Numerical Investigation of Flow and Thermal Behavior in Channels with PCM-filled Thermal Energy Storage Columns for Potential Application in Photobioreactors

Sameed Akber, The University of Western Ontario
Supervisor: Siddiqui, Kamran, The University of Western Ontario
Joint Supervisor: DeGroot, Christopher, The University of Western Ontario
A thesis submitted in partial fulfillment of the requirements for the Master of Engineering Science degree in Mechanical and Materials Engineering
© Sameed Akber 2022

Follow this and additional works at: https://ir.lib.uwo.ca/etd
Part of the Computer-Aided Engineering and Design Commons, Energy Systems Commons, and the Heat Transfer, Combustion Commons

Recommended Citation
https://ir.lib.uwo.ca/etd/8832

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

Microalgae has been identified as a potential source in the production of biofuel. Photobioreactors, which are used for microalgae production, normally experience temperature variations over the diurnal cycle due to changes in ambient conditions. The thermal regulation of photobioreactors to minimize temperature variations will result in a higher yield of microalgae, which are sensitive to such variations. The present research is aimed to investigate a novel approach to thermally regulate photobioreactors using phase change materials (PCM) where the latent heat of the material is exploited as the energy storage. The present research uses a numerical approach to study the flow and thermal behaviors in a rectangular channel with PCM-filled thermal energy storage columns. An open source CFD software, OpenFOAM, is used to numerically simulate the problem. The results show that geometric parameters such as the gap and blockage ratios, column aspect ratio, column shape and column arrangement in the channel influence thermal energy storage in the PCM-filled columns. The results also show that the thermal response of the channel flow, when there is a gradual change in the flow temperature, is influenced by the flow parameters such as the mass flow rate and the rate at which the flow temperature varies.

Keywords

Fluid Mechanics; Computational Fluid Dynamics (CFD); Heat Transfer; Phase Change Materials; Microalgae

Summary for Lay Audience

This thesis project derived its inspiration from the need to maximize microalgae growth inside photobioreactors. Microalgae are microorganisms that photosynthesize to produce biomass which can be converted to biofuel. Photobioreactors that use sunlight as the light source (required for photosynthesis in microalgae) experience temperature variations due to changes in the ambient conditions. Microalgae growth is sensitive to temperature variations, which is why temperature control inside photobioreactors is necessary to maximize microalgae yield. In this thesis, an innovative approach to thermally regulate
photobioreactors using phase change materials as thermal energy storage is proposed. This thermal energy storage would store excess heat throughout the day and release the stored energy back into the photobioreactor during the night. A novel design is proposed where PCM-filled columns are placed inside the photobioreactor channel for temperature control.

The research outlined in this thesis aimed to answer three questions: (1) how does the placement of PCM-filled columns inside a rectangular channel affect the flow and heat transfer behavior in the channel and within the PCM; (2) how do the flow conditions inside the channel and the position of columns as well as the column shape and aspect ratio influence thermal energy storage; and (3) how does thermal energy storage in PCM-filled columns thermally regulate the channel fluid.

The open-source CFD software, OpenFOAM, was used to simulate flow and heat transfer inside a rectangular channel containing PCM-filled columns where the PCM undergoes phase change. The results show that the interaction of flow with the columns influenced the flow velocity and temperature. There was a change in the observed thermo-fluid behavior within the channel when the column arrangement, column shape and flow conditions in the channel were varied. Finally, energy storage in the PCM-filled columns regulated the temperature in the channel such that the higher temperature flow incoming into the channel left the channel at a relatively lower temperature.
Co-Authorship Statement

Thesis:


Authors: Sameed Akber, Kamran Siddiqui, Christopher DeGroot

Status: This thesis will be submitted as one or more manuscripts to different journals
Acknowledgements

I would like to, first and foremost, thank my supervisors, Dr Kamran Siddiqui and Dr Christopher DeGroot for their invaluable guidance and support, and without whose supervision and input, this thesis would not have been possible. I am thankful for the opportunities brought by them, which greatly improved my research horizon, scientific aptitude and learning skills. The scientific knowledge and understanding that I have gained during my time spent working with them will always remain with me.

I would also like to thank my fellow colleagues, department faculty members and other department officials who were at all times ready to extend a helping hand and to offer support. I also thank the engineering administration team, engineering IT department and the engineering finance center for their respective supports.

And finally, I would like to acknowledge the support of the University of Western Ontario and NSERC for funding this work.
Table of Contents

Abstract ........................................................................................................................................ ii
Summary for Lay Audience ........................................................................................................ ii
Co-Authorship Statement ........................................................................................................... iv
Acknowledgements .................................................................................................................... v
Table of Contents ..................................................................................................................... vi
List of Tables ........................................................................................................................ x
List of Figures ........................................................................................................................ xii
List of Appendices .................................................................................................................. xvi
Chapter 1 .................................................................................................................................... 1
  1 Introduction .......................................................................................................................... 1
    1.1 Microalgae as a Renewable Source of Biofuel .............................................................. 2
    1.2 Microalgae Cultivation .................................................................................................. 4
      1.2.1 Thermal Regulation of Photobioreactors ............................................................... 6
    1.3 Thermal Energy Storage ............................................................................................... 9
      1.3.1 Latent Heat-Based Thermal Energy Storage .......................................................... 10
      1.3.2 Melting Behavior of Phase Change Materials ....................................................... 11
    1.4 Flow over Obstacles ..................................................................................................... 16
      1.4.1 Flow over unconfined obstacles ............................................................................ 16
      1.4.2 Influence of the Blockage Ratio .......................................................................... 17
      1.4.3 Influence of the Gap Ratio .................................................................................... 18
    1.5 Motivation and Knowledge Gaps ................................................................................ 20
    1.6 Thesis Objectives ........................................................................................................ 21
    1.7 Thesis Layout ............................................................................................................... 22
Chapter 2 ................................................................................................................................... 23
2 Numerical Model Development for the Characterization of flow and thermal behavior in a rectangular channel containing offset PCM-filled columns ........................................ 23

2.1 Physical Model .................................................................................................. 24

2.2 Mathematical Model .......................................................................................... 26

  2.2.1 Channel Fluid Region ............................................................................... 27

  2.2.2 PCM Region ............................................................................................ 28

  2.2.3 Tube Region ............................................................................................. 31

  2.2.4 Summary of Model Equations .................................................................. 31

2.3 Discretization .................................................................................................... 33

  2.3.1 Transport Equation ................................................................................... 33

  2.3.2 Convective Term Discretization ............................................................... 34

  2.3.3 Diffusive Term Discretization .................................................................. 35

  2.3.4 Source Term Discretization ...................................................................... 36

  2.3.5 Temporal Term Discretization ................................................................ 36

  2.3.6 Complete Discretized Transport Equation ................................................ 37

2.4 Numerical Solution ............................................................................................... 38

  2.4.1 Solution Algorithm ................................................................................... 38

  2.4.2 Solution Control ........................................................................................ 41

  2.4.3 Multi-region solution algorithm ............................................................... 42

2.5 Boundary Conditions ............................................................................................ 44

2.6 Permeability Constant Sensitivity Analysis .......................................................... 45

2.7 Convergence Study ............................................................................................. 47

  2.7.1 Grid Convergence Study .......................................................................... 48

  2.7.2 Time Step Independence Study ............................................................... 50

  2.7.3 Solution Stability ...................................................................................... 50

2.8 Numerical Model Validation ................................................................................ 51
Chapter 3
Numerical investigation of the effects of flow and geometric parameters on thermal energy storage in PCM-filled columns

3.1 Introduction
3.2 Physical Model
3.3 Flow Behavior and Heat Transfer Characterization
  3.3.1 Channel Fluid Flow
  3.3.2 Column Walls
  3.3.3 PCM
3.4 Parametric Analysis of Operating and Geometric Conditions
  3.4.1 Studied Parameters
  3.4.2 Output Metrics
  3.4.3 Influence of Flow Conditions on Energy Storage
  3.4.4 Effect of Geometric Configuration on the Energy Storage
  3.4.5 Effect of Column Aspect Ratio on the Energy Storage
  3.4.6 Effect of Column Shape on the Energy Storage
3.5 Chapter Summary

Chapter 4
Response of a channel flow with PCM-filled thermal energy storage subjected to varying temperatures

4.1 Introduction
4.2 Physical Model
4.3 Thermal Regulation
  4.3.1 Thermal Energy Storage
  4.3.2 Thermal Energy Discharge
4.3.3 Thermal Energy Storage/Discharge Discussion .................................. 100
4.4 Parametric Analysis .............................................................................. 103
  4.4.1 Parameters ..................................................................................... 104
  4.4.2 Output Metrics .............................................................................. 106
  4.4.3 Influence of Mass Flow Rate ....................................................... 108
  4.4.4 Influence of the Rate of Temperature Change ............................. 111
  4.4.5 Influence of the Blockage Ratio .................................................. 114
4.5 Chapter Summary ............................................................................... 118
Chapter 5 .................................................................................................... 121
  5 Conclusions and Recommendations .................................................. 121
  5.1 Chapter 2: Numerical Modeling ....................................................... 121
  5.2 Chapter 3: Influence of flow and geometric parameters on thermal energy storage in PCM-filled columns ............................................. 123
    5.2.1 Characterization of flow and thermal behavior ......................... 124
    5.2.2 Optimization of the flow and geometric parameters to maximize thermal regulation ................................................................. 125
  5.3 Chapter 4: Thermal Response of a channel flow with PCM-filled thermal energy storage subjected to varying temperatures ..................... 127
    5.3.1 Thermal regulation in the presence of a varying flow temperature .... 127
    5.3.2 Parametric study to derive the optimal channel configuration .......... 128
  5.4 Contributions .................................................................................... 129
  5.5 Future Recommendations ............................................................... 130
References .................................................................................................. 132
Curriculum Vitae ....................................................................................... 147
List of Tables

Table 2-1. Thermophysical properties of Rubitherm-26 [89]......................................................... 25

Table 2-2. Conservation equations for the channel fluid, PCM and column wall regions..... 32

Table 2-3. Source terms added to the momentum and energy equations to model buoyancy effects and velocity/enthalpy in the mushy region of the PCM............................................. 32

Table 2-4. Transport equation parameters for the three governing equations..................... 33

Table 2-5. Numerical boundary conditions for the photobioreactor channel ....................... 45

Table 2-6. Percent relative change in grid convergence metric.............................................. 49

Table 3-1. Thermophysical properties of Rubitherm-26 [89]......................................................... 60

Table 3-2. Physical boundary conditions................................................................................ 60

Table 3-3. Variation of flow and geometric parameters in the parametric analysis .............. 72

Table 3-4. The different cases for the parametric study ordered by parameter type .......... 72

Table 3-5. Melting times in seconds for the different flow cases............................................ 79

Table 3-6. Melting times in seconds for different column arrangements......................... 83

Table 3-7. Geometrical properties and numerical results at different AR values............ 85

Table 3-8. The observations of the influence of various flow and geometric parameters on the thermal regulation ............................................................................................................... 89

Table 4-1. Thermophysical properties of Rubitherm-26 [89]......................................................... 94

Table 4-2. Numerical boundary conditions ............................................................................ 95

Table 4-3. Variation of parameters in the parametric analysis ............................................. 105

Table 4-4. Parametric analysis cases .................................................................................... 105
Table 4-5. Melting times at different mass flow rates in the channel...................................... 111

Table 4-6. Melting times at different rates of change in inlet temperature.............................. 114

Table 4-7. Melting times at different blockage ratios in the channel .................................... 118

Table 4-8. Observations of the influence of various parameters on the thermal regulation .... 120
List of Figures

Figure 1-1. The (a) top and (b) side views of the physical model used in experimental study of Toxopeus [43]. The horizontal and lateral offsets between centers of consecutive PCM-filled columns are equal to two and one column diameter(s), respectively........................................ 8

Figure 2-1. Overview of the numerical modeling process where mathematical equations are discretized and solved in OpenFOAM........................................................................................................ 24

Figure 2-2. Top and side views of the physical model, with the (a) top view showing the PCM-filled column inside the channel, and (b) side view showing the channel inlet and outlet. ...................................................................................................................................... 25

Figure 2-3. Solution algorithm for the PCM region equations .............................................. 40

Figure 2-4. Complete solution algorithm for the three-region numerical domain................. 43

Figure 2-5. PCM melt fraction versus time, at C = 103, 105, 106 and 108 ....................... 47

Figure 2-6. Total heat transfer rate from fluid to PCM columns at a specified time............. 48

Figure 2-7. The (a) top and (b) side views of the structured mesh ......................................... 49

Figure 2-8. Total heat transfer rate from fluid to PCM columns at a specified time............. 50

Figure 2-9. Outer column wall temperature at a specific point ................................................. 51

Figure 2-10. Top and side views of the physical model used in experimental study of Toxopeus [43], with the (a) top view showing the column arrangement, and (b) side view showing horizontal spacing between the columns................................................................. 52

Figure 2-11. Validation of the current numerical model against the experimental data of Toxopeus [43]. Outer column wall temperature when the channel inlet temperature is (a) 28C and (b) 33 C ............................................................................................................................... 53

Figure 2-12. The (a) numerical and (b) experimental resultant velocity magnitudes for flow over the first five columns in the channel at a height of 9.57 cm at a mass flow rate of 0.5
liters/min and an inlet temperature of 33 C. Experimental figure adapted from Toxopeus [1]
................................................................................................................................................. 54

Figure 3-1. The (a) top and (b) side views of the (c) physical model. The horizontal and lateral offsets between centers of consecutive PCM-filled columns are equal to two and half column diameter(s), respectively. ........................................................................................................... 61

Figure 3-2. The steady state velocity magnitude contours in the channel at the mid horizontal plane (shown) at Re = 200, for the (a) entire channel length and over the first three columns showing (b) resultant velocity vectors and (c) streamlines..................................................... 63

Figure 3-3. Numerical results for the channel fluid temperature contours in the mid horizontal plane (outlined in the schematic) at 50% PCM melt fraction, at Re = 200. ......................... 64

Figure 3-4. The average column wall temperature (T) and the total heat transfer rate (Q) from the channel fluid to the columns at Re=200........................................................................................................... 65

Figure 3-5. The (a) velocity magnitude and (b) y- velocity contours at 50% melt fraction in the first column at the mid-horizontal plane of y=H/2 (outlined in the schematic)............. 66

Figure 3-6. The (top) melt fraction and (bottom) velocity magnitude contours in the first column at PCM melt fractions of (a) 40%, (b) 60%, (c) 80%, (d) 90%, and(e) 99%........... 68

Figure 3-7. The horizontal (SL) and lateral (ST) offsets between columns......................... 70

Figure 3-8. Channel configuration at a horizontal offset of 1.5D and a lateral offset of (a) 0D, (b) 0.5D, and (c) D.................................................................................................................................................. 70

Figure 3-9. Channel configuration at a lateral offset of 0.5D and a horizontal offset of (a) 1.25D, (b) 1.5D, and (c) 2D............................................................................................................................................... 71

Figure 3-10. The influence of Reynolds number on thermal energy storage at ΔT= (i) 5C and (ii) 10C. The (a) Stored energy fraction, (b) heat transfer rate to the PCM, and (c) channel outlet temperature, versus fractional time................................................................. 78
Figure 3-11. Influence of column lateral offset at $SL = (i) 1.25D$, (ii) 1.5D, and (iii) 2D, on thermal energy storage in PCM-filled columns. (a) Channel outlet temperature, (b) heat transfer rate to the PCM, and (c) Stored Energy fraction, versus fractional time......................... 82

Figure 3-12. The influence of column aspect ratio on thermal energy storage in PCM-filled columns. The (a) Stored energy fraction, (b) heat transfer rate to the PCM, and (c) channel outlet temperature, versus fractional time.................................................................................... 85

Figure 3-13. The influence of column cross section shape on thermal energy storage in PCM-filled columns. The (a) Stored energy fraction, (b) heat transfer rate to the PCM, and (c) channel outlet temperature, versus fractional time. .............................................................................. 87

Figure 4-1. The (a) top and (b) side views of the physical model. The horizontal and lateral offsets between centers of consecutive PCM-filled columns are equal to 1.5D and 0.5D, respectively. ............................................................................................................................ 95

Figure 4-2. The (a) inlet and outlet temperatures at a mass flow rate of 0.375 Kg/min, and (b) the cumulative thermal energy storage in PCM columns during energy storage (i.e. the temperature ramp up). The beginning and end of the melting phase are marked on the outlet temperature curve for reference. ........................................................................................................ 98

Figure 4-3. The (a) inlet and outlet temperatures at a mass flow rate of 0.375 Kg/min, and (b) the cumulative thermal energy storage in PCM columns during energy discharge (i.e. the temperature ramp down). The beginning and end of the solidification phase are marked on the outlet temperature curve for reference. ............................................................................................. 100

Figure 4-4. Thermal response at the channel outlet for the energy storage and discharge cycles..................................................................................................................................... 102

Figure 4-5. Different reference point locations at the mid horizontal (y) plane of the physical model........................................................................................................................................ 103

Figure 4-6. Flow temperature at different reference locations in the channel (outlined in Figure 4-5) during, (a) energy storage and (b) energy discharge. ................................................................. 103
Figure 4-7. The influence of mass flow rate on, (a) stored energy fraction, (b) heat transfer rate, and (c) thermal response, versus fractional time. ................................................................. 110

Figure 4-8. The influence of rate of temperature change on, (a) stored energy fraction, (b) heat transfer rate, and (c) thermal response, versus fractional time.............................................. 113

Figure 4-9. Channel configurations at the blockage ratios of (a) 0.4, (b) 0.5, and (c) 0.6... 116

Figure 4-10. The influence of blockage ratio on, (a) stored energy fraction, (b) heat transfer rate, and (c) thermal response, versus fractional time. ................................................................. 117
List of Appendices

Appendix A: Thermal Energy Discharge ........................................................................ 144
Nomenclature

Abbreviations

AR  Aspect Ratio
BR  Blockage Ratio
GHG Greenhouse gases
GR  Gap Ratio
Gr  Grashof Number
HTF Heat Transfer Fluid
LHS Latent Heat Storage
LHTES Latent Heat based Thermal Energy Storage
Nu  Nusselt Number
PBR Photobioreactor
PCM Phase Change Material
SHS Sensible Heat Storage
TES Thermal Energy Storage
Notations / List of Symbols:

\( C_{p,l} \)  Liquid specific heat capacity

\( C_{p,s} \)  Solid specific heat capacity

\( C_p \)  Specific heat capacity

\( \dot{m} \)  Mass flow rate

\( \Delta H \)  Enthalpy of phase change

\( D \)  Column Diameter

\( f \)  PCM liquid Fraction

\( g \)  Acceleration due to gravity

\( Gr \)  Grashof number

\( H \)  Channel Height

\( h \)  Convective heat transfer coefficient

\( k \)  Thermal conductivity

\( L \)  Channel Length

\( Nu \)  Nusselt number

\( Pr \)  Prandtl number

\( Q \)  Heat transfer rate

\( Ra \)  Raleigh number

\( Re \)  Reynolds number

\( St \)  Strouhal number
t  Time
T  Temperature
W  Channel Width
x/L Dimensionless length (horizontal)
y/H Dimensionless length (vertical)

Subscripts:

s  Solid
l  Liquid
o  Outlet
e  Inlet
1  Initial Value
2  Final Value

Greek Symbols:

\( \beta \)  Volumetric thermal expansion coefficient
\( \nu \)  Kinematic viscosity
\( \alpha \)  Thermal diffusivity
\( \mu \)  Dynamic viscosity
\( \rho \)  Density
Chapter 1

1 Introduction

Contemporary climate change has been linked to the emission of greenhouse gases, most notably carbon dioxide and methane. The major source of these emissions is the burning of fossil fuels for energy production. The awareness and widespread concern surrounding the long-lasting adverse effects of climate change, particularly those caused by global warming, have resulted in an effort to switch away from burning fossil fuels and towards harvesting energy from zero- or low-carbon sources. These alternative sources include solar, wind, geothermal, hydropower, and biomass. It has been shown that such sources favor decentralized energy grids and local solutions that are somewhat independent of the national network [1]. Smaller scale implementations enhance system flexibility and allow for greater adaptability in responding to unpredictable growth and/or changes in energy demand. It is possible for some renewable energy sources to provide thermal energy directly, a prospect which shows potential in the localized space and water heating of residential and commercial buildings, especially when taken into consideration that a large percentage of the total available energy is used for space heating and cooling purposes. In countries with extreme climatic conditions, including Canada, this proportion can reach as high as 40% [2]. One type of the sustainable energy source that has shown potential in local energy production in living/working spaces is biomass [3]. A novel design to integrate photobioreactors within building facades for biomass cultivation has been proposed in recent studies [4]. Building-integrated photobioreactors can help thermally regulate the building, but also bring in new challenges to ensure the thermal conditions in the photobioreactor itself are suitable for the biomass survival. This thesis aims at addressing this challenge. In this thesis, the flow and thermal behaviors in photobioreactors are first characterized. This is followed by investigating, and subsequently optimizing, a design for passive thermal regulation within photobioreactors that could be integrated into building facades. In the following section, the background to relevant established and proposed technologies is discussed.
1.1 Microalgae as a Renewable Source of Biofuel

Biofuel is a carbon neutral alternative to conventional fossil-based fuels. Biofuels are classified as primary or secondary fuels. Primary biofuels such as wood can be used as a source of energy directly, without having to go under any kind of processing. These types of fuels are combusted directly to provide energy for cooking, heating or to produce electricity [5]. Secondary biofuels are produced from some type of processed raw biomass. These can include solid fuels (e.g. charcoal), liquid fuels (e.g. ethanol, biodiesel and bio-oil), or gases (e.g. biogas). Secondary biofuels are further classified as first, second or third generation fuels. First generation liquid biofuels are normally produced from food crops such as corn and wheat [5], and include ethanol, propanol and butanol. First generation biodiesel, for example, is primarily produced from corn oil [6]. Because first generation fuels are produced from agricultural crops that would otherwise be used as a food source, there is a growing need in response to the increasing global population, to move away from active food sources and towards using agricultural feedstock byproducts for biofuel production. Second generation biofuels are produced from agricultural feedstock that is either not a food source or is the waste from food crops [7]. The main advantages of second-generation biofuels are that their production does not require additional land, fertilizers or other agricultural resources that are not already used to grow crops for food. In spite of these advantages over first generation biofuels, there is still concern over competing resources and land use changes [8]. Third generation biofuels are primarily produced from algae [8] and are therefore, unaffected by the common drawbacks of the first- and second-generation biofuels stemming from their reliance on the agricultural feedstock.

Microalgae are unicellular organisms that photosynthesize to produce algal biomass. In 1942, Harder and von Witsch [9] first recommended that microalgae could be a viable source of lipids, which could be used as food or to produce biofuels. Since then, considerable effort has been put into research involving microalgae and their use in the production of third generation liquid biofuels. In recent reviews by Patil et al. [10] and Chisti [11], microalgae were deemed to be the only renewable source of biofuel that was capable of meeting the global demand for transportation fuels, with the potential to
completely displace the use of fossil fuels. Nowadays, microalgae are considered as one of the most promising sources of bioenergy production [12-14]. This can be attributed to a variety of factors, the most prominent of which include the much higher land use efficiency and productivity. For example, palm oil is considered as a high yield vegetable oil for biodiesel, but it has shown that to meet 50% of the fuel demand in the transportation sector of the United States (US) alone, 24% of the farmland in the US needs to be devoted [15]. Contrary to that, it has been shown that the area required to cultivate microalgae to meet 50% of US transportation demand, is less than 3% of the US farmland [16]. Additionally, under optimal growth conditions, some microalgae species can produce and accumulate hydrocarbons up to 30–70% of their dry weight, and the high oil content of such species allow them to produce 1000 times as much oil as that of the soybean grown on the same area of land [17].

In addition to the biofuel production, the by-products of microalgae cultivation can be useful to other industries. The solid waste, for example, can be used to generate animal feed, which would eliminate the carbon footprint associated with its regular production from soy or corn. In fact, with the assumption of 30% residual biomass by weight, the land use efficiency of using biofuel by-product as animal feed is 28 times higher and would result in a 17.3% reduction in greenhouse gas emissions compared to soybean [18]. Microalgae consume carbon dioxide from the atmosphere to grow, which makes their cultivation a biological carbon sequestration process. In contrast to contemporary carbon capture and storage methods, which have shown to be economically infeasible, and whose long-term environmental impacts remain uncertain, biological carbon sequestration through microalgae cultivation is an attractive alternative to minimize the carbon footprint [19]. Other benefits of microalgae include their use as a healthy food, and producers of useful compounds [20], biofilters to remove nutrients and other pollutants from wastewaters [21] and indicators for environmental change. They are also commonly used in space technology and as laboratory research systems [22].
1.2 Microalgae Cultivation

Microalgae utilize the energy from light, as well carbon dioxide and water from the environment to synthesize organic molecules in a process known as photosynthesis; oxygen is released as a by-product. There are two different cultivation systems used for the production of microalgae: open raceways ponds and photobioreactors (PBR). Open raceway ponds are basic cultivation systems. Biomass productivities in open raceway ponds are low, there is a high risk of contamination, and the production is highly dependent on the environment [23]. However, open raceways ponds do have low construction and operating costs [23]. In contrast to open raceways ponds, photobioreactors have more control over the cultivation conditions, which can be optimized to increase the yield of microalgae. Although, one major setback of the photobioreactor is the lack of efficiency with utilizing solar energy for biomass production [24]. Algal growth is affected by several environmental parameters such as temperature, pH, salinity, oxygen concentration, as well as processing parameters such as mixing and light intensity. The optimal conditions tend to be culture specific, and the individual parameters must be tweaked differently depending on the type of microalgae that is being incubated [25].

