it was found that additional do-pant to increase the volumetric absorption of solar radiation was not necessary since it only increased the receiver efficiency by 4.4 %. Assessing the molten glass in the turbulent regime was not required due to its Reynolds number range (from 6.85 up to 180.9). However, it was interesting to note that in this case of the salt dopant were not needed to increase the volumetric absorption of solar radiation, and something that was not performed in this research.

Other important aspects that I needed potential consideration were wave effects for the falling film of molten glass when modeled in a DAR. However, the heat transfer coefficient for evaporation to surrounding saturated vapor of a water film falling over a vertical tube was evaluated experimentally by Chung and [37], Seban [11], and [36] in the laminar and turbulent regimes and they did not observe wave effects up to a Reynolds number of 1600. In my studies, the molten glass Reynolds number goes up to 180 allowing me to justify the need of not including wave effects.

Viskanta and Webb [47] conducted a study to investigate the heat transfer of a gravity-driven semitransparent fluid. Having the physical model a prototypical setup of a DAR in a cavity, absorption and emission in the fluid were included in the analysis. whereas, scattering was neglected. Important factor investigated in the study were substrate emissivity, fluid
layer opacity, spectral nature of incident radiative flux, flow model, and film thickness [24]. Viskanta and Webb performed the study in the turbulent regime. Using a numerical methods with a fully implicit marching scheme, the integro-differential equations were solved first by performing iteration until the Reynolds-dependent diffusivity and velocity profiles were satisfied. The boundary temperatures were guessed. Their results indicated that the most optimal optical thickness for molten salt is 2 (τ=2). This study performed a very complex modeling of the molten salt to find out that the optical thickness of this heat transfer fluid made impacts when above 0 (not transparent) [50]. The same complexity in this research is also implemented to model molten glass as a falling film to transport heat transfer was not required based on justified assumptions, however, they helped me to verify certain approach when treating thermal radiation heat transfer and implementing different optical thicknesses for the molten glass. Wang and Copeland [49] investigated the heat transfer performance of carbonate molten salt as a falling film flow over an insulated inclined flat plate using numerical methods. Wang and Copeland treat the salt film as a laminar flow. Wang et al. found out that the best performance was obtained by having a system with a black wall (ρv=0) and an optical thickness of 1 (τ=1) due to a maximum bulk temperature rise [24].

**Current Techniques to Improve Higher Temperature Collection**

It is known that if the temperature of the source (heat transfer fluid is increased), then, the thermal losses also increase. However, current methods to reduce thermal losses (mainly due to thermal radiation) include to incorporate nanoparticles in the heat transfer fluid [44]. Kameya et al. [25] investigated to addition of Ni nanoparticle suspension by using spectroscopic transmission measurement. The Ni nanoparticles were observed to enhance the absorption coefficient in the visible and near infrared wavelength range of the fluid. For their study, they used alkyl napthalene as the base fluid. The study concluded that by suspension of Ni nanoparticles with an average diameter of 4.9 nm, the absorption coefficient was much higher (100 1/m) in magnitude of the base fluid in the visible and near-infrared wavelength regions, and that in the infrared region, the absorption coefficients remained the same as of the base fluid. This study helped me to assess the main wavelength range of interest to enhance thermal absorption, and why molten glass absorption spectra needs to be address. Also, the addition of nanoparticles might not be needed when using molten glass as a heat transfer fluid.

Volumetric flow receivers were investigated by Veeraragavan et al.[46]. The analysis included the incorporation of nanoparticles to absorb incoming radiation in the volume of fluid by designing compact models to optimize the performance. The heat loss, particle loading, solar concentration, and channel height on receiver efficiency were analytically investigated. The energy equation used a combined radiative and convective heat loss coefficient at the surface. Using dimensionless numbers (Pe and Nu), the analysis provides practical tool to predict the efficiency of any system size. For the case study, Therminol VP-1 was used that had suspended graphite nanoparticles. From their study, the optimal efficiency was found to be 0.35 for a combined efficiency calculation (receiver and power generation and
idealized Carnot efficiency. The efficiency is also calculated as a function of dimensionless parameters (Nu and Re). From this study, volumetric radiative heat generation in the fluid was the technique the impacts of radiative heat transfer when assessing heat transfer fluids. However, in this research, this method to predict Nu and Re numbers cannot be applied since the molten glass has a strong temperature-dependent viscosity.

**Previous Studies Related to The Analysis of the Heat Transfer Process in Molten Glasses**

Previous studies have investigated the heat transfer and flow through molten glass to predict temperature distributions, heat transfer rates and the most important heat transfer mechanisms in molten glass [28]. Eryou et al. [13] analyzed the radiative and conductive heat transfer through a slab of molten glass between two parallel plates by developing an optical method of temperature measurement using helium-neon laser beams. By heating the plates above 2000°F, the glass' absorption coefficients were measured between 2000 and 2300°F. Using diffusive and specular boundary conditions for the walls, their analytical approach follow the methodology developed by Viskanta and Grosh [47]. Their analytical results predicted values for temperature between 5°F and heat fluxes between 10% error with their experimental results. The heat transfer in molten glass was analyzed for glass tank furnaces. Sibiryakov et al. [41] investigated the free convection in a melt and its effect on heat transfer with molten glass in a tank where the molten glass Prandtl number varied between 100 to 10,000. In their studies, they found at the layer close to the walls, conduction was predominant but towards the middle, convective forces were the main heat transfer mechanism based on the Raleigh number range. Pilon et al. [33] analyzed the flow and thermal structures in a glass melting surface for a molten glass bath to evaluate the capability of the furnace operators to control the temperature fields and flow of the molten glass with the firing combustion space. In their studies, they concluded that the heat flux gradient had to be applied in longitudinal direction to generate convective effects of two recirculation loops. Yen et al. [55] numerically study the flow and heat transfer behaviors of an actual glass melting furnace and experimentally verified their results. Using 3D volume of fluids approach, their results showed that the temperature fields trajectory were consistent with their numerical model. Chui et al. [10] modeled a one-dimensional conductive and radiative heat transfer for transient and steady-state analysis to predict the temperature profile of glassmelting tanks. They concluded that it was important to include convective effects as the glass reached temperature above its melting point to reduce their predictions errors to experimental data. Even though the heat transfer in molten glass has been investigated, none of them have investigated molten glass in the context of a heat transfer fluid for a high temperature collection application where conductive, convective and radiative heat transfer mechanisms are expected to be play main roles. In addition, all of the previous mentioned studies used different variations of silicate dioxide as their molten glass with operational temperatures greater than 1200°C. Due to their high melting temperature, thermal radia-
CHAPTER 1. INTRODUCTION

One of the main heat transfer mechanisms. Compared to most silicate glass, Halotechnics phosphorous pentoxide has a lower melting temperature (400°C) and remains as a liquid up to 1200°C enabling the fluid to have a wide operational temperature range. It also exhibits important characteristics such as, its low viscosity, high specific heat (C_p = 1400 J/kg.K), its thermal stability and low in toxicity over its operational temperature range (400 °C to 1200 °C).

Depending on its temperature range, molten glass changes its absorption spectra [14] and [17]. Molten glass is known to be a participating medium or semitransparent material. The assessment of the radiative effects of this glass requires to solve for the radiative transfer equation and to know the absorption coefficients of the material with respect to temperature and wavelength [33] and [31]. Due to the lack of absorption coefficients of this phosphorous pentoxide glass, absorption coefficients of two types of similar phosphorous pentoxide glasses that exhibit low and high absorption coefficients were chosen to assess the radiative effects in the optically thin and thick range [51] and [30].

**Main Objectives for Modeling of Flow and Heat Transfer for High Temperature Collection**

In the research, the assessment of the heat transfer behavior and performance of a phosphorous pentoxide (P_2O_5) base molten glass is investigated. The first step was to model the molten glass in a heat exchanger to investigate its heat transfer performance and unknown thermal material properties that were estimated based on its composition (its thermal conductivity was estimated to be 0.8 W/m/K). The main goal in this first step was to assess the impacts of thermal radiation to predict the thermal energy transfer from the glass to another fluid by comparing the overall heat transfer rates to experimental data provided by Halotechnics [3]. All the details of the approach and the results are in chapter 2. The second step was to model the molten glass in a DAR to investigate its performance at very high temperatures (around 1000°C). By using numerical methods, important flow conditions were implemented when modeling the molten glass as it falls and gets heated, such as, its film thinning effect due to its viscosity variation with temperature. The details of the molten glass falling-film studies are in chapter 3.

1.3 Motivation for Modeling Phase Change Materials in Cold Temperature Thermal Storage

The motivation of this research also focused on the thermal energy transport for low operational temperature range systems. Thermolectric power plants ran with a maximum efficiency of 40 % of the total energy used from the fuel to turn it into electricity. A high amount of the energy is converted into low-grade waste heat. Common ways for power plants to cool down and remove this waste heat is by using water nearby lakes, rivers, or ocean.
By running this water through tubes that surround the condenser, then the cool water then returns at a higher temperature. Regions that have low amounts of water or are limited to cold water sources or when drought conditions are severe, dry-cooling systems are beneficial since instead of using water, air can be used to remove the heat from a plant’s condenser [19].

Current technologies that are using dry-cooling systems lower the efficiency of the power plant; therefore, there is a strong incentive to find ways to improve dry-cooling systems in a power plant condenser without reducing the power plant’s efficiency [6]. Generating new methods that can improve the cooling below ambient temperature during the day and the heat transfer between the air and the condenser so that the efficiency is improved could potential help to decrease the high amounts of water supplies to cool power-plants.

**Current Phase Change Materials for Thermal Energy Storage**

Phase change materials (PCMs) ability of to change phase (e.g. solid to liquid) and to absorb and/or release large amounts of latent heat at nearly a constant temperature makes them attractive to solve thermal energy storage issues in the low-temperature range. Water being the most common material freezes at nearly 0°C and releases when changing phase about 333 J/g of latent heat. However, when other temperatures are desired, then PCMs with higher melting temperatures are required [16].

Phase change materials are currently investigated to moderate and balance thermal energy in several applications from electronics to the automobile industry and buildings [26]. The implementation of PCMs lie more on the heating and cooling type of phenomena for transient applications in electronics cooling, mobile phones, digital videos, solar applications, and thermal energy storage due to their capability to store thermal energy in short terms (for daily applications) and long terms (for seasonal thermal energy storage) [39].

Paraffin based PCMs’s melting temperature (6 to 80°C) are good candidates for practical applications since they have good thermal energy storage capacity. However, due to their low thermal conductivity values (\( k_{\text{solid}} = 0.132 \ \text{W/mK} \) and \( k_{\text{liquid}} = 0.085 \ \text{W/mK} \)), their performance in extraction and charging of thermal energy makes them not practical since it requires more sophisticated techniques and devices to enhance the heat transfer process.

Salt Hydrates are currently the most researched PCMs for latent heat storage materials. They are low in cost (comparable to water and gel packs). However, the most common issues of salt hydrates are that few of them melt between the ranges of 1 and 150 °C, and finding new salts that can melt between those temperatures is pursued (See Fig.1.4).

(a) High Latent Heat: Above 180 J/g

(b) Thermal Cycling Stability : Over the courses of thousands of melts and freeze change phases.

(c) Ideal Melting Temperature
(d) Cost-Effective
(e) Non-Toxic

Macro-encapsulated salts that melt at an appropriate temperature are also being investigated due to their capabilities to melt at desirable temperatures. However, this type of enhancement makes the material more expensive, and the goal is to find economical ways to improve cold thermal energy storage.

