Department of Mechanical Engineering

SIMULATION AND ANALYSIS OF PHASE CHANGE MATERIALS FOR BUILDING TEMPERATURE CONTROL

Author: OLUKAYODE A. OBITAYO

Supervisor: Prof. John Counsell

A thesis submitted in partial fulfilment for the requirement of the degree

Master of Science

Sustainable Energy: Renewable Energy Systems and the Environment

2011
Copyright Declaration

This thesis is the result of the author’s original research. It has been composed by the author and has not been previously submitted for examination which has led to the award of a degree.

The copyright of this thesis belongs to the author under the terms of the United Kingdom Copyright Acts as qualified by University of Strathclyde Regulation 3.50. Due acknowledgement must always be made of the use of any material contained in, or derived from, this thesis.

Signed: Obitayo Olukayode A.  
Date: 9/92011
ABSTRACT

Buildings are designed for the sole purpose of maintaining conducive living standards for the occupants. Their thermal mass plays a vital role in minimising the fluctuations of indoor temperatures. PCM can be used to provide both temperature regulation and additional thermal mass to new and existing structures. This provides lightweight buildings with the advanced thermal properties of their counterparts as well as savings in the amount of energy required to maintain indoor comfort levels. This paper describes a holistic approach to the modelling of the non-linear thermal phase change process of a PCM via volumetric heat capacity discontinuity method in ESL simulation language. Effects of diurnal temperature on the PCM were studied for Glasgow (55N) weather conditions on a school building case study that adopts the CAB building systems. The knowledge for these methods has been transferred from the design of a discontinuous multivariable non-linear aircraft missile. The objectives of the study are to evaluate critically the models and framework relevant to the phase change process, develop an ELS computational model to simulate the sensible and latent regions of a PCM, apply the model to a building case study and formulate recommendations for the implementation of PCM ceiling tiles in buildings construction. The findings from the research show reduced indoor temperature achieved between 0.5K and 1.5K when PCM ceiling tiles was incorporated in the building. Maximum daily storage of a PCM is best achieved with the melting temperature close to the average room temperature. Recommendations for PCM integration into buildings were also proffered based on the results obtained from the simulation.
ACKNOWLEDGMENTS

Firstly, I would like to thank Almighty God for his provision, protection and guidance throughout my course and the completion of the project.

Secondly, I wish to express my gratitude to my supervisor Prof. John Counsell for the support and invaluable advice he proffered during the course of this research. He not only ensured I was going in the right direction but he also challenged me to do a lot of personal thinking.

Thirdly, I would also like to thank Joseph Brindley, for the generous help and support he gave me whilst trying to familiarise myself with the ESL programming phase of the research. Despite the fact that he was very busy writing his PhD thesis, he always made time to go over the model with me.

Finally, I would like to express my deepest sincere gratitude to my parents Mr & Mrs T.T. Obitayo for their glorious support during my study at the University of Strathclyde. Their regular weekly chat with me over the phone made the year feel shorter than it actually is. Without them I would not have been here in the first place. Their words of encouragement were indispensable to me and kept me going throughout my period of study.

To all my former course mates and the friends I met in Glasgow, the sky is not the limit; it’s just the very beginning.
# TABLE OF CONTENTS

Abstract .............................................................................................................................................. i
Acknowledgment ................................................................................................................................. ii
List of Figures ..................................................................................................................................... iii
List of Table ........................................................................................................................................ v
Nomenclature ........................................................................................................................................ vi

Chapter One: INTRODUCTION
1.1 Background ..................................................................................................................................... 1
1.2 Classification of Phase Change materials ......................................................................................... 4
1.3 Phase change materials process in building construction ................................................................. 6
1.4 Research Focus .................................................................................................................................. 7
1.5 Research aim and Objectives ............................................................................................................. 8
1.6 Outline Structure .............................................................................................................................. 9

Chapter Two: LITERATURE REVIEW
2.1 Introduction ....................................................................................................................................... 11
2.2 Phase Change Models ....................................................................................................................... 11
2.3 Development of computational models ............................................................................................. 13
2.4 Conclusion ...................................................................................................................................... 16

Chapter Three: RESEARCH METHODS
3.1 Introduction ....................................................................................................................................... 17
3.2 The Heat Transfer Process ............................................................................................................... 17
  3.2.1 Conduction ............................................................................................................................... 17
  3.2.2 Convection ............................................................................................................................... 18
  3.2.3 Radiation ................................................................................................................................ 19
3.3 The Specific Heat Capacity of the PCM ............................................................................................ 22
  3.3.1 Sensible Heat Region ............................................................................................................... 22
  3.3.2 Latent Heat Region .................................................................................................................. 23
3.4 Numerical Methods for modelling Phase transformation .................................................................... 24
  3.4.1 Effective Heat Capacity Method .............................................................................................. 25
  3.4.2 Enthalpy Method ..................................................................................................................... 26
  3.4.3 Heat Source Method ............................................................................................................... 27
3.5 Discontinuity Analysis of the Phase change process .......................... 28
3.6 ESL Methodology............................................................................ 29

Chapter Four: BUILDING MODEL CASE STUDY
4.1 Introduction ................................................................................. 33
4.2 Description of Building Model....................................................... 33
  4.2.1 Definition of the temperature rates ........................................... 31
4.3 Simulation Cases .......................................................................... 37
  4.3.1 Case one: Heater ONLY without PCM .................................... 34
  4.3.2 Case two: HVAC condition without PCM ............................... 39
  4.3.3 Case Four: HVAC with Varied PCM melting temperature ....... 39

Chapter Five: RESULTS AND DISCUSSIONS
5.1 Introduction .................................................................................. 36
5.2 Results for Case one: Heater only without PCM ........................... 41
5.3 Results for Case Two: HVAC system without PCM ....................... 42
5.4 Results for Case Three: HVAC system with varied PCM melting temperature ......................................................... 43
  5.4.1 Results for RT21 PCM .............................................................. 43
  5.4.2 Results for SP22 A17 PCM ....................................................... 51
5.4 Discussion ...................................................................................... 58
5.5 Summary of results........................................................................ 61

Chapter Six: CONCLUSION AND RECOMMENDATION
6.1 Conclusion and Recommendation .................................................. 62
6.2 Suggestion for future work ............................................................. 63

References .......................................................................................... 66

Appendix A
Modules contained in the ESL code .................................................... 72

Appendix B
Phase Change Material Datasheet............................................................ 73
LIST OF FIGURES

Chapter one

Fig 1.0: Residential Site Energy Consumption by end use 1
Fig 1.1: Trombe Wall system schematics 2
Fig 1.2: PCM transformation phases 3
Fig 1.3: Classification of phase change materials 5

Chapter Three

Fig 3.0: Rate of temperature change in heavy weight and lightweight buildings 19
Fig 3.1: Idealised curve for Enthalpy as a function of Temperature for PCM 20
Fig 3.2: Practical curve for Enthalpy as a function of Temperature for PCM 21
Fig 3.3: Sensible Heat Regions of Phase change process 22
Fig 3.4: Latent Heat Region of Phase change process 23
Fig 3.5: Effective heat capacity method for non-linear 1-D element 26
Fig 3.6: ESL Information flow diagram for the PCM building simulation 30
Fig 3.7: VCH Discontinuity Flow diagram 27
Fig 3.8: VCH discontinuity modelling excerpt 31
Fig 3.9: Rate of change of PCM temperature code excerpt 32

Chapter Four

Fig 4.0: Project design for Clydeview Academy 33
Fig 4.1: Schematic of Building Model Energy flow 34
Fig 4.2: Building model wall Section 32
Fig 4.3: Heat flow through PCM ceiling Tile 34

Chapter Five

Fig 5.0: Weekly comfort temperature Heater ONLY without PCM and HVAC system 41
Fig 5.0a: Weekly comfort temperature without PCM 42
Fig 5.0b: Heat and cooling loads for the building without PCM 42
Fig 5.0c: Hourly comfort temperature with heating inset for control case. 43
Fig 5.1a: Hourly comfort temperature with control case (No PCM) and RT21 PCM (T_m = 21°C) 43
Fig 5.1b: RT21 PCM temperature (T_m = 21°C) 44
Fig 5.1c: Heating and cooling loads for control case (No PCM) and RT21 PCM (T_m = 21°C) 44
Fig 5.2a: Hourly comfort temperature with control case (No PCM) and RT21 PCM ($T_m = 23^\circ C$)  
Fig 5.2b: RT21 PCM temperature ($T_m = 23^\circ C$)  
Fig 5.2c: Heating and cooling loads for control case (No PCM) and RT21 PCM ($T_m = 23^\circ C$)  
Fig 5.3a: Hourly comfort temperature with control case (No PCM) and RT21 PCM ($T_m = 25^\circ C$)  
Fig 5.3b: RT21 PCM temperature ($T_m = 25^\circ C$)  
Fig 5.3c: Heating and cooling loads for control case (No PCM) and RT21 PCM ($T_m = 25^\circ C$)  
Fig 5.4a: Hourly comfort temperature with control case (No PCM) and RT21 PCM ($T_m = 27^\circ C$)  
Fig 5.4b: RT21 PCM temperature ($T_m = 27^\circ C$)  
Fig 5.4c: Heating and cooling loads for control case (No PCM) and RT21 PCM ($T_m = 27^\circ C$)  
Fig 5.5a: Hourly comfort temperature with control case (No PCM) and RT21 PCM ($T_m = 30^\circ C$)  
Fig 5.5b: RT21 PCM temperature ($T_m = 30^\circ C$)  
Fig 5.5c: Heating and cooling loads for control case (No PCM) and RT21 PCM ($T_m = 30^\circ C$)  
Fig 5.6a: Hourly comfort temperature with control case (No PCM) and SP22A17 PCM ($T_m = 21^\circ C$)  
Fig 5.6b: SP22 A17 PCM temperature ($T_m = 21^\circ C$)  
Fig 5.6c: Heating and cooling loads for control case (No PCM) and SP22A17 PCM ($T_m = 21^\circ C$)  
Fig 5.7a: Hourly comfort temperature with control case (No PCM) and SP22A17 PCM ($T_m = 23^\circ C$)  
Fig 5.7b: SP22 A17 PCM temperature ($T_m = 23^\circ C$)  
Fig 5.7c: Heating and cooling loads for control case (No PCM) and SP22A17 PCM ($T_m = 23^\circ C$)  
Fig 5.8a: Hourly comfort temperature with control case (No PCM) and SP22A17 PCM ($T_m = 25^\circ C$)  
Fig 5.8b: SP22 A17 PCM temperature ($T_m = 25^\circ C$)  
Fig 5.8c: Heating and cooling loads for control case (No PCM) and SP22A17 PCM ($T_m = 25^\circ C$)  
Fig 5.9a: Hourly comfort temperature with control case (No PCM) and SP22A17 PCM ($T_m = 27^\circ C$)  
Fig 5.9b: SP22 A17 PCM temperature ($T_m = 27^\circ C$)  
Fig 5.9c: Heating and cooling loads for control case (No PCM) and SP22A17 PCM ($T_m = 27^\circ C$)  
Fig 5.91a: Hourly comfort temperature with control case (No PCM) and SP22A17 PCM ($T_m = 30^\circ C$)  
Fig 5.91b: SP22 A17 PCM temperature ($T_m = 30^\circ C$)  
Fig 5.9c: Heating and cooling loads for control case (No PCM) and SP22A17 PCM ($T_m = 27^\circ C$)  
Fig 5.92a: Annual Heat flow through the RT21 PCM  
Fig 5.92b: Annual Heat flow through the SP22 A17 PCM
# LIST OF TABLES