The most important factor affecting microalgae growth is light intensity, as it relates directly to the photosynthetic rate. The photosynthetic rate increases with light intensity up to a certain saturation point, known as the saturation irradiance. Increasing the light intensity beyond this point causes damage to the microalgae, which leads to photoinhibition, and the algal growth rate slows down. Gonçalves et al. [26] investigated the effects of increasing light intensity on different species of microalgae. It was observed that different species of microalgae have different optimal irradiance levels. A separate study by Nzayisenga et al. [27] involving entirely different species also concluded that there is a great variation in the optimal average light irradiance among different species, with the maximum observed difference being 17% between C. vulgaris and M. aeruginosa. The variation of light wavelength also has pronounced effect on algal growth. The studies by Satthong et al. [28], Sing et al. [29] and Esteve et al. [30] all determined that algal growth after the onset of irradiance, measured in number of
cells/ml, was highest when microalgae species were exposed to white LED light as compared to red or blue LED light.

Temperature has a strong influence on microalgae growth and productivity. The light absorbed by the photobioreactor walls, or by the culture that is not used in photosynthesis is converted into thermal energy, may cause an increase of the culture temperature. The optimal temperature range for algal growth is 20 – 35 degrees Celsius for most species of microalgae, although a few species can survive in temperatures up to 40 degrees Celsius [31]. If the temperature of the culture is lower than this optimal range, then the biomass yield decreases. Conversely, if the temperature is too high, it can cause permanent damage to the microalgae cells [32]. The optimal temperature for *S. almeriensis*, for example, is 35 degrees Celsius and the cells start to die above 40 degrees Celsius [33]. *C. reinhardtii* is most productive in the temperature range of 12 – 36 degrees Celsius [34]. In large scale photobioreactors placed in natural sunlight, temperatures in the system can reach up to 45 – 60 degrees Celsius in the absence of temperature regulation [35]. Temperatures this high would kill most species of microalgae, and artificial temperature control systems have to be set up to avoid overheating [36-37]. In the case of *C. reinhardtii*, it was shown that the growth rate increases by a factor of 1.6 as the temperature is increased from 15 C to 25 C, and by a factor of 2 when the temperature is increased from 18 C to 28 C, or 25 C to 35 C [38]. This positive relationship between temperature and growth rate only applies up to a certain temperature point, which in most cases is in the range 30 – 35 degrees Celsius, and further increasing temperature beyond this point, results in a sharp decrease in growth rate. Microalgae growth is also sensitive to temperature variations. *R. capsulatus*, for example, has twice the productivity when it is exposed to a constant temperature of 30 C compared to the case when the temperature is slowly increased from 15 – 30 C [39]. This suggests that thermal regulation is required to not only keep temperature within an optimal range, but to also dampen temperature variations in the photobioreactor.
1.2.1 Thermal Regulation of Photobioreactors

Thermal regulation of a photobioreactor (PBR) can be achieved in different ways, some of which include, 1) shading the PBR with dark colored paint [40], 2) cooling by spraying water on the PBR panels [41], 3) submerging the PBR in a large amount of water [41], and 4) installing a heat exchanger inside the PBR [42]. Shading the PBR is the most cost-effective method for temperature control but it comes at the cost of restricting the light that is available to microalgae. Spraying water to achieve cooling is a commonly used method but it only works in areas with low air humidity, and it adds to the cultivation costs. Temperature control by partially or fully submerging the PBR in water has the advantages of improved cooling. However, some of the light is absorbed by the external water body which can have adverse effects on microalgae productivity. Additionally, regular water filtration to remove contaminants adds to the maintenance costs [31]. Temperature control using heat exchangers is also commonly employed in photobioreactors. This method requires a secondary flow loop which exchanges thermal energy with the main flow to maintain system temperature, which adds to the equipment and operating costs. All of the aforementioned temperature-control methods employ active thermal regulation. Temperature control in photobioreactors using passive thermal regulation has been proposed in some recent studies.

Uyar and Kapucu [35] experimentally investigated the use of phase change materials (PCM) to passively regulate temperature inside a photobioreactor placed in natural sunlight. The cylindrical photobioreactor was insulated on all sides except at the front and back panels. The front panel was exposed to natural sunlight, and a PCM compartment was attached to the back panel. For the control case, the PCM compartment was removed and the back panel was instead insulated. The minimum and maximum ambient air temperatures over the course of the day were measured to be 20°C and 35°C, respectively. The sunlight intensity was measured to range from 0 to a maximum of 790 W/m² (100 kilo lux). The photobioreactor temperature was found to change in response to variations in the ambient conditions. The maximum culture temperature was 60°C and 45°C in the control and thermally regulated cases, respectively. The 15°C difference between the control and temperature-controlled cases showed considerable thermal energy storage
inside the PCM. The temperature control, however, was not sufficient to keep the PBR temperature within the targeted 20 – 40 C range for optimal culture growth. The authors suggested that temperature control could be further improved by 1) increasing the amount of PCM, 2) increasing the rate of heat transfer between the PBR and PCM compartments, and 3) installing better insulation to the system. The experiment considered a photobioreactor with stagnant fluid. The presence of some kind of flow was hypothesized to achieve greater heat transfer rates between the culture and PCM due to the presence of forced convection and turbulence in the system.

Passive thermal regulation of a photobioreactor using PCM was experimentally investigated by Toxopeus [43]. Figure 1-1 shows the experimental setup to investigate passive thermal regulation in a rectangular channel containing PCM-filled columns. The rectangular channel was insulated on all sides to prevent heat loss. The PCM in the columns was initially subcooled. At the start of the experiment, heated fluid (water) at a constant mass flow rate was circulated through the channel and thermocouples placed at strategic locations in the channel were used to monitor temperature. The study found that there was turbulence generation as a result of flow acceleration in the channel fluid as it passed over the columns and flow separation behind the columns. Flow acceleration, and therefore turbulence in the channel, was found to be influenced by various operating and geometric conditions. Turbulence increased when the mass flow rate in the channel was increased. It was also higher when the horizontal spacing between columns was smaller, and when columns with a square cross section were used in place of circular columns. Of these factors, flow rate was found to have the most pronounced effect on turbulence.

Temperature data obtained from thermocouples revealed that temperatures at the outer column walls increased rapidly as the heated channel fluid from the inlet came into contact with the PCM-filled columns. After this step increase, column wall temperatures continued to rise slowly to approach the temperature of the heated channel fluid. The PCM temperature was found to rise slowly in comparison to the column wall temperature, and it stayed constant at the PCM melting temperature for a considerable time. The heat flux across the column walls, in accordance with the column wall temperature, peaked right after the heated channel fluid made contact with the columns, and it declined rapidly following this peak in response to diminishing temperature
gradients at the column-fluid interface. The peak heat flux at the column walls increased proportionately with an increase in the flow rate and the channel fluid temperature. Heat flux was also higher, albeit to a lesser degree, when square columns were used and when the horizontal distance between columns was smaller. Finally, the total melting time of the PCM was found to be lower at higher flow rates in the channel. The study deduced that thermal energy storage within PCM columns in a rectangular channel is affected by various operational and geometric parameters such as the flow rate, heated fluid temperature, column arrangement and column shape. An in-depth parametric study to determine the optimal column arrangement for maximizing thermal energy storage was left to future work.

Figure 1-1. The (a) top and (b) side views of the physical model used in experimental study of Toxopeus [43]. The horizontal and lateral offsets between centers of consecutive PCM-filled columns are equal to two and one column diameter(s), respectively.
1.3 Thermal Energy Storage

Thermal Energy Storage (TES) is a technology that stores thermal energy to be used at a later time. With the recent breakthroughs in renewable energy technologies such as solar, wind, and biomass, there has been a need to develop efficient and sustainable methods of storing energy from these sources [44]. This has led to the development of efficient TES systems that can be integrated into renewable energy systems with the main purpose of overcoming the mismatch between energy generation and utilization [45-47]. For example, in solar power generation plants, TES systems can store solar energy temporarily for electricity production when sunlight is not available. In this manner, the plant operation can smoothly continue for the entire 24 hours of the day. The advantages of using thermal energy storage include better system efficiency and reliability, energy savings, reduction in recurring costs, and less environmental pollution [48]. It has been estimated that, in Europe, around 1.4 million GWh/year can be saved and 400 million tons of CO2 emissions can be avoided through an extensive use of thermal energy storage for cooling and heating purposes in buildings and the industrial sector [49].

There are two types of thermal energy storage: sensible heat storage (SHS) and latent heat storage (LHS). In SHS, the heat capacity and change in temperature of the storage medium is used to store thermal energy,

$$ Q = m \int_{T_0}^{T_f} c_p \, dT $$

(1.1)

where $m$ is mass, $c_p$ is specific heat, and $T_0$ and $T_f$ are the initial and final temperatures of the storage medium, respectively. LHS refers to thermal energy storage in the form of latent heat during phase change at a constant temperature,

$$ Q = m \Delta H $$

(1.2)

here $m$ is the mass, and $\Delta H$ is the latent heat of the storage medium. Phase change in the context of thermal energy storage can refer to either solid-liquid or liquid-gas transition. The liquid-gas phase transition latent heats are very high, but the large change in volume
makes this process undesirable for TES in most practical cases [50-51]. The solid-liquid phase transition latent heats are sufficiently high and there is limited volume change during phase transition.

Thermal energy storage in latent heat-based systems is a combination of both SHS and LHS, although the fraction of energy stored as sensible heat is relatively low as compared to the energy stored as latent heat. Thermal energy is stored as latent heat during phase change and as sensible heat during temperature change both before and after phase change,

\[ Q_{\text{total}} = Q_s + Q_l = m \left[ \left( \int_{T_0}^{T_m} c_s \, dT \right) + \Delta H + \left( \int_{T_m}^{T_f} c_l \, dT \right) \right] \]  

(1.3)

Where \( c_s \) and \( c_l \) are the PCM specific heats in the solid and liquid phase, respectively, and \( T_0, T_m \) and \( T_f \) are the initial, melting and final temperatures of the PCM, respectively.

### 1.3.1 Latent Heat-Based Thermal Energy Storage

Latent heat-based thermal energy storage systems exploit the latent heat of a material to store thermal energy. Such systems have large energy storage densities due to the large latent heats of phase change materials. In addition, because latent heat storage occurs at a constant temperature, such systems have the potential to maintain the operating temperature of a system in a narrow range around the melting temperature of the PCM [52]. In comparison to sensible heat-based storage systems which are most effective at energy storage in the presence of considerably large temperature gradients, latent-heat-based systems are operable even when temperature gradients between the system and PCM are small. This allows for temperature control not only at a macro level but also as a way to correct small temperature variations in the system.

Phase change materials can be used to regulate the temperature of a system where temperature fluctuates in the presence of heating and cooling cycles. When thermal energy is added to the system, which may cause the system temperature to rise, the PCM absorbs this thermal energy from the system to melt, thus removing excess heat from the
system and maintaining the system temperature. And when the system loses thermal energy (e.g. at night), which may cause the system temperature to fall, the PCM solidifies to release stored thermal energy back to the system to maintain its temperature. In the ideal case of thermal regulation, where heat transfer to and from the PCM is instantaneous, system temperature would always be maintained at a constant level until all the PCM has melted. However, the rate of thermal energy storage is limited by the heat transfer rate to and from the PCM. This is because PCMs have low thermal conductivity, this implies that heat cannot be transferred to or removed from the PCM at sufficiently high rates to maintain the system temperature at a constant level. The phase change (melting and freezing) behavior of PCMs provides an insight into the mechanisms of heat transfer and thermal energy storage.

1.3.2 Melting Behavior of Phase Change Materials

Phase change due to heat transfer creates an interfacial region which separates the solid and liquid regions of the PCM. This interfacial region is termed the active zone [53]. Thermophysical properties of the material differ in solid and liquid regions. Additionally, the primary mode of heat transfer is conduction in the solid region and convection in the liquid region. Hale and Viskanta [54] experimentally studied the melting behavior of paraffin contained within a rectangular enclosure as it was heated from a side wall. The advancement of the melting front suggested that natural convection dictates how the solid-liquid interface advances through the material. Ho and Viskanta [55] experimentally and numerically studied the melting patterns inside paraffin contained within a rectangular cavity. They found that heat transfer occurs purely by conduction in the initial stages of melting up until a large enough accumulation of the liquid phase occurs, after which the buoyant forces become significant and natural convection dictates the melting process and solid-liquid interface movement.

Using a similar setup, Gau and Viskanta [56] experimentally studied the movement of the solid-liquid interface in pure Gallium when heated from a side wall. They found that a thin layer of liquid gallium forms adjacent to the heated wall. At the onset of natural convection, buoyancy force pushes the liquid gallium upwards in this layer, which causes the interface to move outwards, normal to the heated wall. Liquid gallium circulation in
the convective cell continues to push the solid-liquid interface away from the heated wall in the top regions of the enclosure where the heated liquid gallium accumulates. The authors characterized natural convection heat transfer by empirically correlating melt fraction and heat transfer through the use of relevant dimensionless parameters. Rayleigh number represents the ratio of the buoyant forces to the viscous forces in the liquid phase, Nusselt number is a ratio of the convective to conductive heat transfer, and Stefan number is the ratio of sensible to latent heat storage. The authors found that an increase in the Rayleigh and Stefan numbers reduced the total melting time.

Gau et al. [57] considered a heat source at the bottom of a rectangular enclosure containing paraffin wax. They found that the buoyancy driven flow dictates the shape of the solid-liquid interface. Diaz and Viskanta [58] observed that the onset of natural convection in paraffin contained in a rectangular enclosure heated from below depends on the Rayleigh number, and that the formation of small Bernard cells in the liquid PCM is followed by the merging of these cells into one larger convective cell. Prud’Homme et al. [59] numerically investigated the melting behavior inside a vertical adiabatic cylinder heated from below. The authors found that natural convection begins at a critical Rayleigh number and that smaller convective cells in the liquid domain join to form one larger cell.

Bashar and Siddiqui [60] experimentally studied the melting behavior and interface dynamics of paraffin wax contained in a rectangular chamber, where a heat transfer fluid (HTF) passing through a horizontally positioned tube near the bottom of the chamber was the heat source. It was observed that, after the onset of melting, the solid-liquid interface remains mostly linear and progresses upwards at relatively steady speeds when the heat flux across the HTF tube is small, but the interface becomes non-linear in the presence of large spatial fluctuations when the heat flux is increased. It was found that the spatial fluctuations in the interface were the result of bulk motion of the liquid PCM within convective cells, causing acceleration and deceleration of the interface. The temperature measurements suggested that the temperature at a given location rises sharply as it comes into contact with the solid-liquid interface due to convection heat transfer and becomes steady as the location is eventually integrated into the convective cell. Due to this, the
temperature was found to rise at a faster rate close to the HTF tube and at higher heat fluxes.

Bashar and Siddiqui [61] experimentally investigated natural convection melting process in paraffin wax with an embedded U-shaped heat source. A HTF was passed through a U-Tube which was embedded within the solid paraffin in a rectangular chamber. They found the PCM melt fraction increased at a faster rate at higher heat fluxes from the U-shaped heat source. There was a time delay before the increase in PCM melt fraction and this time delay was approximately constant between the different heat fluxes. The convective heat transfer coefficient was found to increase with the heat flux. It was also found to be higher in the region within the U-shaped bend in the rectangular chamber compared to the regions outside of the U-shaped bend close to the chamber walls. The authors characterized natural convection heat transfer using the Raleigh number (Ra). The Raleigh number was found to be highest within the U-shaped bend and it was particularly high in this region near the HTF entry point at the top of the chamber.

Jevnikar and Siddiqui [62] experimentally investigated the influence of heat source orientation on the transient flow behavior during PCM melting in a rectangular enclosure. They found that heat transfer in the PCM through conduction leads to the formation of a thin liquid PCM layer adjacent to the heated wall and this layer remains motionless for a considerable time period over which the viscous forces presumably dominate the buoyancy forces. Conduction was found to be the primary mode of heat transfer up until a large enough amount of the PCM had melted after which buoyant forces became significant and natural convection heat transfer became the dominant mode of heat transfer. The circulation of liquid PCM in a convection cell adjacent to the heated wall resulted in the expansion of the solid-liquid interface near the top of the rectangular enclosure. In the convection cell, heated melted PCM was directed upwards near the heated wall, and slid back down along solid PCM as it cooled. The interface expanded until the entire top region of the PCM had melted, after which melting proceeded in a top-down manner where the top region of the enclosure was fully liquid and the solid region at the bottom diminished over time. The study also found that melting is fastest when there is no tilt to the enclosure.
Tayssir et al. [63] experimentally studied the melting behavior of a paraffin contained in a vertically positioned cylindrical chamber. In the experiment, a HTF at a fixed temperature and volumetric flow rate was forced through a tube embedded within the cylindrical PCM test chamber. Thermocouples were placed at fixed locations radially outwards from the center of the cylindrical chamber to monitor the PCM temperature. They found that melting begins after an initial time delay, and that this delay is independent of HTF flow rate and temperature. After this time delay, the PCM melt fraction increases rapidly due to the onset of natural convection. This initial increase in melt fraction was higher at higher HTF flow rates and temperatures. The authors also found that the total fraction of thermal energy that is stored in the PCM increases with increasing HTF flow rates and temperatures.

Voller and Prakash [64] developed a fixed grid numerical modeling approach for convection-diffusion phase-change problems. In the proposed enthalpy-porosity method, they considered the solid-liquid interface as a porous ( mushy) medium with an associated porosity (liquid fraction) that ranges from 0 (pure solid) to 1 (pure liquid). They recognized that enthalpy and velocity in the mushy region are functions of the liquid fraction and developed formulations for both to be used as source terms in the momentum and energy equations. The velocity source term (Carman-Kozeny equation) inhibits velocity in the solid region (where liquid fraction is zero), and the enthalpy source term adds latent heat of phase change to the energy equation.

Shmueli and Ziskind [65] numerically investigated the melting behavior of subcooled paraffin contained in a vertical cylinder whose wall was kept at a constant temperature. The numerical model of phase change was based on the enthalpy porosity method developed by Voller and Prakash [64]. They found that the permeability constant in the Carman-Kozeny equation [66] affects melting. At low values of the constant, melting is rapid, and at higher values, melting is relatively slower. The authors found that a permeability constant of $10^8$ gives results which best agreed with the experimental data for the case where PCM is contained in a vertical cylinder with heated wall. It was found that the heat transfer rate to the solid PCM is initially uniform across the entire length of the cylinder due to the presence of a uniform radial temperature gradient, but it decreases
rapidly around the top regions of the cylinder due to an accumulation of the heated liquid PCM at the top of the convective cell which results in diminishing temperature gradients. Sridharan et al. [67] numerically investigated the influence of the cylinder dimensions on melting behavior. It was found that with the same amount of PCM mass, an increase in the cylinder aspect ratio (AR) leads to an increase in the melting time up to an AR of 4, after which the melting time becomes independent of the AR.

Mohaghegh et al. [68] studied the melting behavior of paraffin wax in a 2D numerical study. The PCM was confined within a rectangular enclosure. The surface temperature of the walls were suddenly increased to a high temperature and the solid-liquid interface in the PCM was tracked. It was found that during the initial stages of melting, a very fine liquid layer forms adjacent to the container walls, and that this layer remains motionless for a considerable time period over which the viscous forces presumably dominate the buoyancy forces and where conduction is dominant. This layer was found to grow in size starting at the top until the entire top region of the PCM was fully melted due to the natural convection heat transfer. The authors also found that the PCM temperature increases much more rapidly and stays constant at the melting temperature longer in lower regions of the numerical domain, suggesting continued heat storage capacity in the lower PCM region even when top parts have fully melted. Similar numerical studies on the advancement of the solid-liquid front in different shaped enclosures obtained similar results [69-72].

These results lead to a prediction that a similar effect may be observed in the melting of PCM contained in the vertical columns within the heated channel discussed in Chapter 3. That is, the top of the PCM volume should melt first, with a large delay between that and the bottom. There are some differences in heating condition, and geometry that could result in differing behavior.
1.4 Flow over Obstacles

The passive thermal regulation of photobioreactors can be achieved by integrating a latent heat based thermal energy storage into the flow system of the photobioreactor. The numerical and experimental investigations into the melting behavior of phase change materials reveal that the process is almost entirely driven by natural convection heat transfer, and that the buoyancy driven bulk motion of the liquid PCM is responsible for the movement of the solid-liquid interface. Based on this particular melting behavior of PCM and taking into account the generally low thermal conductivity of organic PCMs, it can be hypothesized that PCM melting can be sped up if it is distributed across smaller compartments so as to increase the heat transfer surface area to volume ratio of the PCM, which would result in higher overall heat transfer rates into the storage. A design for the integration of distributed PCM into a photobioreactor channel must take into account the alteration of flow dynamics in the channel due to flow past PCM enclosures. In this section, relevant research on flow past obstacles is highlighted with the aim to better understand flow dynamics in a photobioreactor channel where PCM enclosures are placed in the flow direction. Specifically, the effects of obstacle shape, blockage ratio (BR), gap ratio (GR), and Reynolds number (Re) on flow dynamics and heat transfer in low Re flows past confined obstacles are detailed. Blockage ratio is the ratio of obstacle’s projected width to the channel width, and gap ratio is the ratio of the distance between obstacle and channel wall to the obstacle width. Strouhal number (St) is a dimensionless parameter that is indicative of vortex shedding frequency.

1.4.1 Flow over unconfined obstacles

The flow over an unconfined cylinder at low Re has been numerically investigated by Rajani et al. [73], Thompson et al. [74], Sen et al. [75], and Mittal and Balachandar [76], who categorized this type of flow into different flow regimes based on the flow Reynolds number. These flow regimes are the (1) creeping flow with no separation (Re < 5), (2) flow with fixed pair of symmetric vortices (5 < Re < 40), (3) flow with a laminar vortex sheet (40 < Re < 200), and (4) transition to turbulence in the wake (200 < Re < 300).
1.4.2 Influence of the Blockage Ratio

Chan et al. [77] numerically investigated the effects of Reynolds number and blockage ratio on a circular cylinder centered between two walls. They found that, similar to the unconfined flow case, several flow regimes could be differentiated based on Re and BR. At very low blockage ratios (BR < 0.2), the flow resembles that over an unconfined cylinder (Strouhal number ≈ 0.2) in that there is no interaction between shear layer of the cylinder and boundary layers of the walls. The critical Reynolds number which marks the onset of vortex shedding increased from 50 to 120 when the BR was increased from 0.1 to 0.5. Above the critical Reynolds number in this BR range, the vortex resembled an inverse von Karman vortex sheet and the increase in the shedding frequency was found to be due to the interaction between the cylinder shear layer and boundary layers of the channel walls. The St increased from 0.17 – 0.20 when the Re was increased from 100 to 300 at Br=0.20. The effect of Reynolds number was found to diminish at higher BR values. At a BR of 0.5, St remained steady at 0.35 for Re in the range 150 – 300, and similarly at 0.48 at BR=0.7. Chen et al. [78] found that the increase in BR from 0.1 to 0.5 increases the critical Reynolds number from 51 to 114 but any further increase in BR decreases the critical Re.

Galleti et al. [79] numerically investigated the effects of blockage ratio on a square cylinder confined in a channel. It was found that the onset of vortex shedding occurred at Re > 58 for BR of 0.125 – 0.375. The Strouhal number corresponding to a BR=0.125 increased from 0.12 at Re=50 to 0.144 at Re=150 and it decreased back down to 0.133 at Re=200. Patil and Tiwari [80] numerically investigated the effect of blockage ratio on flow over square cylinders. It was observed that the critical Reynolds number increases with increasing value of the blockage ratio where the rate of increase is much higher up to a BR of 0.26 and then much slower going forward up to a BR of 0.38. For BR > 0.38, the critical Re decreases with increasing value of the blockage ratio. It was also observed that unlike circular blockage, the Strouhal number first increases and then decreases with Re at BR=0.125 but it increases to a constant value at higher BR values (BR = 0.3).

Chakraborty et al. [81] numerically investigated the effect of blockage ratio on the separation angle, and length of the recirculation zone. They found that both the separation
angle and the recirculation zone length decreased linearly as the BR was increased from 0.05 to 0.65. The sensitivity of the recirculation length in this context increased with an increase in Re, while there was no change in the sensitivity of the separation angle. The recirculation length was found to be equal to 5L at Re=50 and BR=0.05, where L is the obstacle’s characteristic length. The recirculation length decreased to 2L at BR=0.65 at Re=50. In a similar manner, at Re=200, the recirculation length decreased from 15L at BR=0.05 to 3.5L at BR=0.65. For square cylinders, the critical Re increased from Re=45 at BR=0.2 to Re=60 at BR=0.38 and then back down to Re=40 at BR=0.5. For a circular cylinder, the critical Re increased from Re=51 at BR=0.1 to Re=125 at BR=0.5, and then decreased back down to Re=111 at BR=0.7. This was the same result produced by Chen et al [78].

Khan and Yovanovich [82] experimentally determined the effects of blockage ratio on heat transfer from a cylinder confined between two parallel planes. They found that heat transfer rates are higher at higher blockage ratios and at higher Reynolds numbers. The average Nusselt number increases by 43% when the Reynold number is increased two-fold at a blockage ratio of 0.8, and it increased by 40% when the blockage ratio was increased from 0.2 to 0.8 at a Reynolds number of 200.

1.4.3 Influence of the Gap Ratio

The influence of the gap ratio or proximity to the channel walls was numerically investigated by Arnal et al. [83], who considered flow past a square cylinder that was attached to a fixed wall. They found that there was no vortex shedding at Re=100 but observed unsteady vortex shedding with St=0.7 at Re=500 and 1000 which was indicative of a weak Re dependence on shedding frequency in this Reynolds number range. For circular cylinders, Zhou et al. [85] observed the critical gap ratio to be GR=0.25. They found that for GR \leq 0.25, vortex shedding was largely suppressed, although there was some wake vortex shedding associated with the upper shear layer of the cylinder. At GR=0, the wake vortex shed from this upper shear layer was observed to break down into smaller vortices. He et al. [86] experimentally investigated vortex dynamics for flow over a circular cylinder placed in close proximity to a wall. They found that flow at GR=0 resembled that over a backward facing step in that flow past the
upper side of the cylinder separated and formed a large separation bubble. The mean recirculation length at GR=0 was x/D = 7. At GR=0.25, flow acceleration through the gap region led to the formation of a jet coming out of the gap region. At GR=0.25, there were two separation bubbles, one directly behind the cylinder and the other on the wall, which was suppressed due to the flow acceleration through the gap. At GR ≥ 0.25, there was considerable vortex shedding in the wake of the cylinder.