**Lithium Nitrate Tryhidrate (LiNO$_3$3H$_2$O) as a Phase Change Material for Cold Thermal Storage**

As previously mentioned, paraffin based PCMs were widely investigated, but due to their low thermal conductivity, a major interest is switching to salt hydrates [?] and [?]. However, few thermo-physical properties are known about these materials with regards to perform computational analysis to assess its thermal energy storage and transfer capabilities. A potential candidate salt hydrate is lithium nitrate trihydrate (LiNO$_3$3H$_2$O). This PCM potential TES contains a high volumetric energy density (about 400 MJ/m$^3$). It melts at about 303 K (30$^\circ$C) comparable to paraffins [38].
Shamberger et al. \cite{Shamberger} reported the thermo-physical properties of solid and liquid nitrate trihydrate for the temperature range of -20°C and 80°C. The study compared them to water and octadene, showing how both types of Lithium Nitrates have high volumetric energy storage density compared to water, paraffin and other types (See Fig. 1.5). Moreover, other important thermo-physical properties like specific energy density, thermal conductivity and thermal diffusivity show to be greater than paraffin (octadecane). Therefore, the potential of using LiNO$_3$ based salts to implement as a thermal energy storage material is very high. However, there is a crucial need to analyze the material such as its performance in devices such as heat exchangers by assessing its heat transfer and melting rates are observed.

![Figure 1.4: Latent Heat of Fusion of Lithium Nitrate Trihydrate versus Water and Paraffin PCMs.](image)

The drive to find materials that can be implemented in thermal energy storage to improve applications such as dry-cooling technologies is very important, and lithium nitrate trihydrate can be one of them. Currently, there are no studies showing its performance in devices such as heat exchangers which are widely used to transfer thermal energy.

### 1.4 Previous Studies that Investigated Phase Change Materials for Cold Thermal Energy Storage

Several studies have been performed to assess the heat transfer of a phase change material. These studies were performed computationally and experimentally. The most valuable part of this literature review is how Fluent was used to model latent heat transfer using the solidification/melting method in ANSYS \cite{Fluent}. In addition, the computational simulations were
validated against experimental data confirming the enthalpy-method and pseudo-porosity used in Fluent to model a phase change heat transfer mechanisms is reliable.

Overview of Studies that Used Fluent/ANSYS to Model Phase Change Materials

Tan et al. [43] studied the natural convection effects of a PCM between Aluminum fins and spiral fins. The aim of their investigation was to understand the PCMs melting behav-iors by observing the natural convection currents movement and melting fronts formation. They used Fluent 6.3 and implemented the enthalpy-porosity formulation to solve a phase change process of PCM to generate visualizations of melting fractions, temperature distribu-tions and flow fields of the melting process. By applying a $\Delta T$ of 10.5 °C above the melting temperature of the PCM, their finding show how adding more spiral fins promotes heat conduction and reduces natural convection at the early stages of melting, but later, the convective effects are enhanced. Their numerical model reached complete melting earlier, shorter phase change period and higher maximum temperature. Therefore, they had to use a volume-correction factor to fix the earlier melting times calculated in their analysis.

Hosseini et al. [20] performed an experimental and computational study on the melting behavior of a phase change storage material. A combined experimental and numerical study is performed aiming to understand the role of buoyancy driven convection during constrained melting of phase change materials (PCMs) inside a shell and tube heat exchanger. A series of experiments is conducted to investigate the effect of increasing the inlet temperature of the heat transfer fluid (HTF) on the charging process (melting) of the PCM. A 22 mm copper tube located centrally in the cylinder was the heat transfer tube through which hot water flows to exchange heat with the PCM. The system consisted of a charging loop, which transferred heat from the hot water to the PCM in the system during the charging process. Heat transfer from the heat exchanger (heat transfer pipe) to the PCM is largely influenced by natural convection at the melting layer section. Based on the melting temperature of the PCM (51°C), Their findings showed that increasing the inlet water temperature from 70°C to 80 °C allowed to decrease the melting of the PCM from 50% to 37%.

Varol et al. [45] performed a Numerical analysis of fin effects. This numerical study aimed to compare the heat transfer during PCM melting in a rectangular container based on two geometrical cases (without fins and consist of five fins). In this study, researchers used an efficient approach to simulate heat transfer during PCM melting in an enclosure including the effects of transient conduction. The paraffin wax used in this study is between 28 to 30 °C. In this study, solidification process has been simulated using ANSYS-FLUENT 12.0 commercial code. A 2D rectangular field was modeled as a container filled with solid wax.
initially without fins. The model also was adjusted to include fins. The dimensions of the rectangle are 100 x 20 cm. In the analysis, thermo physical properties such as, thermal conductivity, density and heat capacity had different values for solid and liquid state of the paraffin wax. The analysis also included buoyancy effects. In their findings, they showed how using 5 fins across the PCM instead of not using fins, enhances the melting rated by about 25%.

Walter et al. [48] modeled the melting and solidification of a sodium nitrate in a vertical arranged energy storage device. The device had two different bi-metal finned tube designs to enhance heat transfer. The study shows the charging and discharging processes using a 3D transient modeled in ANSYS fluent 14.5. They realized that in the 2D modeled the phase change material behavior was not shown correctly. Therefore, their final analysis take place in 3D. During their melting process, their 3D numerical analysis shows that their first period of charging process was mainly due to heat conduction as the main heat transfer mechanism. However as the melting process increased they observed convective effects taking place showing faster melting at the top of their device compared to the bottom. Their results also show that in order to obtain higher melting processes, natural convective effects could be generated if the design of the heat exchanger tubes should be appropriate. Their solidification process showed that heat conduction was the main heat transfer mechanism.

Allouche et al. [2] developed a CFD model for the simulation of a phase change material in a storage tank of 100 L cylindrical tank. The medium of heat transfer was water which flow inside the horizontal tubes. The PCM was a selected slurry with a micro encapsulation. Using a 3D mathematical model, the PCM was modeled using a temperature-dependent thermo physical properties for 3D Navier Stokes with a non-linear temperature. They validated their results, they compared them to experimental data using three different flow rates of the heat transfer fluid during the charging process. Bulk temperatures, heat transfer rates and amount of energy stored are the main parameters compared and indicators of performance. In their comparison to experimental data, their studies predicted results within 5% of error and the energy stored was within 10% of the observed value allowing them to conclude that their computation model predicts experimental model with good accuracy.

All of the previous studies mentioned in this section of the literature review demonstrates how the enthalpy-porosity-method to model phase change heat transfer is reliable even for complex geometries and complex PCMs [1] and [9]. However, they mostly focused on devices in the large scale using PCM are paraffin waxes, which require complex geometries of fins to enhance the heat transfer (making the cost of the heat exchanger much higher). None of the studies quantify overall heat transfer coefficient and mean conductance of their system modeling a unit cell domain for different tubes configuration.
Main Objectives for Modeling Latent Heat Transfer for Low Temperature Applications

In this research, the modeling of a PCM for low temperature thermal energy storage application is performed in a heat exchanger device. The goal is to assess the heat transfer performance of the LiNO$_3$3H$_2$O PCM by using two different configurations of heat exchangers to predict their melting rates, overall heat transfer coefficients and mean conductance. The phase change modeling of the PCM is performed using the enthalpy-porosity technique allowing to model liquid/solid interfaces using a mushy zone. Chapter 4 provides all the details for this study.
Chapter 2

Modeling of Flow and Heat Transfer of Molten Glass in Counter-Flow Heat Exchanger

2.1 Assessing Phosphorous Pentoxide ($\text{P}_2\text{O}_5$) Molten Glass Heat Transfer by Modeling a 3D Annular Counter-Flow Heat Exchanger

In order to investigate the heat transfer performance of this molten glass, it was important to analyze the main mechanisms of heat transfer that govern its behavior. Experimental data was obtained by testing the fluid in a heat exchanger prototype, the heat transfer performance of this phosphorous pentoxide molten glass was initially evaluated by modeling a 3D heat exchanger using computational fluid dynamics software, ANSYS which is based on the finite volume method: Domain is discretized into a finite set of control volumes. Partially differential equations are discretized into a system of algebraic equations and are solved numerically. The heat transfer assessment included the treatment of radiative effects for a participating-absorbing medium. The radiation assessment solved for the radiative transfer equation where the absorption spectra was modeled using a rectangular bandgap model. Since the absorption coefficient spectrum of this molten glass is unknown, the absorption coefficients of two similar phosphorous pentoxide molten glasses were selected to observe its behavior for an optically thick and thin medium. The computational analysis results were then compared to the collected experimental data. This comparison allowed to observe the importance of thermal radiation heat transfer in the temperature range of this study.
Table 2.1: Helical Coil Heat Exchanger Dimensions

<table>
<thead>
<tr>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Helical Coil Inner Diameter</td>
<td>0.6223 cm</td>
</tr>
<tr>
<td>Helical Coil Wall Thickness</td>
<td>0.1651 cm</td>
</tr>
<tr>
<td>Helical Coil length</td>
<td>6.096 m</td>
</tr>
<tr>
<td>Molten Glass Pipe Diameter</td>
<td>1.9 cm</td>
</tr>
<tr>
<td>Molten Glass Pipe Wall Thickness</td>
<td>0.635 cm</td>
</tr>
</tbody>
</table>

Physical Modeling of 3D Counter-Flow Heat Exchanger

Helical-Coil Heat Exchanger: Experimental Test Device

In the heat exchanger of interest, molten glass flows through a single cylindrical flow passage with a circular cross section. Heat from this flow is transferred through a passage wall to air flowing in a counter-flow tube helical-coil wrapping around the tube carrying the molten glass. The helical coil is tightly wound to the inner tube. The helical coil material is Inconel 600 where the air flows, and the inner pipe, where the molten glass flows is made out of graphite. In order to heat up the glass up to 700°C, the glass flows through a recirculation loop. Initially the glass is taken from a cold tank where the glass is at 500°C. The glass, then, gets heated up using radiant electric heaters rated at 3600 watts. These heaters were also used around the heat exchanger section to preheat the piping before the molten glass entered the heat exchanger. The air flows with a Reynolds number of 16,100 calculates using properties evaluated at an average air temperature (300°C) between the inlet and outlet in the heat exchanger (see Figure 2.1 and Table 2.1)

Annular Counter-Flow Heat Exchanger

Exact modeling of the air flow as a flow in a helical coil tube is not necessary since the goal is to explore the heat transfer of the molten glass to the air flow. However, our model must have an equivalent flow and heat transfer behavior to the experimental prototype (See Fig. 2.2 and Table 2.2).

Equivalent Wall Boundary Condition

To have an equivalent flow and heat transfer behavior, the 3D model had to meet three main criteria which imposed an equivalent wall boundary condition for the glass flow. The three main conditions allowed to simplify the 3D model simulation by modeling the flow of the air through an annular passage.

The air mass flow rate in both passages are set equal,

\[ \dot{m}_{\text{air,ann}} = \dot{m}_{\text{air, hc}} \]  (2.1)
Figure 2.1: Experimental Counter-Flow Helical Coil Heat Exchanger.

Figure 2.2: Annular Counter-Flow Heat Exchanger 3D Model.

Table 2.2: 3D Annular counter-flow heat exchanger.