<table>
<thead>
<tr>
<th>Table</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>Qualities of Organic and Inorganic compounds</td>
<td>4</td>
</tr>
<tr>
<td>4.0</td>
<td>HVAC specifications</td>
<td>35</td>
</tr>
<tr>
<td>4.2</td>
<td>Building model wall Section</td>
<td>36</td>
</tr>
<tr>
<td>4.3</td>
<td>Heat flow through PCM ceiling Tile</td>
<td>38</td>
</tr>
<tr>
<td>4.1</td>
<td>Rubitherm PCM properties</td>
<td>38</td>
</tr>
<tr>
<td>4.2</td>
<td>Selected periods for latent for simulation analysis.</td>
<td>40</td>
</tr>
</tbody>
</table>
## NOMENCLATURE

### Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PCM</td>
<td>Phase Change Material</td>
</tr>
<tr>
<td>CAB</td>
<td>Climate adaptive building</td>
</tr>
<tr>
<td>ESL</td>
<td>European Simulation Language</td>
</tr>
<tr>
<td>VHC</td>
<td>Volumetric heat capacity (J·m⁻³·K⁻¹)</td>
</tr>
<tr>
<td>$T_{m1}$</td>
<td>Melting Temperature (°C)</td>
</tr>
<tr>
<td>$T_{m2}$</td>
<td>Temperature at which material is completely liquid (°C)</td>
</tr>
<tr>
<td>$C_{ps}$</td>
<td>Specific Heat Capacity in solid state (kJ/kg K)</td>
</tr>
<tr>
<td>$C_{pl}$</td>
<td>Specific Heat Capacity in liquid state (kJ/kg K)</td>
</tr>
<tr>
<td>$k_s$</td>
<td>Thermal Conductivity in solid state (W/m²K)</td>
</tr>
<tr>
<td>$k_l$</td>
<td>Thermal Conductivity in liquid state (W/m²K)</td>
</tr>
</tbody>
</table>

### Subscripts

<table>
<thead>
<tr>
<th>Subscript</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>s</td>
<td>surface</td>
</tr>
<tr>
<td>e</td>
<td>external</td>
</tr>
<tr>
<td>i</td>
<td>internal</td>
</tr>
<tr>
<td>si</td>
<td>internal surface</td>
</tr>
<tr>
<td>se</td>
<td>external surface</td>
</tr>
<tr>
<td>o</td>
<td>outside</td>
</tr>
<tr>
<td>ft</td>
<td>furniture</td>
</tr>
<tr>
<td>a</td>
<td>air</td>
</tr>
<tr>
<td>l</td>
<td>liquid</td>
</tr>
<tr>
<td>s</td>
<td>solid</td>
</tr>
</tbody>
</table>

### Greek symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda$</td>
<td>Latent Heat of Fusion (kJ/kg)</td>
</tr>
<tr>
<td>$\rho_s$</td>
<td>Density in solid state (kg/m³)</td>
</tr>
<tr>
<td>$\rho_l$</td>
<td>Density in liquid state (kg/m³)</td>
</tr>
<tr>
<td>$\Delta$</td>
<td>Differences values</td>
</tr>
<tr>
<td>$\nabla$</td>
<td>Differential operator</td>
</tr>
</tbody>
</table>
CHAPTER ONE

INTRODUCTION

1.1 BACKGROUND:

One of the fundamental requirements of any home or office is to have an effective temperature control system. A system responsible for maintaining indoor temperatures between the 21°C to 23°C comfort range throughout the year. According to the Chartered Institution of Building Engineers [1] standards, ‘space heating systems should be effectively controlled so as to ensure the efficient use of energy by limiting the provision of heat energy’. Similar conditions are applicable to space cooling during the summer months. Maintaining conducive human comfort in buildings requires a great deal of electrical energy. An estimated 54% of the energy consumption in a residential building is utilised for space heating and cooling [2]. Future global growth in population would tend to increase energy demands. Control systems widely adopted for maintaining indoor comfort are broadly classified as heating and ventilation control (HVAC) systems. These systems are the prime contributors to high energy demands in buildings.

Fig 1.0: Residential Site Energy Consumption by end use [2]
Temperature fluctuation inside buildings can be reduced by the use of thermal mass as a form of passive energy store [3]. The large thermal mass of a concrete wall stores up heat energy during the day and releases it at night, thereby reducing the undulation of perceived indoor temperatures [4]. This provides a less expensive means of building temperature regulation and shift in energy demand to off-peak periods when utility bills are much lower. Application of large thermal masses in buildings for absorbing and releasing heat energy can be seen in the Trombe wall system (Fig 1.1). A reduction in peak day temperatures by as much as 3-5 °K is achievable [48]. However, a building energy storage capacity can be further enhanced by incorporating phase change materials (PCM) into the system configuration.

PCMs are compounds which melt and solidify at narrow temperature intervals and in doing so absorb, store and later release large amounts of heat energy. This energy is known as latent heat energy and occurs during the phase transformations at a fairly constant material temperature whereas sensible heat energy is dependent on the specific heat capacity of the material and the temperature change [5]. The difference in magnitude between sensible and latent heat can be demonstrated by comparing the sensible heat energy of concrete (1.0 kJ/kgK) to the latent heat energy of Calcium Chloride (190.0kJ/kg) during phase change [6]. PCMs therefore possess much greater thermal energy storage property than traditional construction materials and research into ways of harnessing this unique feature would be most beneficial in reducing global environmental pollution via reduced energy demand in buildings.
As shown above in figure 1.2, PCMs can transform their physical structure from solid to liquid or from liquid to gas or vice versa depending on whether the process is an exothermic (release of heat) or endothermic (absorption of heat) reaction. The amount of heat energy stored depends on the melting temperature of the PCM, the temperature range at which it melts and the latent heat capacity per unit area [7].

Solidification can be defined as a process when a fluid is transformed into a solid state whereas fluidification is the reverse process [8]. The Deposition and freezing processes (shown in Fig 1.2) are both examples of the former while sublimation and melting are examples of the latter. The liquid to gas and solid to gas transformation are not practical for use as thermal storage as high pressure and volume changes generated during transformation to the gaseous state are unpredictable and difficult to encapsulate [9-11], hence they are not considered in this paper. Water/Ice PCMs are the most effective and readily available types, but with the fixed freezing temperature of 0°C, they are highly unsuitable for most energy storage systems [12]. Generally, only PCMs within the solid-liquid phase are used as thermal storage devices in the construction sector [10] and this paper seeks to delve deeper into their properties, characteristics and applications.
1.2 CLASSIFICATION OF PHASE CHANGE MATERIALS:

PCMs are broadly classified into several groups namely: organic compounds, inorganic salt hydrates, eutectics of organic or inorganic materials and natural elements [9]. Of these groups, organic and inorganic PCMs are the most widely adopted because of their qualities listed in table 1.0 below:

<table>
<thead>
<tr>
<th>Merits</th>
<th>Inorganic Compounds</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exist in wide temperature range</td>
<td>Low cost and readily available</td>
</tr>
<tr>
<td>Freeze without much super cooling</td>
<td>High Thermal conductivity</td>
</tr>
<tr>
<td>Compatible with conventional building materials</td>
<td>Non-flammable</td>
</tr>
<tr>
<td>Chemically and thermally stable</td>
<td>Sharp phase change</td>
</tr>
<tr>
<td>High Latent heat of fusion</td>
<td>High volumetric latent heat storage capacity (VHC)</td>
</tr>
<tr>
<td>Recyclable</td>
<td></td>
</tr>
<tr>
<td>Non-reactive and safe</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Demerits</td>
<td>Supercooling</td>
</tr>
<tr>
<td>Low thermal conductivity in solid state</td>
<td>High volume change</td>
</tr>
<tr>
<td>Flammable</td>
<td>Segregation</td>
</tr>
<tr>
<td>Low volumetric latent heat storage capacity (VHC)</td>
<td>Reduce in efficiency after repeated use</td>
</tr>
<tr>
<td>Low phase change enthalpy</td>
<td></td>
</tr>
</tbody>
</table>

Table 1.0: Qualities of Organic and Inorganic compounds

Zalba et al [15] classifies 118 organic substances, inorganic substances, organic eutectics, inorganic eutectics, fatty acids and non-eutectic mixtures of inorganic substance with potential for use as PCM. Lane et al, [17] identifies 210 organic, inorganic and eutectic materials that undergo phase change without component separation (segregation), suitable for building temperature regulation. Kuznik et al. [10] outlines 21 experimental research studies performed on PCM wallboards to improve their thermal properties. The selection criteria for PCMs are highly dependent on thermal, physical, chemical and economic characteristics. These characteristics are further elucidated in the paper by Abhat [14].
Phase change materials are often referred to by different nomenclatures such as thermal flywheel, heat of fusion device, latent heat device and fusible mass device. In a report by Alawadhi [16], he frequently referred to them as capacitive insulation types because they slow down the flow of heat through them by absorbing the heat. When incorporated in buildings walls, they act as a heat reservoir, thereby removing excess heat from the building envelope and thus maintaining comfort levels.

Other thermal applications of PCMs include waste heat recovery, spacecraft temperature systems, heat pumps, electrical equipment cooling, transportation of sensitive materials such as blood or chemicals, storage of perishable items, industrial cold store, thermal energy storage and thermal conditioning of buildings, but of particular interest in this research paper is its use in building applications, an area which holds key prospects to improving energy conservation in homes and offices. In construction of concrete application, Betz and Turpin [4] evaluated three ways of application of PCM which include:

- Increasing energy storage capacity of concrete for houses.
- Reducing in temperature rise and subsequent temperature decrease during the first days of hydration of concrete.
- Limiting number of freeze / thaw cycles of bridge deck concrete.
1.3 PCM PROCESS IN BUILDING CONSTRUCTION

The use of PCM in buildings began in the mid 1940s [17] and its application as a type of thermal storage was one of the first studied together with thermal storage tanks [15]. During the 80s, bulk encapsulated PCMs were been manufactured and sold for active and passive applications, including direct gain. They were usually placed adjacent to windows in homes. However, they soon became unsuccessful, as the surface area of the encapsulated PCM products were inadequate to deliver heat to the building passively after the PCM was melted by direct solar radiation [7]. Advancements in technology and research have since propelled studies into some new areas such as integration with walls [10, 18], gypsum wall boards [19], micro-encapsulation in concrete mix [4], thermal solar storage [17] and thermal control of photo voltaics [20].

When PCMs are incorporated into buildings designs as part of the thermal mass, during the day they absorbs heat from the enclosure while melting, thereby reducing the indoor temperature. At night, when the room temperatures are low, the PCM rejects the stored heat into the enclosure, thus preventing the temperature in the room from getting too cold. This cyclic passive process results in a reduction of heat flow from the outdoor to the indoor enclosure [16] which in turn shifts peak cooling loads to off-peak periods, thereby evenly distributing the demand for electricity and avoiding shortages often encountered during the peak periods [5]. The key benefit of this material is that affords structures improved thermal storage capabilities with minimal change to the existing building design. The main methods of incorporating PCMs into building materials are mainly by use of plaster boards [32] and by micro-encapsulation [47].