Ariansyah et al [87] numerically investigated the flow of a heated fluid (T=318 K) over a staggered tube bank initially at a lower temperature (T=306 K). The gap ratio was defined as the ratio between the distance between tubes and the tube diameter, and it was varied by changing the transversal (normal to flow direction) pitch of the tube arrangement. It was found that the channel fluid accelerated as it crossed the gap between the upper and lower tubes in the arrangement. The maximum velocity magnitude in the channel increased by 300% as the gap ratio was reduced by 45% from 3.2 to 1.7. The heat transfer rate between the tube and heated fluid was highest at the lowest gap ratio. There was an 8°C and 3°C drop in the heated fluid temperature across the tube arrangement at GR=1.7 and 3.2, respectively. The heat transfer coefficient was 103, 77, 51 and 45 W/m-K at GR=1.7, 2.7, 2.0 and 3.2, respectively.
1.5 Motivation and Knowledge Gaps

This thesis is part of a larger ongoing project at the University of Western Ontario to develop a novel design for the passive thermal regulation of photobioreactors cultivating microalgae using latent heat-based thermal energy storage. The motivation for this thesis is to investigate the use of phase change materials to thermally regulate a photobioreactor channel. Thermal regulation of photobioreactors is crucial to keep the culture temperature within an acceptable range. Microalgae are most productive within a narrow temperature range. Additionally, if the photobioreactor overheats, the organisms are likely to die. Phase change materials have large thermal energy storage densities and are able to store energy at a constant temperature during phase change, which highlights their potential in providing passive thermal regulation inside photobioreactors.

Toxopeus [1] experimentally investigated the use of PCM-filled columns to thermally regulate flow in a rectangular channel for potential application in photobioreactors. Considering experimental challenges, a numerical approach provides more flexibility to obtain an in-depth understanding of thermal energy storage and thermal regulation in the channel in order to assess the viability of integrating thermal energy storage into a photobioreactor channel. This includes studying and subsequently characterizing the conjugate heat transfer mechanisms, flow dynamics and phase change behavior of the PCM for better understanding of the integrated design. There is a scarcity of studies that consider the effects of flow behavior and heat transfer in bluff body flows on the melting behavior and thermal energy storage within PCM enclosures. The present research is therefore focused on developing a numerical model to effectively study the aforementioned thermo-fluid behaviors.

The influence of geometric parameters pertaining to the arrangement of bluff bodies within a flow has been investigated in a wide array of numerical and experimental work. Similarly, the melting behavior of PCM within different shaped enclosures and subjected to different heating conditions has also been investigated. However, there is a scarcity of studies that consider the effects of bluff body dynamics on the melting behavior and energy storage within bluff bodies filled with PCM. Toxopeus [43] has previously investigated the influence of some of these parameters but a comprehensive parametric
analysis of these parameters could not be carried out experimentally in a feasible manner due to the large number of parameters involved. Hence, in the present study, the parametric analysis is performed numerically to assess the effects of geometric and flow parameters on thermal energy storage. This parametric analysis should act as a reference guide to dictate future design work in the development of viable thermally regulated photobioreactor channel designs.

1.6 Thesis Objectives

The objectives of this numerical study are:

(1) To characterize flow and heat transfer in a rectangular channel with PCM-filled thermal energy storage columns, and to investigate the thermal response of the channel fluid in the presence of these columns

(2) To investigate the influence of geometric parameters such as column offsets, column cross section aspect ratio and column shape as well as operating parameters such as channel flow Reynolds number and temperature, on the thermal energy storage in PCM-filled columns in a rectangular channel.

(3) To investigate passive thermal regulation in the rectangular channel containing PCM-filled columns when the channel fluid temperature varies between heating and cooling cycles.
1.7 Thesis Layout

Chapter 1: An introduction to the work and motivations behind the study. Literature review on topics related to photobioreactors, thermal energy storage, phase change materials, melting behavior and flow dynamics for flow over obstacles. Motivations and gaps in know are addressed to provide context to the thesis work.

Chapter 2: Numerical model development for the characterization of flow and thermal behavior inside a rectangular channel with PCM-filled columns in a staggered formation. The governing equations are presented and boundary conditions are described. The chapter also includes the grid independency analysis and the validation of the numerical model against experimental data.

Chapter 3: The chapter includes a detailed parametric analysis. The numerical model from the previous chapter is used to investigate the effects of geometric and operational parameters in the channel on thermal energy storage in the PCM columns in the presence of a constant temperature heated fluid in the channel. The optimal configuration of the column arrangement in the channel that maximizes thermal energy storage for this flow condition is derived.

Chapter 4: The optimal configuration is used to investigate passive thermal regulation in the channel when the channel fluid temperature varies between heating and cooling cycles. Temperature control in the form of temperature drop across the columns is investigated.

Chapter 5: This chapter provides a summary of results and discussions from the previous chapters and provides conclusion to the work. The extension of the present work is provided in the form of recommendations for the future work.
Chapter 2

2 Numerical Model Development for the Characterization of flow and thermal behavior in a rectangular channel containing offset PCM-filled columns

In the previous chapter, the potential of using latent heat-based thermal energy storage for passive thermal regulation of photobioreactors was discussed. The introduction of thermal energy storage in a flow system for thermal regulation creates a multi-region system that consists of the (flow) fluid, the phase change material (PCM), and the interface that separates the two. Hence, the development of a numerical model to characterize flow and heat transfer in such a system needs to consider (1) conjugate heat transfer across multiple interfaces, and (2) the phase transition of the PCM. This chapter describes the development of a coupled mathematical model that integrates the phase change model into the general numerical model of the multi-region system. The numerical process is shown in figure 2-1, where the mathematical model is solved using the OpenFOAM software library.

OpenFOAM is an open-source CFD software that allows a high level of flexibility in the implementation of discretization schemes and solution algorithms to solve complex flow and heat transfer problems. The first step in the numerical modeling process is the development of a mathematical model that describes the problem through a set of partial differential equations. These differential equations are then discretized into algebraic equations using the Finite Volume Method (FVM) [88]. To solve these algebraic equations for the flow variables, numerical methods must be defined, which apply an iterative method to arrive at the solutions. Finally, a solution algorithm is developed to compute these solutions at each time-step, where solution control mechanisms ensure solution stability and accuracy at each time-step. A convergence study should be conducted to ensure that the numerical solution is sufficiently converged to the “exact” solution of the differential equation for a flow variable. The numerical model should also be validated against experimental data.
Figure 2-1. Overview of the numerical modeling process where mathematical equations are discretized and solved in OpenFOAM.

2.1 Physical Model

The physical model is shown in figure 2-2. It consists of a rectangular channel 30 cm long, 12.5 cm high and 2.54 cm wide. The outlet nozzle is 1 cm in diameter and is placed at a height of 10 cm from the base of the channel. Seven PCM-filled columns are placed along the rectangular channel. The column diameter (D) is half of the channel width (1.27 cm) and the column wall thickness is 1 mm. The horizontal and lateral directions correspond to the streamwise (x) and cross-stream (z) directions, respectively. In the current setup, the channel fluid is considered as water, the columns as copper tubes, and the enclosed PCM as Rubitherm-26 (RT-26). RT-26’s thermophysical properties are listed in table 2-1.
Figure 2-2. Top and side views of the physical model, with the (a) top view showing the PCM-filled column inside the channel, and (b) side view showing the channel inlet and outlet.

Table 2-1. Thermophysical properties of Rubitherm-26 [89]

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>Solid 880 Kg/m$^3$</td>
</tr>
<tr>
<td></td>
<td>Liquid 750 Kg/m$^3$</td>
</tr>
<tr>
<td>Thermal Conductivity</td>
<td>0.2 W/m$^\circ$K</td>
</tr>
<tr>
<td>Viscosity</td>
<td>0.02 Pa-s</td>
</tr>
<tr>
<td>Thermal Expansion Coefficient</td>
<td>0.0005 K$^{-1}$</td>
</tr>
<tr>
<td>Melting Temperature</td>
<td>Solidus ($T_s$) 298.15 K (25 C)</td>
</tr>
<tr>
<td></td>
<td>Liquidus ($T_l$) 299.15 K (26 C)</td>
</tr>
<tr>
<td>Latent Heat of Fusion</td>
<td>180 KJ/Kg</td>
</tr>
</tbody>
</table>
2.2 Mathematical Model

The governing equations for the heat and fluid flow problems are given as [90],

\[
\frac{\partial \rho}{\partial t} = - \nabla \cdot (\rho \vec{u}) \tag{2.1}
\]

\[
\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u} \vec{u}) = - \nabla p + \rho \ddot{g} + \nabla \cdot (\mu \nabla \vec{u}) \tag{2.2}
\]

\[
\frac{\partial H}{\partial t} + \nabla \cdot (\vec{u} H) = \nabla \cdot (\kappa \nabla T) \tag{2.3}
\]

where equation (2.1) is the continuity equation, equation (2.2) is the momentum equation, and equation (2.3) is the energy equation. The variable \( \rho \) is the density, \( \vec{u} \) is the velocity vector, \( p \) is the static pressure, \( \ddot{g} \) is the gravitational acceleration, \( \mu \) is the dynamic viscosity, \( H \) is the enthalpy per unit volume, \( \kappa \) is the thermal conductivity, and \( T \) is temperature.

The fundamental flow equations were simplified in consideration to the present problem. The following assumptions were made:

- **Laminar flow**: Photobioreactor channel flows are typically low Reynolds number flows. The Reynolds number is defined as:

  \[
  \text{Re}_L = \frac{\rho U D_h}{\mu} \leq \text{Re}_{L,\text{crit}}
  \tag{2.4}
  \]

  where \( D_h \) is the channel hydraulic diameter, and the critical Reynolds number in viscous flow in a rectangular duct is \( \text{Re}_{L,\text{crit}} \approx 2300 \) [91].

- **Constant thermophysical properties**: Temperature dependent properties such as thermal conductivity, thermal expansion coefficient, and the specific heat capacity were taken as constant since temperature variations within a photobioreactor are small.
• \textit{Incompressible flow}: Density is assumed to be constant. The Boussinesq approximation accounts for buoyancy effects caused by temperature gradients but ignores density differences elsewhere. Due to low flow rates in photobioreactor channels, buoyant forces can be comparable to inertial forces in the fluid. In the liquid PCM region, buoyant forces tend to far outweigh the inertial forces. Therefore, the Boussinesq approximation can be applied in both channel fluid and PCM regions.

• \textit{Newtonian fluid}: Fluid viscosity is taken as constant. The channel fluid, which was water in the present study, is a Newtonian fluid. The phase change material, which was a paraffin wax in the present study, can be approximated as a Newtonian fluid in liquid state [92].

The aforementioned assumptions were used to simplify the governing flow equations as follows:

\begin{equation}
\nabla \cdot \vec{u} = 0 \tag{2.5}
\end{equation}

\begin{equation}
\frac{\partial \vec{u}}{\partial t} + \nabla \cdot (\vec{u}\vec{u}) = \frac{1}{\rho} \nabla P + \nu \nabla^2 \vec{u} + \vec{g} \tag{2.6}
\end{equation}

\begin{equation}
\frac{\partial H}{\partial t} + \nabla \cdot (\vec{u}H) = \kappa \nabla^2 T \tag{2.7}
\end{equation}

The flow equations (2.5-2.7) were adapted for each of the three regions in the physical domain: channel fluid, PCM and column wall regions.

\section*{2.2.1 Channel Fluid Region}

For fluid flow in the channel, the Boussinesq approximation accounts for buoyancy effects caused by temperature gradients. In this approximation, density has a fixed (reference) part and another that varies linearly with temperature [99]:

\begin{equation}
\rho = \rho_0 - \beta \rho_0 (T - T_0) \tag{2.8}
\end{equation}
where $\rho_0$ is the reference density at the reference temperature, $T_0$, and $\beta$ is the linear coefficient of thermal expansion. This variable density is introduced to the gravitational term of the momentum equation to obtain the Boussinesq source term,

$$\mathbf{S}_b = -\bar{g}\beta (T - T_m)$$

This source term is added to the momentum equation,

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u} \mathbf{u}) = -\frac{1}{\rho_0} \nabla P + \nu \nabla^2 \mathbf{u} + \mathbf{S}_b$$

### 2.2.2 PCM Region

For the phase change material, the momentum and energy equations were modified to account for the phase change. The enthalpy-porosity method developed by Voller and Prakash [64] describes a mushy region in the PCM during phase change. This mushy region is characterized by the PCM liquid fraction, which is calculated as,

$$f(T) = \begin{cases} 0 & T \geq T_i \\ \frac{T - T_s}{T_l - T_s} & T_l > T \geq T_s \\ 1 & T < T_s \end{cases}$$

where $f$ is the liquid fraction, and $T_s$ and $T_l$ are the solidus and liquidus temperatures of the PCM, respectively. Formulations for the mushy region enthalpy and velocity were derived. In the enthalpy-porosity method, enthalpy is described in the following manner [93],

$$H = h + \Delta H$$

where $h = cT$, $c$ is the sensible heat and $\Delta H$ is the latent heat. $\Delta H$ is a function of temperature and can take one of three values depending on the temperature regime [93].

$$\Delta H = f(T) = \begin{cases} L & T \geq T_l \\ L \cdot f & T_l > T \geq T_s \\ 0 & T < T_s \end{cases}$$
where \( L \) is the latent heat of fusion. Equation (2.13) identifies three phases within PCM during phase change: the pure solid phase \( (\Delta H = 0) \), the pure liquid phase \( (\Delta H = L) \) and the mushy (porous) phase \( (0 < \Delta H < L) \). Velocity within the mushy region is described in a similar manner as [93],

\[
\begin{align*}
\mathbf{u} &= f(T) = \begin{cases} 
\mathbf{u}_l & T \geq T_l \\
\mathbf{u}_l f & T_l > T \geq T_s \\
0 & T < T_s
\end{cases}
\end{align*}
\]  
\tag{2.14}

where \( \mathbf{u}_l \) is the actual liquid PCM velocity.

Under the enthalpy-porosity method, governing equations for momentum and energy were modified to account for the conservation of momentum and energy in the mushy region. This was done with the addition of source terms in the governing equations. The Boussinesq approximation accounts for buoyancy effects caused by temperature gradients within the liquid phase of the PCM. The source term was already derived for the fluid region (Eq. 2.9) and was added to the PCM momentum equation.

The Darcy source term models PCM velocity in the mushy region, and is defined as [96],

\[
\vec{S}_u = A \mathbf{u}
\]  
\tag{2.15}

where \( A \) is a parameter that controls the influence of the mushy region on the velocity field, and is a function of the liquid fraction:

\[
A = -C \frac{1 - f^2}{(f^3 + q)}
\]  
\tag{2.16}

where \( C \) is a constant that controls flow permeability in the mushy region, and \( q \) is a constant to avoid a zero-value denominator when the liquid fraction becomes zero. Equation (2.16) implies that the parameter \( A \) tends to zero as the liquid fraction approaches one. On the other hand, if the liquid fraction approaches zero, \( A \) becomes negative and large (because of the large value of constant \( C \)), which forces the velocity field to become zero. This is consistent with the behavior implied in equation (2.14)
where PCM velocity approaches to zero when the PCM is solid and tends to the actual liquid velocity when it is liquid.

An enthalpy source term is required to account for the enthalpy in the mushy region. Equation (2.12) can be expanded in the following manner [94]:

\[ H = \rho (1 - f) \int_{T_0}^{T} c_s(T) \, dT + \rho f \int_{T_0}^{T} c_l(T) \, dT + \rho L \]  

(2.17)

where \( c_l \) and \( c_s \) are the specific heat capacities of the liquid and solid PCM phases, respectively, and \( T_0 \) is a reference temperature. Since the specific heat capacities in the solid and liquid PCM regions are assumed to be equal and constant (\( c_s = c_l = c_p \)), equation (2.17) can be simplified as follows:

\[ H = \rho c_p (T - T_0) + \rho L \]  

(2.18)

Equation (2.18) can be substituted into the energy equation (Eq. 2.3),

\[ \frac{\partial T}{\partial t} + \nabla \cdot (\bar{u}T) = \alpha \nabla^2 T - \frac{1}{c_p} L \frac{\partial f}{\partial t} + \bar{u} \cdot \nabla f \]  

(2.19)

where the new source term that appears in the equation is,

\[ S_h = -\frac{1}{c_p} L \frac{\partial f}{\partial t} + \bar{u} \cdot \nabla f \]  

(2.20)

The source term is a function of the liquid fraction which varies temporally and spatially. Voller and Swaminathan [95] determined that the spatial variations in liquid fraction (Eq. 2.20) are negligible in comparison with the temporal variations, and simplified the source term to:

\[ S_h = -\frac{L}{c_p} \frac{\partial f}{\partial t} \]  

(2.21)
The final forms of the governing equations for PCM become as follows,

\[ \Delta. \vec{u} = 0 \]  \hspace{1cm} (2.22)

\[ \frac{\partial \vec{u}}{\partial t} + \nabla. (\vec{u}\vec{u}) = -\frac{1}{\rho} \nabla P + \nu \nabla^2 \vec{u} + \vec{S}_b + \vec{S}_u \]  \hspace{1cm} (2.23)

\[ \frac{\partial T}{\partial t} + \nabla. (\vec{u}T) = \alpha \nabla^2 T + \vec{S}_h \]  \hspace{1cm} (2.24)

where \( S_b \) is the Boussinesq term to account for buoyancy effects, \( S_u \) is the Darcy source term to account for velocity in the mushy region, and \( S_h \) is the enthalpy source term to account for enthalpy in the mushy region. Both Darcy and enthalpy source terms are functions of PCM liquid fraction and tend to zero as the PCM becomes fully liquid.

### 2.2.3 Tube Region

Finally, for the tubes that constitute the solid columns in the channel, the energy conservation equation (Eq. 2.7) was simplified to the transient heat conduction equation,

\[ \frac{\partial T}{\partial t} = \alpha \nabla^2 T \]  \hspace{1cm} (2.25)

### 2.2.4 Summary of Model Equations

The governing flow and heat transfer equations for the multi-region system are summarized in table 2-2. The Boussinesq, Darcy and enthalpy source term formulations are presented in table 2-3.
Table 2-2. Conservation equations for the channel fluid, PCM and column wall regions

<table>
<thead>
<tr>
<th>Equation</th>
<th>Fluid</th>
<th>PCM</th>
<th>Column</th>
</tr>
</thead>
<tbody>
<tr>
<td>Continuity</td>
<td>$\Delta \vec{u} = 0$</td>
<td>$\Delta \vec{u} = 0$</td>
<td>-</td>
</tr>
<tr>
<td>Momentum</td>
<td>$\frac{\partial \vec{u}}{\partial t} + \nabla \cdot (\vec{u} \vec{u}) = -\frac{1}{\rho} \nabla P + \nu \nabla^2 \vec{u} + \vec{S}_b \frac{\partial \vec{u}}{\partial t} + \nabla \cdot (\vec{u} \vec{u}) = -\frac{1}{\rho} \nabla P + \nu \nabla^2 \vec{u} + \vec{S}_b + \vec{u} \vec{S}_a$</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>Energy</td>
<td>$\frac{\partial T}{\partial t} + \nabla \cdot (\vec{u} T) = \alpha \nabla^2 T$</td>
<td>$\frac{\partial T}{\partial t} + \nabla \cdot (\vec{u} T) = \alpha \nabla^2 T + S_h$</td>
<td>$\frac{\partial T}{\partial t} = \alpha \nabla^2 T$</td>
</tr>
</tbody>
</table>

Table 2-3. Source terms added to the momentum and energy equations to model buoyancy effects and velocity/enthalpy in the mushy region of the PCM

<table>
<thead>
<tr>
<th>Source Term</th>
<th>Formulation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boussinesq</td>
<td>$\vec{S}_b = -\vec{g} \beta (T - T_m)$</td>
</tr>
<tr>
<td>Darcy</td>
<td>$\vec{S}_u = -\frac{C (1 - f^2)}{(f^3 + q)} \vec{u}$</td>
</tr>
<tr>
<td>Enthalpy</td>
<td>$S_h = -\frac{L}{c_p} \frac{\partial f}{\partial t}$</td>
</tr>
</tbody>
</table>
2.3 Discretization

The governing equations for the multi-region problem (see table 1-1) were discretized using the finite volume method (FVM) [88]. In the FVM, the physical domain is divided into finite volumes or cells, and values of the flow variables are stored at cell centers. OpenFOAM uses the finite volume method (FVM) to discretize fluid flow and heat transfer equations. The process of discretizing these equations is described in this section.

2.3.1 Transport Equation

The general transport equation for fluid flow is given as [97],

\[
\int_{V_p} \frac{\partial \rho \phi}{\partial t} dV + \int_{V_p} \nabla \cdot (\rho \vec{u} \phi) dV - \int_{V_p} \nabla \cdot (\rho \Gamma_\phi \nabla \phi) dV = \int_{V_p} S_\phi dV \tag{2.26}
\]

Where \( V_p \) is a control volume, \( \phi \) can be any flow variable, \( \Gamma_\phi \) is the diffusivity of said variable, and \( S_\phi \) is the source term. Table 2-4 shows the equation parameters that correspond to the continuity, momentum, and energy equations.

Table 2-4. Transport equation parameters for the three governing equations

<table>
<thead>
<tr>
<th>Equation</th>
<th>( \phi )</th>
<th>( \Gamma_\phi )</th>
<th>( S_\phi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Continuity</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Momentum</td>
<td>( \vec{u} )</td>
<td>( \nu )</td>
<td>(-\nabla p)</td>
</tr>
<tr>
<td>Energy</td>
<td>( c_p T )</td>
<td>( \kappa )</td>
<td>0</td>
</tr>
</tbody>
</table>

The Gauss (divergence) theorem states that the surface integral of a vector field over a closed surface (flux through the surface) is equal to the volume integral of the divergence over the region contained by the surface:

\[
\iiint_V (\nabla \cdot F) dV = \iint_S (F \cdot \vec{n}) dS \tag{2.27}
\]
Where $S$ is the closed surface bounding the control volume $V_p$, and $dS$ represents an infinitesimal surface element associated with the normal $\vec{n}$ pointing outwards of the surface $S$. This theorem can be used to transform the volume integrals in the general transport equation into surface integrals,

$$\frac{\partial}{\partial t} \int_{V_p} (\rho \phi) \, dV + \int_S (\rho u \phi \vec{n}) \, dS - \int_S (\rho I_{\phi} \nabla \phi \cdot \vec{n}) \, dS = \int_{V_p} S_{\phi}(\phi) \, dV \quad (2.28)$$

The first term on the LHS in equation (2.28) is the temporal term, the second term is the convective term, the third term is the diffusive term, and the term on the RHS is the source term. The discretization process for each of these terms is discussed in this section.

### 2.3.2 Convective Term Discretization

The convective integral in equation (2.28) can be transformed into a discrete algebraic term with the assumption that the flow variable varies linearly across a cell face (between cell centers). Given a total of $N$ faces for a cell, and assigning the subscript ‘$f$’ to represent a face, the Gauss discretization process is as follows [99],

$$\int_S (\rho u \phi \vec{n}) \, dS = \sum_{N} \int_S [\rho u \phi \vec{n}] \, dS \approx \sum_{N} (\rho u \phi_f) S_f \quad (2.29)$$

The term $(\rho u \phi)_f$ is the convective flux of the flow variable, $\phi$, through a cell face. Calculation of this advective term requires an interpolation of the flow variable at the face centroid, $\phi_f$. An upwind interpolation scheme is used,

$$\phi_f = \begin{cases} 
\phi_P & \text{if } F_c \geq 0 \\
\phi_N & \text{if } F_c < 0 
\end{cases} \quad (2.30)$$

where $P$ and $N$ refer to the cells which share a common face, $f$. Equation (2.30) states that the flow variable at the face is equal to the flow variable at the cell center of the upstream cell. With $\phi_f$ known, the advective flux (Eq. 2.29) can be computed.
2.3.3 Diffusive Term Discretization

The diffusive integral in equation (2.28) can be transformed into a discrete algebraic term using the Gauss discretization process as follows [99]:

\[
\iint_S \left( \rho \Gamma \partial \phi \nabla \phi \right) \, dS = \sum_N \int_S \left[ \rho \Gamma \partial \phi \nabla \phi \right] \, dS \approx \sum_N \left( \rho \Gamma \partial \phi \right)_N S_f \tag{2.31}
\]

The term \((\rho \Gamma \partial \phi)_f\) is the diffusive flux of the flow variable through a cell face. Calculation of this discretized diffusive flux requires an interpolation of the diffusive coefficient at the face centroid, \(\Gamma_{\phi,f}\), as well as calculation of the surface normal gradient of the flow variable, \(\nabla \phi\).