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Molten Glass Pipe Diameter</td>
<td>1.9 cm</td>
</tr>
<tr>
<td>Wall Thickness</td>
<td>1 mm</td>
</tr>
<tr>
<td>Annular Passage Outer Diameter</td>
<td>2.1 cm</td>
</tr>
<tr>
<td>Heat exchanger length</td>
<td>73.7 cm</td>
</tr>
</tbody>
</table>
CHAPTER 2. HEAT TRANSFER OF MOLTEN GLASS IN A HEAT EXCHANGER

Eq. 2.1 allows to obtain the same heat capacity rate. The air residence time in the counter-flow heat exchanger is the same as in the helical-coil heat exchanger prototype, the mean axial velocity was set equal:

\[ \bar{u}_{\text{air,ann}} = \bar{u}_{\text{air,hc}} \]  
(2.2)

The gap dimension for the annular section of the air was calculated using Eq.2.1 and 2.2 such as,

\[ \frac{\dot{m}_{\text{air,ann}}}{\rho_{\text{air}} A_{c,o}} = \frac{\dot{m}_{\text{air,hc}} \cos \theta_{hc}}{\rho_{\text{air}} A_{c,hc}} \]  
(2.3)

\[ H = \frac{D_{hc}^2}{4D_o \cos \theta_{hc}} \]  
(2.4)

The thermal resistance in the helical coil and the counter-flow annular side must be equal along the z-axis:

\[ \frac{1}{h_{\text{air,ann}} A_{\text{air,ann}}} = \frac{1}{h_{\text{air,hc}} A_{\text{air,hc}}} \]  
(2.5)

In the helical-coil experimental prototype, the airflows Reynolds number is 16,000 indicating that it is a fully-developed and turbulent flow. Hence, the air flow in the annular counter-flow heat exchanger is also treated as fully-developed and turbulent. Using the Dittus-Boelter correlation for heating a fully-developed and turbulent flow (Reference), the overall heat transfer coefficient can be calculated such as,

\[ Nu_{\text{air,ann}} = 0.00243 Re_{\text{air,ann}}^{0.8} Pr_{\text{air,ann}}^{0.4} \]  
(2.6)

\[ Nu_{\text{air,hc}} = 0.00243 Re_{\text{air,hc}}^{0.8} Pr_{\text{air,hc}}^{0.4} \]  
(2.7)

Using the definition of the Nusselt number, the heat transfer coefficient is expressed as,

\[ h_{\text{air,ann}} = 0.00243 \frac{k_{\text{air,ann}}}{D_{\text{ann}}} Re_{\text{air,ann}}^{0.8} Pr_{\text{air,ann}}^{0.4} \]  
(2.8)

\[ h_{\text{air,hc}} = 0.00243 \frac{k_{\text{air}}}{D_{hc}} Re_{\text{air,hc}}^{0.8} Pr_{\text{air,hc}}^{0.4} \]  
(2.9)

Where the Reynolds number is defined as,

\[ Re_{\text{air,ann}} = \frac{\dot{m}_{\text{air,ann}} D_{\text{ann}}}{\mu D_o H} \]  
(2.10)

\[ Re_{\text{air,hc}} = \frac{\dot{m}_{\text{air,hc}} D_{hc}}{\mu A_{hc}} \]  
(2.11)

and the Prandtl number is defined as,

\[ Pr_{\text{air,ann}} = \frac{c_{p,\text{air}} \mu}{k_{\text{air,ann}}} \]  
(2.12)
Table 2.3: Material properties and adjusted air thermal conductivity

<table>
<thead>
<tr>
<th>Material Property</th>
<th>Molten Glass (at 650°C)</th>
<th>Air (at 300°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>2400 ( \text{kg/m}^3 )</td>
<td>0.60 ( \text{kg/m}^3 )</td>
</tr>
<tr>
<td>Specific Heat</td>
<td>1400 ( \text{J/kg.K} )</td>
<td>1051 ( \text{J/kg.K} )</td>
</tr>
<tr>
<td>Dynamic Viscosity</td>
<td>0.6 ( \text{μ} )</td>
<td>2.95e-5 ( \text{μ} )</td>
</tr>
<tr>
<td>Thermal Conductivity</td>
<td>0.8 ( \text{W/m.K} )</td>
<td>0.087* ( \text{W/m.K} )</td>
</tr>
<tr>
<td>Absorption Coefficient</td>
<td>300 ( \text{m}^{-1} )</td>
<td>0 ( \text{m}^{-1} )</td>
</tr>
</tbody>
</table>

\[
P_{r_{\text{air,hc}}} = \frac{c_{p,\text{air}}\mu}{k_{\text{air}}} \quad (2.13)
\]

\(D_{\text{ann}}\) is defined as the hydraulic diameter of the annular region of the air flow. By definition the hydraulic diameter is defined as,

\[
D_{\text{ann}} = \frac{4A_{\text{flow}}}{\text{perimeter}} \quad (2.14)
\]

\[
D_{\text{ann}} = \frac{4\pi(r_o^2 - r_i^2)}{2\pi(r_o + r_i)} \quad (2.15)
\]

\[
D_{\text{ann}} = 2H \quad (2.16)
\]

Using the thermal resistance relation Eq.2.2 and the average heat transfer coefficient relations for the helical-coil and annular counter-flow model (Eq.2.7 and 2.8), the modified air thermal conductivity in the annular region of the counter-flow heat exchanger follows the equation below,

\[
k_{\text{air,hc}} = k_{\text{air}} \left( \frac{A_{\text{air,hc}}H}{A_{o,hc}L_t} \right)^{5/3} \left( \frac{D_{\text{ann}}}{D_{hc}} \right)^{1/3} \quad (2.17)
\]

Eq. 2.17 shows the modified thermal conductivity for the air in the counter-flow heat exchanger. Its modification includes dimensional ratios between the helical-coil and the annular region heat transfer and cross sectional areas. This modified thermal conductivity imposes the exact wall boundary condition for the glass flow allowing the same heat transfer conditions as in the helical coil heat exchange prototype. The other thermal properties for molten glass and air were evaluated at their average temperature in the heat transfer tests, 695 °C and 300°C, respectively. All the information about the material properties used in the simulations are listed in Table 2.3.

### 2.2 Meshing Method in ANSYS

Due to the geometry of the annular counter-flow heat exchanger, the most suitable meshing method and efficient available in ANSYS is the sweep meshing. The sweep meshing
method requires to have topologically identical source and target faces. In addition, it must have a sweep path that connects the source and target, and the heat exchanger geometry is suitable for this meshing method. This method generates hexahedron and wedge type of elements [47]. Ideally, hexahedron mesh is the most desired since it has a cube topology allowing for shorter simulation times. The air region or the annular region consists of hexahedron elements. The glass region has a combination of hexahedron and wedge elements (wedges elements are mostly at the center of glass region). The division of elements in the glass and air region were set up differently due to their different geometries and thicknesses. Initially, in the glass region, the edge division was set to 25 cells axially and 50 cells radially. In the air region, the edge division was set to 20 cells radially (See Fig. 2.3). In addition, to ensure accurate results, the sizing local mesh controls, known as Bias type and Bias factor in ANSYS, allowed meshing the boundary layer region of both fluids. The Bias type graded the elements in size, and the Bias factor set a ratio between the largest element and the smallest element and a growing rate. For our meshing model, the Bias factor was set to 5 with a growing rate of 1.2 having the thinnest elements at the intersection wall where the heat transfer takes place (See Fig.2.4 and Fig.2.5).

![Figure 2.3: Inner pipe flow sweep mesh profile (glass section).](image)

### Mesh Sensitivity Analysis

An appropriate mesh grid size was selected based on impacts of the heat transfer results. By running the model simulation with conductive and convective heat transfer (explained in the next sections), the glass and the air were imposed with different grid sizes to observe and select the adequate number of elements and nodes to ensure that the analysis yields mesh independent results. Table 2.4 and 2.5 show the overall heat transfer calculation at the interface wall between the glass and air region.
CHAPTER 2. HEAT TRANSFER OF MOLTEN GLASS IN A HEAT EXCHANGER

Figure 2.4: Annular pipe sweep mesh profile (air section)

Figure 2.5: Glass and air fluid modeling in counter-flow heat exchanger

Table 2.4: Mesh Grid Size Assessment for Glass Region

<table>
<thead>
<tr>
<th>Number of Division Across Diameter</th>
<th>No. Elements</th>
<th>No. Nodes</th>
<th>Average Heat Transfer, W</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>32825</td>
<td>35490</td>
<td>748</td>
</tr>
<tr>
<td>50</td>
<td>37800</td>
<td>41080</td>
<td>880</td>
</tr>
<tr>
<td>75</td>
<td>43300</td>
<td>47164</td>
<td>888.8</td>
</tr>
</tbody>
</table>
Table 2.5: Mesh Grid Size Assessment for Air Region

<table>
<thead>
<tr>
<th>Number of Division Across Annular Gap</th>
<th>No. Elements</th>
<th>No. Nodes</th>
<th>Average Heat Transfer, W</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>18300</td>
<td>20644</td>
<td>660</td>
</tr>
<tr>
<td>20</td>
<td>43300</td>
<td>47164</td>
<td>880</td>
</tr>
<tr>
<td>30</td>
<td>56780</td>
<td>60190</td>
<td>890</td>
</tr>
</tbody>
</table>

A sensitivity study was performed to analyze the mesh dependency of the results. In the air region, the number of elements were set to three different sizes: 8, 20 and 30, and in the glass region, the number of elements was increased from 50 to 100. The number of elements were only changed in the radial direction. The heat transfer magnitude with 20 cells increased by 5% as compared to the simulations with 12 cells, and decreased by 1% as compared to the simulation with 25 cells. Increasing the number of cells in the glass region only enhanced the heat transfer by 1%. Therefore, the final results were set to 50 divisions in the glass region and 20 in the air region since the results were observed to not be dependent on the mesh size (approximately).

**Governing Equations**

The modeling of the heat exchanger consists of two regions since we are evaluating two fluids: molten glass and air. The two fluids, which are set as counter flows, are in different flow regimes. Therefore, two sets of governing equations that applies properly to each regime were solved. The general 3D governing transport equations in the heat exchanger, such as, the continuity equation, z-direction momentum transport, and energy equations for the turbulent flow (air) in Cartesian coordinates for steady flow are of the form,

\[
\frac{\partial u}{\partial z} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0
\]  

\[
\rho \left( u \frac{\partial u}{\partial z} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial x} \right) = \rho \left( \frac{\mu}{\rho} + \epsilon_m \right) \left( \frac{\partial^2 u}{\partial z^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 w}{\partial x^2} \right)
\]  

\[
\rho c_p \left( u \frac{\partial T}{\partial z} + v \frac{\partial T}{\partial y} + w \frac{\partial T}{\partial x} \right) = \rho c_p \left( \frac{k}{\rho c_p} + \epsilon_h \right) \left( \frac{\partial^2 T}{\partial z^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial x^2} \right)
\]  

Similar 3-D Cartesian coordinate equations apply for transport of y-momentum and x-momentum. The general transport equations include turbulent momentum and heat diffusivity determined using the \( k \) turbulence model equations when the flow is turbulent. In the model developed here, the air flow is turbulent and fully-developed, whereas, the molten glass flow is laminar and developing thermally. The governing equations in the laminar region to evaluate the molten glass are similar to Eq.(2.18) through (2.20) except \( \epsilon_m \) and \( \epsilon_h \) are
dropped from the momentum and energy equations respectively. The initial heat transfer assessment is performed without thermal radiation. However, the energy equation adds the gradient of the radiative term as shown in the next section.

2.3 Thermal Radiation Assessment

To assess thermal radiation in a participating medium, additional terms are added to the energy equation, such as,

\[ \rho c_v (u \nabla \cdot T) = \nabla \cdot (k \nabla \cdot T) + \nabla \cdot q_r \]  

(2.21)

where,

\[ \nabla \cdot q_r = \kappa \int_0^\Omega \left( I_\lambda d\Omega - 4 \epsilon \sigma T^4 \right) d\Omega \]  

(2.22)

\[ I_\lambda = I_\lambda(0) \exp(-\tau_\lambda) + \int_0^{\tau_\lambda} I_{\lambda b} \exp(-(\tau_\lambda - \tau_\lambda *)) d\tau * \]  

(2.23)

Where \( \Omega \) represents the solid angle of the intensity path.