Modern buildings today are becoming more lightweight structurally and concerns are been raised over indoor comfort due to reduced thermal storage property. These issues are further heightened by global climate change and the continual rise in energy cost. Tension exists between the drive to build better efficient structures with less impact on the environment and the tendency to add more mass to the structure for thermal storage [32]. Studies estimate that 70% of homes in 2050 have already been built and experts warn that unless existing homes are retro-fitted with energy saving devices, targets set for reducing CO₂ emission are unattainable [26]. PCMs store much larger amount of thermal energy
per unit mass than conventional building materials and provide lightweight structures the benefit of increased thermal mass storage [32]. Mehling et al. [40] and Haussmann et al [41] highlight the capabilities of incorporating PCM in such structures to stabilise indoor temperatures.

However, with the cost of energy continually rising globally and amidst growing concerns for reducing environmental pollution resulting from the use of fossil fuels, why have phase change materials not been fully integrated into building constructions, how effective are they and what barriers hinder their development and utilisation. These are some of the questions the author seeks to address in this research paper.

1.4 RESEARCH FOCUS:

There is some confusion about the practicality of integrating PCMs for building temperature control. Serious issues are being raised concerning possible impediments to the successful widespread adoption of PCMs. For example, there have been concerns over the long term stability [15], high cost of material encapsulation [22], flammable nature [42], corrosion and leakages [15, 23]. Baetens et al. [24] suggests that although the principle behind phase change materials holds promise for the future, properties of the current available types are not optimal for general building applications. The need to develop affordable materials with the right melting and freezing points for specific climates is of utmost importance. Heim & Clarke [25] admit that it is difficult to build a PCM plasterboard that regulates room temperature all year round. Kuznik et al. [10] stresses the need for further examination into the use of PCM.

Due to high energy requirements necessary for maintaining present day standards of comfort in buildings and the continual rise in energy utility cost, a research into the application of PCMs in buildings is beneficial to the drive towards reducing global environmental pollution. This study aims to provide an evaluation of the functions of phase change materials in the area of temperature regulation in building. Investigations into the effects of incorporating PCM ceiling tiles into a building façade would also be fully conducted and analysed via a computational model. A building case study would be
applied to the model in order to analyse the effects of real live temperature scenarios on the PCM and recommend specifications for effective temperature regulation.

1.5 RESEARCH AIMS AND OBJECTIVES:

The overall aim of this research is to investigate the impact of temperature changes on PCMs in relation to building temperature control. However, in order to understand building temperature control problems cases, it is necessary to gain insight into the heat transfer control theory and explore thermal properties of PCMs. It would be difficult to comprehend how PCMs affect energy demand in homes without first understanding the governing principles of phase change and the application of PCM as thermal energy storage mass. Given the confusion between those for and against its application, it is all the more important to investigate and clarify the issues that hinder the adoption practices. Furthermore, this research will develop a model to test the properties of some commercial PCMs in order to derive a practical standard property specification for deployment in buildings. Also fully analysed will be a building case study fitted with two commercial PCM ceiling tiles types during winter, spring and summer conditions.

Specifically, within the context of phase change materials used as passive building temperature controls, the objectives of this research are to:

1. Evaluate critically models and frameworks relevant to the phase change process.
2. Develop a computational model to simulate the sensible and latent regions of PCM.
3. Examine the effects of internal temperature changes on the effectiveness of the model.
4. Apply the model to a building case study.
5. Formulate recommendations for the implementation of PCM ceiling tiles in buildings construction.
1.6 OUTLINE STRUCTURE

The research paper contains the following six chapters as outlined below:

**Chapter 1: Introduction**

This chapter provides the reader with background information on the use of PCMs as thermal energy storage mass in buildings, including an illustration of energy demands in residential buildings, the various existing PCM types, qualities and classifications. The focus of the research is discussed, justified and the overall research aim and individual research objectives are identified.

**Chapter 2: Literature Review**

This chapter will outline and examine previous studies that have been conducted on PCMs, focussing on models developed for thermal storage, temperature regulation and space heating in the building sector. Conclusion of findings and the need for research are included at the end of the chapter.

**Chapter 3: Research Methods**

This chapter examines the theory, numerical methods and basic concepts pertaining to the thermal processes of phase change materials. Also described within this chapter is the methodology utilised for developing the computational model which comprises of the governing equations and ESL program codes. The building case study is also presented in detail.

**Chapter 4: Building model Case Study**

This chapter describes a comprehensive study of the effects of incorporating PCMs ceiling tiles into a building case study in ESL simulation language. Simulation cases with two selected Rubitherm PCMs were carried out under varied melting temperatures.

**Chapter 5: Results and discussions**

This chapter presents the results obtained from the ESL simulations defined in the cases in Section 4.3 of Chapter three. Discussions of these results alongside analysis of the temperature and heating load graphs are also offered.
Chapter 6: Conclusion and recommendation

This chapter presents the main conclusion drawn from the research and proffers recommendations for application of PCM for building temperature regulation. The published articles which have been used as references in the report can be found in the Reference section while other relevant details which also pertain to the research are included in the appendices as referrals.
CHAPTER TWO

LITERATURE REVIEW

2.1 INTRODUCTION

This Literature Review will examine critically the models and frameworks from previous studies that have been developed, simulated and applied towards analysing the phase change process. The study within this review of literature focuses on objective 1 as set out in the sub-section 1.5 of the introductory chapter (the second objective will be met through computational developments within the ESL program language, objectives 3 and 4 will be achieved by running simulations on the model, while the final objective –objective 5- is derived as a result of the findings from objectives 1, 2, 3 and 4)

2.1 PHASE CHANGE MODELS

PCMs have been a main topic in research for over 20 years [15]. They have been widely reviewed by many authors in recent times with most focussing on their properties, applications, heat transfer process and material selection aspects [10, 11, 13, 15, 27, 28]. Organic types of PCM are the most widely favoured because they are more thermally stable and easier to encapsulate as shown in experiments by Abat [14] and Hawes et al. [33].

A thorough academic search for relevant literature revealed many existing models to date. Huang et al. [30] studied the use of PCMs to moderate the temperature rise of building integrated photo voltaic systems (BIPV). A two-dimensional finite volume numerical model was validated by comparing the simulations performed with existing experimental results. Although slight variations exist between both results, they suggest that model can still be applied to the study of the phase change process. This is generally acceptable as both results from simulations and experiments cannot always be the same since simulation cases are idealised tests. Application of this model was further utilised in the study of the heat transfer
process through a PCM augmented wall consisting of solid-liquid type PCM bounded by brick and concrete on the outer and inner sides respectively. They varied phase transition temperatures and operational conditions for three days in the month of January to obtain an optimum arrangement of a wall cavity with 100mm concrete block, 110mm clay brick, 20mm Rubitherm GR27 PCM and 20mm air gap. Neeper [7] analysed PCM performance as thermal mass by applying a sinusoidally varying air temperature to an idealised PCM wall. The wall had a large thermal conductivity and an unlimited value for Latent heat at a single melting point. He observed that maximum daily storage occurs at a value of PCM temperature close to the average room temperature of the building. Eight years later, Richardson & Woods [3] also applied the same sinusoidal indoor temperature model to a dimensionless model in order to analyse thermal mass characteristics of PCM. The combined model consists of four dimensionless parameters viz.: diffusivity of the mass, latent heat of the material, melting range of the PCM and convection strength at the mass surface. They observed that by increasing either the diffusivity of the mass or Stefan number, results in a reduction of the maximum surface temperature of the material and an increase in the diurnal energy storage. Increasing the convection heat transfer coefficient is deleterious because maximum surface temperature increases as well as diurnal energy storage. Halford & Boehm [31] discussed the development of a MATHLAB based numerical model that adopts the one dimensional diffusion equation to examine the ability of a RCR configuration to offset peak cooling loads. The Resistive-capacitive-resistive (RCR) configuration consists of a hermatically sealed PCM perlite mixture placed in-between two layers of insulation.

Cabeza et al. [18] studied the use of microencapsulated PCM in concrete walls in order to design a product with the potential of achieving energy savings in buildings. Two test cubicles experimented on in Puigverd of Lleida (spain). They pointed out a major merit of micro over macro encapsulation, as the latter fails due to reduced conductivity of PCM. Experimental results showed an increase in room temperature by 2°C for the cubicles without PCM. They also highlight the effects of thermal inertia which causes a 2h retard in heat wave which consequently reduces electrical consumption due to air-conditioning. By carrying out experiments with the window open, they observed thermal inertia due to phase change freezing was not effective hence inferred that user behaviour was an important issue with respect to effectiveness of PCM. The PCM specs used were: Melting point = 26°C, Phase enthalpy h = 110kJ/kg.
In estimating the thermal behaviour of a wall, the positioning of PCM material is highly important. Alawadhi [16] performed a two dimensional analysis on a 0.25m x 0.15m x 0.15m horizontal brick with several 0.03m cylindrical holes filled with organic PCMs viz.: n-Octadecane, n-Eicosane and P116. He observed that n-eicosane placed in three cylindrical bores at the centreline of the brick achieved a 17.55% reduction in indoor heat flux. Increasing the quantity of the PCM further improved results, although care must be taken while adding more PCMs so as not to diminish the strength of the brick.

An important aspect is the useful life of the PCM systems, the number of cycles they can withstand any degradation of their properties. Gibbs & Hasnain [45] suggests that they have excellent thermal stability and neither the cycles nor contact with metals degrade their qualities. Heim [25] observed a reduction in the PCM characteristics due to overloading after a few weeks of simulation in the summer month of March. Organic paraffin wax have been proven to be durable over longer periods of time when impregnated with concrete [46]. Experiments on two cubicles by Cabeza et al. [18] show that PCMs worked perfectly for six months.

2.3 DEVELOPMENT OF COMPUTATIONAL MODELS

Thermal simulation softwares have also been used to study the phase change phenomenon. Kendrick and Walliman [32] while focussing their research on the area of the use of PCM for passive cooling used a component of IES virtual Environment package called Apache to model PCM plasterboards using conditioned cavity method and observed that having a phase change melting temperature close to the desired average room temperature provides effective thermal storage for both cooling and heating applications. Increasing the value of the latent heat capacity only caused a decrease in indoor temperature and not an increase in the duration of the comfort level i.e there is a limit to the rate of which heat energy can be absorbed by the PCM. They inferred that PCMs are ineffective when operated at similar cooling set points of air conditioners as the material ends up competing with the cooling system. Suggesting that in such cases, they should be placed below the ceiling for effective performance owing to stratification of air temperature within the room. They also showed that the use of PCM has significant advantages for both commercial and residential building applications, 38% to 58% energy savings was achieved for a hot week and well as greater savings at no additional cooling was observed for milder days. By applying low air change night ventilation, further improvement in
PCM performance was obtained. Without this additional cooling technique, the PCM would behave as standard plasterboard having reached its full potential for absorbing excess heat [18, 32].

Betz and Turpin [4] included an excursion into an existing one dimensional finite difference computer code (CONCTEMP) that determines the enthalpy changes during phase transitions by maintaining constant nodal temperature during the latent heat storage process. After the latent process is completed, the nodal temperature was set to vary once more. This program was used to simulate the number of freeze/thaw cycles for bridge decks with different climates. They observed that a 30% reduction in the number of freeze/thaw cycles can be achieved by adding PCM to the concrete. The study also claims that by varying the molecular mass (chain length), the phase transition temperature of Polyethlene glycol can be controlled to obtained improved results.

Rose et al. [35] uses a hygro-thermal simulation package called BSim to evaluate the impact of PCM on cooling and heating demands in Danish buildings. Simulation results were compared with laboratory measurements and it was observed that the model could be used appropriately to predict PCM behaviour in buildings. They expressed concerns about specific heat capacity of PCM been dependent on temperature and the effects of hysteresis on the phase change process. Micronal smart boards were placed on the roof (U-value = 0.155 W/m²K) of a highly insulated lightweight building with the following configurations: thickness 15mm containing 30% (3kg per m²) micro encapsulated Paraffin, specific heat of 1.20kJ/kgK, thermal conductivity of 0.18 W/mK (solid state) and latent heat in transition area of 330kJ/m² were used. Installing these boards in the roof of the building reduced overheating frequency by 33% and also reduced indoor temperatures by 2K when the PCM was loaded. Validation of the model was based on Lab measurements of 270mm thick walls of Micronal smart board i.e. 18 boards of 15mm thickness bolted together on the ceiling board. Numerically, two identical models were developed, one was the reference and the other was used to test different properties of PCM. A list of the settings applied can be seen in the respective journal [35].

Castell et al.[36] evaluates five building modelling programs that can be used to analyse effects of PCMs in buildings namely Trnsys type 232, Trnsys type 241, Trnsys type 204, PCM express (ESP-r) and Energy Plus. Only the last two programs were validated based on functionality for
the purpose for which they were required and general ease of use. Experimental data from Puigverd de Lleida (Spain) site which has four cubicles fitted with PCMs were compared with the simulation results. For PCM express, it was observed that the internal temperatures for the simulation were warmer than those obtained during the experiments. An offset between the actual temperature of the PCM for the simulation and experiment was also noticed for the different cubicles, these deviation was caused by the different types of walls in place i.e. some of the walls have higher thermal resistance. Since the software can’t model HVAC systems, only the free floating condition was simulated so as to verify with experimental results. On utilising Energy Plus, the reverse case was observed. Internal temperatures obtained from the experiments were higher than those of the simulation. This was because the experimental data shows warmer outside temperatures than for the simulation type. This is not the case for the previous software tested. The simulations did not reflect the effect of PCM in the thermal behaviour of the cubicles of free floating conditions.

A paper by Heim and Clarke [25] discusses the development of an ESP-r special materials facility to implement the effects of phase transition into the energy balance equation of a building. Simulations for each day were carried out for varied PCM melt temperature with a phase change temperature range of 1K. However, results showed no appreciable reduction in room temperature owing to the use of a PCM with low latent heat storage of 45kJ/kg. The energy stored by the PCM during daily cycles depends on melting temperature, temperature range which it melts and latent capacity per unit area [7]. A low latent heat storage capacity would make the PCM overcharged during a hot day and at night become incapable of fully discharging its absorbed heat before the start of the next day charge cycle. Situations like this should be avoided because of the adverse effects it has on the performance of the PCMs as this can further introduce unwanted heat energy into the building envelop. Working with ESP-r, Heim [34] further studies two solution methods of heat transfer PCM modelling within whole body dynamic building simulation viz.: “effective heat capacity” and “additional heat source” methods. The effective heat capacity method involves considering heat capacity as a function of temperature in the phase change temperature range while the additional heat source method assumes temperature dependent internal flux corresponds to latent heat energy in the following conditions: negative when the material stores heat, positive when it releases energy and neutral (zero) otherwise.
2.4 CONCLUSION

Developing models to study heat transfer processes in PCM structures are quite complex, particularly when the compound is in the mushy state [25]. Most of the models that have been reviewed in the literature have been validated with experimental data, hence are viable tools for evaluating and predicting the effect of PCM in a building facade. Findings from previous studies show that modelling phase change materials during the transition stages is not adequate. Overall, no existing model incorporates the effects of casual gains from occupants, internal thermal mass (such as furniture) and electrical equipment as well as few utilise real weather data in their models. One point worthy of note is that they don’t fully represent the points of change between phases. This paper aims to design and utilise a volumetric heat capacity discontinuity model in conjunction with the effective heat capacity method in ESL program, which accounts for the likelyhood of “jumps” during the calculations of the previous mentioned methods carried out by Heim [34], to represent the thermal processes of a PCM. By defining points of discontinuity in the phase change process, the Runge-Kutta integration algorithm can be used to practically describe the PCM thermal process.
CHAPTER 3
RESEARCH METHODS

3.1 INTRODUCTION
This chapter examines the process of heat transfer in PCMs and describes the methodology adapted to developing the computational model for the simulations of the phase change process. Numeric methods as well as the approach used to represent the simplified model of the sensible and latent phase regions are described as well.

3.2 THE HEAT TRANSFER PROCESS
Heat is usually transferred across a material by a combination of methods namely: conduction, convection and radiation. The degree of the transfer heavily depend on the temperature and the type of the material been considered. In order to understand the thermal processes of the PCM, the heat transfer modes are considered separately.

3.2.1 CONDUCTION
Conduction can be defined as the transfer of heat through a solid body or fluid at rest [38]. In solids, the heat energy is transferred by the movement of electrons within the lattice of fixed molecules while for fluids, direct molecular interactions occurs since the molecules are free to move in space. Newton and subsequently Fourier developed the fundamental laws of heat conduction from experimental observations on steady state systems. They observed that the heat flow through a material is directly proportional to the temperature difference and normal direction of heat flow. Mathematically this can be represented for the x coordinate direction as:

\[ Q = -kA \frac{\partial T}{\partial x} \]  

(1)

Where Q is rate of heat flow (W), A is the Area normal to the direction of heat flow (m²), \( \frac{\partial T}{\partial x} \) is the temperature gradient in that direction (K/m) and k is the thermal conductivity of the
material (W/mK). In a built environment, conduction heat transfer would take place within existing thermal masses such as walls, equipment and furniture. For a PCM ceiling tile of thickness \((\Delta x)\) of thermal conductivity \(k\), subjected to temperatures \(T_a\) and \(T_{pcm}\) and assuming heat flows only in the x direction, Equation (1) becomes:

\[
Q = kA \frac{(T_a - T_{pcm})}{\Delta x}
\]  

(2)

### 3.2.2 CONVECTION

Convection can be defined as the overall process by which heat is exchanged between a fluid and a bounding area. The nature of the process is highly dependent on the nature of the fluid motion adjacent to the surface where the boundary layer develops. In a built environment, convection heat transfer would take place between the air and the surfaces of the walls. Convection is generally classified in the way in which the fluid motion is generated. When the flow over the transfer surface is generated by external means such as fans, atmospheric winds or pumps, the heat transfer process is referred to as forced convection. When the flow is induced by buoyancy forces arising from the differences in density caused by temperature variations in the fluid in close proximity to the surface, natural convection is said to occur. Newton’s law of cooling is used to express the rate of convection heat transfer as:

\[
Q = hA \Delta T
\]

(3)

Where \(h\) is the convective heat transfer coefficient of the process (W/m\(^2\)K). Considering the rate of convection heat transfer between the PCM ceiling at Temperature \(T_{pcm}\) and the surrounding air of temperature \(T_a\) gives:

\[
Q = hA(T_a - T_{pcm})
\]

(4)
3.2.3 RADIATION

Radiation is a form of heat transfer via electromagnetic waves between two distant surfaces. While the transfer of energy by conduction or convection requires the presence of a material medium, radiation does not. Generally, radiation heat transfer occurs best in a vacuum. The actual amount of energy transmitted by radiation from a body varies with the temperature of the emitting body, the wavelength of the emitted radiation and the nature and area of the surface of the body [38]. The major form of radiation in a built environment is the solar radiation. Effects of this on the temperature of the walls as radiation through the windows are implemented in the building model. Under perfect conditions, the rate of change at which energy is radiated from a body is proportional to the fourth power of its absolute temperature [55]:

\[ Q = \sigma T^4 \]  \hspace{1cm} (5)

Where \( \sigma \) is the Stefan-Boltzmann constant = 5.67 x 10^{-8} \text{ W/m}^2\text{K}^4

Buildings are exposed to ambient conditions that vary randomly with respect to time and these changing environmental conditions consist of parameters that affect the heat transfer process namely: long and short wave solar radiation, air temperature, velocity of the wind, soil earth temperature and relative humidity. The heat loss from a building is proportional to the difference between outdoor and indoor temperatures, integrated over a day [48] and this depends on its thermal mass.

In figure 3.0, within the occupied period of 7am to 6pm, it can be seen that the heat loss is the area between the temperature curves for the external temperature and the building temperature. Heavy weight buildings show a greater amount of heat loss during this period than light weight counterparts.

![Fig 3.0: Rate of temperature change in heavy weight and lightweight buildings](image)

Fig 3.0: Rate of temperature change in heavy weight and lightweight buildings [48]
Heat transfer coefficients and thermal property values are not well defined and change randomly not only with respect to time and space but also with respect to temperature and humidity [44]. This simply connotes that the heat transfer process is non-linear in nature and an appropriate representation of the process in a computational model is quite difficult. PCM exhibit more complex thermal behaviours in their phase change processes especially when in the transition state [34]. This challenge for an accuracy of simulation of the thermal behaviour of a PCM incorporated into building designs is the primary focus of this paper.

When the PCM material is in the solid state and the surrounding air is hotter than it, heat is absorbed from the air as sensible heat. This heat causes a continuous rise in the PCM temperature up till the melting temperature $T_m$ at point B. At this point, the heat being absorbed is solely utilised in breaking down the molecular structure of the solid PCM. The material is said to be in the mushy region here and is capable of absorbing large amounts of latent heat energy from the surroundings without significant rise in its surface temperature. During this phase change, the material exists as a mixture of solid and liquid or mushy (two phase) states. When the PCM melts completely, it becomes fully liquid and it is incapable of latent heat storage. At this condition (point C), the material is completely liquid and experiences a progressive rise in temperature as sensible heat. The latent heat storage occurs only in the mushy region while the sensible heat storage occurs during both the solid and liquid regions. During solidification, these processes are reversed (from point D to point A) for an idealised PCM.

![Fig 3.1: Idealised curve for Enthalpy as a function of Temperature for PCM](image-url)
In practice, two reactions occur during phase transformation. Firstly, the solidification process occurs with a shift in the properties of the thermal mass due to a hysteresis effect. Secondly, the phase change takes place over a range of temperatures as shown in fig 3.2. In order for heat to flow, temperature gradients must exist. For the sake of simplicity, only the latter condition would be implemented in the ESL program model for the study of the PCM thermal properties.

![Diagram](image)

**Fig 3.2:** Practical curve for Enthalpy as a function of Temperature for PCM

The main concern when modelling PCM is the heat capacity’s dependency on temperature [35]. Most studies on PCM process are based on the idealised reversible case shown in figure 3.1. This method classifies the process as a linear time varying process with constant temperature in the latent heat storage region. This paper aims to appropriately define the practical thermal processes by segmenting it into three distinct regions and adopting points of discontinuity within an integration algorithm in the ESL program. For the development of a simplified computational model to study the effects of PCM in a building, the following assumptions were made:

1. The PCM does not undergo hysteresis during thermal processes.
2. PCM material is heterogeneous and gradual nucleation occurs with a slight increase in temperature. Therefore temperature rise width of the mushy phase region value was taken as 2K i.e. $\Delta T = 2K$.
3. Supercooling, undercooling and nucleation effects are assumed not to present in the thermal processes.
3.3 THE SPECIFIC HEAT CAPACITY OF THE PCM

The Specific heat capacity of a substance can be defined as a measure of the capacity to store heat energy per unit mass of a material [38]. It is a property that is temperature dependent and varies non-linearly across the regions of the thermal processes of a PCM. The quantity of heat required to raise the temperature of one kilogram of a PCM by one degree centigrade varies across the thermal processes non-linearly. Although the specific heat capacity during phase change is non-linear in nature, simplified linear relationships models have been developed by many authors for thermal analysis of the phase change process. Alawadhi [16] defined the governing equations for the thermal process using volumetric heat capacity method as follows:

\[
(pC)_{PCM} = \begin{cases} 
\frac{(pC)_S}{2} + \frac{(pC)_L}{2} & \text{Solid Region} \\
\frac{(pC)_S + (pC)_L}{2} & \text{Mushy Region} \\
(pC)_L & \text{Liquid Region}
\end{cases}
\]  

3.3.1 SENSIBLE HEAT REGION:

As previously stated, the sensible storage of heat energy occurs during the solid and liquid region. Although its effect in a PCM is quite minimal compared to latent energy, it is also important and has been considered in the model. The values for the specific heat capacity of

---

Fig 3.3: Sensible Heat Regions of Phase change process
some PCM vary during these regions and this was implemented in the VHC discontinuity procedure. The governing equation for sensible heat energy of the PCM is given as:

\[ Q = \int_{T_i}^{T_f} mC_p dT \]  

(7)

\[ Q = mC_p(T_f - T_i) \]  

(8)

Where \( Q \) is rate of heat flow (W), \( T_i \) is the initial temperature (°C), \( T_f \) is the final temperature (°C), \( C_p \) is specific heat capacity at constant pressure (kJ/kg), \( m \) is mass of the material (kg)

3.3.2 LATENT HEAT REGION

Latent heat energy is the quantity of heat required to convert a unit mass from the first state to the second state without any change in temperature [48]. Latent heat accumulates in a material before a phase change process, thus it is the energy necessary for a process change to take place. Practically, a slight rise in temperature occurs during the phase change process. Latent heat energy for the model is defined as:

\[ Q = \int_{T_{m1}}^{T_{m2}} mC_{pm} dT \]  

(9)

\[ T_{m2} = T_{m1} + \Delta T \]  

(10)
Where $T_{m1}$ is the Initial melting temperature, $T_{m2}$ is the Final melting temperature, $\Delta T$ is melting temperature range (taken as 2K), $C_p$ is specific heat capacity in solid or liquid region

Therefore the total heat flow through the PCM is given as:

$$Q = \int_{T_m}^{T_{m1}} mC_{ps}dT + \int_{T_{m1}}^{T_{m2}} mC_{pm}dT + \int_{T_{m2}}^{T_f} mC_{pl}dT$$  \hspace{1cm} (11)

The $1^{st}$ integral on the right hand side of the equation represents the sensible heat gained from the solid state, the $2^{nd}$ term is the latent heat of fusion from the mushy state and the third is the sensible heat gain in the liquid state. Since mass remains constant throughout the phase transformation, equation (11) can be written as:

$$Q = m \left[ \int_{T_m}^{T_{m1}} C_{ps}dT + \int_{T_{m1}}^{T_{m2}} C_{pm}dT + \int_{T_{m2}}^{T_f} C_{pl}dT \right]$$  \hspace{1cm} (12)

### 3.4 Numerical Methods for Modelling Phase Transformation

Phase change transformations occur in cases such as melting, solidification, vaporisation and condensation. A transformation of phase from solid to gas or vice versa consists of two phase transformations. Such a system of more than one phase is complex to represent mathematically as a whole. However, the entire transformation process can be broken down into segments of each phase. A simplified analysis of the whole system can then be undertaken by considering the thermodynamic properties of each segment. Two phase transformations are generally not applicable to the design PCMs. This is because of the unpredictable high pressure and volumes generated during transformation to the gaseous state. Single phase transformations such as melting (solid to liquid) and solidification (liquid to solid) are most desirable modes of the transformation for phase change devices.

Melting and solidification are transformation processes which accompany absorption of heat and release of heat respectively. A moving boundary condition exist between the two phase transformations [52]. A simple case of a moving boundary condition is the one phase, one dimensional melting-ice problem studied by Stefan in 1890 [56]. The solidification of ice
problem involves considering the conservation of energy in the $\Omega$ domain and dividing it into two separate sub domains in the liquid ($\Omega_l$) and solid state ($\Omega_s$). The overall domain $\Omega$ is the sum of these two sub domains and the energy conservation defined for the liquid state ($\Omega_l$) is [52]:

$$\rho_l C_l \frac{\partial T}{\partial t} = \nabla . k_l \nabla T$$

(13)

and for solid state ($\Omega_s$)

$$\rho_s C_s \frac{\partial T}{\partial t} = \nabla . k_s \nabla T$$

(14)

Where $T$ is the temperature, $k$ is the thermal conductivity, $\rho$ is the density, $c$ is the specific heat capacity, subscripts $l$ and $s$ represent liquid and solid respectively.

The absorption and release of heat energy is primarily governed by the latent heat energy of the material. Several methods have been used to represent the latent heat energy during phase transformation. These methods are generally divided into one domain (fixed mesh) and two domain (moving mesh) methods. One domain technique comprises of a solution of a continuous system with an implicit representation of the phase change process while two domain techniques involves the separate representation of the solid and liquid regions as well as considering the phase change interface explicitly as a moving boundary [52]. Overall, the two dimensional method offers a greater accuracy of the representation of the phase change thermal processes but cannot readily be applied in the case of a material freezing over a range of temperatures. One dimension methods are generally preferred because of their simplicity and that they account for the phase change implicitly. However, they tend to be less accurate around the phase change boundary [53]. Some of the commonly used methods are hereby discussed in the following subsections.

### 3.4.1 EFFECTIVE HEAT CAPACITY METHOD

The effective heat capacity method is one of the earliest and widely adopted methods of analysing phase change processes. Heim, in [54] presented applications of this method and later in [34] utilises the technique in modelling the thermal phase processes of a PCM incorporated into a building model in ESP-r software. This method is governed by a single energy conservation equation written as [52]:

$$\frac{\partial H}{\partial t} = \nabla . k \nabla T$$

(15)
Where the effective heat capacity $C_{eff}$ is given as

$$C_{eff} = \frac{dH}{dT}$$  (16)

For the following boundary conditions of a phase change over an interval of temperatures:

$$C_{eff} = \rho C_s \quad (T < T_s)$$
$$C_{eff} = \rho C_f + \frac{L}{T_l - T_s} \quad (T_s \leq T \leq T_l)$$
$$C_{eff} = \rho C_l \quad (T > T_l)$$  (17)

According to Heim and Clarke [25], effective heat capacity is a highly non-linear function of temperature within phase change temperature range. A drawback of this procedure as shown in figure 3.6 below is that in order to directly apply effective specific heat, it would require that the selected temperature interval be maintained for the period of the latent heat energy. Therefore this method cannot fully represent an isothermal phase change process due to its range of temperature restriction.

![Figure 3.5: Effective heat capacity method for non-linear 1-D element](image)
3.4.2 ENTHALPY METHOD

This method of phase change representation eliminates the problems linked with the effective heat capacity method. The enthalpy method involves reformulation of Stefan problem in terms of the enthalpy property by considering it to be the primary variable while the temperature \( T = T(h) \) is solved simultaneously with the enthalpy equation [52]. The general form of an enthalpy formulation is:

\[
\rho \frac{\partial h}{\partial t} = \nabla [k(\nabla T)]
\]  

(18)

Where \( T \) is the temperature, \( k \) is the thermal conductivity, \( t \) is the time, and \( \rho \) density.

The type of phase change determines the nature of the relationship between temperature and enthalpy [58]. Although, the enthalpy method is simpler and accurate, it has some limitations such as:

1. Takes longer time for the computer to simulate owing to the small spatial and temporal size requirements for ideal analysis.
2. The latent heat energy absorbed and rejected during a phase change is not fully represented in this method.
3. Due to the reliance on a temperature range for the analysis of the latent heat energy, isothermal phase changes cannot be represented appropriately.
4. Oscillations in temperature occur close to the boundary conditions.

In order to eliminate temperature oscillations, Ayasoufi [55] applied the space time conservation element (CE) and solution element (SE) methods to solid / liquid phase change problems as an alternative to the enthalpy method.

3.4.3 HEAT SOURCE METHOD

The heat source method is similar to the enthalpy method but lacks the mathematical theory which supports the enthalpy method as well as its simplicity [52]. Despite this, the heat source method does not suffer from the demerits of the enthalpy method listed above. It is an efficient and flexible method for representing phase change processes. Heim [34] also adopted this method as a second approach in the modelling of the thermal phase processes of a PCM incorporated into a building in ESP-r software. The main drawback of this method is the lack of smoothness of the temperature profile for coarse meshes and large time steps.
3.5 DISCONTINUITY ANALYSIS OF PHASE CHANGE PROCESS

A discontinuity is a break in physical continuity or sequence in time, mathematically it is a point at which a function is discontinuous or undefined [43]. In mathematical terms the function is piece-wise continuous with a discontinuity representing an abrupt change in state variable, or its first or higher derivative. In ESL program, a discontinuity can be defined as an event which causes the algebraic or differential equations representing the system to suffer a ‘jump’ or ‘step change’ in one or more modelling variables. Such events are very common in real systems and also exist in the thermal phase change processes of a PCM. The most significant non-linear behaviour of a PCM thermal process is when the material undergoes latent heat storage. During this condition, the property variables change values to accommodate the new state. The PCM’s specific heat capacity and density vary across each phase change state.

For the phase change modelling of the thermal processes, two discontinuity points were defined in order to represent the segments for sensible heat storage (Fig 3.3) and latent heat storage regions (Fig 3.4). These points occur at the boundary of the change of phase. The first instance is at the point when the PCM starts to melt i.e. when the temperature is at $T_{m1}$ (point B as shown in Fig 3.2). The second point of discontinuity occurs when the PCM has completed the melting process and is now fully liquid at temperature $T_{m2}$ (point D). These two points can be easily obtained from laboratory tests with a differential scanning calorimeter (DSC). For the simplified model in this study, an assumed temperature rise of 2K during the two defined discontinuity points was used during the simulation run.

In order to determine the rate of heat flow through the PCM, an overall integration step must be performed across the curve (Fig 3.2) which represents the thermal process. Integration algorithms cannot effectively represent the rate of heat flow in the presence of discontinuities. A discontinuity within an integration step invalidates the Runge-Kutta representation of the step. ESL incorporates an integration-discontinuity control mechanism which accurately and efficiently detects and locates discontinuities, thus preventing a discontinuity to occur within an integration step. By applying the representation of the effect of phase change transition via the effective heat capacity method and defining the points of discontinuity as described earlier, an appropriate model of the PCM can be developed for the study of the thermal effects on a building temperature. The discontinuity feature of ESL would be utilised alongside the fourth
order Runge-Kutta integration Algorithm to represent the phase change processes. RK4 is an explicit iterative method for the approximation of solutions of ordinary differential equations based on the rate of heat transfer $\dot{Q}$.

3.5 ESL METHODOLOGY

The European Space Agency general simulation tool ESL has been in widespread use for a wide range of engineering problems which involve the simulation of dynamic systems such as thermal vibrations in the Hubble Space Telescope, battery simulation in Earth Resources Satellite and rapid gravity water filter simulations. Brindley et al. [50] describes the use of the discontinuity feature of the ESL program to simulate a non-linear multivariable model of a high performance missile. He stressed that the ESL programming structure is an ideal tool that simplifies the approach to modelling multiple discontinuities present in complex dynamic systems. All the modelling and simulation presented in this paper was done using the ESL simulation language and solver. The results files were exported to MATLAB for graphical display and analysis of the results. The structure of the program was broken down into models and sub models as shown in program flow chart in Fig 3.6. The program consist of one main model called zone_40 which was linked with five sub models namely: sm_pc, sm_environment, sm_build, sm_controller and sm_actuatorfull. A full description of the models and sub models including the code embedded in them can be seen in Appendix B.
The following method describes the processes involved in developing the PCM model in ESL simulation language. The first modelling challenge was to ensure that the phase regions are appropriately represented during the run of the simulation. The solid, liquid and mushy regions must be clearly defined in order to simulate the thermal effects of PCMs. The volumetric heat capacity method was applied according to the flow chart in fig 3.7. The latent storage region starts at the point when the melt temperature of the PCM is reached; a conditional code statement acts as a trigger at this point and applies the necessary calculations (equation 6) in line with latent heat energy condition. The solid and liquid sensible regions undergo a similar process within the program. Computational modelling of the thermal process of the PCM involved the use of multiple IF statements which define the condition of the state of the equations used to calculate the rate of flow of heat through the PCM. It is the logical expressions in the flow diagram shown in Figure 3.7 below, that generates the discontinuity functions.

Fig 3.6: ESL Information flow diagram for the PCM building simulation
The following code excerpt shows the implementation of the volumetric heat capacity method using the multiple IF clause statement:

```c
48  --Apply discontinuity condition when buffer is called to determine (PC_pcm)
49  PC_pcm:= If Tpcm >= Tm1 and Tpcm <= Tm2 Then
50      (((Dpcm_s * Cpcm_s) + (Dpcm_l * Cpcm_l))/2) + (((Dpcm_s +Dpcm_l)/2)*(Lpcm / 2.0))
51  Else If Tpcm > Tm2 Then
52      Dpcm_l * Cpcm_l
53  Else
54      Dpcm_s * Cpcm_s;
```

Fig 3.8: VHC discontinuity procedure code excerpt

The Second problem was to ensure that this VHC method was activated just at the right instance of calculating the rate of change of temperature of the PCM. In order to achieve this, a buffer variable PC_pcm was placed in the equation for rate of change of temperature as
shown in the ESL code excerpt in Fig 3.8. Thus when the PCM temperature differential equation is called by the solver, the routine is paused and VHC conditional procedure (Fig 3.7) is activated. The Runge-Kutta fourth order integration algorithm was adopted for the model with a communication interval of 60 seconds, minimum step size of 10 for each communication interval and the maximum integration step-size was 6.

```
57  --Temperature rate of change for Phase Change Material
58  Tpcm' := (1.0/(V *PC_pcm))*(Qd_pcm + 0.0*Qfree);
59
60
61  --Rate of Heat flow through PCM
62  Qd_pcm := U*(Ap_cm*(Ta-Tpcm));
63
64
```

Fig 3.9: Rate of change of PCM temperature code excerpt
CHAPTER FOUR

BUILDING MODEL CASE STUDY

4.1 INTRODUCTION
This chapter describes a comprehensive study of the effects of incorporating the PCM model developed in Chapter three into a building case study. Simulation cases with two selected Rubitherm PCMs were carried out under different material configurations. This study aims to evaluate indoor comfort temperature levels as well as space heating and cooling loads.

4.2 DESCRIPTION OF BUILDING MODEL
The model was based on a classroom section of Clydeview Academy in Gourock, Inverclyde which is currently under construction using CAB philosophy. A conceptual model is illustrated in Fig 4.0. The school is been designed to incorporate the fundamental elements of sustainable design such as natural ventilation and energy efficiency. The academy is rated as BREEAM very good status with a score of 69.14% [51].

Fig 4.0: Project design for Clydeview Academy [37]
Chapter 4: Case Study

The area been considered is a section of a single classroom block on the second floor of the building bounded by other similar rooms on its sides. The exterior wall consists of two windows each with an area of 8.45m$^2$ spaced 1.83m apart. Opposite this wall lies an interior wall of dimension 8.60m x 5.86m, two side walls and an inclined roof as shown in the building sketch (Fig 4.1). The specific heat capacity of the walls are 1000 J/kgK and its cavity consist of concrete brick of thermal conductivity 0.1 W/m$^2$K coated on both sides by textured acrylic wall finish (Fig 4.2). The roof has an area of 44.4m$^2$ and is completely covered with PCM ceiling tiles on the interior side. Total surface area of the structure is 85.6m$^2$. The total thermal mass of furniture which comprises of chairs, desks, tables and other classroom materials is 8000 kg, at an internal mass area of 138m$^2$ with a specific heat capacity of 900 J/kgK. Mass flow rate of air in the dwelling was 0.02m$^3$/s and specific heat capacity of air 1012 J/kgK. An initial number of six (6) pupils were set to occupy the room between the hours of 7am to 5pm. Specific heat transfer coefficient of the furniture is 2W/m$^2$K. The specific heat capacity of the structure is 1000 J/kgK, walls are of 50mm with and thermal conductivity of 0.1W/m$^2$K. Effective ventilation openings area is 0.01m. The HVAC control system specifications are enumerated in table 4.0 below.

![Fig 4.1: Schematic of Building Model Energy flow](image)

1. Heat Conduction through walls.
2. Heat gained from lighting $Q_L$
3. Phase Change Material under ceiling $Q_{d,pcm}$
4. Air out, $Q_{mv}$
5. Internal Long wave radiation from structure $Q_s$
6. Casual gain from occupants $Q_{oc}$
7. Casual gain from equipment $Q_{free}$
8. Gain from internal mass
9. Under floor heating $Q_f$
10. Electrical Appliance $Q_h$
11. Direct and diffuse solar radiation $Q_{sol}$
12. Air infiltration $Q_{inv}$
The defined heat transfer coefficients of the buildings are:

- Roof = 1.5 W/m²K
- Windows = 1.5 W/m²K
- Floor = 0.2 W/m²K
- Furniture = 2.0 W/m²K

<table>
<thead>
<tr>
<th>Rating</th>
<th>10kW</th>
</tr>
</thead>
<tbody>
<tr>
<td>Overall Thermal Capacitance</td>
<td>4500 J/K</td>
</tr>
<tr>
<td>Overall Transmittance area factor</td>
<td>40 J/sK</td>
</tr>
<tr>
<td>Heat transfer coefficient in duct</td>
<td>8.33 W/m²K</td>
</tr>
<tr>
<td>Heat transfer coefficient in ambient</td>
<td>16.6 W/m²K</td>
</tr>
<tr>
<td>Mass of duct model</td>
<td>38.42 kg/m</td>
</tr>
<tr>
<td>Specific Heat capacity of duct material</td>
<td>41827 J/kg.K</td>
</tr>
<tr>
<td>Temperature Set point</td>
<td>21°C</td>
</tr>
</tbody>
</table>

Table 4.0: HVAC specifications

### 4.2.1 Definition of temperature rates:

(a) The temperature equation that fully describes the indoor temperature $T_a$ is

$$\frac{dT_a}{dt} = \frac{1}{\rho_a V_a c_{pa}} \left[ \dot{Q}_h + \dot{Q}_{free} - \dot{Q}_s - \dot{Q}_f - \dot{Q}_r - \dot{Q}_w - \dot{Q}_{d,pcm} - \dot{Q}_{fv} - \dot{Q}_w - \dot{Q}_t \right]$$

Where,

- $\dot{Q}_h$ = Heat from HVAC control system
- $\dot{Q}_{free}$ = Sum of heat gain from equipment and occupants
- $\dot{Q}_s$ = Heat gained from structure
- $\dot{Q}_f$ = Heat from under floor heating
- $\dot{Q}_r$ = Heat from roof
- $\dot{Q}_w$ = Window heat transfer
- $\dot{Q}_{d,pcm}$ = PCM heat energy
- $\dot{Q}_{fv}$ = Heat gained from forced convection
\begin{align*}
\dot{Q}_\text{nv} &= \text{Heat gained from natural ventilation} \\
\dot{Q}_\text{ft} &= \text{Heat absorbed by furniture mass}
\end{align*}

(b) The structure of the wall was divided into two segments viz: internal and external parts as shown in the figure below for the analysis of the thermal processes.

![Building model wall Section](image)

\text{Fig 4.2: Building model wall Section}

In order to determine the rate of heat flow through the entire wall section, the temperature rate of change was calculated in two stages of heat transfer. For the external surface, temperature rate of change \( T_{se} \) is as follows:

\begin{equation}
\frac{dT_{se}}{dt} = \frac{1}{M_{se}c_{p,se}} \left[ (k \times A_s \times (T_{si} - T_{se}) - \dot{h}_e \times A_s (T_{se} - T_o)) \right] \tag{20}
\end{equation}

Similarly, the internal wall surface temperature is as follows:

\begin{equation}
\frac{dT_{si}}{dt} = \frac{1}{M_{si}c_{p,si}} \left[ \dot{h}_i \times A_s (T_a - T_{si}) - (k \times A_s \times (T_{si} - T_{se})) \right] \tag{21}
\end{equation}

(c) The rate of change of temperature of the furniture mass in the building model is as follows:

\begin{equation}
\frac{dT_{ft}}{dt} = \frac{1}{M_{ft}c_{p,ft}} \left[ U_{ft} \times A_{ft} (T_a - T_{ft}) \right] \tag{22}
\end{equation}

(d) Rate of change of PCM ceiling tiles temperatures:
Where $V_{pcm}$ is the volume of the PCM ceiling tiles derived from:

$$V_{pcm} = \text{thickness} \times \text{Area of PCM} \quad (24)$$

Heat transfer through the PCM

$$\dot{Q}_{d,pcm} = U_{pcm}A_{pcm}(T_a - T_{pcm}) \quad (25)$$

It is worthy to note that the negative sign of $\dot{Q}_{d,pcm}$ in equation (19) defines the manner in which heat flow is been transferred between the PCM and the surrounding air particles. When air temperature $T_a$ is greater than PCM temperature $T_{pcm}$, the value of $\dot{Q}_{d,pcm}$ in equation (25) is positive. When the value for $Q$ is placed in equation (19) it becomes negative, this indicates that heat is been absorbed by the PCM from the indoor air temperature. When PCM temperature $T_{pcm}$ is greater than the air temperature $T_a$, the reverse is the case.

### 4.3 SIMULATION CASES

Having developed the VHC discontinuity model in ESL program, it would be incorporated into the simulation cases of the building case study. A selection of commercially available Rubitherm PCMs would be applied in the study and analysis of the temperature effects on comfort and energy demand in the projected school building for a period of January 1st to Aug 31st 2000 (240 days). The table 4.1 lists the properties of the PCM ceiling tiles used in the research paper. Additional characteristics and company specifications for the selected PCMs are included in Appendix C.

An ESL communication interval of 60 seconds and an integral step of 10 were used for all the simulations presented in this report. Values for the temperature, space cooling and heating loads, PCM temperature and the latent heat of phase change were recorded to an Excel .csv file. To appropriately analyse the effects of the PCM in the building model, the results were presented in weekly time periods for the three seasons (winter, spring and summer).
Theoretically the coefficient of heat transfer for the figure 4.3 above is given as:

\[ \frac{1}{U} = \frac{1}{R_1} + \frac{1}{R_2} = \frac{1}{h_a} + \frac{k}{l} \]  \hspace{1cm} (26)

<table>
<thead>
<tr>
<th>Properties</th>
<th>Phase change material</th>
</tr>
</thead>
<tbody>
<tr>
<td>RT 21</td>
<td>SP 22 A17</td>
</tr>
<tr>
<td>Melting Temperature $T_{m1}$</td>
<td>21</td>
</tr>
<tr>
<td>Latent Heat capacity $\lambda$</td>
<td>134</td>
</tr>
<tr>
<td>Specific Heat capacity $C$</td>
<td>2000</td>
</tr>
<tr>
<td>Density in solid phase $\rho_s$</td>
<td>880</td>
</tr>
<tr>
<td>Density in liquid phase $\rho_l$</td>
<td>770</td>
</tr>
<tr>
<td>Thermal conductivity $k$</td>
<td>0.2</td>
</tr>
</tbody>
</table>

Table 4.1: Rubitherm PCM properties

Weather data for Glasgow ($55^0\text{N}$) in 2000 was used to define the climate conditions for the simulations. The average ambient air temperature for the summer months of July, August and September were 13.3$^0\text{C}$, 18.5$^0\text{C}$ and 19.4$^0\text{C}$ respectively. Annual value for wind speed is
The following outlined cases were simulated in developed building computational ESL model:

4.3.1 CASE ONE: Heater ONLY without PCM and HVAC system
Case one involves a simulation case where the 10kW radiator heaters are the only space regulation devices present in the building throughout the year. This case is similar to the existing condition in most UK residential homes where cooling units are absent. These houses are prone to overheating in the summer months if alternative means of cooling such as natural ventilation i.e. opening windows, are not applied. The heater is set to maintain the indoor temperatures at 21°C.

4.3.2 CASE TWO: HVAC condition without PCM
Case two incorporates into the model the use of a HVAC system which control both space cooling and heating. This case was carried out without PCM ceiling tiles. Reason for this are to observe the changes in indoor air temperature and assess the total heating and cooling loads utilised in the building without the inclusion of PCMs. This was necessary so as to investigate the effects of ambient air conditions on indoor temperatures throughout the different weather seasons. This case would act as a control case for comparison with the other cases.

4.3.3 CASE THREE: HVAC with varied melting temperatures of the PCM
Case three involves simulation with the inclusion of the PCMs listed in table 4.1 at different melt temperatures. A uniform material thickness of 15mm and U-value 1.5W/m²K was applied to both Rubitherm PCM ceiling tiles types. Five weekly periods were selected to coincide with the beginning of the melting procedure of the varied temperature of the selected PCM i.e. points at which the indoor air temperature is greater than the PCM melting temperature. This was done so as to analyse the effects of the latent heat storage during these periods. The periods are presented in the table 4.2 below:
<table>
<thead>
<tr>
<th>PCM Melting Temperature (°C)</th>
<th>Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>21</td>
<td>9-16 April</td>
</tr>
<tr>
<td>23</td>
<td>4-11 June</td>
</tr>
<tr>
<td>25</td>
<td>1-8 August</td>
</tr>
<tr>
<td>27</td>
<td>8-15 January</td>
</tr>
<tr>
<td>30</td>
<td>11-18 March</td>
</tr>
</tbody>
</table>

Table 4.2: Selected periods for latent for simulation analysis.
Chapter 5: Results and Discussions

CHAPTER FIVE

RESULTS AND DISCUSSIONS

5.0 INTRODUCTION
This chapter presents the simulation results of the simulation cases defined in the sections 4.3.1 to 4.3.3 in Chapter 4. The research concentrates on the temperature effects as well as the space heating and cooling load effects when incorporating the two types of (RT21 and SP22 A17) Rubitherm PCMs into the ceiling tiles of the school building model. Total duration for the simulation was from January 1st to August 31st 2000 (240 days). Discussions on the results obtained are also offered alongside temperature and heating load graphs.

5.1 RESULTS FOR CASE ONE: Heater ONLY without PCM

Fig 5.0: Weekly comfort temperature Heater ONLY without PCM and HVAC system
5.2 RESULTS FOR CASE TWO: HVAC system without PCM

Fig 5.0a: Weekly comfort temperature without PCM

Fig 5.0b: Heat and cooling loads for the building without PCM
Fig 5.0c: Hourly comfort temperature with heating inset for control case.

5.4 RESULTS FOR CASE THREE: HVAC system with varied melting temperatures for the PCMs

5.4.1 RT 21 PCM

Fig 5.1a: Hourly comfort temperature with control case (No PCM) and RT21 PCM (T_m = 21°C)
Fig 5.1b: RT21 PCM temperature ($T_m = 21^\circ C$)

Fig 5.1c: Heating and cooling loads for control case (No PCM) and RT21 PCM ($T_m = 21^\circ C$)
Fig 5.2a: Hourly comfort temperature with control case (No PCM) and RT21 PCM ($T_m = 23^\circ C$)

Fig 5.2b: RT21 PCM temperature ($T_m = 23^\circ C$)
Fig 5.2c: Heating and cooling loads for control case (No PCM) and RT21 PCM ($T_m = 23^\circ C$)

Fig 5.3a: Hourly comfort temperature with control case (No PCM) and RT21 PCM ($T_m = 25^\circ C$)
Fig 5.3b: RT21 PCM temperature ($T_m = 25^\circ$C)

Fig 5.3c: Heating and cooling loads for control case (No PCM) and RT21 PCM ($T_m = 25^\circ$C)
Fig 5.4a: Hourly comfort temperature with control case (No PCM) and RT21 PCM ($T_m = 27^0C$)

Fig 5.4b: RT21 PCM temperature ($T_m = 27^0C$)
Fig 5.4c: Heating and cooling loads for control case (No PCM) and RT21 PCM ($T_m = 27^{\circ}C$)

Fig 5.5a: Hourly comfort temperature with control case (No PCM) and RT21 PCM ($T_m = 30^{\circ}C$)
Chapter 5: Results and Discussions

Fig 5.5b: RT21 PCM temperature ($T_m = 30^\circ C$)

Fig 5.5c: Heating and cooling loads for control case (No PCM) and RT21 PCM ($T_m = 30^\circ C$)
5.4.2 SP22A17 TYPE

Fig 5.6a: Hourly comfort temperature with control case (No PCM) and SP22A17 PCM \( (T_m = 21^0\text{C}) \)

Fig 5.6b: SP22 A17 PCM temperature \( (T_m = 21^0\text{C}) \)
Fig 5.6c: Heating and cooling loads for control case (No PCM) and SP22A17 PCM ($T_m = 21^\circ C$)

Fig 5.7a: Hourly comfort temperature with control case (No PCM) and SP22A17 PCM ($T_m = 23^\circ C$)
**Chapter 5: Results and Discussions**

**Fig 5.7b:** SP22 A17 PCM temperature ($T_m = 23^0C$)

**Fig 5.7c:** Heating and cooling loads for control case (No PCM) and SP22A17 PCM ($T_m = 23^0C$)
Fig 5.8a: Hourly comfort temperature with control case (No PCM) and SP22A17 PCM ($T_m = 25^0C$)

Fig 5.8b: SP22 A17 PCM temperature ($T_m = 25^0C$)
Fig 5.8c: Heating and cooling loads for control case (No PCM) and SP22A17 PCM ($T_m = 25^\circ C$)

Fig 5.9a: Hourly comfort temperature with control case (No PCM) and SP22A17 PCM ($T_m = 27^\circ C$)
Chapter 5: Results and Discussions

Fig 5.9b: SP22 A17 PCM temperature ($T_m = 27^\circ$C)

Fig 5.9c: Heating and cooling loads for control case (No PCM) and SP22A17 PCM ($T_m = 27^\circ$C)
Fig 5.91a: Hourly comfort temperature with control case (No PCM) and SP22A17 PCM ($T_m = 30^\circ$C)

Fig 5.91b: SP22 A17 PCM temperature ($T_m = 30^\circ$C)


5.4 DISCUSSIONS

The first simulation run (case one in section 4.3.1) for the 10kW heater in the building clearly shows high frequency of the number of overheating days most especially during the summer weeks. Indoor comfort temperature reaches a peak of 34.4°C on week 25. Situations when the indoor diurnal temperatures are above the level of comfort are most unsatisfactory to the occupants in the building and it is therefore imperative that the room be fitted with a cooling (HVAC) system which would maintain comfort temperature by heating as well as cooling the indoor air temperatures when necessary.

The second simulation run (case two in section 4.3.2) shows improved levels of comfort with the inclusion of 10kW HVAC system. Average indoor temperature of 21°C was roughly maintained throughout the year by the HVAC systems especially during the hot summer weeks (between 23rd to 34th week). Although, space cooling loads are high during this period as shown in graph of the heating and cooling loads (Fig 5.0b). Days of overheating were predominantly observed during the winter period as shown in the weekly comfort temperature graph (Fig 5.0c). During this overheating period, comfort temperatures range between 28°C to 31°C. Total space heating and
cooling load observed was 22557 kWh. A value largely due to the high amount of energy (15487 kWh) used for heating the building during the winter period.

The third set of simulations (case three in section 4.3.3) results for varied melting temperature of the two PCMs under consideration are shown from figures 5.1a to 5.5c for RT21 PCM and figures 5.6a to 5.91c for SP22 A17. The following paragraphs analyse the individual PCM in detail.

Figure 5.1a, 5.2a, 5.3a, 5.4a and 5.5a show the variation of indoor comfort temperature for RT21 PCM melting temperatures of 21°C, 23°C, 25°C, 27°C and 30°C respectively. At the melting point of 21°C, the RT21 PCMs show a decrease in the indoor air temperature by about 0.5K to 1.0K. The latent storage property was active for most days of the week considered as shown in Figure 5.1b. For the week (4th to 11th June) selected for the 23°C melting temperature, difference of about 0.1K in indoor comfort temperature was observed. Analysis of the PCM temperature (Fig 5.2b) shows that the material often undergoes sensible heat storage during that week, thus less heat energy is stored and released into the room in comparison to the energy from the latent heat storage region. The heating loads are noticeable reduced on all days except on the 3rd day (7th June) as shown in Fig 5.2c. At 25°C melt temperature, comfort temperatures reduced by a difference of about 0.05K was observed between the periods of 1st to 8th August. The PCM does not undergo latent storage during the week since the melt temperature is not attained as shown in fig 5.3b. For the overheating period in the winter season (8th to 15th January), the RT21 PCM with melting temperature of 27°C was able to absorb and release latent heat energy for the last three days. The PCM with the melting temperature at 30°C seldom experienced latent heat storage for the winter period considered.

The SP22 A17 PCM types showed greater degree of difference in comfort temperature for the melting temperature of 21°C. Differences in comfort temperatures ranged from about 1.0K to 1.2K across the week (Fig 5.6a). The difference is most noticeable during at night time when the temperature drops and the PCM rejects portion of the stored heat back into the room. Thus keeping the room from getting to cold at night. PCM temperature show frequent days of latent heat energy thermal storage (Fig 5.6b) across the week. At melting temperature of 23°C, indoor comfort temperatures range between 0.8K to 1.0K despite the fact that PCM melt temperature was not attained during this period (Fig 5.7b). Slight savings in heating loads were observed on the 1st, 4th and 7th days of the selected week. Minimal difference in the indoor comfort levels for the 25°C PCM melting temperature was observed as 0.2K. Latent heat storage did not occur for the 27°C and
30°C melting temperature. Although, the sensible heat exchange was responsible for decreasing the indoor comfort temperature by about 1K in both cases. The 5\textsuperscript{th} of the 300°C melting temperature PCM showed a reduction in the hourly fluctuations of indoor temperature in comparison to the case of no PCM (Fig 5.91a).

Analysis of the annual energy stored by the two types of PCM for varied melting temperature showed maximum amounts of heat flow through the PCM at a melting temperature of 21°C for the both PCMs. The SP22 A17 PCM exhibited higher diurnal energy storage property due to its higher latent heat energy and specific heat capacity. The heat flow graphs are shown below.

Fig 5.92a: Annual Heat flow through the RT21 PCM
Chapter 5: Results and Discussions

5.5 SUMMARY OF RESULTS

In summary, it was observed that PCMs function at best when installed with a melting temperature within the range of the average room temperatures. When the melting is set above the average room temperature, only sensible heating and cooling processes occur in the solid state. If the melting point is set below the room temperature, sensible heat process would occur only in the liquid state. The heat energy during sensible heating is just a fraction of the amount of heat energy that is stored during the latent energy state. It was also observed that when the PCM melting temperature was higher than the room temperature, more work was done by the HVAC system to maintain conducive temperature in the room. An instance of this was observed on the 5th day of the use of the SP22 A17 at 27°C melting temperature in figure 5.91c. Both PCM showed slight improvements in reducing the level of overheating experienced in the room. This may be due to the fact that it was only the ceiling area (44m²) that housed the PCMs. Additional application of PCM to the all the walls of the building is expected to provide improved comfort temperature results.
CHAPTER 6

CONCLUSION AND RECOMMENDATION

6.0 CONCLUSION AND RECOMMENDATIONS

Phase change heat transfer has been critically reviewed and an ESL computational model has been developed to study the latent and sensible regions. The effects on indoor comfort temperatures, heating loads as well as heat energy stored have also been analysed in a building model with inclusion of two types of PCMs at varied melting temperatures. It was observed that the most essential properties that govern the PCM functionality when incorporated into a building design for the purpose of indoor temperature regulation are the melting temperature, the amount of latent heat energy that can be stored and the transitional temperature range.

From the simulations carried out, it was observed that maximum daily storage occurred for both PCMs at a melting temperature of 21°C. This is in agreement with Neeper’s [7] observation that PCMs function optimally when their melting temperature is close to the room temperatures. Although, Kendrick and Walliman [32] observed that the effectiveness of a PCM is affected when the melting temperature is fixed at the set point of the HVAC equipment. A condition which they further suggest can be resolved by placing the PCM in the ceiling. It then becomes effective because of the thermal stratification of temperature in the enclosure.

Designing a PCM that would function effectively throughout the year is quite challenging [25]. Temperature fluctuations in the building envelop need to be kept at an acceptable range for the PCM to work. In order to achieve this, the following recommendations need to be implemented prior to incorporating PCMs into the building environment:

1. The building should be properly insulated from the external environment. This is necessary so as to enable the PCM with a fixed melting temperature to be selected for operation throughout the year. Minimising the effect of the ambient weather conditions on the indoor temperature would reduce the temperature fluctuations experienced in the enclosure.
2. Strict occupancy behaviours should be enforced. For example, windows should be controlled automatically by opening and closing at specific times or when the outdoor temperatures are at a predefined temperature level.

3. Tests such as the computational fluid dynamics (CFD) analysis need to be performed prior to installation of the PCM so as to analyse the air flow regimes and nodal temperature variations of the building.

6.1 SUGGESTIONS FOR FUTURE WORK

This study is the first step in the integration of the VHC discontinuity method into the effect heat capacity method to represent the phase change thermal processes of a PCM. The initial building model implemented in ESL simulation language, used to analyse the effects of inclusion of PCM ceiling tiles performed as expected but further refinements are required. The research was limited by the availability of experimental data for the selected PCM. It is therefore recommended that the model be validated via experimental studies. Incorporation of a PCM temperature controller which could increase the efficiency of the material by providing night time cooling for the device so as to improve the thermal storage capacity and eliminate chances of overloading before the next day charge cycle will need to be incorporated into the model in the future.
REFERENCES


Appendix A

MODULES CONTAINED IN THE ESL CODE

The description and functions of the models and sub models contained in the PCM code are given in this section. The subroutines contained in these modules are also listed and described. They include:

1. **zone_40**
   The zone_40 model is the top level program module of the simulation which defines the interconnections between the submodels. In ESL it is referred to as the study. It is here that other submodels are linked with one another with the “INCLUDE” statement. The dynamic region of the model contains the calls to submodels input and output variables specified in the argument list. The integration algorithm (RK4), communication intervals, start and finish times as well as integration steps are defined in this model.

2. **sm_pc**
   The zone submodel defines the electrical devices present in the building model. Some examples of such devices include PC, projectors and monitors. It contains a procedural switch stamen that controls the ON and OFF times of the appliances in the building model.

3. **sm_environment**
   The sm_environment submodel contains the code to read the weather data .csv file into the program. The external lux and wind speeds are also read into the program.

4. **sm_build**
   The sub model contains the dynamic code for the temperature rate of change for the building and PCM as well as VHC discontinuity logical code and other PCM calculations such as the volume of the material and rate of heat flow through the material. The PA_PARAMERS package is linked to the sub model by the “USE” statement. This package contains defined parameters for the PCM as well the necessary ones for the building. The initial section of the program contains the values for the initialising the state variables such as temperature parameters for the building and the PCM. The PCM was set to an initial temperature of the temperature of the air at 15°C.

5. **sm_actuatorfull**
   The sm_actuator full contains the code for controlling the HVAC control system in the building model. For the model in this paper, the set control temperature was 21°C and the rated power of the system was 10kW.
Appendix B
Phase Change Materials Data Sheets

RUBITHERM® SP

Latent Heat Blend

The creation of the latent heat blend RUBITHERM SP has lead to a new and innovative class of low flammability PCM. RUBITHERM SP consists of a unique composition of salt hydrates and organic compounds. This combination unites the advantages of both classes of PCM, salt hydrate based as well as latent heat paraffin based.

RUBITHERM SP is preferably processed into sustaining and/or absorptive structure (e.g. foams). Material densities of 1.0 kg/l and more can be achieved. These properties make RUBITHERM SP the preferred PCM used in the construction industry. Passive and active cooling is now possible e.g. in wall elements and air conditioners.

Properties:
- Stable performance throughout the phase change cycles
- High thermal storage capacity
- Limited supercooling
- low flammability
- non toxic
- Different melting temperatures between 18°C und 29°C are available
<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting area</td>
<td>22 - 24</td>
</tr>
<tr>
<td>Congealing area</td>
<td>21 - 19</td>
</tr>
<tr>
<td>Typical being: 23°C</td>
<td></td>
</tr>
<tr>
<td>Heat storage capacity</td>
<td>150</td>
</tr>
<tr>
<td>Temperature range 13°C to 28°C</td>
<td></td>
</tr>
<tr>
<td>Density solid at 15°C</td>
<td>1.49</td>
</tr>
<tr>
<td>Density liquid at 35°C</td>
<td>1.43</td>
</tr>
<tr>
<td>Volume expansion with phase change and ΔT= 20 K</td>
<td>4.03</td>
</tr>
<tr>
<td>Heat conductivity</td>
<td>0.6</td>
</tr>
<tr>
<td>Kin. Viscosity at 55°C</td>
<td>111.1</td>
</tr>
<tr>
<td>corrosion</td>
<td>Corrosive compared to metal</td>
</tr>
<tr>
<td>Water hazard</td>
<td>Water hazard class (WGK): 1, low hazardous to waters (self-classification)</td>
</tr>
</tbody>
</table>

Note: The product is hygroscopic. If stored in a not completely self contained container the material may absorb moisture. This could result in other than the given physical properties.
RUBITHERM® RT

Phase Change Material based on n-Paraffins and Waxes

A new generation of ecological heat storage materials utilizing the processes of phase change between solid and liquid (melting and congealing) to store and release large quantities of thermal energy at nearly constant temperature.

The RUBITHERM® phase change materials (PCM’s) provide a very effective means for storing heat and cold, even when limited volumes and low operating temperature differences are applicable.

We look forward to discussing your particular questions, needs and interests with you.

Properties:

- High thermal energy storage capacity
- Heat storage and release take place at relatively constant temperatures
- No supercooling effect
- Long life product, with stable performance through the phase change cycles
- Ecologically harmless and non-toxic
- chemically inert
- Melting temperature range between approx. –4 °C and 100 °C
## Data Sheet

**RUBITHERM® RT 21**

(based on: RT 20)

### Typical Values

<table>
<thead>
<tr>
<th>Property</th>
<th>Unit</th>
<th>Value</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting area</td>
<td>°C</td>
<td>18 - 23</td>
<td>typical being: 21°C</td>
</tr>
<tr>
<td>Congealing area</td>
<td>°C</td>
<td>22 - 19</td>
<td>typical being: 22°C</td>
</tr>
<tr>
<td>Heat storage capacity</td>
<td>kJ/kg</td>
<td>134</td>
<td></td>
</tr>
<tr>
<td>temperature range 15°C to 50°C</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Density solid at 15°C</td>
<td>kg/l</td>
<td>0.88</td>
<td></td>
</tr>
<tr>
<td>Density liquid at 25°C</td>
<td>kg/l</td>
<td>0.77</td>
<td></td>
</tr>
<tr>
<td>Volume expansion</td>
<td>%</td>
<td>14</td>
<td></td>
</tr>
<tr>
<td>In phase change range</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Heat conductivity</td>
<td>W/(m*K)</td>
<td>0.2</td>
<td></td>
</tr>
<tr>
<td>Kin. Viscosity at 50°C</td>
<td>mm²/s</td>
<td>25.71</td>
<td></td>
</tr>
<tr>
<td>Flash point (PCM)</td>
<td>°C</td>
<td>154</td>
<td>chemically inert with respect</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>to most materials</td>
</tr>
<tr>
<td>corrosion</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>water hazard</td>
<td></td>
<td>Water hazard class (WGK) 1</td>
<td></td>
</tr>
</tbody>
</table>