The face gradient, \((\nabla \phi)_f\), can be interpolated from the cell centered gradients, \((\nabla \phi)_P\) and \((\nabla \phi)_N\), where P and N refer to the cells which share a common face, f.

\[
(\nabla \phi)_f = f_x (\nabla \phi)_P + (1 - f_x) (\nabla \phi)_N \tag{2.32}
\]

\[
f_x = \frac{||fN||}{||PN||} \tag{2.33}
\]

where \(||fN||\) is the distance from the cell face to the center of cell N, and \(||PN||\) is the total distance between the centers of cells P and N. The cell centroid gradient terms in equation (2.32) are discretized using the gauss theorem:

\[
(\nabla \phi)_P = \frac{1}{V_P} \sum_N S_f \phi_f \tag{2.34}
\]

Equation (2.34) can then be substituted into equation (1.31) to expand the cell centroid gradient terms to obtain a simplified expression:

\[
(\nabla \phi)_f = \frac{\phi_N - \phi_P}{||PN||} \tag{2.35}
\]
Equation (2.35) applies when the mesh is fully orthogonal i.e. if the vector connecting the cell centers is orthogonal to the face. If this is not the case, then a correction must be applied to equation (2.35) to account for non-orthogonality in the mesh. The correction scheme modifies equation (2.35) by applying underrelaxation to it and adding an explicit correction term as follows:

\[
(\nabla \phi)_f = \alpha \frac{\phi_N - \phi_P}{\|\vec{P}\N\|} + \left(\hat{n} - \alpha \vec{P}\N\right) \cdot (\nabla \phi)_f
\]  

(2.36)

\[
\alpha = \frac{1}{\cos(\theta)}
\]  

(2.37)

where \(\hat{n}\) is the normal vector to the face, and \(\theta\) is the angle between the face normal and the vector connecting cell centers. In the case where \(\theta = 0\) (i.e. \(\hat{n} \perp \vec{P}\N\)), equation (2.36) simplifies to equation (2.35). Equation (2.36) is solved iteratively.

The diffusive coefficient, \(\Gamma_{\phi,f}\), is interpolated at the face centroid using a linear scheme as follows:

\[
\Gamma_{\phi,f} = f_x \Gamma_{\phi,P} + (1 - f_x) \Gamma_{\phi,N}
\]  

(2.38)

With \(\Gamma_{\phi,f}\) and \((\nabla \phi)_f\) known, the diffusive flux (Eq. 2.30) can be computed.

### 2.3.4 Source Term Discretization

The source term volume integral is discretized by applying the mean value theorem [96]:

\[
\int_{V_p} S_\phi \, dV \approx S_P V_p
\]  

(2.39)

### 2.3.5 Temporal Term Discretization

The discretization of the temporal term is as follows [96]:

\[
\int_{t}^{t+\Delta t} \int_{V_p} \frac{\partial \phi}{\partial t} \, dV \, dt = \rho \left(\phi_{p+\Delta t}^{t} - \phi_{p}^{t}\right) V_p
\]  

(2.40)
The convection and diffusion terms can be integrated with respect to time as follows:

\[ \int_{t}^{t+\Delta t} \phi(t) \, dt = \omega \phi^{t+\Delta t} \Delta t + (1 - \omega) \phi^{t} \Delta t \quad (2.41) \]

where \( \phi(t) \) is any time-dependent flow variable, and \( \omega \) is a weighting function that controls the assumed variation of the integrand over the timestep. A fully implicit, first order accurate scheme provides solution stability in phase change problems [92], and is obtained by setting \( \omega = 1 \) in equation (2.41):

\[ \int_{t}^{t+\Delta t} \phi(t) \, dt = \phi^{t+\Delta t} \Delta t \quad (2.42) \]

### 2.3.6 Complete Discretized Transport Equation

The final form of the discretized transport equation is as follows:

\[ \int_{t}^{t+\Delta t} \left[ \frac{\partial \rho \phi_p}{\partial t} v_p + \sum_{N} (\rho u \phi_f) S_f \right] \, dt = \int_{t}^{t+\Delta t} \left[ \sum_{N} (\rho \Gamma_\theta \nabla \phi_f) S_f + S_p v_p \right] \, dt \quad (2.43) \]

When the first order Implicit (Euler) time scheme (Eq. 1.40) is applied:

\[ \rho \frac{\phi_p^{t+\Delta t} - \phi_p^{t}}{\Delta t} v_p + \sum_{N} (\rho u \phi_f^{t+\Delta t}) S_f = \sum_{N} (\rho \Gamma_\theta \nabla \phi_f^{t+\Delta t}) S_f + S_p v_p \quad (2.44) \]

Equation (1.43) can be written in a more concise form for a control volume as follows:

\[ a_p \phi_p^{t+\Delta t} + \sum_{nb} a_{nb} \phi_{nb}^{t+\Delta t} = b_\theta \quad (2.45) \]

where the sum over \( nb \) refers to the sum over all neighboring cells that share the same faces as cell \( P \). In equation (2.45), the suffix \( nb \) refers to the values at the centroid of neighboring cells, and \( b_\theta \) stands for all known terms. Equation (2.45) can be written for every control volume in the numerical domain to obtain a set of algebraic equations that can be represented as:
\[ A\vec{x} = \vec{b} \]  

(2.46)

where \( A \) is the matrix of the \( a_p \) coefficients. Equation (2.46) can be solved iteratively to arrive at a (flow variable) solution that is within specified tolerances.

### 2.4 Numerical Solution

The linear system of equations for a flow variable (Eq. 2.46) was solved in OpenFOAM. The implementation of solution algorithms in OpenFOAM is discussed in this section. Solutions algorithms for the fluid, PCM and column regions were developed independently and linked together to form the complete multi-region solution algorithm. The solution algorithm for the PCM region is explained first and in most detail on account of it involving the phase change.

#### 2.4.1 Solution Algorithm

The solution algorithm for the PCM region is shown in figure 2-3. The algorithm starts by applying the specified boundary and initial conditions to the numerical domain. Temperature is used to compute the liquid fraction. Temperature and liquid fraction are then used to compute the Darcy (DT), Boussinesq (BT) and Enthalpy (ET) source terms (table 2-3). The solution algorithm then enters the first time-step. The following explanation is for a general time-step in the solution process.

In the momentum predictor stage, the momentum equation is solved for the velocity field using pressure from the previous time step (or initial pressure field). This velocity field does not satisfy the continuity equation. The velocity field from the previous time step (or initial velocity field) is used to solve the pressure (Poisson) equation. This newly calculated pressure is then used to correct the velocity field that was previously calculated in the momentum predictor stage. This corrected velocity field does satisfy the continuity equation. At this point, the algorithm enters the Pressure-Implicit with Splitting of Operators (PISO) loop where the corrected velocity field is used to calculate a new pressure field, which is then used to correct the velocity field. Any number of iterations can be used in the PISO loop.
Once the PSIO loop exits, the energy equation is solved. The temperature field is used to compute the liquid fraction. The liquid fraction and temperature are then used to compute the Darcy (DT), Boussinesq (BT) and enthalpy (ET) source terms. At this point, the solution algorithm enters another loop. If the difference in values of the computed liquid fraction and the old liquid fraction is less than a specified tolerance, the solution algorithm proceeds ahead. Otherwise, the energy equation is solved again. At each iteration, the liquid fraction and source terms are recomputed.

The algorithm proceeds forward to check the velocity, pressure and temperature field residuals. If they are within the specified tolerances, the solution control goes to the next time step. Otherwise, the solution control returns to the momentum predictor step. At this point a second iteration in the Semi-Implicit Method for Pressure Linked Equations (SIMPLE) [100] loop begins (i.e. $i = 1$). In the momentum predictor stage, the momentum equation is solved for a velocity field using pressure from the last SIMPLE iteration. The velocity field from the last SIMPLE iteration is used to solve the pressure equation for a new pressure field, which is then used to correct the velocity field calculated in the momentum predictor stage. Hereafter, the second SIMPLE iteration proceeds in a similar manner to the first iteration. The SIMPLE loop keeps repeating until the pressure, velocity and temperature field residuals become lower than their respective specified SIMPLE tolerances. When the SIMPLE and PISO loops are incorporated into one solution algorithm as in the present study, the resulting algorithm is termed the PIMPLE algorithm.
Figure 2-3. Solution algorithm for the PCM region equations
2.4.2 Solution Control

The momentum and energy equations in the outlined solution algorithm were solved using the bi-conjugate gradient method. The pressure equation was solved using the multigrid (MG) method. Both of these linear methods are iterative in nature. At the end of each solver iteration, the residual is calculated by substituting the current solution into the equation (Eq. 2.46) and taking the magnitude of the difference between left- and right-hand sides:

\[ Ax = b \]  
\[ r = b - Ax \]

The residual in equation (2.47) is scaled using a normalization procedure. With each solver iteration, this scaled residual is recalculated until one of three conditions is met:

- The residual falls below the provided tolerance
- The ratio of current to initial residuals falls below the specified relative tolerance
- The number of iterations reaches the specified maximum number of iterations

Residuals are also calculated in the same manner at the end of each SIMPLE iteration. If these residuals are within the specified SIMPLE tolerances, solution algorithm proceeds to the next time step. Otherwise, another SIMPLE iteration begins.

Under-relaxation factors are applied within each SIMPLE iteration to stabilize calculations by limiting the rate of change of flow fields and equations. Under-relaxation works by limiting the amount by which a variable can change from one iteration to the next,

\[ \phi^p_n = \gamma \phi^p_n + (1 - \gamma)\phi^p_{n-1} \]

where \( \phi^p_n \) is the computed value of the flow variable not subjected to under-relaxation, \( \phi^p_{n-1} \) is the value at the previous iteration, and \( \phi^p_n \) is the value at the current iteration after under-relaxation. The relaxation factor, \( \gamma \), limits the influence of the current computation.
on the flow variable’s value. Lower values of the under-relaxation factor result in higher stability, whereas higher values of the factor lead to faster convergence.

2.4.3 Multi-region solution algorithm

The complete solution algorithm is shown in figure 2-4. At each time step, the channel fluid region equations are solved first followed by the PCM region and column region equations. At the interface between the channel fluid and column wall regions, the heat flux entering one region must equal the heat flux leaving the other:

\[ Q_{\text{fluid}} = -Q_{\text{column}} \]  \hspace{1cm} (2.50)

Equations (2.50) is used to derive a boundary condition at the interface for the channel fluid and the column regions:

\[ k_{\text{fluid}} \frac{dT_{\text{fluid}}}{dn} = -k_{\text{column}} \frac{dT_{\text{column}}}{dn} \]  \hspace{1cm} (2.51)

where \( \vec{n} \) represents the direction normal to the interface, and \( k_{\text{fluid}} \) and \( k_{\text{column}} \) are the thermal conductivities of the fluid and column wall regions, respectively. Equation (2.51) imposes a fixed temperature gradient boundary condition on both regions at the interface. When the fluid energy equation is solved, the column temperature is used to define the heat flux (Eq. 2.51) at the interface. And when the column wall energy equation is subsequently solved, the fluid temperature is used to define the heat flux (Eq. 2.51) at the interface. In this manner, the fluid and column equations are coupled. The same formulation of the boundary condition is used to couple the PCM and column wall equations.
Figure 2-4. Complete solution algorithm for the three-region numerical domain
2.5 Boundary Conditions

The resolution of a numerical problem requires that boundary and initial conditions are defined in accordance with the physical problem that is being modeled. These conditions provide a starting point, both in time and space, in the computation of the discretized flow equations. Before numerical boundary conditions can be set, physical boundary conditions need to be formally defined. The physical boundary conditions correspond to the physical model outlined at the beginning of this chapter (Fig. 2-2).

From the physical model, the following physical boundaries can be defined:

- **Inlet**: Constant mass flow rate through the inlet. Temperature is also constant. Therefore, a constant velocity, and constant temperature boundary conditions are applied.
- **Outlet**: It is assumed that the flow is fully developed at the outlet. Therefore, zero-gradient velocity and temperature boundary conditions are applied.
- **Top (Free Surface)**: It is a free surface that is exposed to the surroundings. Therefore, convection and slip boundary conditions are applied.
- **Channel Walls**: Channel walls are insulated. Therefore, zero heat flux and no-slip boundary conditions are applied.

The three types of numerical boundary conditions were used in the study:

- **Dirichlet boundary condition**: value of a variable is fixed at a boundary.
- **Von Neumann boundary condition**: gradient of a variable is fixed at boundary.
- **Robin boundary condition**: a linear combination of the variable’s gradient and its flux at a boundary.

Table 2-5 lists the numerical boundary conditions. The initial system temperature was set at just below the melting temperature of the PCM. And the initial flow velocity in the channel was equal to the inlet velocity.
Table 2-5. Numerical boundary conditions for the photobioreactor channel

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Numerical Boundary Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet</td>
<td>( u = U_{IN} )</td>
</tr>
<tr>
<td></td>
<td>( T = T_{IN} )</td>
</tr>
<tr>
<td>Outlet</td>
<td>( \frac{\partial u}{\partial x} = 0 )</td>
</tr>
<tr>
<td></td>
<td>( \frac{\partial T}{\partial x} = 0 )</td>
</tr>
<tr>
<td>Free Surface</td>
<td>(-k \frac{\partial T}{\partial y} = h[T - T_\infty])</td>
</tr>
<tr>
<td>Channel Walls</td>
<td>( u = 0 )</td>
</tr>
<tr>
<td></td>
<td>( \nabla T \cdot \vec{n} = 0 )</td>
</tr>
</tbody>
</table>

2.6 Permeability Constant Sensitivity Analysis

The permeability constant, \( C \), in the Kozeny equation dictates fluid flow permeability in the porous (solid-liquid) region defined in the enthalpy-porosity method. The Kozeny equation is repeated here,

\[
A = -C \frac{(1 - f^2)}{(f^3 + q)} \tag{1.15}
\]

Where \( f \) is the liquid fraction in the mushy region. The values reported for the permeability constant in literature generally range between \( 10^4 \) and \( 10^8 \) [105]. Ebrahimi et al. [105] numerically showed that, in the case of isothermal phase change, the mushy zone constant has no effect on melting behavior if a reasonably fine grid is used. For the non-isothermal melting case, as in the present study, Ebrahimi et al. [105] observed that sensitivity of the numerical solution to the permeability constant increased with (a)
mushy zone thickness and (b) fluid flow velocities adjacent to the solid-liquid interface. The mushy zone thickness increases with an increase in the melting temperature range, and can be estimated as:

\[ m_t = \frac{\Delta T_m}{|\nabla T|} \]  

(1.51)

Where \( \Delta T_m \) is the PCM temperature melting range. The fluid flow in the PCM can alter the mushy zone thickness when convective heat transfer is significant. This can be expressed through the Peclet number, which is defined as the ratio between the rate of heat advection and heat diffusion, and is given as:

\[ Pe = \frac{|\nabla|}{\alpha} \frac{m_t}{\alpha} \]  

(1.52)

Where \( |\nabla| \) is the magnitude of interface-adjacent fluid velocity in the PCM. Large values of the Peclet number (\( Pe >> 1 \)) indicate a strong sensitivity of the solution to the permeability constant while smaller values indicate insensitivity to the constant [105]. In the present study, the effect of the permeability constant on melting time was investigated. The difference in the PCM melting fraction (Fig. 2-6) was negligible between the four cases. The average Peclet number in the PCM was found to be around one, across all time steps in the numerical simulation, which explains the observed insensitivity of the solution to the permeability constant. These results match up with the observations of Ebrahimi [105] where it was deduced that a smaller melting temperature range (1°C in present study) leads to a smaller interface thickness which in turn leads to a smaller sensitivity of the solution to the permeability constant. Therefore, in the absence of any significant difference in the numerical results, the permeability constant of \( 10^5 \) was selected for use in the numerical model.
2.7 Convergence Study

A numerical solution is converged when the difference between the numerical solution and the exact solution of the differential equation is less than some specified tolerance. The discretization error, in both time and space, is a measure of the discrepancy between the numerical and differential equations, and is given as follows:

\[ \epsilon_T = O(\Delta t^q, \Delta x^p, \Delta y^r, \Delta z^s) \quad (2.52) \]

Where \( \Delta x, \Delta y, \) and \( \Delta z \) are the cell lengths in the \( x-, y-, \) and \( z- \) directions, respectively, \( \Delta t \) is the time-step, and \( q, p, r, \) and \( s \) are the orders of error. The numerical solution can be deemed convergent when,

\[ \lim_{\Delta x, \Delta y, \Delta z, \Delta t} \epsilon_T = 0 \quad (2.53) \]

That is when the truncation error tends to zero as the space and time steps tend to zero. A grid size and time step independence studies were performed to ensure that the convergence condition (Eq. 2.53) is satisfied.
2.7.1 Grid Convergence Study

Five different sized grids were used in the grid convergence study, which is used to assess discretization error. Figure 2-6 shows a plot of the total heat transfer rate to the PCM columns at a specified time for different grid sizes. The percent relative change in the convergence metric between the grids is presented in table 2-6. The trend in the plot shows that the heat transfer rate converges to a value with increasing grid size. There is a less than 0.5% change in heat transfer rate between the fourth and fifth grids. Therefore, the solution becomes grid independent at the fourth grid. This grid is shown in figure 2-7. A structured hexahedral mesh topology was used and O-grid meshing was generated within and around the columns. Mesh refinement was performed close to the channel walls and the free surface.

![Figure 2-6. Total heat transfer rate from fluid to PCM columns at a specified time](image)
Table 2-6. Percent relative change in grid convergence metric

<table>
<thead>
<tr>
<th>Grid Size (Millions)</th>
<th>Heat Transfer Rate [W]</th>
<th>Percent Relative Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.3</td>
<td>15.42</td>
<td>-</td>
</tr>
<tr>
<td>0.5</td>
<td>15.61</td>
<td>1.23</td>
</tr>
<tr>
<td>0.8</td>
<td>15.78</td>
<td>1.04</td>
</tr>
<tr>
<td>1.5</td>
<td>15.88</td>
<td>0.63</td>
</tr>
<tr>
<td>2.5</td>
<td>15.94</td>
<td>0.38</td>
</tr>
</tbody>
</table>

Figure 2-7. The (a) top and (b) side views of the structured mesh
2.7.2 Time Step Independence Study

A similar convergence study was conducted for the time-step size. Figure 2-8 shows a plot of the total heat transfer rate to the PCM columns at a specified time for different time step sizes. The heat transfer rate increases by less than 1% going from a time step size of 0.025s to 0.01s. A time step size of 0.025s was selected for further analysis.

![Heat Transfer Rate vs. Time Step Size](image)

**Figure 2-8. Total heat transfer rate from fluid to PCM columns at a specified time**

2.7.3 Solution Stability

A solution of a numerical scheme is stable when the error between this solution and the exact solution of the numerical scheme is bounded at all time-steps. The solution stability was checked by monitoring a flow variable (temperature) at a specific location over time. Figure 2-9 shows numerical results for the temperature at a specific point on the outer column wall. It is shown that the temperature converges to a specific value (33 C) after some time and there are no major fluctuations in the temperature profile. This is an indicator of solution stability. Moreover, the steady state temperature approaches the channel inlet temperature (33 C), which gives physical consistency to the results.
2.8 Numerical Model Validation

Toxopeus [43] studied the flow behavior and heat transfer in a rectangular channel containing offset PCM-filled columns. The physical model is shown in figure 2-10. Seven vertical PCM-filled columns were confined to the walls of a rectangular channel. The spacing between the centers of the columns was equal to one column diameter in the lateral direction and two column diameters in the horizontal direction. The channel width was equal to two column diameters. Fluid at a constant mass flow rate and temperature was let into the channel from the inlet. The side walls of the channel were insulated and the free surface was exposed to the surrounding air. Thermocouples were placed at specific locations on the columns’ outer walls to monitor the temperature. The experiment was run until the PCM in all columns had melted.
Figure 2-10. Top and side views of the physical model used in experimental study of Toxopeus [43], with the (a) top view showing the column arrangement, and (b) side view showing horizontal spacing between the columns

2.8.1 Temperature Data

Figure 2-11 shows the temperature at a specific point on the outer wall of a column. The agreement between numerical results and experimental data was quantified by the relative mean absolute error as follows:

\[
\text{Relative MAE} = \frac{1}{n} \sum_{i=1}^{n} \frac{|T_{i,\text{num}} - T_{i,\text{exp}}|}{T_{i,\text{exp}}}
\]  

(2.54)

The relative MAE for the case when the inlet temperature was 28 C was 0.02 (2%). And the relative MAE for the case when the inlet temperature was 33 C was 0.01 (1%). Numerical results show the greatest deviation from experimental data in the initial increase in outer column wall temperature. The much more abrupt transition to a stable temperature in experimental data can be explained by the initial conditions in the channel. At the start of the experiment, the channel was empty and it was slowly filled up to the top height. The process of filling up the channel is highly turbulent and flow mixing in
the channel increases the initial heat transfer rate to the PCM columns, causing the sudden temperature jump seen in the experimental data. In the numerical model however, flow velocity in the channel was initialized as the inlet velocity. Therefore, there was no significant turbulence generation in the initial flow, and the temperature increase was far more gradual. After the initial discrepancy, numerical results become in sync with the experimental data especially with the temperature approaching the same steady state value in both cases. The numerical model is therefore considered to be validated against experimental data.

![Figure 2-11. Validation of the current numerical model against the experimental data of Toxopeus [43]. Outer column wall temperature when the channel inlet temperature is (a) 28 C and (b) 33 C](image)

2.8.2 PIV Data

Figure 2-12 shows the velocity magnitude distribution in the channel for flow over the first five columns at a height of 9.57 cm. In the numerical model, the flow accelerates as it passes over the columns, which results in a gradual increase in the mean flow velocity. The maximum velocity magnitude is around 0.03 m/s and it occurs as the flow passes over the fifth column. A similar velocity magnitude distribution is observed in the
experimental velocity data from Toxopeus [1] where there is also a similar velocity pattern for flow over the columns, and where the maximum velocity magnitude is also around 0.03 m/s for flow over the fifth column. In the absence of discrete velocity data, a qualitative comparison between the velocity magnitudes shows that the flow behavior is similar in both the numerical model and the PIV data. Therefore, the numerical model is further validated against the velocity data.

![Figure 2-12](image-url)

**Figure 2-12.** The (a) numerical and (b) experimental resultant velocity magnitudes for flow over the first five columns in the channel at a height of 9.57 cm at a mass flow rate of 0.5 liters/min and an inlet temperature of 33 C. Experimental figure adapted from Toxopeus [1]
Chapter 3

3 Numerical investigation of the effects of flow and geometric parameters on thermal energy storage in PCM-filled columns

Latent heat-based thermal energy storage (LHTES) can be used to thermally regulate a photobioreactor channel. A novel design for passive thermal regulation of photobioreactors using latent heat-based is proposed, wherein PCM-filled columns are placed inside a photobioreactor channel, and the thermal energy storage inside the PCM provides thermal regulation in the photobioreactor. Thermal energy is stored primarily as latent heat in the phase change material contained in each column. This chapter aims to numerically investigate the mechanisms of heat transfer and thermal energy storage in a rectangular channel containing PCM-filled columns when a step increase in the channel inflow temperature is introduced. The thermal response of flow in the channel in the presence of these columns is investigated. In addition, the effects of varying the column arrangement, column shape and column aspect ratio, as well as the operating parameters such as the channel flow temperature and the channel flow rate on the thermal energy storage is also investigated. The optimal configuration of these geometric and operating parameters that maximizes thermal regulation in the channel is derived. The validated numerical model for simulating flow and heat transfer in a rectangular channel containing PCM-filled columns that was developed in the previous chapter will be used in this parametric study.

3.1 Introduction

Thermal energy storage in PCM-filled columns in a channel occurs as a result of the heat exchange between the channel fluid and the columns. This heat exchange requires the presence of a temperature gradient across the channel fluid-column wall interface. Changes in this temperature gradient affect the heat transfer rate and therefore the energy storage process. Toxopeus [43] experimentally determined that, for heated flows over cylindrical columns, there is a step increase in the column wall temperature when the heated channel fluid comes into contact with the columns. In correspondence with this
temperature increase, a step increase in the heat flux across the column walls was also observed. With the increase in the column wall temperature, the temperature gradient across the fluid-wall interface was found to diminish very rapidly and the high initial heat transfer rate decreased rapidly. Toxopeus [43] found that an increase in the mass flow rate at low Reynolds numbers (Re=50-100) led to a higher step increase in column temperature and the heat flux. They also reported an uneven distribution of the heat flux along the column height, where buoyancy effects in the channel fluid led to higher heat fluxes in the top sections of the columns relative to the bottom sections. The column arrangement and column cross section shape were found to influence the flow behavior and thermal energy storage in the channel. A decrease in the horizontal spacing between the columns led to higher turbulence in the channel, higher thermal energy storage rates and lower PCM melting times. The switch from a circular column cross section shape to a square one led to higher flow mixing in the channel and higher thermal energy storage rates.

The influence of blockage and gap ratios on flow behavior and heat transfer in flows over confined cylinders have been investigated in a wide array of numerical and experimental work. Khan and Yovanovich [82] experimentally investigated the effects of blockage ratio on heat transfer for flow over a confined cylinder. They found that heat transfer rates were higher at higher blockage ratios (BR) and at higher flow Reynolds numbers (Re). The average Nusselt number increased by 43% when the Re was increased two-fold at a BR of 0.8, and it increased by 40% when the BR was increased from 0.2 to 0.8 at a constant Re. Chan et al. [77] reported on the influence of blockage ratio (BR) on flow over a circular cylinder centered between two walls. They found that the critical Re marks the onset of unsteady vortex shedding in the wake of a circular cylinder. This critical Re was found to increase with an increase in the BR for BR ≤ 0.5.

He et al. [86] experimentally investigated the effects of gap ratio (GR) on the flow behavior over a circular cylinder. They found that vortex shedding was suppressed for GR ≤ 0.25. For a wall-confined cylinder (GR=0), the flow resembled that over a backward facing step where flow separation occurred with a mean recirculation length of x/D = 7. For a wall confined (GR=0) square cylinder, Arnal et al. [83] observed that there
was no vortex shedding at a Re=100 but there was unsteady vortex shedding at the higher Re of 500 and 1000. The effect of gap ratio on flow behavior and heat transfer in a staggered tube arrangement was numerically investigated by Ariansyah et al. [87], who considered the flow of a heated fluid over a bank of tubes. It was found that the heat transfer coefficient and the temperature drop across the bank of tubes were highest when the gap between the rows of tubes was the smallest.