The radiative gradient term account for the sum of each radiation intensity from all the direction over the whole solid angle (absorbed radiation) minus the emitted thermal radiation. The intensity is represented as the radiative transfer equation (RTE) and is solved in fluent using the discrete ordinates model (DO). Fluent solves for the RTE (See Eq. 2.23) by discretizing space in finite control volumes following the mesh (similarly to the flow and energy equations) and directions are discretized in control angles for any type of optical thickness as shown. The RTE is calculated at each octant (since the fluent modeling is in 3D) based on the solid angle discretization. The angular discretization is given by \( N_\theta \times N_\phi \) such as,

Azimuthal angle (\( \phi \)), \( 0 < \phi < \pi / 2 \)
Polar angle (\( \theta \)), \( 0 < \theta < 2\pi \)

\[ \Omega = \int \int_S \sin \phi d\theta d\phi \]  

(2.24)

**Phosphorous Pentoxide Glass Absorption Coefficient Data**

The lack of measurements of the absorption coefficients for this molten glass required searching absorption coefficients data for similar phosphorous pentoxide. The wavelength range of interest for this study was determined by following Planck’s law, such as,

\[ B_\lambda = \frac{2hc^2}{\lambda^5} \frac{1}{\exp \left( \frac{hc}{\lambda k_B T} \right) - 1} \left( \frac{W}{sr m^3} \right) \]  

(2.25)
Based on the operational temperature range of the molten glass, from 650 to 727°C, the maximum absorption and emission as a blackbody was between 1 to 8 \( \mu \text{m} \) (as observed by the area under the curve when plotting Planck blackbody distribution versus wavelength),

![Planck's Distribution with Wavelength at 700 °C](image)

Figure 2.6: Planck’s Distribution with Wavelength at 700 °C

The absorption coefficient data found in the literature covered wavelength ranges from the visible range up to the near infrared range. The average absorption coefficient was calculated between their maximum and minimum values. The average absorption coefficient was then applied to the wavelength range between 1 and 8 \( \mu \text{m} \) for this study even though the absorption coefficients in the literature were between 0.4 and 1.6 \( \mu \text{m} \) (See Table 2.6 and 2.7). The absorption coefficients data for the similar phosphorous pentoxide glasses had a wide range of values, and two specific phosphorous pentoxide with absorption coefficients that yielded profiles in the optically thin and thick were selected to understand the radiative effects in the extreme regimes of the intensity absorption along its path [8 and 9] (See Table (2.6)). The DO method allows to input absorption coefficients as a function of wavelength. The absorption spectra was set up using three bandgaps representing wavelength ranges as shown in Table 2.6. Most glasses are assumed to be transparent (very low in optically thickness) in the visible wavelength range to be opaque (high in optically thickness) in the far infrared region. ANSYS requires to input absorption coefficients for a wide wavelength range; nevertheless, it sets it as zero. We arbitrarily chose a high absorption coefficient for each glass for bandgap 3 since it is in the far infrared region, and not exact absorption coefficient data for phosphorous pentoxide was available in this wavelength region.
Table 2.6: Phosphorous pentoxide glass absorption spectra

<table>
<thead>
<tr>
<th>Material Composition</th>
<th>$\lambda$</th>
<th>$\kappa$</th>
<th>$\tau$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_2O_5$ (41.86 %), BaO(14.47 %), SrO (10.33 %) $K_2O$ (9.54 %), $Al_2O_3$ (6.47 %),$Er_2O_3$ (0.21 %)</td>
<td>1-6 $\mu$m</td>
<td>0.0105 cm$^{-1}$</td>
<td>0.1</td>
</tr>
<tr>
<td>CuO (50 %), $P_2O_5$ (50 %)</td>
<td>1-5 $\mu$m</td>
<td>7.75 cm$^{-1}$</td>
<td>75.1</td>
</tr>
</tbody>
</table>

Table 2.7: Bandgap Method Modeling for Optical thickness Assessment

<table>
<thead>
<tr>
<th>$\lambda$, $\mu$m</th>
<th>$\tau$ for O. Thick</th>
<th>$\tau$ for O. Thin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Visible and Near Infrared Wavelength Range</td>
<td>0.4 -1</td>
<td>0</td>
</tr>
<tr>
<td>Mid-Range and Far Infrared</td>
<td>1 - 8</td>
<td>75.1</td>
</tr>
</tbody>
</table>

Flow Conditions

The incoming molten glass at an inlet temperature of 727°C (as measured in the experiments) transfer energy through a graphite pipe wall to incoming air flow at 20°C. The two streams are flowing in counter-current mode. The molten glass (hot fluid) has an inlet mean velocity of 0.027 m/s, and the air has an inlet mean velocity of 63 m/s. The mean velocities are calculated to match the mass flow rates measured in the experiments of both fluids. At the wall interface of the two fluids, radial and shell heat transfer conduction boundary is applied as part of the option in ANSYS for couple walls. Adiabatic (i.e. zero heat flux) is applied at the outer wall (air region). No-slip conditions are assumed at the interface of the solid/fluid regions. The pressure is assumed constant throughout the pipe. For the radiative boundary conditions, the inner pipe wall was assumed to be diffusive with an emissivity of 1.

Results

Initially, the heat transfer was analyzed without assessing the radiative effects of the glass. Fig.2.7 shows the temperature profiles at the center plane ($yz$ plane, $x=0$) of the pipe. The development of the thermal boundary layer is observed by comparing the temperature profiles across the pipe. The temperature profile does not reach a fully developed parabolic profile by the time it exits the pipe. On the other hand, the velocity profiles show the glass reaches a fully hydrodynamically developed profile by comparing the profiles close to the inlet and
by the exit of the pipe (Fig 2.7). The flow behavior follows an expected pattern due to their high Prandlt number and low Reynolds number of this glass ($\text{Pr} = 368.9$ and $\text{Re} = 6.85$). The local heat transfer coefficient (Fig 2.8) shows a traditional profile for a laminar flow ($\text{Re} = 6.85$). The temperature distribution of the glass is shown in Fig. 2.9. With a small thermal diffusivity and large momentum diffusivity ($k \rho c_p = 2.38 \times 10^{-4} \text{mm}^2/\text{s}$, $\nu = 0.088 \text{mm}^2/\text{s}$), the thickness of molten glass thermal boundary layer is about one third of the pipe radius (6 mm) at the exit of the pipe. The viscosity of the glass changes radically with temperature. However, for the temperature range in the heat exchanger, evaluating the viscosity at the average temperature (695°C) is adequate since the viscosity increases by about twice in magnitude from the inlet to the outlet (159 cP at 727°C and 325 cP at 650°C). The small deviation of the overall heat transfer (about 7% of the experimental helical coil results) indicates that the adjusted air thermal conductivity calculated to model the thermal resistance of the air and physical dimensions of the pipes in the experimental helical coil heat exchanger prototype were made appropriately, and using a viscosity evaluated at an average temperature is appropriate for a temperature drop less than 100°C. When radiative effects are added in the optically thick ($\tau=75.1$) and thin ($\tau=0.1$), the temperature profiles do not deviate significantly compared to when the heat transfer is analyzed using pure conduction and convection (See Fig. 2.12). The mean bulk and wall temperatures also show similar
CHAPTER 2. HEAT TRANSFER OF MOLTEN GLASS IN A HEAT EXCHANGER

Figure 2.8: Molten Glass Local Heat Transfer Predictions without Radiation ($\tau=0$) and with Radiation in The Optically Thick ($\tau=75.1$) and Optically Thin ($\tau=0.1$).

Figure 2.9: Temperature Distribution of Molten Glass and Air Flow in a 2D YZ Plane with no Radiation ($\tau=0$).
CHAPTER 2. HEAT TRANSFER OF MOLten GLASS IN A HEAT EXCHANGER

Figure 2.10: Temperature Distribution of Molten Glass and Air Flow in a 2D YZ Plane with Radiation in the Optically Thick region ($\tau=75.1$).

Figure 2.11: Temperature Distribution of Molten Glass and Air Flow in a 2D YZ Plane with Radiation Optically Thin region ($\tau=0.1$).
behaviors for both types of optical thicknesses (Fig. 2.15). The local heat transfer coefficient (Fig. 2.8) trends show similar behaviors for the optically thick and no radiation cases. This confirms that the optically thick case approaches the Rosseland. On the other hand, the optically thin case shows a trend of fluctuation with decreasing and increasing curves, but by the exit of the pipe, all three profiles reached the same local heat transfer value (250 W/m² K). The overall heat transfer values when using radiation in both regimes show no significant enhancement as compared to the experimental results. Using radiation with an optical thick and thin approach, yields a percent error compared to the experimental of 4 and 5% respectively.

The overall heat transfer percent error when using no radiation indicates a percent error of about 5.2% (See Table 2.8). One of the main assumptions was to use a constant viscosity at the average value between the inlet and outlet temperature of the glass. For the operational temperature range of the glass in the heat exchanger, evaluating the viscosity at the average temperature (695°C) is adequate since the viscosity decreases by about half in magnitude.
from the inlet to the outlet (159 cP at 727°C and 321 cP at 650 °C) for a temperature drop less than 100°C. In addition, the adjusted air thermal conductivity calculated (Eq. 2.17) provided the necessary (within a 5.2 percent error) wall boundary condition for the glass flow to make our 3D annular counter-flow heat exchanger model equivalent to the helical-coil heat exchanger prototype.

Figure 2.13: Molten Glass Temperature Distribution Difference between the Optically Thick Radiative and Non Radiative Effects Predictions.

Figure 2.14: Molten Glass Temperature Distribution Difference between the Optically Thin Radiative and Non Radiative Effects Predictions.

Thermal radiation effects were assessed by comparing both optical thickness behaviors, optically thick (τ = 73.6) and thin (τ = 0.1), to the non-radiative effects analysis. The first assessment was performed by calculating the local temperature differences between the radiative and non-radiative values. Fig.2.13 shows the difference between the optically thick and non-radiation temperature fields. The highest temperature difference (Δ T = 7.06 °C) is about 10.4 % of the total temperature difference of the molten glass from the inlet and outlet mean temperatures for the optically thick case (T_{inlet} - T_{outlet} = 69.8°C). The temperature difference between the optically thin and non-radiation temperature fields show
Table 2.8: Non-Radiative and Radiative Heat Transfer for Air Outlet Temperature and Overall Heat Transfer from Molten Glass to Air Predictions Comparison to Experimental Data.

<table>
<thead>
<tr>
<th></th>
<th>No Radiation</th>
<th>$\tau=75.1$</th>
<th>$\tau=0.1005$</th>
<th>Experimental Data Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molten Glass Mean Outlet Temperature</td>
<td>659.2°C</td>
<td>659°C</td>
<td>662°C</td>
<td>660°C</td>
</tr>
<tr>
<td>Air Mean Outlet Temperature</td>
<td>700°C</td>
<td>715.7°C</td>
<td>717°C</td>
<td>664.4°C</td>
</tr>
<tr>
<td>Overall Heat Transfer</td>
<td>886 W</td>
<td>890 W</td>
<td>888 W</td>
<td>919.8 W</td>
</tr>
</tbody>
</table>

slightly higher temperature differences ($\Delta T = 10.22 ^\circ C$) and 13.8 % of the total temperature difference of the molten glass from the inlet and outlet mean temperatures for the optically thin case ($T_{inlet} - T_{outlet} = 68.7^\circ C$). They are mostly observed to take place in the middle region of the pipe which indicated that the thermal boundary layer development is affected by the radiative terms. The thermal boundary layer starts to develop a slight longer distance when radiative effects are taken into account, but the final thermal boundary layer height is very close to each other (3.2 mm, see Fig 2.15). Although the optically thin radiative case has higher wall temperatures (see Fig.2.14) which enhances the local heat transfer coefficients (Eq. 2.8) from the middle region toward the end region of the pipe (Fig 2.8), it only enhances the overall heat transfer by about 1.4 % as compared to the non-radiative overall heat transfer amount (see Table 2.8). Hence, the overall heat transfer values when using radiation show no significant enhancement as compared to the non-radiation heat transfer amount. The enhancement when using radiative effects are less than 2 % improving the simulation results from 5.2 % to 3.8 %. It can be also observed from Fig.2.15, 2.15 and 10 that the optical thick radiative case behaves in a similar way to the non-radiative case since it approaches the diffusive behavior (Rosselands approach) showing how an effective thermal conductivity can assess both radiative and conductive heat transfer.