In the presence of PCM thermal energy storage columns, in addition to flow dynamics and heat transfer in the channel, the evolution of heat transfer mechanisms in the PCM also affect the dynamics of the thermal energy storage. Gau and Viskanta [56] experimentally determined that heat transfer in the PCM adjacent to a heated wall, for PCM contained in a rectangular enclosure, is initially through conduction until a significant portion of the PCM melts, after which natural convection is responsible for the continued melting process and movement of the solid-liquid interface. Tayssir et al. [63] expanded on this work by considering a vertical cylinder with heated wall containing paraffin. They found that significant melting in the cylinder occurs only after a certain time delay and that the primary mode of heat transfer switches from conduction in a thin liquid PCM film close to the cylinder to natural convection in the convection cell that forms as this initially thin liquid film expands radially towards the cylinder center. Shmueli and Ziskind [65] numerically determined that natural convection driven melting of PCM in a vertical cylinder with heated wall proceeds in such a way that the PCM in the top regions of the cylinder melts first, leaving an inverse cone of solid PCM that extends from the top of the cylinder to the bottom. Sridharan et al [67] numerically determined that in vertical cylinders with high aspect ratios, natural convection heat transfer through the liquid PCM in the top region of the cylinder is mostly radial which results in the formation of a long inverse solid PCM cone which decreases in length as the convection cells continue to grow in size.

Jevnikar and Siddiqui [62] experimentally investigated the influence of heat source orientation on the transient flow behavior during PCM melting in a rectangular enclosure. They found that heat transfer in the PCM through conduction leads to the formation of a thin liquid PCM layer adjacent to the heated wall and this layer remains motionless for a
considerable time period over which the viscous forces presumably dominate the buoyancy forces. Conduction was found to be the primary mode of heat transfer up until a large enough amount of the PCM had melted after which buoyant forces became significant and natural convection heat transfer became the dominant mode of heat transfer. The circulation of liquid PCM in a convection cell adjacent to the heated wall resulted in the expansion of the solid-liquid interface near the top of the rectangular enclosure. In the convection cell, heated melted PCM was directed upwards near the heated wall, and slid back down along solid PCM as it cooled. The observations from this work are relevant to the case of vertical cylinders in the present study due to the axisymmetry of the cylinders.

Although the influence of geometric and flow parameters on flow behavior and heat transfer in flows over confined cylinders has been previously studied, such effects have only been considered in isolation and not as part of a comprehensive latent heat based thermal energy storage system. Moreover, the numerical and/or experimental studies that have dealt with heat transfer and melting behavior in PCM do not consider the effects of varying the external geometric and flow conditions. This chapter numerically investigates the influence of flow and geometric parameters on the thermal energy storage in the PCM in a comprehensive parametric analysis that considers the effects of such parameters in conjugation with the aim to derive a configuration that maximizes thermal regulation in the channel.

3.2 Physical Model

The physical model is shown in figure 3-1. It consisted of an open rectangular channel 30 cm long (L), 12.5 cm high (H) and 2.54 cm wide (W). The channel was bounded on all sides by insulated walls except for the top surface which was exposed to the atmosphere. The long outlet pipe was 1 cm in diameter and was placed at a height of 10 cm from the base of the channel. 7 PCM-filled columns were placed along the rectangular channel. The column diameter (D) was half of the channel width (1.27 cm). The horizontal distance between the centers of any two consecutive columns was initially set equal to two column diameters (2D). The lateral offset between the centers of any two consecutive columns was initially set equal to 0.5D. The gap ratio (GR), defined as the distance
between columns and the channel wall, was set equal to 0.25D. The blockage ratio (BR), defined as the column diameter divided by the channel width, was set equal to 0.5D. The horizontal and lateral axes correspond to the direction parallel to flow (x) and normal to flow (z), respectively.

In the current setup, the channel fluid was water, the columns were copper tubes, and the PCM was Rubitherm-26 (RT-26). RT-26’s thermophysical properties are listed in table 3-1. The numerical model developed in Chapter 2 was used to simulate flow and heat transfer in the channel. The initial temperature in the channel was set as 24°C. There was a uniform velocity of 3.4 mm/s at the inlet. At this inlet velocity, the mass flow rate in the channel was equal to 0.65 Kg/min. At the start of the simulation, the inlet temperature was increased to 34°C. This represented a step increase of 10°C in the channel fluid temperature over the initial system temperature:

$$\Delta T = T_{\text{inlet}} - T_0$$ (3.1)

where $T_{\text{inlet}}$ and $T_0$ are the channel inlet and initial system temperatures, respectively.

The boundary conditions are summarized in table 3-2. The simulation was run until the PCM in the columns had fully melted. The results of this numerical simulation were used to characterize flow behavior and heat transfer in the channel.
### Table 3-1. Thermophysical properties of Rubitherm-26 [89]

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Density</strong></td>
<td></td>
</tr>
<tr>
<td>Solid</td>
<td>880 Kg/m³</td>
</tr>
<tr>
<td>Liquid</td>
<td>750 Kg/m³</td>
</tr>
<tr>
<td><strong>Thermal Conductivity</strong></td>
<td>0.2 W/m-K</td>
</tr>
<tr>
<td><strong>Viscosity</strong></td>
<td>0.02 Pa-s</td>
</tr>
<tr>
<td><strong>Thermal Expansion Coefficient</strong></td>
<td>0.0005 K⁻¹</td>
</tr>
<tr>
<td><strong>Melting Temperature</strong></td>
<td></td>
</tr>
<tr>
<td>Solidus (T_s)</td>
<td>298.15 K (25 C)</td>
</tr>
<tr>
<td>Liquidus (T_l)</td>
<td>299.15 K (26 C)</td>
</tr>
<tr>
<td><strong>Latent heat of fusion</strong></td>
<td>180 KJ/Kg</td>
</tr>
</tbody>
</table>

### Table 3-2. Physical boundary conditions

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet</td>
<td>(T = 34\ C); (M=0.65\ Kg/min); (u=3.44\ mm/s)</td>
</tr>
<tr>
<td>Outlet</td>
<td>Fully Developed Flow</td>
</tr>
<tr>
<td>Free (top) surface</td>
<td>Slip Condition</td>
</tr>
<tr>
<td></td>
<td>Convection ((h = 10\ W/mK))</td>
</tr>
<tr>
<td>Channel Walls</td>
<td>(U = 0) (No Slip)</td>
</tr>
<tr>
<td></td>
<td>(\nabla T \cdot \vec{n} = 0) (Insulated)</td>
</tr>
</tbody>
</table>
Figure 3-1. The (a) top and (b) side views of the (c) physical model. The horizontal and lateral offsets between centers of consecutive PCM-filled columns are equal to two and half column diameter(s), respectively.
3.3 Flow Behavior and Heat Transfer Characterization

3.3.1 Channel Fluid Flow

Figure 3-2a shows the steady-state velocity magnitude contours in the mid horizontal plane (y=H/2) of the rectangular channel at Re = 200. Figure 3-2b shows the resultant velocity vectors for flow over the first three columns. The velocity at the channel and column walls was zero due to the no slip condition at the walls. The flow accelerated as it passed over the columns. The flow acceleration over each column resulted in an increase in the velocity magnitude of the flow as it passed through the channel. The velocity magnitude adjacent to the last downstream column was 175% higher compared to the inlet flow velocity. Figure 3-2c shows streamlines for the flow over first three columns. At Re=200, flow separation occurred at around $\theta = 100^\circ$ and, in the presence of adverse pressure gradients, there was a backflow in the wake of the columns. The backflow velocities were higher for the downstream columns due to higher bulk flow velocities.
Figure 3-2. The steady state velocity magnitude contours in the channel at the mid horizontal plane (shown) at Re = 200, for the (a) entire channel length and over the first three columns showing (b) resultant velocity vectors and (c) streamlines
Figure 3-3 shows temperature contours in the channel at the mid horizontal (y=H/2) plane at the time when 50% of the solid PCM had melted (same Reynolds number as in Figure 3-2). A consistent drop in the channel flow temperature was observed across the column arrangement. The temperature increase relative to the step temperature increase at the channel inlet ($\Delta T=10^\circ C$) in the region between a pair of columns can be calculated as:

$$\Delta T_{\text{change}} = \frac{T_{\text{gap}} - T_0}{T_{\text{inlet}} - T_0} = \frac{T_{\text{gap}} - T_0}{10^\circ C} \quad (3.2)$$

where $T_{\text{gap}}$ is the temperature at the midpoint on the line connecting the centers of two columns, and $T_0$ and $T_{\text{inlet}}$ are the initial and inlet temperatures, respectively. The relative temperature increase between each successive pair of columns was found to be 0.96, 0.90, 0.84, 0.72, 0.62 and 0.47. The overall relative temperature change at the outlet was 0.33. This means that, in response to the temperature increase of 10 C at the inlet, the outlet temperature increased by only 3.3 C ($0.33 \times 10^\circ C$) over its initial value at the time when 50% of the solid PCM had melted. This relative increase in the outlet temperature increases with time due to the finite energy storage capacity of the columns and, if the numerical simulation is run for a long time, the outlet temperature converges to the inlet temperature.

3.3.2 Column Walls

Figure 3-4 shows the average (across all columns) column wall temperature and the total heat transfer rate from the channel fluid to the column walls. There was an initial rapid increase in the heat transfer rate to the columns when the hot channel fluid from the inlet made contact with the columns that were at a lower initial temperature. Due to the high
thermal conductivity of the columns walls, there was an immediate increase in the average column wall temperature corresponding to the increase in the heat transfer rate. There was a gradual decrease in the heat transfer rate over time due to diminishing temperature gradients between the channel fluid and the columns. With the decrease in the heat transfer rate, there was also a decrease in the rate at which the average column wall temperature increased. As the column temperature approached the channel fluid temperature (34 C), the heat transfer rate approached zero. There was a sudden increase in the average column wall temperature at 700s, which corresponds to the time when the PCM in all columns had fully melted. The heat transfer rate into the columns is related to the PCM melting behavior and energy storage mechanics which are discussed next.

![Graph](image)

**Figure 3-4. The average column wall temperature (T) and the total heat transfer rate (Q) from the channel fluid to the columns at Re=200.**

### 3.3.3 PCM

Figure 3-5a shows the contours of the liquid PCM velocity magnitude contours in the first column at the time when 50% of the PCM had melted. The velocity magnitude was zero at the column wall due to the no slip condition. Figure 3-5b shows the contours of the vertical (y) velocity in the same region. The positive (upwards) velocity close to the column wall is the result of heated liquid PCM rising upwards along the column wall due to buoyancy. The negative (downwards) velocity is the colder PCM falling to the bottom.
of the column. This implies that the liquid PCM is circulated through the entire height of the column in the form of a convective cell. The PCM was fully solid in the center of the column, and there was no velocity in this region.

Figure 3-5. The (a) velocity magnitude and (b) y-velocity contours at 50% melt fraction in the first column at the mid-horizontal plane of y=H/2 (outlined in the schematic).

Figure 3-6 shows the PCM velocity magnitude at different melt fractions (MF) in the first column in the vertical plane at z=0.375W. The melt fraction refers to the fraction of the PCM that is in the liquid form. The solid and liquid PCM regions are shown in red and blue, respectively. In the initial stages of melting, a very thin layer of liquid PCM forms adjacent to the column wall and it remains motionless over a considerable time period (MF < 0.20). The heat transfer through this layer occurs by conduction as velocity magnitudes in this layer are negligible. Once a significant fraction of the PCM melts close to the column wall, the buoyant forces become significant and natural convection dictates the melting process and solid-liquid interface movement. A convection cell develops in which the heated liquid PCM rises to the top of the column and the colder liquid PCM sinks to the bottom (see figure 3-6). The accumulation of heated liquid PCM at the top of the column moves the solid-liquid interface in this region away from the column wall and towards the center of the column until the interface merges at the very top of the column at around MF=0.75. Once this occurs, the melting proceeds in a top-down manner where the liquid PCM sits atop an inverse cone of solid PCM that extends downwards from a point near the top of the column. This inverse cone of solid PCM
decreases in height as the PCM melt fraction increases. The corresponding velocity magnitude contours are shown in figure 3-7. The velocity close to the column wall is directed upwards in the convection cell. The heated liquid PCM that rises along the column wall loses heat as it slides back down along the solid PCM. The velocity contours at MF=0.90 show that the liquid PCM accelerates as it slides down along the inverse cone of solid PCM.

The observed melting behavior is supported by the experimental investigation of Jevnikar [62] on the melting behavior of PCM heated from a side wall. In the experimental study, it was found that, similar to the findings of the present study, heat transfer in the PCM through conduction led to the formation of a thin liquid PCM layer adjacent to the heated wall and this layer remained motionless for a considerable time period over which the viscous forces presumably dominate the buoyancy forces. In the experimental study, similar to the present results, it was found that the circulation of liquid PCM in a convection cell adjacent to the heated wall resulted in the expansion of the solid-liquid interface near the top of the rectangular enclosure. This behavior is also supported by the work of Shmueli and Ziskind [65] who numerically investigated the melting behavior of subcooled paraffin contained in a vertical cylinder whose wall was kept at a constant temperature. It was found that the heat transfer rate to the solid PCM in the cylinder was initially uniform across the entire height of the cylinder due to the presence of a uniform temperature gradient, but the heat transfer decreases rapidly around the top regions of the cylinder due to an accumulation of the heated liquid PCM at the top of the convective cell which results in diminishing temperature gradients. This uneven heat transfer was found to facilitate faster melting at the top of the cylinder and the formation of an inverse cone of solid PCM extending to the bottom of the cylinder.

As stated above, when the PCM initially melts, there is a formation of a thin liquid PCM layer adjacent to the column wall. This layer remains motionless for a considerably large time period during which heat conduction is the primary mode of heat transfer in the PCM. Since organic PCMs have a very low thermal conductivity (0.2 for RT-26), it takes a long time for enough PCM to melt in the thin liquid layer before significant natural convection begins. Once natural convection begins, the heat transfer process accelerates.
Figure 3-6. The (top) melt fraction and (bottom) velocity magnitude contours in the first column at PCM melt fractions of (a) 40%, (b) 60%, (c) 80%, (d) 90%, and (e) 99%.
3.4 Parametric Analysis of Operating and Geometric Conditions

Thermal energy storage in PCM-filled columns placed in a rectangular channel was hypothesized to be influenced by the flow conditions and column arrangement. The flow parameters include the fluid temperature and mass flow rate. The mass flow rate dictates the rate at which thermal energy is supplied to the channel. The flow temperature affects the magnitude of temperature gradients at the columns’ walls. The column arrangement affects blockage and gap ratios in the channel, both of which have been shown to affect the flow behavior and heat transfer rate [43]. Since almost of all these parameters work in conjugation to influence the flow behavior and the heat transfer in a channel containing PCM-filled columns, these parameters cannot be studied in isolation but as part of detailed parametric study aimed to identify the configuration that maximizes the thermal energy storage in PCM-filled columns.

3.4.1 Studied Parameters

Table 3-3 lists the parameters that are varied in the parametric analysis. The offsets between columns are given in multiples of the column diameter, D.

The channel flow Reynolds number (Re) is calculated as:

\[ \text{Re} = \frac{\rho V D_h}{\mu} \]  \hspace{1cm} (3.3)

where \( V \) and \( D_h \) are the channel inlet flow velocity and channel hydraulic diameter, respectively. The \( \text{Re} \) was varied by changing the mass flow rate. The step increase in temperature (\( \Delta T \)) is defined as,

\[ \Delta T = T_{\text{inlet}} - T_0 \]  \hspace{1cm} (3.4)

where \( T_{\text{inlet}} \) and \( T_0 \) are the channel inlet and the initial system temperatures, respectively. \( \Delta T \) was varied by changing the channel inlet temperature.
Figure 3-7 defines the horizontal ($S_L$) and lateral ($S_T$) offsets between the centers of consecutive columns. The horizontal offset was varied by changing the horizontal (x direction) distance between the columns. The lateral offset was varied by changing the lateral (z direction) distance between the columns. Figure 3-8 shows the channel configurations at the three lateral offsets. A vertical offset ($S_T$) of 0 means that the columns are aligned in a straight line in the center of the channel. An $S_T$ of 0.5D means that the columns are displaced a distance of 0.25D away from the channel walls. An $S_T$ of D means that the columns are wall bound and there is no gap between the columns and channel walls. Figure 3-9 shows the channel configurations at the three horizontal offsets. The horizontal offsets of $S_L$=1.25D, 1.5D and 2D correspond to horizontal distance between the centers of columns of 1.25D, 1.5D and 2D, respectively.

Figure 3-7. The horizontal ($S_L$) and lateral ($S_T$) offsets between columns.

Figure 3-8. Channel configuration at a horizontal offset of 1.5D and a lateral offset of (a) 0D, (b) 0.5D, and (c) D
The change of column cross section shape from circular to square was done in such a manner that there was no difference in the PCM mass or in the gap and blockage ratios in the channel. The column aspect ratio (AR) is defined as,

\[ AR = \frac{H}{D} \]  \hspace{1cm} (3.5)

where H and D are the column height and column diameter, respectively. The AR was varied by changing the column height and diameter in such a manner that the total PCM mass in each column as well as the gap and blockage ratios remained the same. In order to keep the same PCM mass per column, the only way to increase the AR is to increase the column length and decrease the diameter in such a way that the column volume remains the same. An increase in the column length also means that the channel height increases by the same amount. Similarly a decrease in the column diameter means that the channel width also decreases such that the blockage ratio remains the same. In the parametric study, only one parameter was varied at a time. Tables 3-4 summarizes different cases in the analysis where each row represents one simulated case.
Table 3-3. Variation of flow and geometric parameters in the parametric analysis

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Channel Flow Reynolds number</td>
<td>Re = 50, 100, 200, 400</td>
</tr>
<tr>
<td>Temperature Step Increase</td>
<td>ΔT_{step} = 5C, 10C</td>
</tr>
<tr>
<td>Column horizontal Offset</td>
<td>S_L = 1.25D, 1.5D, 2D</td>
</tr>
<tr>
<td>Column lateral Offset</td>
<td>S_T = 0, 0.5D, 1D</td>
</tr>
<tr>
<td>Column cross-section Shape</td>
<td>Circular, square</td>
</tr>
<tr>
<td>Column Aspect Ratio</td>
<td>AR = 2.5, 5, 10, 20</td>
</tr>
</tbody>
</table>

Table 3-4. The different cases for the parametric study ordered by parameter type

<table>
<thead>
<tr>
<th>Parameter Type</th>
<th>Re</th>
<th>ΔT [°C]</th>
<th>S_L</th>
<th>S_T</th>
<th>AR</th>
<th>Shape</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flow Condition</td>
<td>50, 100, 200, 400</td>
<td>5,10</td>
<td>2D</td>
<td>0.5D</td>
<td>10</td>
<td>Circular</td>
</tr>
<tr>
<td>Column Arrangement</td>
<td>200</td>
<td>10</td>
<td>1.25D, 1.5D, 2D</td>
<td>0, 0.5D, D</td>
<td>10</td>
<td>Circular</td>
</tr>
<tr>
<td>Column Aspect Ratio</td>
<td>200</td>
<td>10</td>
<td>2D</td>
<td>0.5D</td>
<td>2.5,5,10,20</td>
<td>Circular</td>
</tr>
<tr>
<td>Column Shape</td>
<td>200</td>
<td>10</td>
<td>2D</td>
<td>0.5D</td>
<td>10</td>
<td>Circular, Square</td>
</tr>
</tbody>
</table>
3.4.2 Output Metrics

The thermal response of the channel flow in the presence of PCM columns was characterized using three defined metrics: heat transfer rate, stored energy fraction and thermal response. The heat transfer rate is the rate at which thermal energy is transferred to the PCM columns. It is equal to the total heat conduction rate into the PCM columns at the channel fluid – column wall interface:

\[ \dot{Q} = -k \int \nabla T \cdot \vec{n} \, dA \]  

(3.6)

where the local wall heat fluxes are integrated over the entire column surface area to obtain the total heat transfer rate. The heat transfer rate is affected by temperature gradient at the channel fluid – column wall interface. In the ideal energy storage case where the PCM has an infinitely large thermal conductivity, the heat that is transferred from the fluid to the columns is stored in the PCM instantaneously, leading to a constant temperature gradient at the channel fluid-column wall interface until all the PCM melts. In reality, however, organic PCMs generally have low thermal conductivity, which leads to a low heat transfer rates at the column walls. The energy storage rate is also affected by the total column surface area (Eq. 3.6).

The stored energy fraction is the fraction of supplied thermal energy that is stored in the PCM. The thermal energy that is stored in the PCM is calculated as:

\[ E_{\text{PCM}} = \rho \Delta H \int \alpha \, dV + \rho c_p \int (T - T_0) \, dV \]  

(3.7)

where \( \alpha \) is the PCM melt fraction, \( m \) is the total PCM mass, \( \Delta H \) is the PCM latent heat, and \( T_0 \) is the initial PCM temperature. The first and second terms on the RHS of equation (3.7) are the PCM latent heat storage and PCM sensible heat storage, respectively. The thermal energy that is supplied to the channel is calculated as:

\[ E_{\text{SUPPLIED}} = \int_0^t (\dot{m} h_e - \dot{m} h_o) \, dt \]  

(3.8)
where $h_e$ and $h_o$ are the mass flow averaged channel inlet and outlet enthalpies, respectively, and $\dot{m}$ is the constant mass flow rate. The energy storage fraction can then be calculated as:

$$E_{\text{fraction}} = \frac{E_{\text{PCM}}}{E_{\text{SUPPLIED}}}$$  \hspace{1cm} (3.9)

It should be noted that the stored energy fraction defines the energy storage efficiency relative to the available energy in the channel and not relative to the excess thermal energy at the inlet. The thermal response relative to the excess thermal energy in the flow is defined by the thermal response:

$$\Delta T_R = \frac{T_{\text{outlet}} - T_0}{T_{\text{inlet}} - T_0}$$  \hspace{1cm} (3.10)

where $T_{\text{outlet}}$, $T_{\text{inlet}}$ and $T_0$ are the channel outlet, channel inlet and initial temperatures, respectively. $\Delta T_R$ is the change in channel outlet temperature relative to the step increase in the inlet temperature. A small $\Delta T_R$ means that there is a small change in the outlet temperature in response to the high temperature flow from the inlet. A high $\Delta T_R$ indicates a greater sensitivity to the heated channel flow from the inlet. It should be noted that $\Delta T_R$ will always approach a value of 1 eventually since the PCM columns have a finite energy storage capacity and cannot thermally regulate the flow indefinitely.

Since the bulk of thermal energy is stored in the form of latent heat in the PCM, the time scales in all three metrics were normalized by the total melt time to analyze the change in the defined metrics with respect to the PCM melt fraction. Hereafter, the term ‘fractional time’ (FR) refers to this normalized time. A metric that changes slowly over a large FR means that the rate of change in this metric is slow relative to the PCM melting.
3.4.3 Influence of Flow Conditions on Energy Storage

Figure 3-10 shows the influence of the flow parameters (Re and ΔT) on the studied parameters. As mentioned earlier, Re is the channel flow Reynolds number and ΔT is the step increase in the inlet temperature. Figure 3-10a shows the influence of Re and ΔT on the stored energy fraction. The fraction increased with an increase in Re. At ΔT = 5C, the stored energy fractions at FR=0.1 were 0.082, 0.115, 0.150 and 0.175 for Re=50, 100, 200 and 400, respectively. At FR=0.40, the respective energy storage fractions were 0.302, 0.306, 0.313 and 0.319. The difference in storage fraction between Re=50 and Re=400 decreased from 113% at FR=0.1 to 5% at FR=0.4. At FR>0.6, the energy storage fraction became almost equal for all Re values. The energy storage fraction decreased with an increase in ΔT for all Re values. At Re=200, the energy storage fraction at FR=0.1 for ΔT=5C was 150% higher compared to the energy storage fraction at ΔT=10C. At FR=0.4, this increase in storage fraction was 65%. The energy storage fractions at 100% melt times (FR=1) were 0.40 and 0.26 at ΔT=5C and 10C, respectively.

Figure 3-10b shows the influence of Re and ΔT on the heat transfer rate (HTR). There was an increase in HTR to a peak value in the early stages of melting. The peak HTR increased with an increase in Re. The peak HTR also occurred at higher fractional times for lower Re values, where the peak HTR value decreased with a decrease in Re. For ΔT=5C, the peak heat transfer rates were 13.7W (FR=0.14), 18.7W (FR=0.09), 25.3W (FR=0.054) and 37.2W (FR=0.032) at Re=50, 100, 200 and 400, respectively. The time averaged heat transfer rates were also higher at higher Re values. At ΔT=5C, the average heat transfer rates were 4W, 6W, 7W and 7.5W at Re=50, 100, 200 and 400, respectively. The increase in ΔT from 5 C to 10 C resulted in an approximate two-fold increase in the peak HTR at each Re. For Re=50 and 400, the average heat transfer rates at ΔT=10C were 75% and 115% higher, respectively, than those at ΔT=5 C for the same Re.

Figure 3-10c shows the influence of Re and ΔT on the thermal response. The results show that there was a delayed thermal response at the outlet at lower Re values and this delay decreased monotonically with an increase in Re. For ΔT=5C, the delays in thermal response at Re=50, 100, 200 and 400 were FR= 0.10, 0.05, 0.025 and 0.0125,
respectively. The thermal response was faster for higher Re values. At FR=0.3, the thermal response was 0.75, 0.90, 0.95 and 0.97 at Re=50, 100, 200 and 400. With the progression of PCM melting, the differences in thermal response between the different Re cases diminished. At FR=0.80, the thermal response was 0.93, 0.97, 0.98 and 0.99 at Re=50, 100, 200 and 400, respectively. The increase in $\Delta T$ from 5C to 10C led to a two-fold increase in the thermal response delay. For example, at Re=50, this delay increased from FR=0.1 at $\Delta T=5$C to FR=0.2 at $\Delta T=10$C. The increase in $\Delta T$ also led to a decrease in the thermal response at all Re values. At Re=50, the thermal response at FR=0.4 decreased from 0.84 at $\Delta T = 5$C to 0.67 at $\Delta T = 10$C.