2.4 Summary of Findings

Based on the predictions for a high Prandtl number and low Reynolds number fluid such as this phosphorous pentoxide molten glass, the thermal boundary layer shows its slow development in an inner pipe flow as compared to its velocity boundary layer as observed in Fig.2.9. Using absorption coefficients from two similar phosphorous pentoxide molten glass (copper oxide and barium oxide) with different absorption spectra is a useful way to assess the impact of radiation effects. It shows that the radiative heat transfer effects are
negligible when the phosphorous pentoxide molten glass is in the optically thin or thick range (low and high absorption coefficients) for the temperature ranges in this study. The local temperature differences fields are within 13% or less of the total the glass temperature drop indicating that the thermal radiative effects are not make a significant impact to the temperature fields. The overall heat transfer when using thermal radiation with both optical thicknesses only enhance heat transfer by less than 2% as compared to the amount of heat transfer when using no radiation in the analysis. The equivalent wall boundary condition imposed in the 3D annular counter-flow heat exchanger model that imposed an equivalent residence time, heat capacity rate and thermal resistance of the air as in the experimental heat exchanger prototype was accurately implemented since the the percent errors calculated for the overall heat transfer were within 5%, and the mean outlet temperature of the air were within 10%. In addition, the manufacturer recommended thermal conductivity value of 0.8 W/m/K yielded predictions in close agreement with the heat transfer rates measured in the experimental prototype tests. Since the molten glass temperature drop (from inlet to outlet) was less then 100°C, using material properties including viscosity at an average temperature (695°C and 300°C respectively) was adequate based on the percent errors level to the experimental prototype. Nevertheless, the radiative effects are expected to become more significant if the operational temperature of this molten glass increases ($T > 900^\circ$C).
A temperature-dependent viscosity and other adequate absorption coefficients based on the operational temperature to perform a heat transfer assessment will be required.
Chapter 3

Transient Heat Transfer Modeling of A Phase Change Cold Thermal Energy Storage System

3.1 Objective of Melting a PCM in a Cold Thermal Energy Storage System

In this study, the transient numerical analysis of melting a phase change material previous described as lithium nitrate trihydrate is performed (See Chapter 3, section 3.2). The main objective is to assess its performance to absorb thermal energy carried by a running hot fluid, such as water, by changing phase from solid to liquid. This study reflects the cooling effect in a cold storage system (See Fig. 3.1). A cold storage system is potentially expected to increase its cooling performance by melting a PCM held in place by a heat exchanger.

The transient modeling is carried over using a commercial software (ANSYS-Fluent) CFD package which is based on the finite volume method: Domain is discretized into a finite set of control volumes. Partially differential equations are discretized into a system of algebraic equations and are solved numerically. From previous studies, CFD simulations to design latent heat transfer energy storage systems have shown to be an efficient way to save money and time and to perform optimization of the system to find maximum efficiency [39-47].

Mathematical Approach to Model Latent Heat Transfer of A Phase Change Medium in Fluent

Initially, the melting was solved with pure conduction setting the energy equation as,

\[ h = h_{ref} + \int_{T_{ref}}^{T} c_p \Delta T \]  \hspace{1cm} (3.1)
CHAPTER 3. HEAT TRANSFER MODELING OF A PHASE CHANGE SYSTEM

Figure 3.1: Thermal Energy Storage Design: Rectangular and Round Tube Water Flow Passage with Rectangular Fins.

\[
\left( \rho \frac{\partial \bar{H}}{\partial t} \right) + \nabla (\rho v \bar{H}) = \nabla (k \nabla T) \tag{3.2}
\]

\(\bar{H}\) is the enthalpy, which is expressed as,

\[
\bar{H} = h + \Delta \bar{H} \tag{3.3}
\]

\[
\dot{\gamma} = \frac{T - T_s}{T_l - T_s}, T_l > T > T_s \tag{3.4}
\]

\[
\dot{\gamma} = 0, T < T_s, \tag{3.5}
\]

\[
\dot{\gamma} = 1, T > T_s, \tag{3.6}
\]

\[
\dot{\gamma} = \frac{\Delta \bar{H}}{L_{PCM}}, \tag{3.7}
\]

The solidification/melting method in Fluent uses a model called enthalphy-porosity technique to model melting and solidification process in a phase change medium. In this type of modeling, the melt interface is not tracked as in the typical phase change equations. Instead, a quantity known as liquid fraction is assigned in each finite volume cell. This liquid fraction is solved at every iteration in the enthalpy balance. In the model setup, there exits an area called mushy zone, where the liquid fraction is from 0 to 1. This mushy zone is a pseudo-porous medium. In the porous medium or mushy zone, as the material changes phase, the liquid fraction changes from 0 to 1 in the case of melting.
\( \Delta \overline{H} \) is the enthalpy change during the phase change (latent heat), which varies from 0 when the PCM is solid to \( L_{PCM} \) (latent heat of the material) when the PCM becomes liquid. The liquid fraction, \( \hat{\gamma} \), changes according to the temperature in the PCM (See Eq.3.4). The values of \( T_l \) and \( T_s \) determine the size of the mushy zone. In this study, \( T_l \) and \( T_s \) were set very few decimals away from the melting temperature to ensure a very fine thickness in the mushy zone. An iteration between the energy equation (Eq.3.2) and the liquid fraction (Eq.3.4) is carried over at each finite volume cell for the calculation of the local temperature field. If the liquid fraction (Eq. 3.4) is calculated directly, the energy equation yields very poor convergence residuals (inaccurate results). In Fluent-ANSYS R16.0, the pressure-correction solver is used along with the PISO algorithm to solve transient cases. The first order upwind difference scheme (UDS) is used to discretized the momentum and energy equations.

### 3.2 Rectangular Fin Geometry for Rectangular Tube Design

The first geometry used to enclose the PCM is a fin with rectangular shape surface area. The PCM is placed between parallel fins.

Figure 3.2: Thermal Energy Storage Device with Rectangular Tubes and Side View to Demonstrate The PCM Region.

The fin length was set to 9.65 mm and the depth to 6mm Fig. 3.4 yielding a surface fin area \( (A_{\text{fin,cell}}) \) of 57.9 mm\(^2\). The fin gap (the distance between fins where the PCM is enclosed), was a variable parameter as shown in Table 3.1

Where the \( A_{\text{tube,cell}} \) is the area of contact between the PCM and the pipe with the hot water. When modeling the PCM as it was located between rectangular fins, the fin thickness
Table 3.1: PCM Gap Variation for a Fin Length of 9.65 mm, Volume of PCM in Unit Cell, Area of Contact with Tube (unit cell area)

<table>
<thead>
<tr>
<th>PCM Gap Enclosure, mm</th>
<th>PCM Unit Cell Volume, m³</th>
<th>A_{tube,unitcell}, m²</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>2.895*10⁻⁸</td>
<td>3*10⁻⁶</td>
</tr>
<tr>
<td>1</td>
<td>5.79*10⁻⁸</td>
<td>6*10⁻⁶</td>
</tr>
<tr>
<td>1.5</td>
<td>8.69*10⁻⁸</td>
<td>9*10⁻⁶</td>
</tr>
<tr>
<td>2</td>
<td>1.158*10⁻⁷</td>
<td>1.2*10⁻⁵</td>
</tr>
<tr>
<td>3</td>
<td>1.737*10⁻⁷</td>
<td>1.8*10⁻⁵</td>
</tr>
</tbody>
</table>

was assumed to have a thickness of 0.5 mm (to yield fin efficiency of 95%). It is important to indicate that the unit cell represents half of the PCM domain or distance between fins as observed in Fig.3.2. Therefore, in the real design, the fin distance is twice the length of the PCM gap dimension used to design the unit cell to reduce convergence times. The PCM unit cell modeling is shown in Fig. 3.2 and 3.3.

![Figure 3.3: Unit Cell 3D Model for Rectangular Tube Thermal Energy Storage Design.](image)

**Mesh Sensitivity Analysis Using Hexahedron Elements**

Appropriate assessment of the transient modeling of this PCM melting is key to ensure good quality results. The time that is required to melt the PCM depends on the geometry encasing the PCM (heat transfer surface area), the PCM material properties and the
temperature difference between the heated bounding surfaces and the melting temperature of the PCM. Therefore, selecting the adequate mesh grid size and time step for this transient modeling is key to model the melting interface and obtain good transient heat transfer results. The most adequate element used to mesh the rectangular 3D geometry that represents the PCM bounded by the rectangular fin was the hexahedron element. It was very important to ensure that the mesh was very fine to allow convergence (especially to model the solid/liquid interface). The first step was to select the appropriate mesh grid division. This was performed for each PCM dimension as shown in Table 3.2.

The time step was also assessed in the same manner. Table 3.3 shows the time step selection for the 1.5mm PCM gap, and similarly, all other PCM gap cases time step selection was assessed.

The final mesh grid for each PCM gap case and time step were set as shown in Table 3.4,

**Benchmark Study of Phase Change Analysis**

Initially, the melting method was assessed its solution by running a simple semi-infinite case. The solution was then compared to the exact solution by Stefan for a constant temperature boundary application. The analysis was run in 3D using the dimensions as for the rectangular fin shape (See Fig. 3.4). Stefan’s exact solution predicts the temperature profiles
Table 3.2: Mesh Grid Sizing Selection For Each PCM Gap Dimension of Unit Cell.

<table>
<thead>
<tr>
<th>PCM gap of 0.5 mm</th>
<th>No. Elements</th>
<th>No. Nodes</th>
<th>Complete melting time ($\hat{\gamma}=1$),s</th>
</tr>
</thead>
<tbody>
<tr>
<td>30000</td>
<td>34463</td>
<td></td>
<td>11.56</td>
</tr>
<tr>
<td>60000</td>
<td>68926</td>
<td></td>
<td>15.24</td>
</tr>
<tr>
<td>90000</td>
<td>103389</td>
<td></td>
<td>15.71</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>PCM gap of 1.5 mm</th>
<th>No. Elements</th>
<th>No. Nodes</th>
<th>Complete Melt Time ($\hat{\gamma}=1$),s</th>
</tr>
</thead>
<tbody>
<tr>
<td>90000</td>
<td>100738</td>
<td></td>
<td>75</td>
</tr>
<tr>
<td>180000</td>
<td>201476</td>
<td></td>
<td>139.3</td>
</tr>
<tr>
<td>270000</td>
<td>302214</td>
<td></td>
<td>140.5</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>PCM gap of 3 mm</th>
<th>No. Elements</th>
<th>No. Nodes</th>
<th>Complete Melt Time ($\hat{\gamma}=1$),s</th>
</tr>
</thead>
<tbody>
<tr>
<td>180000</td>
<td>200151</td>
<td></td>
<td>480</td>
</tr>
<tr>
<td>360000</td>
<td>400301</td>
<td></td>
<td>553.33</td>
</tr>
<tr>
<td>540000</td>
<td>600453</td>
<td></td>
<td>558.78</td>
</tr>
</tbody>
</table>

Table 3.3: Time Step Selection for Transient Modeling of PCM for 1.5mm

<table>
<thead>
<tr>
<th>Time Step ($\Delta t$), s</th>
<th>Complete melting time ($\hat{\gamma}=1$),s</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0001</td>
<td>104</td>
</tr>
<tr>
<td>0.00001</td>
<td>120</td>
</tr>
<tr>
<td>0.000001</td>
<td>139.3</td>
</tr>
<tr>
<td>0.0000005</td>
<td>140</td>
</tr>
</tbody>
</table>

Table 3.4: Final Mesh for Rectangular Tubes Design

<table>
<thead>
<tr>
<th>PCM Gap Enclosure, mm</th>
<th>Time step $\Delta t$, s</th>
<th>No. Elements</th>
<th>No. Nodes</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>$1*10^{-6}$</td>
<td>60000</td>
<td>68926</td>
</tr>
<tr>
<td>1</td>
<td>$1*10^{-6}$</td>
<td>120000</td>
<td>135201</td>
</tr>
<tr>
<td>1.5</td>
<td>$1*10^{-6}$</td>
<td>180000</td>
<td>201476</td>
</tr>
<tr>
<td>2</td>
<td>$5*10^{-6}$</td>
<td>216000</td>
<td>241241</td>
</tr>
<tr>
<td>3</td>
<td>$5*10^{-6}$</td>
<td>360000</td>
<td>400301</td>
</tr>
</tbody>
</table>
with length for a semi-infinite solid. However, the fin gap is a very short distance, therefore, the comparison were applied at very short times. Stefan’s solution predicts the temperature field at a given time when the system is initially at the melting temperature. Therefore, in Fluent, the model was setup to start at the melting temperature.
Table 3.5: Material Properties for Lithium Nitrate Trihydrate

<table>
<thead>
<tr>
<th>Material Property</th>
<th>Quantity</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>1425</td>
<td>kg/m³</td>
</tr>
<tr>
<td>Specific Heat</td>
<td>2245</td>
<td>J/kgK</td>
</tr>
<tr>
<td>Thermal Conductivity</td>
<td>0.584</td>
<td>W/mK</td>
</tr>
<tr>
<td>Dynamic Viscosity</td>
<td>0.00507</td>
<td>N.s/m²</td>
</tr>
<tr>
<td>Thermal Coefficient of Expansion</td>
<td>0.0008</td>
<td>1/K</td>
</tr>
<tr>
<td>Melting Temperature</td>
<td>30</td>
<td>ºC</td>
</tr>
</tbody>
</table>

Stefan’ solution comparison were made for different times to observe the agreement and deviation. In Fig. 3.6, at time 1 second, the temperature profile calculated in fluent matches perfectly for the fin gap of 1.5 mm. However, as time increases, e.g. at 10 seconds, the temperature profile deviate much farther since the slope that the exact solution predicts higher temperature profiles as compared to the solidification and melting method in Fluent. The benchmark results are expected since the exact solution is for a semi-infinite plane. This results indicate that the melting analysis are going to be reliable when running melting cases ahead. In addition, in the literature review for using Fluent when solving melting of phase change materials was well studied and compared to experimental data. The literature review indicated how the percent errors found in these studies were below 5%.