Table 3-5 lists the melting times for different cases. There was a two-fold decrease in the melting time at each Re value when $\Delta T$ was doubled from 5C to 10C. At $\Delta T=5$C, the melting time decreased by 13%, 10% and 8% as Re was doubled from 50 to 100, 100 to 200 and 200 to 400, respectively.

The results show that the heat transfer rate increases to a maximum value as the heated channel fluid makes contact with the PCM-filled columns. The rapid increase in the heat transfer rate at the column walls results in a rapid increase in thermal energy storage within the PCM. At a higher mass flow rate (or Re), the heated channel fluid is able to make contact with a greater amount of column surface area in a short amount of time which leads to the higher initial column heat transfer rates at higher Re. The heat transfer occurs at the fluid-column interface across a temperature gradient. Since the PCM has a low thermal conductivity, heat from the column cannot be transferred to the PCM at sufficiently high rates to maintain a steady temperature gradient at the column-PCM interface. This causes the column wall temperature to increase rapidly, which results in diminishing temperature gradients at the channel fluid-column wall interface. These diminishing gradients result in a reduction in the heat transfer rate following the peak value. Since the overall heat transfer rate is limited by heat transfer within the PCM, the heat transfer rates at all Re values decrease to the same value. This occurs at FR=0.20 at $\Delta T=5$C and at FR=0.40 at $\Delta T=10$C. Since heat transfer rate to the PCM is the primary indicator of thermal energy storage, it can be deduced that, beyond the initial stages of heat transfer, continued energy storage in the PCM is limited by thermal conductivity of
the PCM and, at the same $\Delta T$, is independent of the mass flow rate. Because of this limitation, the stored energy fraction at the time when the PCM fully melts is equal at all Re values for a specific $\Delta T$.

Thermal regulation in the channel is also related to this limitation. Since the heat transfer rate into the columns is limited, increasing the flow rate would result in the bulk of thermal energy passing through the columns without being stored. At lower flow rates, the flow is afforded more time to exchange heat with the columns before reaching the outlet. This results in a delayed thermal response at the outlet and the rate of outlet temperature increase is also smaller. It can be deduced that the rate of supplied energy should match the rate of energy storage rate for the effective thermal regulation in the channel. A two-fold increase in $\Delta T$ leads to a proportional increase in the column heat transfer rate due to the presence of higher temperature gradients across the channel fluid – column wall interface. For a fixed mass of PCM, the same amount of thermal energy is stored at both $\Delta T$ conditions and the additional thermal energy in the channel in the higher temperature flow case leads to a reduction in the stored energy fraction and the overall energy storage efficiency. It can be deduced from this result that incremental increases in the channel fluid temperature over a long time period would allow for better thermal regulation in the channel since energy losses, in the form of thermal energy exiting the channel, would be smaller.
Figure 3-10. The influence of Reynolds number on thermal energy storage at $\Delta T = (i)$ 5°C and (ii) 10°C. The (a) Stored energy fraction, (b) heat transfer rate to the PCM, and (c) channel outlet temperature, versus fractional time.
Table 3-5. Melting times in seconds for the different flow cases.

<table>
<thead>
<tr>
<th>Reynolds Number (Re)</th>
<th>$\Delta T = 5 \text{ C}$</th>
<th>$\Delta T = 10 \text{ C}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>1930</td>
<td>1005</td>
</tr>
<tr>
<td>100</td>
<td>1670</td>
<td>825</td>
</tr>
<tr>
<td>200</td>
<td>1496</td>
<td>660</td>
</tr>
<tr>
<td>400</td>
<td>1382</td>
<td>642</td>
</tr>
</tbody>
</table>

3.4.4 Effect of Geometric Configuration on the Energy Storage

Figure 3-11 shows the influence of lateral and horizontal offsets between consecutive columns on the thermal energy storage. Three lateral and three horizontal offsets were investigated for a total of 9 cases pertaining to the geometric configuration of the column arrangement. Figure 3-11a shows the influence of column offsets on the stored energy fraction in the PCM. For the same horizontal offset, there was an increase in the stored energy fraction for a lateral offset of $S_T=0.5D$ over $S_T=0$ and $S_T=D$ during the initial stages of energy storage. At $S_L=1.25D$ and $FR=0.10$, the energy storage fractions were 0.06, 0.09 and 0.07 at $S_T=0$, 0.5D and D, respectively. The stored energy fraction at $S_T=0.5D$ remained consistently higher compared to the other two cases until FR= 0.80, after which the storage fractions at all three lateral offsets became equal. The stored energy fraction at the time when the PCM fully melts was 0.25 for all three cases. For the same lateral offset, no difference in energy storage fraction was observed across the three horizontal offsets of $S_L=1.25D$, 1.5D and 2D.

Figure 3-11b shows the influence of the column offsets on the total heat transfer rate to the columns. For the same horizontal offset, there was an increase in the heat transfer rate at a vertical offset of 0.5D compared to the other two cases. At $S_L=1.25D$, the peak heat transfer rate at $S_T=0.5D$ was 50% higher compared to $S_T=0$ and $S_T=D$. For the same lateral offset, the peak heat transfer rate was highest at the intermediate horizontal offset.
of \( S_L = 1.5D \). At \( S_T = 0.5D \), the peak heat transfer rate at \( S_L = 1.5D \) was 10\% and 25\% higher compared to \( S_L = 1.25D \) and 2D, respectively. At \( FR \geq 0.20 \), the heat transfer rates across all 9 offset cases became equal, and the heat transfer rate became independent of the column arrangement.

Figure 3-11c shows the influence of column offsets on the thermal response. For the same horizontal offset, the thermal response was marginally delayed at a lateral offset of zero compared to the other two cases, suggesting slightly better thermal regulation at this offset. At \( S_L = 1.25D \) and \( FR = 0.10 \), the outlet temperature at \( S_T = 0 \) was 6.5\% and 1.23\% higher compared to \( S_T = 0.5D \) and D, respectively. This difference became progressively smaller when \( S_L \) was increased to 1.5D and 2D, respectively. In all 9 column offset cases, the outlet temperature reached within 95\% of the inlet temperature at \( FR \geq 0.20 \).

Table 3-6 shows the melting times for the corresponding cases presented in figure 3-11. For the same \( S_L \), there was a decrease in melting time when \( S_T \) was increased from 0 to 0.5D but an increase in the melting time when \( S_T \) was further increased to D. These differences in melting times were amplified at a horizontal offset of \( S_L = 1.5D \) compared to \( S_L = 1.25D \) and 2D. For the same \( S_T \), changing \( S_L \) had a negligible effect on the melting time.

These results show that the storage of thermal energy in PCM-filled columns is influenced by the column arrangement in the channel. In the initial stages of melting, the rate of energy storage is higher when the lateral offset between consecutive columns is \( S_T = 0.5D \). This also corresponds to the much higher peak heat transfer rate (see figure 3-11b). At \( S_T = D \), the columns are wall bound and the heat transfer is limited to the column surfaces that are exposed to the heated channel fluid. At \( S_T = 0.5D \), the columns are placed at some distance from the column walls which allows fluid flow through the gap regions between the columns and the channel walls. There is an increase in the total column surface area available for heat transfer. At \( S_T = 0 \), the columns are placed in a single line at the center of the channel. There is little flow resistance in the large gaps on either side of the columns once the flow splits into two streams at the first upstream column. The absence of any significant flow between the columns lowers the heat transfer rate. These
results show that the column offset relative to the channel walls is a significant factor affecting the thermal energy storage. The effect of horizontal column offset was to amplify the lateral offset differences in the heat transfer rate. The percentage difference in peak heat transfer rate at $S_T=0.5D$ compared to $S_T=0$ and $D$ increased from 35% at $S_L=2D$ to 55% at $S_L=1.5D$. 
Figure 3-11. Influence of column lateral offset at $S_L = (i) \ 1.25D$, (ii) $1.5D$, and (iii) $2D$, on thermal energy storage in PCM-filled columns. (a) Channel outlet temperature, (b) heat transfer rate to the PCM, and (c) Stored Energy fraction, versus fractional time.
Table 3-6. Melting times in seconds for different column arrangements

<table>
<thead>
<tr>
<th></th>
<th>$S_L = 1.25D$</th>
<th>$S_L = 1.5D$</th>
<th>$S_L = 2D$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_T = 0$</td>
<td>712</td>
<td>716</td>
<td>712</td>
</tr>
<tr>
<td>$S_L = 0.5D$</td>
<td>651</td>
<td>644</td>
<td>660</td>
</tr>
<tr>
<td>$S_L = D$</td>
<td>702</td>
<td>690</td>
<td>718</td>
</tr>
</tbody>
</table>

3.4.5 Effect of Column Aspect Ratio on the Energy Storage

Figure 3-12 shows the influence of the column aspect ratio on the thermal energy storage. Figure 3-12a shows the influence of the aspect ratio on the thermal energy storage. The fraction of stored energy increased with a decrease in the aspect ratio. The stored energy fraction in the fully melted PCM was 0.31, 0.28, 0.24 and 0.22 at AR=2.5, 5, 10 and 20, respectively. The difference in stored energy fraction was greatest when AR was doubled from 10 to 20, followed by the increase from 5 to 10 and 2.5 to 5.

Figure 3-12b shows the influence of the column aspect ratio on the heat transfer rate to the columns. There was an increase in the peak heat transfer rate with an increase in the aspect ratio. The peak heat transfer rate at AR=20 was 88%, 52% and 18% higher than the peak heat transfer rates at AR=2.5, 5 and 10, respectively. The decrease in the heat transfer rate following the peak value occurred at a comparable rate in all three cases such that the differences in heat transfer rates between the cases were carried over until the PCM had fully melted. The time-averaged column heat transfer rate at AR=20 was 275%, 160% and 129% higher than that at AR=2.5, 5 and 10, respectively.

Figure 3-12c shows the influence of the column aspect ratio on the thermal response. The rate of increase in the outlet temperature was higher at lower values of AR. The outlet temperature reached within 95% of the inlet temperature at FR=0.08, 0.11, 0.16 and 0.45 for AR=2.5, 5, 10 and 20, respectively.
Table 3-7 lists the geometric properties associated with different AR values. The column surface area is equal to the number of columns multiplied by the surface area of one column \((n \times \pi DH)\). The increase in the aspect ratio generally led to faster melting and higher peak heat transfer rates (peak HTR). The melting time decreased by 44%, 70% and 46% when the AR increased from 2.5 to 5, 5 to 10 and 10 to 20, respectively. The greater reduction in melting time from AR=5 to AR=10 also corresponds to the higher percentage increase in both the column surface area (40%) and peak heat transfer rate (29%).

The results show that the thermal energy storage in the PCM-filled columns is influenced by the column aspect ratio. For a fixed column volume, an increase in the aspect ratio leads to an increase in the surface area. Table 3-7 lists the column surface area for each case. The column surface area increases by 30% when the AR increased from 2.5 to 5, by 40% when the AR increased from 5 to 10, and by 25% when the AR increased from 10 to 20. The total heat transfer rate from the heated channel fluid to the columns is a function of column surface area. The increase in surface area at higher AR values leads to higher heat transfer rates. The biggest difference in the peak heat transfer rate occurred when the AR was increased from 5 to 10 since this change entailed the greatest percent increase in the column surface area (40%). There is an increase in the column diameter with a decrease in the aspect ratio. The column diameter decreases by 23% when the AR is increased from 2.5 to 5, by 28% when the AR is increased from 5 to 10, and by 27% when it is increased from 10 to 20. For a fixed horizontal \((y)\) plane in the rectangular channel, an increase in the diameter directly corresponds to an increase in the interface length over which the heat transfer occurs. The interface length, for one plane in the channel, is calculated as the perimeter of the columns: \(P = \pi D\). An increase in the interface length implies that heat transfer occurs over a larger distance as the channel fluid flows over a column. This increases the fraction of thermal energy in the channel that is stored in the columns, which leads to a higher overall energy storage efficiency. The decrease in the diameter and an increase in the heat transfer rate with increasing values of AR also affects thermal regulation in the channel. A column with a smaller diameter would experience faster melting as the heat transfer to the center of the column would be faster (table 3-7). A faster melting rate means that in the same amount of time,
more energy is stored in the columns between the inlet and the outlet, which leads to a slower increase in the outlet temperature.

**Figure 3-12.** The influence of column aspect ratio on thermal energy storage in PCM-filled columns. The (a) Stored energy fraction, (b) heat transfer rate to the PCM, and (c) channel outlet temperature, versus fractional time.

**Table 3-7. Geometrical properties and numerical results at different AR values**

<table>
<thead>
<tr>
<th>AR</th>
<th>Diameter (mm)</th>
<th>Column Surface Area (mm²)</th>
<th>Peak HTR (W)</th>
<th>Melting Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5</td>
<td>17.9</td>
<td>2740</td>
<td>42</td>
<td>1548</td>
</tr>
<tr>
<td>5</td>
<td>14.2</td>
<td>3560</td>
<td>52</td>
<td>1075</td>
</tr>
<tr>
<td>10</td>
<td>10.7</td>
<td>4987</td>
<td>67</td>
<td>660</td>
</tr>
<tr>
<td>20</td>
<td>8.5</td>
<td>6283</td>
<td>79</td>
<td>452</td>
</tr>
</tbody>
</table>
3.4.6 Effect of Column Shape on the Energy Storage

Figure 3-13 shows the influence of the column cross sectional shape on the thermal energy storage in PCM-filled columns. Figure 3-13a shows the influence of column cross sectional shape on the stored energy fraction. There was a marginal increase in the stored energy fraction for the square columns during the intermediate stages of the melting process. The stored energy fraction for the fully melted PCM was 1.5% higher for square columns. Figure 3-13b shows the influence of the column shape on the heat transfer rate to the columns. The column heat transfer rate showed that the peak heat transfer rate was 15% higher for the square columns. There was a convergence in the heat transfer rates during the later stages of melting and the heat transfer rates for the two cases became almost equal at FR=0.75. This was also evident in the comparable time-averaged heat transfer rates of 12W and 13W for the circular and square column shapes, respectively. Figure 3-13c shows the influence of the column shape on the thermal response. The thermal response was found to be marginally lower during the initial to intermediate phases of the melting process (FR<0.50) for the square column. Beyond this, the difference in the thermal response was negligible between the two cases. The time to melt was 660s and 601s for the circular and square columns, respectively.

The results show that the thermal energy storage in the PCM-filled columns is influenced by the column shape, although this influence was found to be weaker than the effects of other geometric parameters such as the column aspect ratio and column arrangement in the channel. The sharp edges of square columns provide relatively higher level of turbulence and flow mixing in the channel as compared to circular columns. Flow agitation in this manner increases the heat transfer rate at the fluid-channel wall interface. This results in the slight increase in the peak heat transfer rate. It is important to note that while the square columns provides slightly better thermal performance, they cause higher flow losses that lead to higher operating cost.
Figure 3-13. The influence of column cross section shape on thermal energy storage in PCM-filled columns. The (a) Stored energy fraction, (b) heat transfer rate to the PCM, and (c) channel outlet temperature, versus fractional time.

3.5 Chapter Summary

The influence of flow and geometric parameters on thermal energy storage in PCM-filled columns in a rectangular channel have been investigated. The flow parameters were found to affect the thermal regulation in the channel. At low flow rates, the flow interacts with the columns for a longer time as it flows through the channel. This allows a greater portion of the thermal energy to be stored in the columns which results in a greater drop in the fluid temperature across the columns. There was a decrease in the thermal response of 25% (at 50% fractional time) when the Reynolds number was decreased from 400 to 50, which suggests an increase in thermal regulation with a decrease in Re. For the same flow rate, a larger number of columns along a longer channel would therefore result in a higher temperature drop. Conversely, for the same number of PCM columns in the channel, a lower flow rate would result in a higher temperature drop. Therefore, the flow rate must be adjusted according to the number of columns in the channel. For the current setup, the lowest tested flow rate which corresponds to the flow Reynolds number of 50, resulted in the lowest thermal response at the outlet. At low channel fluid temperatures,
the temperature gradient between the channel fluid and the column walls is small, and therefore the heat transfer rate to the columns is also small. At higher channel fluid temperatures, the heat transfer rate is higher, but the energy storage efficiency was not found to increase proportionally in order to keep the stored energy fraction at a comparable level to the lower channel fluid temperature case. The heat transfer rate at a step temperature of 10°C was 100% higher than that at a step temperature of 5°C but the energy storage efficiency was 60% lower. For a fixed mass of PCM in the channel, the storage efficiency was found to be higher at lower channel flow temperatures. Therefore, the flow temperature conditions must be selected in accordance to the channel design to ensure a high energy storage efficiency. In the current study, the lower tested channel inlet temperature of 29°C was found to provide a higher energy storage efficiency.

The column arrangement influenced thermal energy storage in the columns. The heat transfer rate is highest when the columns are placed at some lateral offset from each other such that the columns are close to the channel walls but not confined to them. The heat transfer rate at the lateral offset of 0.5D was 35% higher than the heat transfer rates at lateral offsets of 0 and D. At this lateral offset, the heat transfer rate was 25% higher at a horizontal offset of 1.5D compared to that at 2D. The heat transfer rate is highest and the thermal response is lowest at higher column aspect ratios. An increase in the aspect ratio from 5 to 10 leads to an increase in the surface area of 40%, which results in an increase in the heat transfer rate of around 40% and a corresponding decrease in the thermal response, which is an indication of higher thermal regulation in the channel. However, the energy storage efficiency decreased with an increase in the aspect ratio. The storage efficiency at AR=10 was 20% lower than that at AR=5. There is a trade-off between the thermal regulation and storage efficiency in this case. The column shape was found to have a marginal effect on the thermal energy storage and thermal regulation. The square columns had a marginally higher energy storage rate (9% higher) compared to the circular columns, although there was no considerable difference in the storage efficiency and thermal regulation. Due to the higher operating cost of using square columns (due to higher flow losses), circular columns were selected for use as they provide a comparable level of thermal regulation with lower operating cost. The results of the parametric study are presented in table 3-8 which lists the influence of flow and geometric parameters on
thermal energy storage. These results provide an understanding of how different parameters influence thermal energy storage, which is essential in the development of a viable design for the photobioreactor.

Table 3-8. The observations of the influence of various flow and geometric parameters on the thermal regulation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Observation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reynolds number</td>
<td>Lower thermal response at lower Re</td>
</tr>
<tr>
<td>Step temperature increase</td>
<td>Much higher energy storage efficiency at higher $\Delta T$</td>
</tr>
<tr>
<td>Column Offsets</td>
<td></td>
</tr>
<tr>
<td>Horizontal</td>
<td>High heat transfer rate at $S_L = 1.5D$</td>
</tr>
<tr>
<td>Lateral</td>
<td>High heat transfer rate at $S_T = 0.5D$</td>
</tr>
<tr>
<td>Column Aspect Ratio</td>
<td>Higher heat transfer rate and lower thermal response at lower storage efficiency at higher AR</td>
</tr>
<tr>
<td>Column Shape</td>
<td>Marginally higher heat transfer rate for square columns</td>
</tr>
</tbody>
</table>
Chapter 4

4 Response of a channel flow with PCM-filled thermal energy storage subjected to varying temperatures

In the previous chapter, flow and heat transfer behavior in a rectangular channel containing PCM-filled thermal energy storage columns were numerically characterized. This was followed by a parametric analysis, where the effects of various flow and geometric parameters on thermal energy storage were investigated, and the optimal configuration to maximize energy storage was derived. This preceding analysis was performed in the presence of a step increase in the channel flow temperature, where the excess thermal energy in the channel fluid was stored in the PCM-filled columns. Photobioreactors placed under natural sunlight experience temperature variations over the diurnal cycle due to changes in ambient conditions [101]. These temperature variations include a gradual increase in photobioreactor channel temperature during the peak sunlight hours and a gradual decrease in the temperature during night time. A latent heat based thermal energy storage system must be able to thermally regulate a photobioreactor channel in the presence of such temperature variations and maintain the temperature ideally at a constant level over the entire operational cycle. This chapter aims to numerically investigate thermal regulation in a rectangular channel containing PCM-filled thermal energy storage columns when the channel flow temperature is gradually varied in both heating (temperature increase) and cooling (temperature decrease) cycles. The effects of varying the channel flow conditions such as the mass flow rate and the rate of change in flow temperature on thermal regulation were investigated. The effect of varying the geometric parameters such as the blockage ratio in the channel on the thermal response were similarly investigated. The optimal configuration of these geometric and flow parameters that maximizes thermal regulation in the channel were derived. The optimal channel design that was derived in chapter 3 was used in this study. The validated numerical model for simulating flow and heat transfer in a rectangular channel containing PCM-filled columns that was developed in chapter 2 was used in the present numerical study.
4.1 Introduction

Sunlight is the most economical option for outdoor microalgae cultivation [102] but variations in the weather, day-night cycles, and seasonal changes affect light intensity [101], which can negatively affect microalgae growth [103,104]. Photobioreactor temperature is directly related to solar irradiance. The light absorbed by the photobioreactor walls, or by the culture that is not used in photosynthesis is converted into thermal energy, which may cause an increase in the culture temperature. The optimal temperature range for algal growth is 20 – 35 degrees Celsius for most species of microalgae, although a few species can survive in temperatures up to 40 degrees Celsius [31]. If the temperature of the culture is lower than this optimal range, then the biomass yield decreases. Conversely, if the temperature is too high, it can cause permanent damage to the microalgae cells [32]. The optimal temperature for S. almeriensis, for example, is 35 degrees Celsius and the cells start to die above 40 degrees Celsius [33]. C. reinhardtii is most productive in the temperature range of 12 – 36 degrees Celsius [34].

In large scale photobioreactors placed in natural sunlight, temperatures in the system can reach up to 45 – 60 degrees Celsius in the absence of temperature regulation [35]. Temperatures this high would kill most species of microalgae, and artificial temperature control systems have to be set up to avoid overheating [36-37]. Microalgae growth is also sensitive to temperature variations. R. capsulatus, for example, has twice the productivity when it is exposed to a constant temperature of 30 C compared to the case when the temperature is slowly increased from 15 – 30 C [39]. This suggests that thermal regulation is required to not only keep temperature within an optimal range, but to also dampen temperature variations in the photobioreactor.

Thermal regulation of a photobioreactor can be achieved in different ways, some of which include, 1) shading the PBR with dark colored paint [40], 2) cooling by spraying water on the PBR panels [41], 3) submerging the PBR in a large amount of water [41], and 4) installing a heat exchanger inside the PBR [42]. These active thermal regulation methods have the disadvantages of recurring costs in the form of equipment and operating costs. Temperature control in photobioreactors placed under natural sunlight using passive thermal regulation has been proposed in some recent studies, although there
is a scarcity in studies exploring the potential of latent heat based thermal energy storage systems to thermally regulate photobioreactors. Uyar and Kapucu [35] experimentally investigated the use of phase change materials (PCM) to passively regulate temperature inside a photobioreactor placed in natural sunlight. The cylindrical photobioreactor was insulated on all sides except at the front and back panels. The front panel was exposed to natural sunlight, and a PCM compartment was attached to the back panel. The photobioreactor temperature was found to change in response to variations in the ambient conditions. The maximum culture temperature was 15 °C lower compared to the control case where no PCM was used. This temperature difference between the control and temperature-controlled cases showed considerable thermal regulation in the presence of temperature fluctuations. The temperature control, however, was not sufficient to keep the PBR temperature within the targeted 20 – 40 °C range for optimal culture growth. The authors suggested that temperature control could be further improved by 1) increasing the amount of PCM, 2) increasing the rate of heat transfer between the PBR and PCM compartments, and 3) installing better insulation to the system.

The variations in the sunlight intensity over the day-night cycle as well as the variations in weather conditions lead to varying temperatures in the photobioreactor. The effect of an increase in the sunlight intensity is the gradual increase in photobioreactor temperature while a decrease in the light intensity leads to a gradual decrease in the photobioreactor temperature. This chapter aims to numerically investigate thermal regulation in a rectangular channel containing PCM-filled thermal energy storage columns when the channel flow temperature is gradually varied.

### 4.2 Physical Model

The physical model is shown in figure 4-1. The geometrical properties of the model were derived from the parametric study in chapter 3 which aimed to maximize thermal energy storage. The gap and blockage ratios as well as the column shape and aspect ratio from
the optimal configuration were used in the current physical model. The model consisted of a rectangular channel 1.05 m long, 0.4 m high and 0.1 m wide. The channel was bounded on all sides by insulated walls except for the top surface which was exposed to the surroundings. The outlet pipe was 0.03 m in diameter and was placed at a height of 0.35 m from the base of the channel. Ten PCM-filled circular columns were placed along the rectangular channel. The column diameter (D) was equal to half of the channel width (1.27 cm). The horizontal distance between the centers of any two consecutive columns was equal to 1.5 times the column diameter (1.5D). The lateral offset between the centers of any two consecutive columns was equal to 0.5D. The gap ratio (GR), defined as the distance between columns and the channel wall, was equal to 0.25D. The blockage ratio (BR), defined as the column diameter divided by the channel width, was equal to 0.5D. The horizontal and lateral directions correspond to the parallel to flow (x) and normal to flow (z) directions, respectively. In the current setup, the channel fluid was water, the columns were copper tubes, and the PCM was Rubitherm-26 (RT-26). RT-26’s thermophysical properties are listed in table 4-1.

From the physical model, the following physical boundaries can be differentiated:

- **Inlet:** there was a uniform velocity equal to 0.156 mm/s at the inlet. At this velocity, the mass flow rate through the channel was equal to 0.375 Kg/min. The flow temperature was time-dependent and it changed over time from the initial system temperature to a higher temperature in the case of energy storage (PCM melting) or to a lower one in the case of energy discharge (PCM solidification). This temperature change can be formally defined as,

\[
T_{\text{inlet}} = T_0 + R t
\]

(4.1)

where \(T_0\) is the initial system temperature and \(R\) is the time rate of change of temperature. The initial system temperature was 24°C for energy storage and 27°C for energy discharge; \(R\) was +0.1 for energy storage and -0.1 for energy discharge such that there was an increase in inlet temperature with time for the energy storage case and a decrease in inlet temperature with time for the energy discharge case.
• Outlet: the flow was fully developed at the outlet. Therefore, zero-gradient velocity and temperature boundary conditions were applied.