Heat Transfer Assessment

The modeling of the melting process of the lithium nitrate trihydrate in this study allows to assess the performance of latent heat content extraction from the PCM. The thermo-physical properties of lithium nitrate trihydrate PCM used in this study are shown in Table 3.5,

Main Assumptions and Idealizations

Important assumptions and idealizations were made to setup our phase change model, such as,

1. The molten PCM is a Newtonian fluid, and its flow is laminar.
2. The change in volume when changing phase is neglected.
3. The liquid phase of the LiNO₃3H₂O is incompressible.
4. The liquid and solid phases in the PCM are homogeneous and isotropic.
5. The melting process is symmetric.
Table 3.6: Boundary Conditions and Initial Conditions for Rectangular Tube Geometry

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Quantity</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{\text{init}}$</td>
<td>29.9 °C</td>
</tr>
<tr>
<td>$T_{\text{wall}}$</td>
<td>37.4 °C</td>
</tr>
<tr>
<td>$T_s$</td>
<td>29.9 °C</td>
</tr>
<tr>
<td>$T_l$</td>
<td>30.1 °C</td>
</tr>
</tbody>
</table>

**Boundary and Initial Conditions for Rectangular Tube Geometry**

Due to the symmetry of the unit cell design of the PCM (see Fig. 3.2), all symmetry surfaces were set as adiabatic. The areas of contact with the solid encasing the PCM (the area of contact with the tube, $A_{\text{tube,cell}}$, and the area of contact with the fin, $A_{\text{fin,cell}}$) were set with a constant temperature of 37.4 °C (7.4 °C above the melting temperature of the PCM). The shape of the constant wall temperature boundary condition forms a L-shape temperature increase on the PCM geometry. To allow the system to converge and solve the energy and liquid fraction equations with the assigned mesh grid and time step, the $T_l$ and $T_s$ were assigned to be few decimals away from the actual melting temperature of the PCM (See Table 3.6).

### 3.3 Overall Heat Transfer Coefficient and Mean Conductance Assessment

A parameter that allowed to quantify the heat transfer performance of the melting process for each PCM gap design study is the overall heat transfer coefficient. This parameter allows to compare all designs regardless of their melting conditions (Temperature difference, melting time, and surface area of heat transfer). For the L-shape boundary condition, the total heat input to melt the unit cell is defined as,

$$U = \frac{Q_t}{A_{\text{tube,cell}}(T_w - T_m)} \quad (3.8)$$

Eq.3.8 is the overall heat transfer coefficient, and Eq. 3.9 is the mean conductance,

$$UA = \frac{Q_t}{(T_w - T_m)} \quad (3.9)$$
Table 3.7: Unit Cell Dimension Assessment for Rectangular Tube TES Device ($\Delta T = 7.4^\circ C$, $A_{base, fin} = 3 \text{mm}^2$ and $A_{fin, cell} = 5.79 \text{mm}^2$)

<table>
<thead>
<tr>
<th>Fin Gap, mm</th>
<th>$A_{tube, cell}$, $m^2$</th>
<th>PCM Unit Cell Volume, $m^3$</th>
<th>Total melt time, s</th>
<th>Time step, s</th>
<th>$U$, W/m$^2$K</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>$3\times10^{-6}$</td>
<td>$2.895\times10^{-8}$</td>
<td>15.24</td>
<td>0.000001</td>
<td>48589.4</td>
</tr>
<tr>
<td>1</td>
<td>$6\times10^{-6}$</td>
<td>$5.79\times10^{-8}$</td>
<td>60.14</td>
<td>0.000001</td>
<td>12137.14</td>
</tr>
<tr>
<td>1.5</td>
<td>$9\times10^{-6}$</td>
<td>$8.69\times10^{-8}$</td>
<td>139.3</td>
<td>0.000001</td>
<td>5723.03</td>
</tr>
<tr>
<td>2</td>
<td>$1.2\times10^{-5}$</td>
<td>$1.158\times10^{-7}$</td>
<td>246.32</td>
<td>0.000005</td>
<td>3343.7</td>
</tr>
<tr>
<td>3</td>
<td>$1.8\times10^{-5}$</td>
<td>$1.737\times10^{-7}$</td>
<td>553.33</td>
<td>0.000005</td>
<td>1586.19</td>
</tr>
</tbody>
</table>

$Q_t$ is the total heat input in the system over time defined as,

$$Q_t = \left( \int_0^t \dot{q}_{w, fin}dt \right) * A_{fin, cell} + \left( \int_0^t \dot{q}_{w, tube}dt \right) * A_{tube, cell}$$  \hspace{1cm} (3.10)

The $A_{tube, cell}$ varied with PCM enclosure gap. The overall heat transfer coefficient and mean conductance values are shown in Table 3.7. The area to calculate $UA$ was the total area of the tube cell and the fin thickness, such as,

$$A = A_{tube, cell} + A_{base, fin}$$  \hspace{1cm} (3.11)

where, the $A_{base, fin}$ was fixed to $3 \text{mm}^2$ and The $A_{fin, cell}$ was fixed to $5.79 \text{mm}^2$.

As observed in Fig. 3.7, the heat transfer performance when melting the PCM decreases as fin gap increases. Based on Fig. 3.8, to make the devices as low cost and efficient, the PCM gap should be at least of 1.5 mm for the rectangular fin shape geometry. Fig. 3.14 show the melting progress from 30% (at 11.5 seconds) to 80% (at 83 seconds) and the mean temperature of the PCM being $32^\circ C$ and $34.5^\circ C$ (2 and $4.5^\circ C$) above the melting temperature. After the PCM reaches 80%, the material takes longer to melt making the heat transfer less efficient since it takes about 83 seconds to melt up to 80% and 139 seconds to melt at 100%. The process indicates that most of the heat transfer is due to latent heat and small portion to sensible heat transfer given the fact that the system presents a Stefan Number of 0.05, the main mechanism of heat transfer due to phase change is expected.

**Critical Onset Buoyancy Effects Assessment**

The next step was to investigate the impacts of including buoyancy effects in the heat transfer analysis to verify how the extraction of thermal energy from the PCM is enhanced. By using the Boussinesq approach (See Eq.3.12), Table 3.5 shows the value used for the
CHAPTER 3. HEAT TRANSFER MODELING OF A PHASE CHANGE SYSTEM

Figure 3.7: Overall Heat Transfer Coefficient, $U$, of LiNO$_3$3H$_2$O for Rectangular Tube TES device ($A_{\text{tube, cell}}$ is per unit length) at $\Delta T = 7.4\, ^\circ\text{C}$.

Figure 3.8: Mean Conductance, $UA$, of LiNO$_3$3H$_2$O for Rectangular Tube TES device ($A_{\text{tube, cell}}$ is per unit length) at $\Delta T = 7.4\, ^\circ\text{C}$.
Figure 3.9: Interface Contour Graphs for 9.65mm x 1.5mm Unit Cell Domain Varying with Time (only conduction) for Rectangular Tube TES Device Δ T=7.4 °C

thermal coefficient of expansion found for this material [47]. The viscosity was taken at an average temperature since no significant fluctuation was observer between the temperatures of interest.

\[
(\rho - \rho_m) g = \rho \beta (T - T_m) g
\]  

(3.12)

The Raleigh number definition is known as,

\[
Ra = \frac{g \beta}{\nu \alpha} (T_s - T_{ref}) L_{fin}^3
\]  

(3.13)

In the literature it was found that the onset buoyancy critical Raleigh number was about 569 for two parallel plates when heating one plate to melt a phase change material. Therefore, in order to assess a critical Raleigh number and find any observation of buoyancy motion as the PCM turns into liquid, the case study was setup, such as the Raleigh number was above this critical Raleigh number. By keeping the same dimension as in the rectangular fin model and using a fin gap of 1.5mm, the temperature difference (ΔT) was double. This allowed to have a Ra number of 604 (higher than 569) [46]. Due to the non-linearity added by incorporating the gravity and buoyancy approach, the simulations in 3D required extremely long times, and it was more efficient to run the buoyancy effects assessment using a 2D
model. By modeling a cross-section of the rectangular PCM enclosure, the plane dimensions were similar (9.65 mm by 1.5 mm).

The non-linearity required the simulations to run for several days to melt the PCM with the stated dimensions. Therefore, only one set-up of dimensions were run to observe the differences in the velocity fields, melt times, and mean conductance values. Two assessments were performed. First, buoyancy effects were investigated by applying a $\Delta T$ of 7.4 °C similar to the rectangular tubes configuration boundary condition. Then, to validate the critical Raleigh number calculated in the literature, only the vertical ($L_{fin} = 9.65$ mm) was heated up by applying a constant temperature. Table 3.10 shows all important parameters and results for the three different cases.

Buoyancy effects were investigated as part of the assessment of how it could impact the heat transfer as the PCM turns into liquid. The onset critical Ra number is above 569 [46]. This indicates that above that number, liquid motion might be seen. As shown in Tab. 3.10. However, no fluid motion enhancing heat transfer were observed for the rectangular tubes configuration boundary condition at $\Delta T = 7.4$°C. To obtain a higher Ra than 569 with a PCM gap of 1.5 mm, the $\Delta T$ was increased from 7.4 to 14.8 °C (See Table 3.10). Fig.3.15 and 3.17 show the liquid melting, temperature and velocity profiles of the buoyancy effects. The
CHAPTER 3. HEAT TRANSFER MODELING OF A PHASE CHANGE SYSTEM

Table 3.8: Critical Raleigh Number Assessment Input Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Quantity</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal Coefficient of Expansion, $\beta$</td>
<td>0.0008</td>
<td>1/K</td>
</tr>
<tr>
<td>$T_w - T_m, \Delta T$</td>
<td>14.8</td>
<td>°C</td>
</tr>
<tr>
<td>Dynamic Viscosity, $\mu$</td>
<td>5.07*10^{-3}</td>
<td>Pa.s</td>
</tr>
<tr>
<td>Kinematic Viscosity, $\mu$</td>
<td>3.56*10^{-6}</td>
<td>m²/s</td>
</tr>
<tr>
<td>Specific Heat Capacity, $c_p$</td>
<td>2245</td>
<td>J/kgK</td>
</tr>
<tr>
<td>Thermal Conductivity, $k$</td>
<td>0.584</td>
<td>W/mK</td>
</tr>
<tr>
<td>Thermal Diffusivity, $\alpha$</td>
<td>1.83e^{-7}</td>
<td>m²/s</td>
</tr>
</tbody>
</table>

Figure 3.11: Temperature Contour Graphs for 9.65mm x 1.5mm Unit Cell Domain Varying with Time (conduction and convection) for Rectangular Tube TES Device $\Delta T= 7.4$°C

Table 3.9: Critical Raleigh Number Assessment Cases for Rectangular Tube TES Device ($\Delta T= 7.4$ °C 9.65mm x 1.5mm)

<table>
<thead>
<tr>
<th>Case No</th>
<th>Fin Gap, $mm$</th>
<th>$T_w - T_m$, °C</th>
<th>Melt Time, $s$</th>
<th>$\beta$, 1/K</th>
<th>Ra</th>
<th>$U$, W/m²K</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.5</td>
<td>7.4</td>
<td>136.7</td>
<td>0.0008</td>
<td>150</td>
<td>5750</td>
</tr>
<tr>
<td>2</td>
<td>1.5</td>
<td>7.4</td>
<td>139.3</td>
<td>0</td>
<td>150</td>
<td>5723.03</td>
</tr>
</tbody>
</table>
Figure 3.12: Temperature Contour Graphs for 9.65mm x 1.5mm Unit Cell Domain Varying with Time (only conduction) for Rectangular Tube TES Device $\Delta T = 7.4^\circ C$

Figure 3.13: Interface Contour Graphs for 9.65mm x 1.5mm Unit Cell Domain Varying with Time (conduction and convection) for Rectangular Tube TES Device $\Delta T = 7.4^\circ C$
Figure 3.14: Temperature Contour Graphs for 9.65mm x 1.5mm Unit Cell Domain Varying with Time (only conduction) for Rectangular Tube TES Device $\Delta T = 7.4^\circ C$

Table 3.10: Critical Raleigh Number Assessment Cases ($\Delta T = 14.8 \, ^\circ C$ on Vertical Wall, 9.65mm x 1.5mm)

<table>
<thead>
<tr>
<th>Case No</th>
<th>Fin Gap, mm</th>
<th>$T_w - T_m, ^\circ C$</th>
<th>Melt Time, s</th>
<th>$\beta$, 1/K</th>
<th>Ra</th>
<th>Overall Heat Transfer Coefficient, W/m²K</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>1.5</td>
<td>14.8</td>
<td>65.04</td>
<td>0.0008</td>
<td>604</td>
<td>4568.72</td>
</tr>
<tr>
<td>4</td>
<td>1.5</td>
<td>14.8</td>
<td>68.7</td>
<td>0</td>
<td>604</td>
<td>4130.5</td>
</tr>
</tbody>
</table>
3.4 Cylindrical Unit Cell PCM design for an Array of Round Tubes

The next configuration to explore is the cylindrical fin shape and place the PCM in between the fin around the inner tube. This configuration is very promising for commercial heat exchangers since they could potentially enhance heat transfer in a minimum volume. In this configuration, the extraction of thermal energy is analyzed by modeling the fin and PCM
CHAPTER 3. HEAT TRANSFER MODELING OF A PHASE CHANGE SYSTEM

Figure 3.16: Temperature Contour Graphs for 9.65mm x 1.5mm Unit Cell Domain Varying with Time (only conduction) for Rectangular Tube TES Device when applying $\Delta T = 14.8 \, ^\circ C$ only on vertical wall.

together and using symmetry to allow for faster convergence. Based on the buoyancy effects found in the previous study, the cylindrical shape only includes conduction heat transfer. The geometry and dimensions selected can be observed in Fig.3.19. The fin is in the center surrounded by the PCM.

**Meshing Method**

For the cylindrical fin shape geometry, the sweep meshing method was used. The sweep meshing method requires to have topologically identical source and target faces. In addition, it must have a sweep path that connects the source and target, and the heat exchanger geometry is suitable for this meshing method. This method generates hexahedron and wedge type of elements. Ideally, hexahedron mesh is the most desired since it has a cube topology allowing for shorter simulation times. The PCM region or the annular region consists of hexahedron elements. The fin region has a combination of hexahedron and wedge elements (wedges elements are mostly at the center of the fin region).
Mesh Sensitivity Analysis

The division of elements in the PCM and fin region were set up differently due to their different geometries and thicknesses. A mesh sensitivity analysis was performed by finding the appropriate mesh grid sensitivity for each fin gap dimensions (see Table 3.11).

The final mesh division was set to 30 cells axially and 50 cells radially in the PCM region. In the fin region, the edge division was set to 30 cells radially (See Fig. 3.19).

The final mesh for each configuration was based on a sensitivity analysis after performing calculations and observing how the results were mesh independent. Table 3.12 shows the final number of elements and nodes for each PCM width.

The time step was also assessed in the same manner. Table 3.13 shows the time step selection for the 1.5mm PCM gap, and similarly, all other PCM gap cases time step selection was assessed.

Heat Transfer Assessment for Cylindrical PCM Geometry

Similarly to the rectangular PCM enclosure, the main goal was to calculate the overall heat transfer coefficients and mean conductance for different PCM gap dimensions.

The PCM material properties are the same as shown in Table 3.5. The boundary conditions and initial conditions were the same in the rectangular fin case (See Table 3.6). The
Figure 3.18: Temperature Contour Graphs for 9.65mm x 1.5mm Unit Cell Dimension Varying with Time (only conduction) for Rectangular Tube TES Device when applying $\Delta T = 14.8 \degree C$ only on vertical wall.

Table 3.11: Mesh Grid Sizing Selection For Each Cylindrical Annular Unit Cell.

<table>
<thead>
<tr>
<th>PCM gap of 1 mm</th>
<th>No. Elements</th>
<th>No. Nodes</th>
<th>Complete melting time ($\hat{\gamma}=1$), s</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>50800</td>
<td>70134</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>101600</td>
<td>108222</td>
<td>117</td>
</tr>
<tr>
<td></td>
<td>203200</td>
<td>240876</td>
<td>117.8</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>PCM gap of 1.5 mm</th>
<th>No. Elements</th>
<th>No. Nodes</th>
<th>Complete melting time ($\hat{\gamma}=1$), s</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>90000</td>
<td>100738</td>
<td>210</td>
</tr>
<tr>
<td></td>
<td>180000</td>
<td>201476</td>
<td>234.9</td>
</tr>
<tr>
<td></td>
<td>270000</td>
<td>302214</td>
<td>235.2</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>PCM gap of 2 mm</th>
<th>No. Elements</th>
<th>No. Nodes</th>
<th>Complete melting time ($\hat{\gamma}=1$), s</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>169092</td>
<td>176590</td>
<td>389</td>
</tr>
<tr>
<td></td>
<td>304050</td>
<td>317934</td>
<td>414.9</td>
</tr>
<tr>
<td></td>
<td>610890</td>
<td>700890</td>
<td>415.9</td>
</tr>
</tbody>
</table>
Figure 3.19: Unit Cell PCM Mesh for an Array of Round Tubes.

Table 3.12: Final Mesh for Cylindrical Unit Cells PCM design.

<table>
<thead>
<tr>
<th>Fin Gap, mm</th>
<th>No. Elements</th>
<th>No. Nodes</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>101600</td>
<td>108222</td>
</tr>
<tr>
<td>1.5</td>
<td>180000</td>
<td>201476</td>
</tr>
<tr>
<td>2</td>
<td>304050</td>
<td>317934</td>
</tr>
</tbody>
</table>

Table 3.13: Time Step Selection for Transient Modeling of PCM for 1.5mm Cylindrical geometry

<table>
<thead>
<tr>
<th>Time Step ($\Delta t$), s</th>
<th>Complete melting time ($\dot{\gamma}=1$), s</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0005</td>
<td>230.4</td>
</tr>
<tr>
<td>0.00001</td>
<td>234.9</td>
</tr>
<tr>
<td>0.000001</td>
<td>235.1</td>
</tr>
<tr>
<td>0.0000005</td>
<td>235.4</td>
</tr>
</tbody>
</table>
annular gap of the PCM was varied to calculate important parameters ($U$ & $UA$), temperature and liquid melting fractions were calculated. The cases analyzed are described in Table 3.14.

The overall heat transfer coefficients as described in Eq.3.8.

Based on the findings of that buoyancy effects were negligible for the temperature difference of 7.4 °C for our melting studies, the cylindrical shape fin heat transfer assessment was performed without any buoyancy effects (the non-linearity of the equations make the time to solve 10 times greater yielding to results that do not have potential impacts). The melting rate is represented in Fig. 3.22 and 3.23. It can be observed that the melting rates are slower when the cylindrical fins are used instead of a rectangular case. For example, in the rectangular case it took about 11.3 seconds to melt at about 30% as compared the cylindrical case (fin thickness of 0.8 mm) that it takes 15 seconds, and for 50% liquid melted, it takes about 30 seconds using the cylindrical as compared to the rectangular case that it takes 27 seconds. Even though, the amount of PCM is less in the cylindrical, the radial phase change (heating from an inner rod towards the PCM) requires more time and therefore, it decreases its efficiency. However, the cylindrical shape requires a more compact design for good performance (from this study, a PCM annular gap of 0.5 mm is ideal). The performance can be very well observed in Fig. 3.21 & 3.20. The order of magnitudes of the $UA$ values

#### Table 3.15: $U$ with unit cell domain for Round Tubes Geometry $\Delta T= 7.4 \, ^\circ C$

<table>
<thead>
<tr>
<th>Fin Gap, mm</th>
<th>Volume, $m^3$</th>
<th>Melt time, s</th>
<th>Overall Heat Transfer Coefficients, $W/m^2K$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>5.0957*10^{-9}</td>
<td>32.058</td>
<td>912249</td>
</tr>
<tr>
<td>1</td>
<td>1.41*10^{-8}</td>
<td>117</td>
<td>2510.14</td>
</tr>
<tr>
<td>1.5</td>
<td>2.705*10^{-8}</td>
<td>234.88</td>
<td>969.526</td>
</tr>
<tr>
<td>2</td>
<td>4.56*10^{-8}</td>
<td>414.9</td>
<td>725</td>
</tr>
<tr>
<td>3</td>
<td>6.56*10^{-8}</td>
<td>600</td>
<td>480</td>
</tr>
</tbody>
</table>
are 10 times smaller compared to the rectangular fin. However, they are more compact and allows less encasement material (lowering the cost of the device). From the different PCM encasement gaps, the design of the heat exchanger has to have thin fin rods (0.8 mm or thinner) and keep the PCM gap shorter (No bigger than 0.5 mm).

Figure 3.20: Overall Heat Transfer Coefficient, $U$, (W/m$^2$K) of LiNO$_3$3H$_2$O for Round Tubes TES Device ($A_{\text{tube,cell}}$ is per unit length) at $\Delta T = 7.4$ °C.

Figure 3.21: Mean Conductance, $UA$, (W/K) of LiNO$_3$3H$_2$O for Round Tubes TES Device ($A_{\text{tube,cell}}$ is per unit length) at $\Delta T = 7.4$ °C.
Figure 3.22: Temperature Profiles as melting time increases in LiNO$_3$3H$_2$O for a Unit Cell domain of 1mm for Round Tubes TES ($A_{tube,cell} = 2.82\text{mm}^2$) at $\Delta T = 7.4 \ ^\circ\text{C}$

Figure 3.23: Liquid Melting Fraction as melting time increases in LiNO$_3$3H$_2$O for a Unit Cell domain of 1mm for Round Tubes TES ($A_{tube,cell} = 2.82\text{mm}^2$) at $\Delta T = 7.4 \ ^\circ\text{C}$
Table 3.16: Thermal Resistance in Rectangular and Round tubes Configuration at $\Delta T = 7.4$ °C (A of unit cell and tube are per unit length)

<table>
<thead>
<tr>
<th>Fin Gap, mm</th>
<th>$1/(UA)_{rec}$, K/W</th>
<th>$1/(UA)_{cyl}$, K/W</th>
<th>$1/(UA)<em>{rec} + 1/(hA)</em>{rec}$, K/W</th>
<th>$1/(UA)<em>{cyl} + 1/(hA)</em>{cyl}$, K/W</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>3.43</td>
<td>86.2</td>
<td>52.75</td>
<td>113.32</td>
</tr>
<tr>
<td>1</td>
<td>9.154</td>
<td>129.46</td>
<td>58.49</td>
<td>156.58</td>
</tr>
<tr>
<td>1.5</td>
<td>15.5</td>
<td>145.5</td>
<td>64.87</td>
<td>172.66</td>
</tr>
<tr>
<td>2</td>
<td>19.93</td>
<td>152.5</td>
<td>69.26</td>
<td>179.64</td>
</tr>
<tr>
<td>3</td>
<td>30.02</td>
<td>600</td>
<td>79.34</td>
<td>184.9</td>
</tr>
</tbody>
</table>

Table 3.17: Fully Developed Average Heat Transfer Coefficients for Rectangular and Round Tubes Inner Flows of Water at $T = 37.4$ °C

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Rectangular Tube</th>
<th>Round Tube</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_h$</td>
<td>0.0045m</td>
<td>0.0045m</td>
</tr>
<tr>
<td>Re</td>
<td>2190.1</td>
<td>2207.1</td>
</tr>
<tr>
<td>Pr</td>
<td>3.77</td>
<td>3.77</td>
</tr>
<tr>
<td>$L/D_h$</td>
<td>222.22</td>
<td>222.22</td>
</tr>
<tr>
<td>$Nu_{FD}$</td>
<td>3.97</td>
<td>3.68</td>
</tr>
<tr>
<td>$h_{ave,FD}$, W/m²K</td>
<td>563.23</td>
<td>521.97</td>
</tr>
</tbody>
</table>

**Heat Transfer Performance Comparison Between Rectangular Tubes and Array of Round Tubes TES**

To analyze the overall heat transfer from the hot water flow to the PCM through the metal encasement and fins, both configuration of heat exchangers are compared by calculating their total thermal resistance. In the PCM, the thermal resistance is calculated as $1/UA_{unit,cell}$ for the rectangular and round tubes configuration. In the water flow, the thermal resistance, due to convection, is defined as $1/hA$, where the area of the tube is per unit length (assumed to be 1m in length). The convective heat transfer coefficient is calculated using correlations of fully developed and laminar flow for rectangular and round tubes. The thermal resistance in through the walls of the tubes is assumed negligible due to the high thermal conductivity (aluminum) of the material, and the thickness of walls are assumed to be 1mm.
3.5 Summary of Findings

Based on Fig. 3.8, to make the device low cost and efficient, the PCM gap should be at least of 1.5 mm (3mm in the real design) for the rectangular fin shape geometry. From Fig. 3.14, it can be observed that most of the heat transfer and latent heat releases performs best in up to 80% melting liquid fraction instead of melting at 100% since the PCM melting rate decreases with time not allowing to make the charging process to be as efficient. Fig. 3.14 shows the melting progress from % 30 (at 11.5 seconds) to % 80 (at 83 seconds) and the mean temperature of the PCM being 32°C and 34.5°C (2 and 4.5 °C) above the melting temperature. Therefore, to make a heat exchanger device lower in cost and more efficient the melting process should be stopped at 80% to take advantage of most of the latent heat transfer release.

No fluid motion enhancing heat transfer were observed for the rectangular tubes configuration boundary condition at ΔT=7.4°C when applying buoyancy effects (Bousinessq approach). The enhancement of the heat transfer was only significant when using a ΔT of 14.8 °C at the vertical wall of about 10% when using buoyancy effects compared to no buoyancy effects (See Table 3.10). Therefore, Ra numbers above the predicted onset Ra number can enhance heat transfer with the LiNO$_3$3H$_2$O, however, with the PCM gap dimensions selected for adequate performance and a ΔT =7.4°C (Ra = 102), the buoyancy effects are not significant.

The cylindrical shape fin heat transfer assessment was performed without any buoyancy effects (the non-linearity of the equations make the time to solve 10 times greater yielding to results that do not have potential impacts). The melting rates are slower when the cylindrical fins are used instead of a rectangular case. For example, in the rectangular case it took about 11.3 seconds to melt at about 30% as compared the cylindrical case (fin thickness of 0.8 mm) that it takes 15 seconds, and for 50% liquid melted, it takes about 30 seconds using the cylindrical as compared to the rectangular case that it takes 27 seconds. Fig. 3.21 and 3.20 show the order of magnitudes of the UA values, which are 10 times smaller for the round tubes compared to the rectangular fin.

The total thermal resistance predictions using fully developed correlations for round and rectangular tubes (See Table3.17) [56] to calculate the fully developed convective heat transfer coefficient for inner flow of water show that total thermal resistance improves (smaller values) when the fin gap is kept as small as 1mm (0.5 in unit cell domain). In addition, the total resistance values demonstrate that the improvement of smaller fin gaps as of 1mm compared to 6mm (3mm in unit cell domain) are about 33.5% and 38.3% less in magnitude for the rectangular and round tubes configuration respectively. If comparing both configurations, rectangular and round tubes, the total thermal resistance are much smaller when using rectangular tubes. Using the same hydraulic diameter and fully developed average heat transfer coefficients (563.23 W/m²K and 521.97 W/m²K) for rectangular and round tubes respectively, the total resistance in rectangular tubes when a PCM surrounds them to enhance heat transfer are about 42.5% to 46.6% smaller compared to the total resistance in rectangular tubes.
Chapter 4

Concluding Remarks

In this dissertation, thermal energy transport in the high temperature range (> 800 °C) and low temperature range (> 30 °C) was investigated. Regardless of the temperature range of a system, thermal energy transport can take place to improve the overall efficiency of a system. The different types of thermal energy transport in this study (sensible and phase change) was applied to different material to take advantage of their capabilities to transport thermal energy from one medium to another in an efficient way.

*Molten Glass Heat Transfer Assessment for High temperature Collection*

In order to investigate the heat transfer performance of this molten glass, it was important to analyze the main mechanisms of heat transfer that govern its behavior. Experimental data was obtained by testing the fluid in a helical coil counter-flow heat exchanger prototype. The heat transfer performance of the molten glass was initially evaluated by modeling a 3D annular counter-flow heat exchanger using computational fluid dynamics software, Fluent-ANSYS. The heat transfer assessment included the treatment of radiative effects for a participating-absorbing medium. The radiation assessment solved for the radiative transfer equation where the absorption spectra was modeled using a rectangular bandgap model. Since the absorption coefficient spectrum of this molten glass is unknown, the absorption coefficients of two similar phosphorous pentoxide molten glasses were selected to observe its behavior for an optically thick and thin medium. The computational analysis results were then compared to the collected experimental data. This comparison allowed to observe the importance of thermal radiation heat transfer in the temperature range of this study.

The investigation in high collection consisted on analyzing molten glass as a heat transfer fluid. The first step was to assess its performance in a heat exchanger to transfer heat to another fluid, such as air. Due to technical difficulties and appropriate equipment, its thermal conductivity is not available. Halotechnics estimated its thermal conductivity based on its material composition (mainly phosphorous pentoxide). The temperature of operation in the experimental heat exchanger was between 650°C and 727°C, and thermal radiative heat
transfer is a mechanism to investigate in the study to quantify its impact. By modeling a 3D heat exchanger using computational fluid dynamics software, ANSYS, thermal conductivity and absorption coefficients were obtained from the literature of similar phosphorous pentoxide molten glasses. The expected behavior of a high Prandlt number (\(Pr = 368.9\)), its thermal boundary layer was thermally developing which indicated the validity of the computational model. Thermal radiative effects were assessed by allowing the glass to behave as an optically thick and thin medium. Even though, it is very well known that glass is opaque in the infrared wavelength range, the absorption coefficient found for the wavelength ranges of interest in this study (1 though 8 \(\mu\)m) shows a wide spectrum of its optical thickness. ANSYS allows to solve for the radiative transfer equation using a Direct Ordinate method. Three different behaviors were analyzed and compared: no radiation, optically thin (transparent), and optically thick (opaque).

The overall heat transfer when using thermal radiation with both optical thicknesses only improved the predictions by less than 2\% as compared to the amount of heat transfer when using no radiative heat transfer. The 3D modeling of the heat exchanger as an annular flow instead of a swirl for the air flow as the experimental helical coil heat exchanger prototype imposed the wall boundary condition by calculating the appropriate gap dimension of the annular region and the adjusted air thermal conductivity that allowed equivalent thermal resistance were accurately implemented since the percent errors calculated for the overall heat transfer were within 5\%, and the mean outlet temperature of the air were within 10\%. The manufacturer recommended thermal conductivity value of 0.8 W/m/K yielded predictions in close agreement with the heat transfer rates measured in the experimental prototype tests. Since the molten glass temperature drop (from inlet to outlet) was less than 100°C, using material properties including viscosity at an average temperature (695°C and 300°C respectively) was adequate based on the percent errors level to the experimental prototype.

**Transient Modeling of a Phase Change Cold Thermal Storage System**

The main goal of the study of a transient modeling of a phase change material for a cold thermal energy storage system was to investigate lithium nitrate trihydrate’s (\(LiNO_3\cdot3H_2O\)) capability to increase the dry-cooling effect of various applications. This was assessed by modeling of a unit cell of two different heat exchanger designs, melting rates, the overall heat transfer coefficient and mean conductance were calculated. The PCM was represented by the unit cell that melted at rates based on the temperature difference of 7.4 °C above the PCM’s melting temperature. The unit cell was varied with different dimensions representing the fin space geometry. of the gap between the fins where the PCM is located is varied for each configuration allowing to observe the impacts in their mean conductance values for the melting process of the PCM (charging).

The overall heat transfer coefficient about 5 order of magnitude for the fin gap of 1mm
for the rectangular fin geometry compared to the 1mm annular gap between round tubes. However, the overall heat transfer coefficient orders of magnitude decrease with increasing fin gap (for 6mm, rectangular fins $U$ is only twice higher than the 6mm cylindrical annular gap for an array of tubes). In the rectangular tube design heat exchanger design, the maximum mean conductance, $U_A$, was calculated to be 0.28 W/K at a fin gap of 1mm (0.5mm in unit cell domain). Increasing the fin gap to 2mm and 3mm (1mm and 1.5mm for unit cell design) decreases the $U_A$ by 40% and 28% orders of magnitude (0.11 and 0.076 W/K). Similarly, increasing the annular gap dimension to 2mm and 3mm (1mm and 1.5mm in unit cell domain) decreased $U_A$ magnitude by 35% (0.0077 W/K) and 40% (0.0065 W/K) respectively. The highest mean conductance was found at the unit cell annular dimension of 1mm (0.5mm in simulation due to symmetry) with a magnitude of 0.012 W/K.

The total thermal resistance predictions ($1/(U_A)_{unit,cell} + 1/(h_A)_{conv,water}$) using correlations for fully developed flows in round and rectangular tubes (See Table 3.17) to calculate average convective heat transfer coefficients demonstrate that its magnitude improved in smaller fin gaps (1mm or 0.5mm in unit cell domain). The smaller thermal resistance is about 33.5% less when the fin gap is 1mm compared to 6mm (3mm in unit cell domain) in the rectangular tube configuration. Similarly, the total thermal resistance is observed for round tubes with smaller thermal resistance in smaller tube gaps (1mm or 0.5mm in unit cell domain) of 38.3% less in magnitude compared to 6mm (3mm in unit cell domain) tube gaps (See Table 3.16). This indicates that for laminar and fully developed water flows in rectangular and round tubes, the heat transfer performance is significantly improved when the phase change material is configured in a smaller gap as compared to a wider gap (in this study from 1mm to 6mm), and this is clearly observed in both rectangular and round tubes configurations. However, If comparing both configurations, rectangular and round tubes, the total thermal resistance are much smaller when using rectangular tubes. Using the same hydraulic diameter and fully developed average heat transfer coefficients (563.23 W/m²K and 521.97 W/m²K) for rectangular and round tubes respectively, the total resistance in rectangular tubes when a PCM surrounds them to enhance heat transfer are about 42.5% to 46.6% smaller compared to the total resistance in rectangular tubes.

This analysis framework contributes to the improvement of dry-cooling technologies by providing the means of establishing the most effective tube design for a thermal energy storage device to melt a PCM and cool the temperature of water by 7.4°C effectively. This initial step could potentially enhance the implementation of this technology to other areas where cool thermal energy storage allows controlling a desired temperature.
Bibliography


[38] Patrick J. Shamberger and Timothy Reid. “Thermophysical properties of lithium nitrate trihydrate from (253 to 353) K”. In: Journal of Chemical and Engineering Data 57.5 (2012), pp. 1404–1411. ISSN: 00219568. DOI: 10.1021/je3000469.