• Top (Free Surface): it was a free surface that was exposed to the surroundings. Therefore, convection \((h=10 \text{ W/m-K})\) and slip boundary conditions were applied.

• Channel Walls: channel walls were insulated. Therefore, zero heat flux and no-slip boundary conditions were applied.

The numerical model developed in chapter 2 was used to simulate flow and heat transfer in the channel under the above listed flow and thermal conditions. The numerical boundary conditions are listed in table 4-2.

### Table 4-1. Thermophysical properties of Rubitherm-26 [89]

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td></td>
</tr>
<tr>
<td>Solid</td>
<td>880 Kg/m³</td>
</tr>
<tr>
<td>Liquid</td>
<td>750 Kg/m³</td>
</tr>
<tr>
<td>Thermal Conductivity</td>
<td>(0.2 \text{ W/m-K})</td>
</tr>
<tr>
<td>Viscosity</td>
<td>0.02 Pa-s</td>
</tr>
<tr>
<td>Thermal Expansion Coefficient</td>
<td>0.0005 K(^{-1})</td>
</tr>
<tr>
<td>Melting Temperature</td>
<td></td>
</tr>
<tr>
<td>Solidus ((T_s))</td>
<td>298.15 K (25 C)</td>
</tr>
<tr>
<td>Liquidus ((T_l))</td>
<td>299.15 K (26 C)</td>
</tr>
<tr>
<td>Latent Heat of Fusion</td>
<td>180 KJ/Kg</td>
</tr>
</tbody>
</table>
### Table 4-2. Numerical boundary conditions

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Numerical Boundary Condition</th>
</tr>
</thead>
</table>
| **Inlet**           | \( u = 0.156 \text{ mm/s} \)  
                      | \( T = 24 + 0.1t \) (energy storage)  
                      | \( T = 27 - 0.1t \) (energy discharge)                                                |
| **Outlet**          | \( \frac{\partial u}{\partial x} = 0; \frac{\partial T}{\partial x} = 0 \)                |
| **Free Surface**    | \( -k \frac{\partial T}{\partial y} = h[T - T_\infty]; \ h = 10\text{W/mK} \)             |
| **Channel Walls**   | \( u = 0; \nabla T \cdot \vec{n} = 0 \)                                                    |

---

**Figure 4-1.** The (a) top and (b) side views of the physical model. The horizontal and lateral offsets between centers of consecutive PCM-filled columns are equal to 1.5D and 0.5D, respectively.
4.3 Thermal Regulation

4.3.1 Thermal Energy Storage

The effect of a slow increase in the channel fluid temperature at the inlet on the thermal energy storage and thermal regulation in the channel is investigated in this section. In the previous study, it was observed that an increase in the channel flow Reynolds number leads to a faster thermal response at the outlet. Therefore, the thermal response was found to be lowest at the lowest Reynolds number of Re=50. In order to be consistent with the previous study, the flow rate associated with the Reynolds number of 50 was selected, which corresponds to a mass flow rate of 0.375 Kg/min in the current study. The value for the rate of change in the inlet temperature was selected in accordance with the findings of Uyar and Kapucu [35]. They found that photobioreactors placed under direct sunlight over the course of a day experience temperature variations and, in the absence of thermal regulation, the internal temperatures can reach as high as 60 C (from around 20 C) over 6-7 hours, which translates to a rate of change in photobioreactor temperature of around 0.1 C/min. Figure 4-2a shows the channel outlet temperature at a mass flow rate of 0.375 Kg/min when the channel inlet temperature was ramped up at a rate of 0.1 C/min. The channel inlet temperature was increased linearly from an initial temperature of 24 C to a final temperature of 60 C over a period of 360 min (6 hours). The difference in channel inlet and outlet temperatures is an indicator of thermal regulation in the channel as it shows how much of the thermal energy in the channel is stored within the PCM before the flow reaches the outlet. The numerical results show that there was no significant increase in the channel outlet temperature until 75 min. At 75 minutes, the difference in the inlet and outlet temperatures was 7.25 C. Between 75 and 200 minutes, the outlet temperature increased at a relatively slow rate from 24 C to 28C. At 200 minutes, the difference between the inlet and outlet temperatures was the highest at 15.5 C. Following the completion of the melting period (i.e. latent heat storage period) indicated in the figure, the channel outlet temperature increased from 28 C to 37 C within a short time period between 200 and 250 minutes, and the difference between the inlet and outlet temperatures decreased from 15.5 C to 11 C. After 275 minutes, the outlet
temperature increased linearly at approximately the same rate as the inlet temperature, as the thermal energy is stored as sensible heat.

Figure 4-2b shows the corresponding thermal energy storage in the PCM columns over time. The stored thermal energy is the sum of sensible heat and latent heats. The numerical results show that the thermal energy storage during the first 40 minutes occurred only as sensible heat storage and the stored energy during this time accounted for less than 1% of the total stored energy. Between 50 and 100 minutes, there was a considerable increase in thermal energy storage due to the increase in latent heat storage, corresponding to the increase in PCM melt fraction from 0.01 to 0.25. The latent heat storage increased almost linearly between 100 and 200 minutes at a rate of 5.5 KJ/min corresponding to an increase in the PCM melt fraction of 0.70 from 0.25 to 0.95. The sensible heat storage increased linearly at a much slower rate of 0.20 KJ/min during the same time period. There was a decrease in the latent heat storage rate as the PCM melt fraction approached 1 between 200 and 225 minutes. From 225 to 360 minutes, thermal energy storage occurred only as sensible heat storage at an approximate rate of 0.9 KJ/min. At 360 minutes, the cumulative sensible and latent energy storages accounted for 25% and 75% of the total stored thermal energy, respectively.
4.3.2 Thermal Energy Discharge

Figure 4-3 shows the effects of a decrease in the channel inlet temperature on thermal regulation and thermal energy discharge in the rectangular channel containing PCM-filled columns. Figure 4-3a shows the channel outlet temperature at a mass flow rate of 0.375 Kg/min when the channel inlet temperature was ramped down at a rate of 0.1 C/min. The
channel inlet temperature was decreased linearly from an initial temperature of 27°C to a final temperature of -9°C over a period of 360 min (6 hours). It should be noted that water freezes at a temperature of 0°C and ramping the temperature down to -9°C isn’t realistic but was done so nonetheless to be consistent with the ramp up case. The numerical results show that, similar to the energy storage case, there was no significant decrease in the channel outlet temperature for the first 75 minutes. At 75 minutes, the difference in the inlet and outlet temperatures was 7.34°C. Between 75 and 200 minutes, the outlet temperature decreased by only 4°C compared to the inlet temperature which decreased by 13°C over the same time period. At 200 minutes, the difference between the inlet and outlet temperatures was the highest at 15.6°C. Following the PCM freezing period i.e. the latent heat discharge period indicated in the figure, the channel outlet temperature decreased from 22.8°C to 14°C within a short time period between 200 and 250 minutes, and the difference between the inlet and outlet temperatures decreased from 15.5°C to 11°C. After 275 minutes, the outlet temperature decreased linearly at approximately the same rate as the inlet temperature due to the release of sensible heat.

Figure 4-3b shows the corresponding thermal energy discharge from the PCM columns over time. Thermal energy discharge is the sum of sensible heat and latent heat discharges. The numerical results show that thermal energy discharge during the first 40 minutes occurred only as a sensible heat release and the stored energy release during this time accounted for less than 1% of the total stored energy. Between 50 and 100 minutes, there was a considerable increase in thermal energy discharge due to the increase in the latent heat release, corresponding to a decrease in the PCM melt fraction from 0.98 to 0.75. The latent heat release increased almost linearly between 100 and 200 minutes at a rate of 5.5 KJ/min corresponding to a decrease in the PCM melt fraction from 0.75 to 0.05. The sensible heat release increased linearly at a much slower rate of 0.20 KJ/min during the same time period. There was a decrease in the latent heat release rate as the PCM melt fraction approached 0 between 200 and 225 minutes. From 225 to 360 minutes, thermal energy discharge occurred only as sensible heat release at an approximate rate of 0.9 KJ/min. At 360 minutes, the cumulative sensible and latent energy discharges amounted to 25% and 75% of total discharged thermal energy, respectively.
4.3.3 Thermal Energy Storage/Discharge Discussion

Thermal regulation in the channel depends on heat transfer between the flow and PCM columns. A difference between the column and flow temperatures results in heat transfer between the two regions, which results in temperature change of the PCM until it reaches the melting (or solidification) temperature. The change in PCM temperature leading up to

Figure 4-3. The (a) inlet and outlet temperatures at a mass flow rate of 0.375 Kg/min, and (b) the cumulative thermal energy storage in PCM columns during energy discharge (i.e. the temperature ramp down). The beginning and end of the solidification phase are marked on outlet temperature curve for reference.
the phase change temperature is linked to sensible heat storage or discharge. Because the initial temperature of the PCM (24°C) was only 1°C lower than the PCM melting temperature (25°C) in the case of energy storage, or 1°C higher (27°C) than the solidification temperature (26°C) in the case of energy discharge, sensible heat storage/release occurred very briefly before latent heat storage/release was initiated at the melting/solidification temperature. During the latent heat storage/discharge period, the PCM temperature remained within the melting temperature range since it stored or discharged thermal energy as latent heat. Due to the large latent heat storage density of the PCM, it is able to store a large amount of thermal energy within a narrow temperature range. The process of charging or discharging the PCM within this narrow temperature range is therefore the main driving force behind thermal regulation in the channel. During this time, due to the increased level of thermal regulation, the outlet temperature changed by only 4°C compared to the 13°C change in the inlet flow temperature for both the energy storage and discharge cases. As the PCM phase change fraction approaches 1, the latent heat storage/discharge rate decreases, and the thermal regulation capacity of the PCM also decreases. The continued sensible heat storage/discharge occurs in conjunction with a steady change in the PCM temperature, and the corresponding reduced level of thermal regulation in the channel results in a steady change in the channel outlet temperature in response to the change in the flow temperature at the inlet. Over a period of 360 min (6 hours) of a linear change in the flow temperature (ramp up or ramp down), latent heat storage/discharge occurred over 40% of the total time and was responsible for 75% of the total energy exchange in the channel. Figure 4-4 shows a plot of the temperature change at the outlet where the time scale is normalized by the time when the PCM fully transitions between phases. The temperature change at the outlet \(T_{out}\) relative to temperature change at the inlet \(T_{IN}\) is termed the thermal response, \(\Delta T_r\), and, given an initial temperature of \(T_0\), is defined as:

\[
\Delta T_r = \frac{T_{OUT} - T_0}{T_{IN} - T_0}
\]  

(4.2)
Figure 4-4. Thermal response at the channel outlet for the energy storage and discharge cycles.

Both thermal energy storage and energy discharge cycles show similar profiles for the thermal response. In the case of energy storage, $t_{\text{phase}}$ refers to the total melting time and in the case of energy discharge, it refers to the total solidification time. The relative temperature change at the channel outlet is limited during the latent heat storage/discharge part ($t/t_{\text{phase}} \leq 1$) of the heat exchange process. As seen in the figure, the thermal response becomes stable during the latent heat storage/discharge process during which there is no significant change in the thermal response. As the PCM is close to fully transitioning between phases ($t/t_{\text{phase}} = 1$), the latent heat storage/discharge rate decreases and the rate of change in the outlet temperature increases. Figure 4-5 shows different reference points along the channel at the mid horizontal (y) plane. Figure 4-6a shows the temperature at these reference points as the flow passes over the PCM columns during the charging of the thermal energy storage. Figure 4-6b shows the temperature at the same points during the thermal energy discharge. Since most of the energy is stored/released as latent heat, the data is shown only up to the point when all the PCM melts/solidifies. It was observed that near the channel inlet, the change in temperature closely followed the change in the inlet temperature with some time delay, while far from the inlet, temperature change occurred at a slower rate. At the point C2, the rate of change in temperature was the same as that at the inlet. At the point C4, there was an
increase in the time delay before there was a change in the temperature. There was also some curvature in the temperature profile which developed into a region of stability at the point C6. Temperature change over this region occurred relatively slowly. Between C6 and the outlet, this region expanded and became progressively flatter such that, at the outlet, temperature change within this region was largely suppressed across a considerably large fraction of time relative to the time to a complete phase change.

**Figure 4-5. Different reference point locations at the mid horizontal (y) plane of the physical model**

**Figure 4-6. Flow temperature at different reference locations in the channel (outlined in Figure 4-5) during, (a) energy storage and (b) energy discharge.**

### 4.4 Parametric Analysis

Thermal energy storage in the PCM occurs primarily through latent heat storage as the PCM undergoes phase change. Due to the low thermal conductivity of most organic PCMs, heat transfer in PCMs is a slow process and it is driven by convection during the phase change. The rate of thermal energy storage is therefore limited by the melting behavior of the PCM. The rate of thermal energy that is brought into the channel is a
function of the mass flow rate. In the previous chapter it was observed that a higher mass flow rate does in fact lead to higher heat fluxes at the column walls but also results in a lower storage efficiency since a large portion of the available thermal energy simply passes through the channel without being stored. Due to this observation, the effect of mass flow rate on thermal regulation was investigated in this study. In the previous chapter, the flow temperature at the inlet was kept constant and two different inlet temperatures were considered. It was found that the column heat flux during energy storage increased with an increase in the inlet temperature but the overall energy storage efficiency was higher at lower inlet temperatures. From this observation, it was hypothesized that higher flow temperatures reduce the energy storage efficiency since the heat transfer rate to the columns does not increase proportionally with an increase in the flow temperature to guarantee the same level of storage efficiency. In this study, the effect of varying the rate of temperature change at the inlet on thermal regulation and energy storage was investigated. The parametric analysis in the previous chapter led to the development of an optimal geometric configuration of the channel that maximized thermal regulation and heat transfer rate. The same optimal channel design was used in the current parametric analysis.

### 4.4.1 Parameters

Table 4-3 shows the parameters that were varied in the parametric analysis. The mass flow rate was varied by changing the channel inlet condition in the numerical model (table 4-1). For consistency with the previous study, the mass flow rates that were selected for the current analysis correspond to channel flow Reynolds numbers that are similar to those in the previous study. The channel inlet temperature was previously defined in equation (4.1). The rate of change in temperature was varied by changing the ‘R’ variable in equation (4.1). The values for this R variable were selected in accordance with the findings of Uyar and Kapucu [35], which as mentioned earlier, was translated into a value of 0.1 C/min. Therefore, in the current study, the baseline temperature change rate was selected to be 0.1 C/min. This value was doubled and halved to obtain two additional values for the parametric analysis. Blockage ratio is defined as the ratio of the column diameter, D, to the channel width. For a fixed column diameter, the blockage
ratio was varied by changing the distance between the columns and the channel walls. In the parametric study, only one parameter was varied at a time. Table 4-4 summarizes the different cases in the analysis where each row represents one simulated case.

**Table 4-3. Variation of parameters in the parametric analysis**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass Flow Rate (Kg/min)</td>
<td>M = 0.1875, 0.375, 0.75, 1.5</td>
</tr>
<tr>
<td>Temperature change rate (°C/min)</td>
<td>R = 0.05, 0.1, 0.2</td>
</tr>
<tr>
<td>Blockage Ratio</td>
<td>BR = 0.4, 0.5, 0.6</td>
</tr>
</tbody>
</table>

**Table 4-4. Parametric analysis cases**

<table>
<thead>
<tr>
<th>Parameter Type</th>
<th>Mass Flow Rate (Kg/min)</th>
<th>Temperature Change Rate (°C/min)</th>
<th>Blockage Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass Flow Rate</td>
<td>0.1875</td>
<td>0.1</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td>0.375</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.75</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Temperature Change Rate</td>
<td>0.75</td>
<td>0.05</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.1</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.2</td>
<td></td>
</tr>
<tr>
<td>Blockage Ratio</td>
<td>0.75</td>
<td>0.1</td>
<td>0.4, 0.5, 0.6</td>
</tr>
</tbody>
</table>
4.4.2 Output Metrics

As discussed in a preceding section, there is no significant difference in thermal response and energy storage patterns between the melting and solidification cases (see Figure 4-4). Therefore, parametric analysis is restricted to energy storage (PCM melting case). The results for the energy discharge case are presented in Appendix A.

Thermal energy storage in the PCM-filled columns was characterized using three defined metrics: heat transfer rate, stored energy fraction and thermal response. The heat transfer rate is the rate at which thermal energy is transferred into the PCM columns. It is equal to the total heat conduction rate at the channel fluid – column wall interface:

\[ Q = -k \int \nabla T \cdot n \, dA \]  

(4.3)

where the local wall heat fluxes are integrated over the entire column surface area to obtain the total heat transfer rate. The heat transfer rate is affected by temperature gradient at the channel fluid – column wall interface. In the ideal energy storage case where the PCM has an infinitely large thermal conductivity, the heat transfer rate between the channel fluid and PCM across the column walls would be consistently high until the PCM fully melts. In reality, however, organic PCMs generally have low thermal conductivity, which leads to low heat transfer rates which become even smaller as the PCM phase change fraction approaches 1. The heat transfer rate is also affected by the total column surface area (Eq. 4.3).

The stored energy fraction is the fraction of thermal energy in the channel that is stored in the PCM. It is indicative of the energy storage efficiency in the channel. A low stored energy fraction indicates a low energy storage sensitivity. The thermal energy that is stored in the PCM is calculated as:

\[ E_{\text{PCM}} = \rho \Delta H \int \alpha \, dV + \rho c_p \int (T - T_0) \, dV \]  

(4.4)

where \( \alpha \) is the PCM melt fraction, \( \Delta H \) is the PCM latent heat, and \( T_0 \) is the initial PCM temperature. The first and second terms on the RHS of equation (4.4) are the PCM latent
heat storage and PCM sensible heat storage, respectively. The thermal energy that is supplied to the channel is calculated as:

\[
E_{\text{SUPPLIED}} = \int_0^t (\bar{m}h_e - \bar{m}h_o) \, dt \tag{4.5}
\]

where \( h_e \) and \( h_o \) are the mass flow averaged channel inlet and outlet enthalpies at a specific time, respectively, and \( \bar{m} \) is the constant mass flow rate in the channel. The energy storage fraction can then be calculated as:

\[
E_{\text{fraction}} = \frac{E_{\text{PCM}}}{E_{\text{SUPPLIED}}} \tag{4.6}
\]

It should be noted that the stored energy fraction defines the energy storage efficiency relative to the available energy in the channel and not relative to the excess thermal energy at the inlet. The thermal response relative to the excess thermal energy in the flow is defined by the thermal response:

\[
\Delta T_R = \frac{T_{\text{outlet}} - T_0}{T_{\text{inlet}} - T_0} \quad \text{(4.7)}
\]

where \( T_{\text{outlet}} \), \( T_{\text{inlet}} \) and \( T_0 \) are the channel outlet, channel inlet and initial temperatures, respectively. \( \Delta T_R \) is the change in channel outlet temperature relative to the increase in inlet temperature. A small \( \Delta T_R \) means that thermal regulation along the channel results in only a small change in the outlet temperature relative to a high temperature flow from the inlet. A high \( \Delta T_R \) at earlier stages in the melting process indicates a greater sensitivity to the heated channel flow from the inlet. It should be noted that \( \Delta T_R \) will always approach a value of 1 eventually since the PCM columns have a finite energy storage capacity and cannot thermally regulate the flow indefinitely.

Since the bulk of thermal energy is stored in the form of latent heat in the PCM, the time scales in all three metrics were normalized by the total melt time to analyze the change in the defined metrics with respect to the PCM melt fraction. Hereafter, the term ‘fractional
time’ (FR) refers to this normalized time. A metric that changes slowly over a large FR means that the rate of change in this metric is slow relative to PCM melting.

4.4.3 Influence of Mass Flow Rate

Figure 4-7 shows the influence of the mass flow rate on the output parameters. The stored energy fraction increased with an increase in the mass flow rate (see Figure 4-7a). The peak stored energy fraction was higher at higher mass flow rates, and the peak values occurred at higher fractional times at higher mass flow rates. The peak stored energy fractions were 0.3 (FR=0.4), 0.35 (FR=0.55), 0.38 (FR=0.65) and 0.40 (FR=0.75) at mass flow rates of 0.1875, 0.375, 0.750 and 1.5 Kg/min, respectively. The final stored energy fraction at 100% melt time was 0.28, 0.30, 0.34 and 0.36 at mass flow rates of 0.1875, 0.375, 0.750 and 1.5 Kg/min, respectively. The heat transfer rate (Figure 4-7b) was higher at higher mass flow rates. The peak heat transfer rates increased by 52%, 40% and 20% as the mass flow rate was increased from 0.1875 to 0.375 Kg/min, 0.375 to 0.750 Kg/min, and from 0.750 to 1.5 Kg/min, respectively. The average heat transfer rates were 59W, 81W, 107W and 133W at the respective mass flow rates. The thermal response (see Figure 4-7c) was slower at lower mass flow rates. At FR=0.4, the thermal response was 0, 0.05, 0.20 and 0.40 at mass flow rates of 0.1875, 0.375, 0.750 and 1.5 Kg/min. And at FR=0.8, the thermal response was 0.075, 0.175, 0.375 and 0.55 at the respective mass flow rates. The thermal response at the time of complete melting was 0.22, 0.40, 0.60 and 0.68 at the respective mass flow rates. Table 4-5 lists the melting times for different mass flow rate cases. There was a decrease in the melting times with an increase in the mass flow rate. The melting time at a mass flow rate of 1.5 Kg/min was 62%, 43% and 22% lower than the melting times at mass flow rates of 0.1875, 0.375 and 0.750 Kg/min, respectively.

At high mass flow rates, there is an increase in the convection heat transfer rate in the channel due to higher flow velocities around the columns. Consistently high heat transfer rates lead to a higher fraction of the available thermal energy in the channel to be stored in the PCM columns which leads to a high energy storage efficiency. A high energy storage efficiency only indicates the energy storage sensitivity and it does not take into account the energy losses in the form of excess energy at the inlet passing through the
channel without being stored. At high mass flow rates, energy storage occurs over a small time period as the flow moves faster through the columns to reach the outlet within a small time period. This leads to an increase in the energy losses and a higher thermal response at the outlet. And at high mass flow rates, even during the latent heat storage period, there is a consistent increase in the outlet temperature. This difference in the magnitude of the thermal losses is evident in the thermal response where the response is much slower and occurs after a much longer delay at smaller mass flow rates. The increase in the thermal response between mass flow rates is, however, not consistent. The increase in thermal response at the lowest mass flow rate as it is doubled, for example, is only 50% of the increase in the response when it is doubled again. The same trend is also observed in the increase in the stored energy fraction and heat transfer rate as the mass flow rate is increased. Therefore, there is a trade-off between energy storage efficiency and thermal regulation in the channel, where a higher mass flow rate leads to a higher energy storage efficiency and a lower one leads to a lower thermal response.
Figure 4-7. The influence of mass flow rate on, (a) stored energy fraction, (b) heat transfer rate, and (c) thermal response, versus fractional time.
Table 4-5. Melting times at different mass flow rates in the channel

<table>
<thead>
<tr>
<th>Mass Flow Rate (Kg/min)</th>
<th>Melting Time (minutes)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1875</td>
<td>345</td>
</tr>
<tr>
<td>0.375</td>
<td>230</td>
</tr>
<tr>
<td>0.750</td>
<td>167</td>
</tr>
<tr>
<td>1.500</td>
<td>130</td>
</tr>
</tbody>
</table>

4.4.4 Influence of the Rate of Temperature Change

Figure 4-8 shows the influence of the rate of temperature change (R) at the channel inlet on the output parameters. Figure 4-8a shows that the stored energy fraction increased with a decrease in R. The peak stored energy fraction at R=0.05 C/min was 17% and 40% higher compared to R=0.1 C/min and R=0.2 C/min, respectively. The peak energy storage fractions occurred at FR=0.78, 0.75 and 0.72 for R=0.05, 0.1 and 0.2 C/min, respectively. The final energy storage efficiencies were 40%, 32% and 27% at R=0.05, 0.1 and 0.2 C/min, respectively. Figure 4-8b shows an increase in the heat transfer rate with an increase in R. The peak heat transfer rate at R=0.2 C/min was 92% and 38% higher compared to R=0.05 and 0.1 C/min, respectively. The average heat transfer rates were 76W, 108W and 151W at R=0.05, 0.1 and 0.2 C/min, respectively. Figure 4-8c shows that the thermal response was slower at higher R values. At FR=0.6, the thermal response at R=0.2 C/min was 45% and 90% lower compared to R=0.1 and 0.05 C/min, respectively. At 100% melt time, these differences were reduced to 25% and 50% at R=0.1 and 0.05 C/min, respectively. The melting times for the different cases are listed in table 4-6. The melting time decreased with an increase in R. There was a percentage reduction in the melting time of 25% when R was increased from 0.05 to 0.1 C/min and a reduction of 23% when it was further increased from 0.1 to 0.2 C/min.
As the rate of change in flow temperature is increased, a greater amount of excess thermal energy enters the channel within a specified time interval, which leads to a higher heat transfer rate into the columns and faster melting of the PCM. However, the energy storage rate does not increase proportionally with the excess thermal energy in the channel which leads to a reduction in the energy storage efficiency. The distinguishing feature of thermal regulation at lower R values is the establishment of a region of stability during which the increase in thermal response is minimal (see Figure 4-8c). As the inlet temperature is slowly increased, there is a time period over which there is no significant increase in the thermal response (stable thermal response). This is due to consistently high latent heat storage rates during this specific time period. As the rate of change in temperature is increased, the mismatch between the energy storage rate and the rate of supplied thermal energy grows which leads to a consistent increase in the thermal response at all times. Since thermal regulation is concerned with a stability in the channel temperature, the system performs better at lower R values since the outlet temperature remains within a very narrow range over a considerably large fraction of the total melting time. It should be noted that thermal response as a whole is lower at higher R values. This low thermal response should not be mistaken for better thermal regulation since even a low thermal response at a high R value translates to a high absolute increase in the outlet temperature.
Figure 4-8. The influence of rate of temperature change on, (a) stored energy fraction, (b) heat transfer rate, and (c) thermal response, versus fractional time.
Table 4-6. Melting times at different rates of change in inlet temperature

<table>
<thead>
<tr>
<th>Rate of temperature Change (C/min)</th>
<th>Melting Time (minutes)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05</td>
<td>218</td>
</tr>
<tr>
<td>0.1</td>
<td>162</td>
</tr>
<tr>
<td>0.2</td>
<td>125</td>
</tr>
</tbody>
</table>

4.4.5 Influence of the Blockage Ratio

Figure 4-9 shows the channel configurations at the three considered blockage ratios of 0.4, 0.5 and 0.6. Figure 4-10 shows the influence of these blockage ratio on the output parameters. The results in Figure 4-10a show that there was an increase in the stored energy fraction with an increase in the blockage ratio (BR). The peak stored energy fraction at BR=0.6 was 60% and 22% higher compared to BR=0.4 and 0.5, respectively. The stored energy fraction at 100% melt time at BR=0.6 was similarly 53% and 23% higher compared to BR=0.4 and 0.5, respectively. Figure 4-10b shows that the heat transfer rate increased with an increase in the blockage ratio. The change in heat transfer rate was much higher with the increase in BR from 0.4 to 0.5 as compared to the increase from 0.5 to 0.6. The peak heat transfer rate at BR=0.6 was 3% and 16% higher compared to BR=0.4 and 0.5, respectively. The time averaged heat transfer rates were 96W, 108W and 111W at BR=0.4, 0.5 and 0.6, respectively. Figure 4-10c shows that the thermal response was the slowest at BR=0.5 followed by BR=0.4 and 0.6. At FR=0.6, the thermal response at BR=0.5 was 10% and 28% lower compared to BR=0.4 and 0.6, respectively. The melting times for the three cases are listed in table 4-7. The melting times decreased with an increase in the blockage ratio. The melting time at BR=0.6 was 15% and 2.5% lower compared to BR=0.4 and 0.5, respectively.

The behavior observed in Figure 4-10 can be explained based on the channel configurations for these blockage ratios as shown in Figure 4-9. At a blockage ratio of 0.6, the PCM columns are in contact with the channel walls and there is flow only
through the gaps between the columns in the absence of any gaps between the columns and channel walls. In this configuration (BR=0.6), since the channel width is small, the flow velocity is high (for a constant mass flow rate) and the flow acceleration in the gaps between the columns leads to a high convection heat transfer rate and a very small total melting time for the PCM. Furthermore, since the flow is restricted to only one path through the gaps between the columns, the energy losses are minimized as a greater fraction of the total flow is in close vicinity to the energy storage interface (fluid–column interface). This results in a high energy storage efficiency. As the channel walls are moved away from the columns on either sides with a decrease in the blockage ratio (BR=0.5), there is flow both between the columns and in the gaps between the channel walls and columns. An increased surface area over which heat transfer occurs results in a high heat total heat transfer rate. However, since the channel width is higher than before, there is a greater fraction of the total flow that is farther away from direct contact with the columns. This results in a reduction in the energy storage efficiency. And if the channel walls are moved further away from the columns (BR=0.4), the channel width is increased even more and the flow velocity decreases (for the same mass flow rate in the channel). A reduction in the velocity results in a reduction in convection heat transfer rate and an increase in the PCM melting time. Furthermore, since the flow is even more spread out, a much larger fraction of the total flow remains far from the columns and the energy in this fraction of the flow is not stored in the columns which results in a further decrease in the energy storage efficiency. Even with a high energy storage efficiency at BR=0.6, the thermal response is low. This is because the flow is streamlined as it flows through the mean flow path through the columns, and even though the energy losses are comparatively small, the mean flow reaches the outlet at a higher speed. In contrast, at BR=0.5 and 0.4, there is more flow resistance in the channel and there is no mean flow path as the flow is through both between columns and in the gaps between the channel walls and the columns. This results in a higher flow mixing in the channel which results in a greater temperature drop between the inlet and the outlet. Between BR=0.5 and 0.4, thermal regulation is higher at BR=0.5 as the temperature increases comparatively slower during the latent heat storage period (stable thermal response).
Figure 4-9. Channel configurations at the blockage ratios of (a) 0.4, (b) 0.5, and (c) 0.6.
Figure 4-10. The influence of blockage ratio on, (a) stored energy fraction, (b) heat transfer rate, and (c) thermal response, versus fractional time.
Table 4-7. Melting times at different blockage ratios in the channel

<table>
<thead>
<tr>
<th>Blockage Ratios</th>
<th>Melting Time (minutes)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.4</td>
<td>185.6</td>
</tr>
<tr>
<td>0.5</td>
<td>162</td>
</tr>
<tr>
<td>0.6</td>
<td>158</td>
</tr>
</tbody>
</table>

4.5 Chapter Summary

In this chapter, thermal regulation in a rectangular channel containing PCM-filled thermal energy storage columns was numerically investigated in the presence of gradual changes in the flow temperature. The thermal energy storage in the PCM columns when the channel flow temperature is gradually increased, and the thermal energy discharge from the PCM columns when the channel flow temperature is gradually decreased have both been investigated numerically. The numerical results showed similar trends for the PCM melting and solidification cases. The thermal response at the channel outlet was the same in both melting and solidification cases. There was an initial change in the outlet temperature until the PCM reached the phase transition temperature after which the change in outlet temperature was largely suppressed due to a consistently high latent heat exchange rate between the columns and the channel fluid. As the phase transition fraction approached 1, there was a gradual change in the outlet temperature. When there is a gradual change in the inlet temperature, the thermal response becomes stable during latent heat exchange in comparison to the steady increase in the thermal response when the inlet temperature is kept constant at a high temperature (Chapter 3). This difference in the thermal response highlights the importance of a parametric study in the current chapter even though the flow and geometric parameters that are considered are similar.

The flow parameters that include the mass flow rate and the time rate of change in the inlet temperature affected thermal energy storage in the PCM filled columns. At low
mass flow rates, the thermal response at the outlet was low and there was a slower increase in the thermal response during the latent energy exchange. For example, the thermal response at a mass flow rate of 0.1875 Kg/min was 80% lower than that at a mass flow rate of 1.5 Kg/min. The heat transfer rates between the columns and the channel fluid were relatively smaller which resulted in smaller energy storage/discharge efficiencies. The peak heat transfer rate at 0.1875 Kg/min was 160% lower than that at 1.5 Kg/min. The heat transfer and thermal response results in this study were consistent with the results of the preceding study (Chapter 3). However, there was a difference in the energy storage efficiency. When the inlet temperature is kept constant (Chapter 3), there is no significant difference in the energy storage efficiency. However, if the inlet temperature is slowly changed as in the present study, there is an increase in the efficiency when the mass flow rate is increased.

At low rates of change in the inlet temperature, the heat transfer rates between the channel fluid and the columns were small but the energy exchange efficiency was higher. The thermal response at the outlet was also found to increase at a slower rate during latent heat exchange in comparison to the steady increase in the thermal response at higher rates of change in inlet flow temperature. For example, the peak heat transfer rate at a temperature change rate of 0.05 C/min was 95% lower than that at 0.2 C/min. The energy storage efficiency was 50% higher at 0.05 C/min, however. The heat transfer rate and energy storage efficiency results were consistent with the results of Chapter 3 where the inlet temperature was kept constant. The thermal response results are also similar in that the thermal response was lower when the inlet temperature was higher (see Chapter 3) and when the rate of change in the inlet temperature was higher (current Chapter). However, there was a clear stability in the thermal response during latent heat exchange only at lower temperature change rates, which was not observed in the results of Chapter 3.

The investigated geometric parameter was the blockage ratio. The thermal regulation and energy exchange efficiency was found to be influenced by the proximity of PCM columns to the channel walls. When the columns were touching the channel walls (BR=0.6), the energy exchange efficiency and the heat transfer rate were found to be high
but the rapid thermal response at the outlet indicated a faster change in the outlet temperature. As the channel walls were moved away from the columns (BR=0.5), the energy exchange efficiency was found to decrease but the thermal response was smaller and temperature regulation was spread out over a longer time period. And finally, when the channel walls were moved even further away from the columns (BR=0.4), the energy efficiency became much lower and there was little thermal regulation in the channel which resulted in a consistent change in the outlet temperature.

Thermal regulation in the channel, assessed by the outlet temperature response, was highest at a mass flow rate of 0.1875 Kg/min when the time rate of change in the inlet temperature was 0.05 C/min and when the blockage ratio in the channel was 0.5. However, the energy storage efficiency was highest at a mass flow rate of 1.5 Kg/min when the rate of change in the inlet temperature was 0.05 C/min and at a blockage ratio of 0.5. The influences of all three parameters are summarized in table 4-8. Even with the results of the parametric study being consistent with the results of the preceding study (Chapter 3), some significant differences were observed which makes the current results a great resource in the development of a potential design for the photobioreactor where there is a gradual change in the temperature.

Table 4-8. Observations of the influence of various parameters on the thermal regulation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Observation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass Flow Rate</td>
<td>Low thermal response at low mass flow rates</td>
</tr>
<tr>
<td>Rate of change in inlet temp</td>
<td>Slow change in thermal response and a high energy storage efficiency at low temperature change rates</td>
</tr>
<tr>
<td>Blockage Ratio</td>
<td>Slow change in thermal response at BR=0.5</td>
</tr>
</tbody>
</table>
Chapter 5

5 Conclusions and Recommendations

The conclusions of the works in chapters 2-4 are discussed in this chapter and recommendations for future works are detailed.

5.1 Chapter 2: Numerical Modeling

In this chapter, a numerical model to characterize flow and thermal behavior in a rectangular channel containing PCM-filled thermal energy storage columns was developed. The methodology can be summarized as:

(1) A physical model for the problem was defined. The physical model consisted of a rectangular channel containing PCM-filled columns. The columns were placed vertically in a staggered arrangement along the channel. There were three regions in the physical model: channel fluid, PCM and columns. The channel fluid (water) was circulated through the channel at a constant mass flow rate. The columns were thin walled (copper) tubes. The PCM (Rubitherm-26) was enclosed within these columns.

(2) A mathematical model to describe the problem was developed. The fundamental flow equations [90] were simplified with the assumptions of laminar flow in the channel, constant thermophysical properties, incompressible flow and Newtonian fluids. The simplified flow equations were modified for each region as follows:

a. Channel Fluid: A Boussinesq source term was added to the momentum equation to model buoyancy effects in the channel.

b. PCM: A Boussinesq source term was added to the momentum equation to model buoyancy effects. The enthalpy-porosity method developed by Voller and Prakash [64] was used to model phase change in the PCM. This method describes a mushy (porous) region where the PCM is partially liquid (porous region). The mushy zone is therefore characterized by the liquid fraction. The momentum and energy equations were modified to
account for velocity and enthalpy in the mushy zone. The Darcy source term was added to the momentum equation to limit the velocity in regions where the liquid fraction is very small such that the velocity is forced to zero in the fully solid regions. An enthalpy source term was added to the energy equation to account for the enthalpy of phase change during phase transition.

c. Columns: The energy equation was simplified to the transient heat conduction equation for a solid.

(3) The mathematical equations were discretized using the Finite Volume Method (FVM). The volume integrals in the advective and diffusive terms were converted to surface integrals using the divergence theorem. The surface integrals were subsequently converted to algebraic sums over cell faces using the gauss theorem. The flow variables at cell faces were interpolated using the first order upwind scheme. The face gradients were interpolated from the adjacent cell center gradients. The source terms were discretized using the mean value theorem. The first order accurate Euler scheme was used to resolve the time integrals. The final form of the algebraic formulation for a flow variable was of the form, $A\bar{x} = \bar{b}$ which is a set of linear algebraic equations where each equation corresponds to one control volume (cell) in the grid.

(4) The boundary conditions in the channel were defined. These included the constant mass flow rate uniformly mapped over the channel inlet, a fully developed flow condition at the outlet, a zero-heat flux and no slip conditions at the channel walls, a no slip condition at the column walls, and a convection boundary condition at the free (top) surface of the channel. The channel inlet temperature condition was a constant temperature that was higher than the initial system temperature. This temperature condition was used in chapter 3 but a time varying temperature condition was used in chapter 4.

(5) OpenFOAM was used as the computational platform to solve the algebraic equations using a set of defined linear solvers. A convergence criterion was
outlined to limit the iterative solution process to a finite number of steps where the solution residual (for a flow variable) is gradually reduced until it falls below a specified tolerance. The pressure-velocity coupling was achieved using the PISO algorithm which corrects the velocity field a specified number of times in one time step. The SIMPLE algorithm was also implemented which goes through the entire solution process a specified number of times in a time step. Within each iteration of the SIMPLE algorithm, the flow variables were underrelaxed by a specified amount to achieve solution stability and improve convergence. The channel fluid and column wall regions were linked by equating the heat flux leaving one region and that entering the other. The same formulation was used for the column wall and PCM regions.

(6) A convergence study was performed to investigate solution convergence. The solution was found to converge with decreasing grid element and time step sizes. The numerical model was validated against the experimental data of Toxopeus [43]. The column wall temperature at a specific point was used as the validation metric. Aside from an initially large error over a very small fraction of the total simulation time, the numerical results were in very close agreement with the experimental data.

5.2 Chapter 3: Influence of flow and geometric parameters on thermal energy storage in PCM-filled columns

In this chapter, flow behavior and heat transfer in channels with PCM-filled thermal energy storage columns were numerically investigated using the numerical model that was developed in chapter 2. The flow and thermal behavior in the channel, the heat transfer through the columns and the melting behavior of PCM were first investigated. This was followed by a parametric study to derive the optimal configuration that maximized thermal regulation in the channel.
5.2.1 Characterization of flow and thermal behavior

The flow and thermal behaviors in the channel in the presence of PCM-filled columns were numerically characterized. The channel inlet temperature was higher compared to the initial system temperature. At a Reynolds number of Re=200, the channel fluid was found to accelerate as it passed over the columns such that there was a steady increase in the mean flow velocity along the channel. There was flow separation for the flow over the columns with a separation angle of around 100 degrees. The backflow velocities were found to be higher in the wake of the downstream columns. At Re=200, there was no vortex formation in the channel. There was a consistent drop in the channel flow temperature across the columns, with the maximum temperature drop, relative to the inlet temperature, occurring at the channel outlet.

The heat transfer between the channel fluid and columns was investigated. There was a rapid increase in the total heat transfer rate to the columns corresponding with the heated channel fluid from the inlet coming into contact with the columns. In response to the increase in the heat transfer rate, there was an increase in the channel wall temperature. The heat transfer rate decreased at a rapid rate following the peak value. The heat transfer rate eventually approached zero as the channel wall temperature began to stabilize as it approached the hot channel fluid temperature (inlet temperature).

The melting behavior of the PCM in vertical columns was investigated. It was found that a solid-liquid interface forms after the onset of melting and, for a considerable amount of time, this interface moves radially away from the column walls as heat is conducted through the liquid PCM region. When a considerable amount of the PCM had melted, natural convection in the liquid PCM was observed where the heated liquid PCM close to the column walls moved to the top of the column. The accumulation of the PCM at the top pushed the interface in the top regions of the columns way from the column walls at a faster rate compared to the bottom regions of the columns. This resulted in the interface merging at a point at the top of the columns and melting occurred in a top-down manner after that where the liquid PCM filled the top region of the columns and slowly made its way down until the entirety of the PCM I the column had melted.
5.2.2 Optimization of the flow and geometric parameters to maximize thermal regulation

A parametric study was performed to derive the optimal configuration that maximizes thermal regulation in the channel. Seven parameters were varied in the parametric study: flow Reynolds number (Re), channel inlet temperature, horizontal offset between columns ($S_L$), lateral offset between columns ($S_T$), column aspect ratio (AR), and the columns shape. The influence of each of these parameters was assessed using three output parameters: stored energy fraction, heat transfer rate and the thermal response.

The flow Reynolds number was found to influence the energy storage rate in the columns and the thermal response. The stored energy fraction increased monotonically with an increase in Re. The thermal response was slower at smaller values of the Re. The convection heat transfer rate was found to be higher at higher values of the Reynolds number due to the higher flow velocities around the columns. At higher flow velocities, however, the channel flow was found to reach the outlet at a faster speed which resulted in an increase in the outlet temperature much earlier and at a faster rate compared to low Re flows.

The heat transfer rate was found to increase proportionally with an increase in the inlet temperature but the energy storage efficiency was lower at higher channel inlet temperatures. The heat transfer rate was higher due to higher temperature gradients at the channel fluid – column interface. The increase in thermal energy in the channel at higher channel inlet temperatures was found to not result in a proportional increase in the energy storage, primarily due to there being a fixed mass of the storage medium, which resulted in a lower energy storage efficiency.

The geometric placement of the columns was found to influence the heat transfer rate to the columns. The heat transfer rate was highest when the columns were placed at some lateral distance away from the channel walls such that there was flow between the columns and also in the gaps between the channel walls and the columns ($S_T=0.5D$). The horizontal offset of $S_L=1.5D$ was found to have the highest heat transfer rate due to flow
acceleration between the gap regions. There were no observed differences in either the energy storage efficiency or thermal response between the different offset cases.

The increase in the aspect ratio was found to result in an increase the heat transfer rate and a decrease in the thermal response at the outlet. The increase in the heat transfer rate was found to be due to an increase in the total surface area of the columns (higher surface area per volume ratio at higher AR values). The energy storage efficiency was lower at higher AR values, however. This was found to be the result of a smaller column circumference at higher values of AR. The interface length over which heat transfer occurs around a column is equal to the column circumference. A reduction in the circumference means that the length over which heat transfer occurs decreased and a lower amount of the thermal energy in the channel was stored in the columns.

The influence of column shape on thermal energy storage was less pronounced compared to the other geometric parameters. There was only a marginal increase in the heat transfer rate to the columns due to higher flow resistance and flow mixing in the channel. An optimal configuration was proposed based on the parametric analysis. In this optimal configuration, the flow Reynolds number was 50, the horizontal offset between columns was equal to 1.5D, the lateral offset between columns was equal to 0.5D, the column aspect ratio was 10 and the column shape was circular.
5.3 Chapter 4: Thermal Response of a channel flow with PCM-filled thermal energy storage subjected to varying temperatures

In this chapter, thermal regulation in the rectangular channel in the presence of a varying flow temperature was numerically investigated. This was followed by a parametric study to determine the effects of various parameters on thermal energy storage in the channel.

5.3.1 Thermal regulation in the presence of a varying flow temperature

Thermal energy storage during a steady increase in the channel inlet temperature and thermal energy discharge in the presence of a steady decrease in the channel inlet temperature were both investigated. It was found that the thermal response at the outlet was the same in both cases. There was a steady change in the outlet temperature during the sensible heat exchange period after some time delay. The outlet temperature change was largely suppressed shortly after the onset of latent heat exchange. This corresponded with the time during which the PCM phase change fraction increased from around 0.25 to 0.95. During this time, the latent heat storage/discharge increased approximately linearly and thermal regulation in the channel was consistently high. As the phase change fraction approached a value of 1, the increase in latent heat storage/discharge approached zero and the energy exchange between the PCM and channel fluid was limited to sensible heat exchange. In this phase, in the absence of significant thermal regulation, there was a steady change in the outlet temperature in response to the change in the inlet temperature. At any specific time in the latent heat exchange period, there was a steady increase in the thermal response along the channel. Near the channel inlet, the change in temperature closely followed the change in inlet temperature. And near the channel outlet, the temperature change was largely suppressed due to the flow experiencing continuous energy exchange across the columns.
5.3.2 Parametric study to derive the optimal channel configuration

A parametric study was performed to derive the optimal channel configuration to maximize thermal regulation in the channel. The influence of mass flow rate, the rate of change in inlet flow temperature and the blockage ratio were investigated in the parametric study. Thermal energy storage in the channel was assessed using three output parameters: stored energy fraction, heat transfer rate and the thermal response.

The energy storage efficiency and heat transfer rate were found to increase with the mass flow rate. The thermal response was however much slower at lower mass flow rates. At higher mass flow rates, the convection heat transfer rate was higher, and consistently high convection heat transfer rates resulted in a high fraction of the total available thermal energy in the channel to be stored in the PCM, which resulted in an increase in energy storage efficiency. At high mass flow rates however, energy storage occurred over a small time period as the flow accelerated through the columns to reach the outlet within small time periods. This led to an increase in the energy losses and an increase in the thermal response at the outlet.

There was a decrease in the energy storage efficiency with an increase in the rate of change in the flow temperature. There was an increase in the heat transfer rate with an increase in the rate of change in flow temperature. As the rate of change in flow temperature was increased, a greater amount of excess thermal energy entered the channel within a specified time interval, which led to a higher heat transfer rate into the columns and faster melting of the PCM. However, due to a finite mass of the storage medium (PCM), the greater amount of thermal energy in the channel at higher flow temperature cases could not be stored in the PCM at consistently high rates. This led to a decrease in the overall energy storage efficiency at higher rates of change in the flow temperature. The thermal response at higher rates of change in flow temperature was found to increase consistently with time as opposed to lower rates of change in temperature where there was a region of time when the thermal response stayed approximately constant. As the rate of change in temperature was increased, the mismatch between the energy storage rate and the rate of supplied thermal energy grew, which led to a consistent increase in the thermal response at all times.
The energy storage efficiency and heat transfer rate were found to increase with an increase in the blockage ratio. At higher blockage ratios, the channel fluid was in close proximity to the columns which resulted in an increase in the energy storage efficiency and heat transfer rate. As the blockage ratio was increased, the gaps between the columns and channel walls increased which resulted in a larger fraction of the channel fluid to be farther away from the columns. This led to a decrease in the total heat transfer rate and energy storage efficiency. The increased flow resistance at moderately high blockage ratios (small gaps between channel walls and columns) resulted in a higher thermal regulation in the channel.

An optimal configuration was proposed based on the parametric study to maximize thermal regulation in the channel while maintaining a sufficient energy storage efficiency. In this optimal configuration, the mass flow rate was 0.375 Kg/min, the rate of change in flow temperature was 0.05 C/min and the blockage ratio was 0.5.

5.4 Contributions

This thesis research is focused on a novel design for a photobioreactor with an integrated latent heat-based thermal energy storage system with the purpose of regulating temperature in the photobioreactor channel. The flow and thermal behaviors in a channel with such an integrated energy storage system have only recently been characterized by Toxopeus [3] who experimentally investigated flow over circular columns in a rectangular channel. The present research focuses on the numerical investigation of the thermo-fluid behavior in a channel with PCM-filled thermal energy storage columns. Heat transfer in a phase change material and in flow systems have been previously studied in isolation but conjugate heat transfer in an integrated Multiregion system such as the one in the present study has not been numerically investigated before. Therefore, the development of a numerical model to characterize flow and heat transfer in such a system and to study the thermos-fluid processes involved in it are the main contributions of the present research to scientific knowledge.
The results of this study highlight some interesting relations between thermal energy storage in PCM-filled columns in a rectangular channel and various flow and geometric parameters such as the flow rate, geometric arrangement of columns, gap and blockage ratios in the channel and the columns shape. The observation that almost all of these parameters worked in conjugation to produce different numerical results indicates to future researchers continuing this research to test additional configurations to optimize thermal regulation.

5.5 Future Recommendations

This thesis work is a significant step in the numerical characterization of the complex thermo-fluid behavior in channels with PCM-filled thermal energy storage columns. In addition, significant work on the influence of various flow and geometric parameters on thermal energy storage in the presence of both a constant and a varying flow temperature has been detailed in this thesis. There are aspects of this work that can be expanded upon:

1. Implement a radiation model for heating the photobioreactor channel

Photobioreactors placed under direct sunlight experience temperature variations due to changes in the light intensity over the 24-hour cycle. The light that is not used by the microalgae is converted to thermal energy that heats up the photobioreactor. Therefore, a radiation model that takes into account the varying light intensity over the complete operational cycle of the photobioreactor would provide the most accurate heating condition in the photobioreactor.

2. Expand the numerical model to include microalgae

Since the integration of latent heat based thermal energy storage columns in a photobioreactor channel has been shown to thermally regulate the photobioreactor channel, the next step would be to numerically study the effects of thermal regulation and flow behavior on microalgae growth and health.

3. Investigate the channel design to incorporate additional columns
In the present study, only one row in the staggered arrangement of PCM-filled columns was considered. More columns can be added with additional rows of columns and/or with additional columns along the channel. Such design modifications should be investigated for a complete understanding of thermal regulation in the channel containing a staggered arrangement of columns.

There are many other iterations of the numerical study that would constitute valuable additions to the state of science.
References


[58] L.A. Diaz and R. Viskanta, “Visualization of the solid-liquid interface morphology formed by natural convection during melting of a solid from below,”


Appendix A: Thermal Energy Discharge

Figure A-1. The influence of mass flow rate on thermal energy discharge. The (a) stored energy fraction, (b) heat transfer rate, and (c) thermal response, versus fractional time.
Figure A-2. The influence of rate of change in flow temperature on thermal energy discharge. The (a) Stored energy fraction, (b) heat transfer rate, and (c) thermal response, versus fractional time.
Figure A-3. The influence of rate of blockage ratio on thermal energy discharge. The (a) Stored energy fraction, (b) heat transfer rate, and (c) thermal response, versus fractional time.
Curriculum Vitae

Name: Sameed Akber

Post-secondary Education and Degrees:
- University of Toronto, Toronto, Ontario, Canada, 2015-2019 BSc.
- The University of Western Ontario, London, Ontario, Canada, 2020-2022 MESc.

Related Work Experience:
- Teaching Assistant, The University of Western Ontario, 2020-2022

Publications: