Universitat de Lleida

TESI DOCTORAL

Simulation-based optimization of thermal energy storage (TES) materials for building and industry applications

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Memòria presentada per optar al grau de Doctor per la Universitat de Lleida
Programa de Doctorat en enginyeria i tecnologies de la informació

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(2017)

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Acknowledgements

I would first like to thank my thesis advisors Prof. Dr. Luisa F. Cabeza of the Polytechnic Superior School at University of Lleida, and Dr. Alvaro de Gracia of the Mechanical Engineering department at University of Rovira i Virgili.

The doors to Prof. Dr. Luisa F. Cabeza and Dr. Alvaro de Gracia offices were always open whenever I ran into a trouble spot or had a question about my research or writing. They consistently allowed this thesis to be my own work, but steered me in the right direction whenever they thought I needed it. Without their precious support it would not be possible to conduct this research.

Also, I wish to acknowledge the assistance and support of Dr. Martin Belusko and Dr. Alemu Alemu from Barbara Hardy Institute at University of South Australia (UniSA), who provided me an opportunity to join their team as visiting research student under INNOSTORAGE project.

Furthermore, I would like to particularly extend his thanks to his colleagues and friends at GREiA Innovació Concurrent from University of Lleida, and all of my friends at University of South Australia for all the fun, for the good moments that we have had, and for their very kind collaboration during these years.

I would like to acknowledge all the funding institutions that have supported this research: including the Catalan Government for the quality accreditation given to GREA research group (2009 SGR 534, 2014 SGR 123), the Spanish Government (ENE2011-28269-C03-02 and ENE2015-64117-C5-1-R (MINECO/FEDER)), the European Commission Seventh Framework Programme (FP/2007-2013) for Grant agreement No. PIRSES-GA-2013-610692 INNOSTORAGE, the European Union's Horizon 2020 research and innovation programme for grant agreement No. 657466 INPATH-TES, and the city hall of Puigverd de Lleida.

Finally, I must express my very profound gratitude to my parents and to my sister for providing me with unfailing support and continuous encouragement throughout my years of study and throughout the process of researching and writing this thesis. This accomplishment would not have been possible without them. Thank you.

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Mohammad Saffari

Summary

A substantial amount of energy is used in building and industry sectors for heating and cooling purposes. Thermal energy storage (TES) materials can offer important short-term and long-term energy, economic, and comfort benefits to residential, commercial, and industrial buildings.

In residential buildings, providing the thermal comfort for occupants is of a high importance whether in mechanically or naturally ventilated buildings. The application of innovative thermal energy storage (TES) materials such as phase change materials (PCM) offers an attractive solution to increase the thermal mass of buildings envelopes, thus reducing the temperature fluctuation in buildings. In the industry sector, on the other hand, new energy policies are encouraging the consumers to use solar photovoltaic (PV) for electricity generation and also to increase the flexibility of their systems by integrating TES systems.

TES materials have the potential to reduce the cooling and peak electricity demands in building and industry sectors, however, in order to properly implement this technology to maximize the economic benefits, numerical simulation and optimization techniques are necessary. The present thesis has gone towards enhancing the understanding of using and implementing TES materials in residential and commercial buildings. Different energy-related aspects due to the application of TES materials will be investigated.

The significant original contribution emerges from the present thesis is the use of numerical simulation and optimization methods to advance the application of TES technology in the industrial and building sector. To achieve this, a review will be presented regarding the use of whole-building energy simulation tools to analyse buildings passively enhanced with TES materials.

Further on, to control the HVAC system in PCM-enhanced buildings, a new methodology based on Fanger thermal comfort algorithm is presented to simulate the occupants behaviour and their influence in energy conservation.

Additionally, simulation-based optimization will be performed based on an innovative enthalpy-temperature function to find out the optimum PCM melting temperature for building applications.

Besides, the energy performance of buildings enhanced with PCM will be analysed for cooling, heating, and total annual heating and cooling under cooling dominant climates, heating dominant climates, and climates with both heating and cooling demands.

Moreover, the influence of PCM to decrease the cool roof membrane heat stress and to improve its performance in buildings will be studied based on simulation and optimization techniques. Also, optimization techniques and advanced control strategies will be applied to couple TES with solar PV to reduce and shift peak electricity load of cooling and refrigeration processes for industrial purposes.

Resumen

Una cantidad substancial de energía se utiliza en los sectores de la edificación y de la industria para los propósitos de la calefacción y de la refrigeración. Los materiales de almacenamiento de energía térmica (TES) pueden ofrecer importantes beneficios energéticos y económicos a los edificios residenciales, comerciales e industriales.

En edificios residenciales, proporcionar la comodidad térmica o confort para los ocupantes es de una alta importancia. La aplicación de materiales innovadores de TES como los materiales de cambio de fase (PCM) ofrecen una solución única para aumentar la masa térmica de los cerramientos de los edificios, lo que reduce la fluctuación de la temperatura en los edificios. En el sector industrial, por otra parte, las nuevas políticas energéticas alientan a los consumidores a utilizar energía solar fotovoltaica (PV) para la generación de electricidad y también a aumentar y mejorar la flexibilidad de sus sistemas mediante la integración de sistemas de TES.

Los materiales de TES tienen el potencial para reducir las demandas de enfriamiento y de la electricidad máxima en sectores de la edificación y de la industria; sin embargo, con el fin de implementar adecuadamente esta tecnología para maximizar los beneficios económicos, se necesitan técnicas de simulación y optimización numérica. La presente tesis ha ido encaminada a mejorar la comprensión del uso e implementación de materiales de TES en edificios residenciales, comerciales e industria. Se investigarán diferentes aspectos relacionados con la energía debido a la aplicación de los PCMs.

La importante contribución original que emerge de la presente tesis es el uso de métodos de simulación numérica y optimización para avanzar la aplicación de la tecnología TES en los sectores residenciales e industriales. Para ello, se presentará una revisión con respecto al uso de herramientas de simulación de energía para el desarrollo de edificios para analizar pasivamente los materiales realzados con TES.

También, para controlar el sistema de climatización en los edificios mejorados por PCM, se presenta una nueva metodología basada en el algoritmo de confort térmico de Fanger para simular el comportamiento de los ocupantes y su influencia en la conservación de la energía.
Además, la optimización basada en la simulación se llevará a cabo en base a una innovadora función de entalpía de temperatura para encontrar la temperatura óptima de fusión del PCM para el enfriamiento, la calefacción, y el rendimiento anual de la energía de calefacción y enfriamiento total bajo refrigeración dominante, calefacción dominante, y climas con las demandas de calefacción y refrigeración.

Adicionalmente, la influencia del PCM para disminuir el estrés térmico de la membrana del techo fresco y mejorar su rendimiento en los edificios se estudiará en base a técnicas de simulación y optimización.

Por otra parte, se aplicarán técnicas de optimización y estrategias avanzadas de control para acoplar TES con PV solar a la reducción y desplazamiento de la carga eléctrica máxima de refrigeración y procesos de refrigeración para fines industriales.

Resum

Una quantitat substancial d'energia s'utilitza en els sectors de l'edificació i de la indústria per als propòsits de la calefacció i de la refrigeració. Els materials d'emmagatzematge d'energia tèrmica (TES) poden oferir importants beneficis energètics i econòmics als edificis residencials, comercials i industrials.

En edificis residencials, proporcionar la comoditat tèrmica o confort per als ocupants és d'una alta importància. L'aplicació de materials innovadors de TES com els materials de canvi de fase (PCM) ofereixen una solució única per augmentar la massa tèrmica dels tancaments dels edificis, el que redueix la fluctuació de la temperatura en els edificis. En el sector industrial, d'altra banda, les noves polítiques energètiques encoratgen als consumidors a utilitzar energia solar fotovoltaica (PV) per a la generació d'electricitat i també a augmentar i millorar la flexibilitat dels seus sistemes mitjançant la integració de sistemes de TES.

Els materials de TES tenen el potencial per reduir les demandes de refredament i de l'electricitat màxima en sectors de l'edificació i de la indústria; però, per tal d'implementar adequadament aquesta tecnologia per maximitzar els beneficis econòmics, es necessiten tècniques de simulació i optimització numèrica. La present tesi ha anat encaminada a millorar la comprensió de l'ús i implementació de materials de TES en edificis residencials, comercials i indústria. S'investigaran diferents aspectes relacionats amb l'energia a causa de l'aplicació dels PCMs.

La important contribució original que emergeix de la present tesi és l'ús de mètodes de simulació numèrica i optimització per avançar l'aplicació de la tecnologia TES en els sectors residencials i industrials. Per a això, es presentarà una revisió pel que fa a l'ús d'eines de simulació d'energia per al desenvolupament d'edificis per analitzar passivament els materials realçats amb TES.

També, per controlar el sistema de climatització en els edificis millorats per PCM, es presenta una nova metodologia basada en l'algoritme de confort tèrmic de Fanger per simular el comportament dels ocupants i la seva influència en la conservació de l'energia.

A més, l'optimització basada en la simulació es durà a terme d'acord amb una innovadora funció d'entalpia de temperatura per trobar la temperatura òptima de fusió del PCM per al refredament, la calefacció, i el rendiment anual de l'energia de calefacció i refredament total sota refrigeració dominant, calefacció dominant, i climes amb les demandes de calefacció i refrigeració.

Addicionalment, la influència del PCM per disminuir l'estrès tèrmic de la membrana del sostre fresc i millorar el seu rendiment en els edificis s'estudiarà en base a tècniques de simulació i optimització.

D'altra banda, s'aplicaran tècniques d'optimització i estratègies avançades de control per acoblar TES amb PV solar a la reducció i desplaçament de la càrrega elèctrica màxima de refrigeració i processos de refrigeració per a fins industrials.

Nomenclature

ACO	Ant Colony Optimization
CIP	Constraint Integer Programming
ConFD	Conduction Finite Difference
COV	Coefficient of Variability
CP	Constraint Programming
DE	Differential Evolution
DSM	Demand Side Management
EP	Evolutionary Programming
FDM	Finite Difference Method
GA	Genetic Algorithms
GP	Genetic Programming
HS	Harmony Search
MILP	Mixed-Integer Linear Programming
PCM	Phase Change Material
PSO	Particle Swarm Optimisation
PV	Photovoltaic
SA	Simulated Annealing
SAT	Satisfiability
TES	Thermal Energy Storage
UHI	Urban Heat Island

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1. Introduction

1.1. Energy use in building and industry sectors

Most of the observed global warming is very likely due to human activities such as burning fossil fuels, oil, gas, and deforestation. Our societies have been combusting increasing amounts of fossil fuels for electricity generation, air conditioning of buildings, and transportation, especially in developed and industrialized nations. These activities induce releasing huge amounts of greenhouse gases into the atmosphere which is boosting the greenhouse effect. The most common greenhouse gas produced by human activities is carbon dioxide (CO_2) which accounts for about 64% of human-caused global warming [1,2]. Globally, a considerable energy is used in the building sector for heating, ventilation, and air conditioning systems to provide thermal comfort for occupants [3], hence, offering a specific potential for sustainable energy investment [4]. For example in 2011, the building sector dedicated 14% of global primary energy use to itself (Figure 1). Besides, the share of the industry sector in primary energy use in the same year was about 22%. In addition, building and industry sectors produced 8% and 26% of global CO_2 emissions in 2011 (Figure 1).

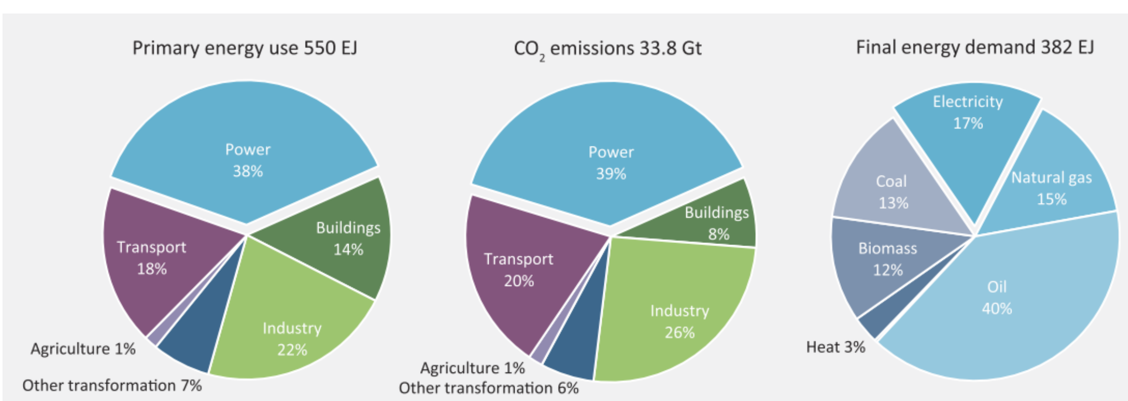

Figure 1. Primary energy use by sector, CO_2 emissions by sector, and final energy by fuel in 2011 [5].

Electricity plays an important role in the global energy system. Almost 40% of global primary energy is used to generate electricity, making electricity a core commodity in the energy system [5]. For example in 2011, 17% of the global final energy demand was belonged to electricity use which shows the high dependency of the global energy system to electric energy (Figure 1). Later on, in 2014 building (residential) and industry sectors consumed about 7000 TWh and 6000 TWh of electricity, respectively. According to World Energy Outlook 2016 [6], the electricity consumption in building and industry sectors will rise to about 40% and 30% in 2040, respectively (Figure 2).

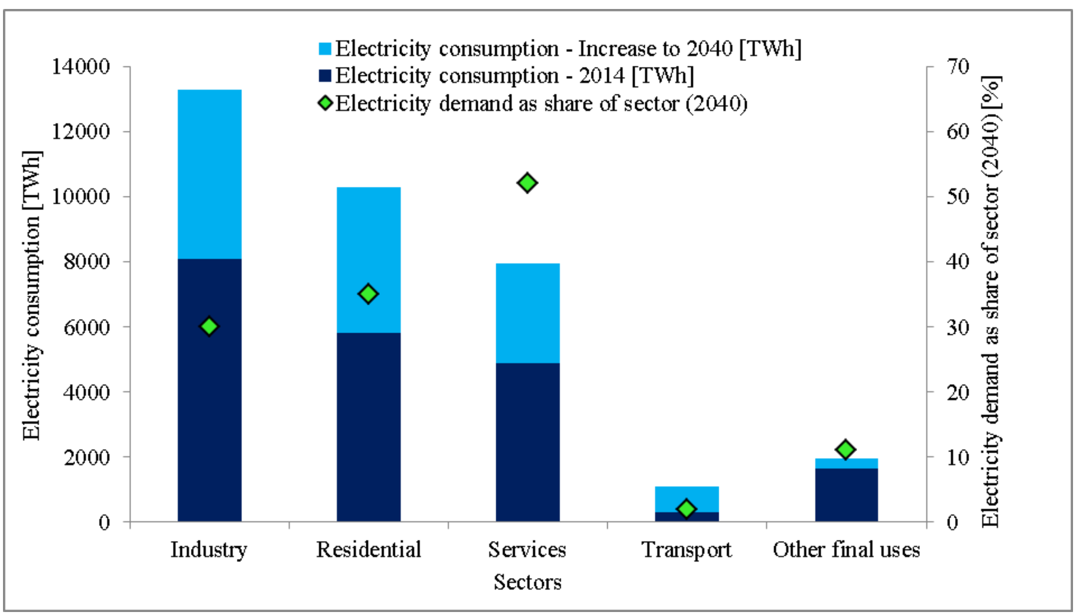

Figure 2. Growth in global electricity demand by sector and electricity´s share of sector demand in New Policies Scenario, adopted from [6].

In the industry sector peak electricity demand at on-peak or high-demanding hours is a big concern. Electricity storage in a large scale is not feasible; therefore electricity has to be consumed in real time covering the demand. On the other hand, since generation plants with different supply sources such as thermal, solar photovoltaic (PV), hydro, wind, and other renewables of variable efficiency are used to meet demand, the cost of electricity varies hour to hour, day to day, and month to month [7]. Additionally, variability in both demand profiles and renewable energy sources makes the energy management of the grid more difficult and increases the cost of electric power generation [8].

To overcome these global concerns, policy makers are endeavouring to put effective solutions on the table to decrease these problems. As an example, the European Commission has defined a cost-effective pathway for achieving high emission reductions by 2050. Roadmap 2050 long-term policy is seeking to a more sustainable way to use resources. The Roadmap aims to cut off EU emissions to 80% below 1990 levels just through domestic reductions; to achieve this goal it sets out milestones in a cost-effective way to reduce emissions up to 40% by 2030 and 60% by 2040. Also it indicates how the main responsible sectors for greenhouse gas emissions in Europe such as power generation, industry, transport, building and construction, and agriculture can lead to a low-carbon economy with a minimum cost [1,9,10]. Among the possible solutions on the table, passive cooling and heating using thermal energy storage (TES) technology and renewable electricity generation are of very high priority and importance.

1.2. Thermal energy storage

Today, almost in all low-carbon energy scenarios, TES is a key element. This technology is an effective way to enhance the energy efficiency and to reduce the energy use in building and industry sectors [11]. TES technologies are valuable components in the most energy systems and can be essential tools to approach a low-carbon future [12]. The major advantages of TES systems are increasing energy efficiency, system performance, thermal comfort, economic benefits, reduction of CO_2 emissions, and capital and operational costs [13]. In general, TES can narrow the gap between the global energy demand and the supply in various applications [14]. Energy could be stored physically or chemically. In physical processes energy is stored as sensible or/and latent heat, on the other hand thermochemical energy storage takes place when a chemical reaction with high heat of reaction happens [15]. For building applications, mostly sensible heat storage and latent heat storage are considered; however, today thermochemical energy storage is gaining more interest within researchers [16].

Sensible heat storage is one of the most typical methods for heat storage since it has two main advantages: first, it is cheap and second, no toxic materials are used in it. Additionally, the material used to store energy is contained in vessels as bulk material which facilitates the system design [17]. Sensible heat storage happens by increasing or decreasing the temperature of the material and the amount of stored energy could be calculated according to the following equation:

$$dQ = m \,.\, C_p \,.\, \Delta T \qquad (1)$$

where Q stands for the amount of sensible heat stored in the material (J), m is the mass of the storage material (kg), C_p is the specific heat of the storage material (J/kg·K), and ΔT is the temperature change (K) [13,15].

The sensible heat storage could be achieved by solid materials (such as concrete, brick, and stone) and liquid materials (such as water). However, a disadvantage of using sensible heat storage in the building sector is the high volume that it requires depending on the amount of desired heat stored from the active or passive technology [17].

Latent heat storage takes place by phase transition of the storage material. When heat is transferred to the storage material, melting takes place within a small range of temperature, storing a large quantity of heat, which is called melting temperature or phase change temperature. After this stage, further increase of heat results in an addition of sensible heat storage. This heat then dissipates by solidification of the storage material. The latent heat stored over the phase change process is calculated according to Eq. (2):

$$dQ = \mathrm{dH} = m \, . \, dh \qquad (2)$$

where dQ stands for the amount of latent heat stored to the material and dH the enthalpy difference between the solid and liquid phase.

1.3. PCM for residential, commercial, and industrial applications

Research on the utilization of PCM dates back to the 1970s and 1980s, when it was incorporated into the storage tank and building structure for heating and cooling purposes [18]. Recent developments in thermal energy storage field, pointedly PCM have led to a renewed interest in application of the PCM for building energy saving aspects in terms of new building envelope technologies together with proper passive cooling and heating strategies. PCM based on their properties and mainly melting temperature could be utilized in various areas such as solar heating and cooling systems [19,20], heat pump [21] and heat exchanger [22], water storage tank [23], concrete slab and floor systems [24,25], ventilated façade [26], residential attics [27], cementitious composite [28], and so forth.

For several years a great effort has been devoted to the study of PCM for building applications. With this regard, previous studies documented and classified different types of PCM and their main characteristics for building applications and renewable heating and cooling systems [29,30].

PCMs are classified into two categories: organic and inorganic. Examples of the organic PCMs are paraffin, fatty acids, and the polyethylene glycol (PEG), and examples of inorganic PCMs are salt hydrates [31]. The both organic and inorganic PCMs have some advantages and disadvantages which are listed in Table 1.

Table 1. Different types of PCM and their features [29,31,32].

	Organic PCM	Inorganic PCM
Advantages	-No corrosive -Negligible or none subcooling -Chemical and thermal stability -Availability in a wide-range temperatures -Congruent melting -Self-nucleating properties -Compatible with construction materials -No segregation, high heat of fusion -Safe and non-reactive , recyclable	-Higher heat of fusion -High volumetric latent heat storage capacity -Cheap and easy availability -Steep phase change -High thermal conductivity -Non flammable
Disadvantages	-Low phase change enthalpy -Low thermal conductivity -Flammability -Low volumetric latent heat storage capacity	-Subcooling -Corrosion -Phase change separation -Phase segregation -Lack of thermal stability -High volume change

PCM can be incorporated into building construction materials by direct incorporation, immersion, shape-stabilized PCM, form-stable composite PCM, and encapsulation [33,34], however, PCM has to be encapsulated to avoid the movement of liquid-phase PCM and to prevent its contact with surrounding materials which may adversely influence their performance. Encapsulations are categorized into macroencapsulation and microencapsulation. Macroencapsulation means inclusion of PCM in a macroscopic containment (usually larger than 1 cm) such as tubes, pouches, spheres, panels or other containers. In microencapsulation, solid or liquid particles of 1 μm-1000 μm are encapsulated in a thin, high molecular weight polymeric film. Then, the enclosed particles can be incorporated in any matrix that is adaptable with the encapsulating film. In fact, the film must be adoptable with both PCM and the matrix [15,29,33].

In most applications, PCM are microencapsulated [29]. The main advantages of microencapsulation of PCM are improvement of heat transfer to the surrounding due to large surface to volume ratio of the capsules and the enhancement of cycling stability because phase separation in microscopic distances is less frequent. Further on, the leakage and evaporation problems are solved in this method and the loss of PCM under construction work e.g. cutting the wallboard or screwing is very small. In addition, they could be integrated into other materials to form composite materials [15].

Some popular applications of PCM are their integration into gypsum plasterboard with microencapsulated paraffin [35] which is a popular way to enhance thermal capacity of lightweight buildings, plaster with microencapsulated paraffin [36] that could be applied on the surface of the walls, concrete with microencapsulated paraffin [37], shape-stabilized paraffin panels [38], PCM bricks [39], and wood with PCM [40]. Additionally, PCMs have vast applications for building components such as slabs [41], floors [42], blinds and windows [43,44], and cool roof [45].

Further on, recently, special importance has been given to improve cool roofs performance with PCM integration since roofs represent about the 20%-25% in the urban area and are also characterized by a higher view factor to the incoming solar radiation, especially during summer season. Hence, cool roofs have a great potential for both building energy saving and urban heat island (UHI) mitigation, when efficiently designed [46].

Cool roof coatings and paintings increase the solar reflectance, thus absorbing less heat gains from solar radiation, nevertheless, an important issue that influences the efficiency and workability of cool roof membranes is extreme temperature fluctuations and heat stress from solar radiation and repetitive freeze and thaw cycles. From here the importance of TES technology to improve cool roof performance begins. For instance, Pisello et al. [45] experimentally analysed the application of PCM with polyurethane-based cool roof membrane to enhance the heat stress in the cool roof membrane. However, further research is needed to investigate the impact of PCM characteristics and different climate regions on the improvement of cool roof membrane.

Another important aspect of TES application is in industry sector for cooling and refrigeration purposes. Both sensible and latent TES could be integrated into a system to supply heat or cold of commercial and industrial buildings by means of a heat or cold storage tank. However, the different supply and demand situations have a great influence on the integration concept [15]. The first case to consider is when there is no overlap in time between loading from the supply and unloading to the demand. In this case, the storage system can match different times of supply and demand; in addition, in many cases, the storage system can match different supply and demand power, and even supply and demand locations, with transport of the storage medium. If there is a partial or total overlap in time, it is possible to smooth out fluctuations of the supply and/or the demand. Thus, the principal goals of TES integration are temperature regulation, power matching, and peak load reduction.

The value of TES technologies is found in the services that they provide at different locations in the energy system. These technologies can be used throughout the electricity grid, in dedicated heating and cooling networks, and in distributed system and off-grid applications. To ensure reliable off-grid energy supplies and to support increasing levels of local resources use, energy storage can be used to fill gaps between variable supply resources and demand together with an optimized demand side management system (DSM). Furthermore, they can provide infrastructure support services across supply, transmission and distribution, and demand portions of the energy system. Generally speaking, they can serve as valuable tools for operators in systems with supply and/or demand-side variability. The latter has historically been part of the energy system. The former is an increasing concern in a transition to increased penetration of variable renewables. In the current literature, there has been little discussion about integration of TES and renewable generation such as solar PV for energy management and electricity peak load reduction according to the new tariff structures and further simulation and optimization studies are essential to further investigate in aspect of TES application.

Currently, in available literature, little discussion has been made on the energy optimization of PCM-enhanced passive buildings addressing the appropriate melting point temperature of PCM taking into account various climate conditions. This shows the necessity of carrying out further numerical simulation and optimization in this field.

1.4. Whole-building energy simulation

Numerical simulation can model and predict an outcome based on what has happened in the past or on current trends, and it is critical to success in many fields such as aircraft manufacture, space exploration, and the planning, design, construction, and operation of buildings and energy systems. Modelling allows evaluation of alternative designs, technologies, or processes without having to for example constructing a whole building which is costly. On the other hand, some technologies require models to assess performance relative to competing options. For example, building and energy engineers use dynamic simulation tools to evaluate buildings passive and active energy performance. So that, it is more economically beneficial to create a model of the underlying physical processes and test alternative configurations than to build a real prototype and have to change it later based on trial and error [47].

Reliable whole-building energy simulation tools can numerically facilitate design, analysis and optimization of the PCM-enhanced building component with no need to set up expensive and time consuming whole-building field experiments [48]. Further on, computer-based simulation tools help designers and engineers to evaluate potential decisions and achieve long-term targets. For example, some researchers developed thermal load predictive models of commercial buildings using building energy simulation software [49]. In another study, whole-building simulation was used for the benchmarking of residential buildings [50]. Additionally, the validated model can always be employed for parametric or optimization studies and it has more general applications than an experimental work.

Analysing and computing the heat transfer phenomenon in the building envelope and the dynamic interactions between the outdoor and indoor environment, the HVAC system, thermal comfort of the occupants and their behaviour, is a complex task especially when PCM is incorporated into the building envelope. Additionally, application of PCM requires special attention to choose proper materials, the location, and the quantity of PCM [51]. In this regard, dynamic building simulation is required to measure energy performances coming from new designs and technologies applied to the building and it is a cost effective method to analyse the performance of the buildings [52]. Simulation has various advantages such as studying the effects of different parameters and optimization scenarios affecting energy performance of the building and thermal satisfaction of the occupants in different climatic zones. Simulation is highly appreciated since it is the cheapest and the fastest way to analyse the effects of new technologies such as PCM on the energy performance of the building.

A considerable amount of literature has been published on Building Energy Simulation (BES) taking into account the PCM effects [53]. There are numerous building energy simulation programs that are accurate and capable of carrying out dynamic energy simulation [54] but there are few whole building energy simulation programs that can simulate the effects of PCM on the energy performance of the building and comfort level of the occupants [53]. EnergyPlus [55–58], TRNSYS [59–61], ESP-r [62–64] and BSim [65,66] are those popular simulation software that can handle phase change material modelling in the building. Furthermore, there are some other simulation programs with limited capabilities that can simulate PCM in buildings that are mentioned in literature [53]. However, in order to make use of these featured capabilities one must have strong enough background and conscience in building technologies, materials science, and heat transfer phenomenon.

1.5.Optimization

Optimization is referred to as “the action of making the best or most effective use of a situation or resource”. Furthermore, the optimization approach makes sure that the search is done as efficiently as possible. From the general standpoint of searching for the best available design, optimization can be defined as follows: “Mathematical optimization is the process of maximizing and/or minimizing one or more objectives without violating specified design constraints, by regulating a set of variable parameters that influence both the objectives and the design constraints”. It is important to realize that in order to apply mathematical optimization; the objective(s) and the design constraint(s) should be expressed as quantitative functions of the variable parameters. These variable parameters are also known as design variables or decision variables [67]. In recent years using optimization techniques applied to renewable energy researches has been increased substantially (Figure 3).

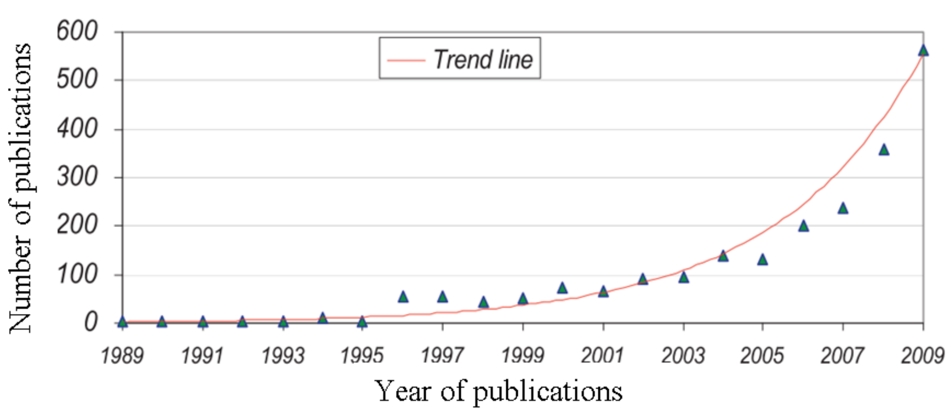

Figure 3. The trend of applying optimization algorithms in renewable energy researches for 20 years, adopted from [68].

Computational optimization can be defined as the process of designing, implementing and testing algorithms for solving a large variety of optimization problems. Computational optimization includes the disciplines of mathematics to formulate the model, operations research to model the system, computer science for algorithmic design and analysis, and software engineering to implement the model. Today, researchers can solve real-life problems that in the past were thought to be unsolvable with the help of new technological developments in algorithms and computer hardware [68].

The general mathematical description of an optimisation problem can be written as Eq. 3 [69]:

$$\textit{Minimise or Maximise } F(x_1, x_2, \dots, x_n) \tag{3}$$
$$G(x_1, x_2, \dots, x_n) \geq 0$$
$$X_i \in S_i$$

There could be one or more than one objective functions F, which could be minimized or maximized. There are a number of functional constraints G, which by convention must be greater than or equal to zero. Each design variable x_i is constrained to certain values S_i, defined either as discrete or continuous values. Objectives and constraints may be interchangeable, depending on how the problem is formulated.

1.5.1. Optimisation algorithms

Different optimisation algorithms could be used for optimisation of building energy technologies. Heuristic methods do not guarantee to arrive at the true optimum, but offer an efficient method that has a high probability of finding the optimum or of getting close to it. References are given either to the work that proposed them or to a more recent discussion of their use. ‘Direct search’ covers methods that compare trial solutions with the best found so far, with a strategy based on results so far for determining the next trial. Generally, these methods are efficient but can get trapped in local optima. Examples used in building optimisation include [69]:

- Pattern search, e.g. Hooke and Jeeves [70]: each dimension in turn is trialled; when no further improvement is possible, the step size is halved.
- Linear programming, including the simplex method/Nelder and Mead [71]: if the objective function and all constraints are linear, the optimum must fall on an extremal point.
- Non-linear programming: a range of extensions to allow non-linear objectives and constraints (e.g. the interior point method, which traverses a feasible region defined by barrier functions). Evolutionary algorithms are a common meta-heuristic optimisation algorithm. They apply the Darwinian principle of survival of the fittest by maintaining a population of solutions of which the poorest are eliminated each generation. Common 'operators' applied to generate new solutions include mutation (introducing random changes) and crossover (switching elements from different solutions).

Different types of evolutionary algorithms are namely: Genetic Algorithms (GA) [72], Evolutionary Programming (EP) [73] and Genetic Programming (GP) [74], Covariance Matrix Adaptation Evolutionary Strategy (CMA-ES) [75], and Differential Evolution (DE) [76].

Meta-heuristic algorithms that mimic other natural processes include: Harmony Search (HS) [77], Particle Swarm Optimisation (PSO) [78], Ant Colony Optimisation (ACO) [79], and Simulated Annealing (SA) [80]. Figure 4 shows characteristics and features of different optimization algorithms.

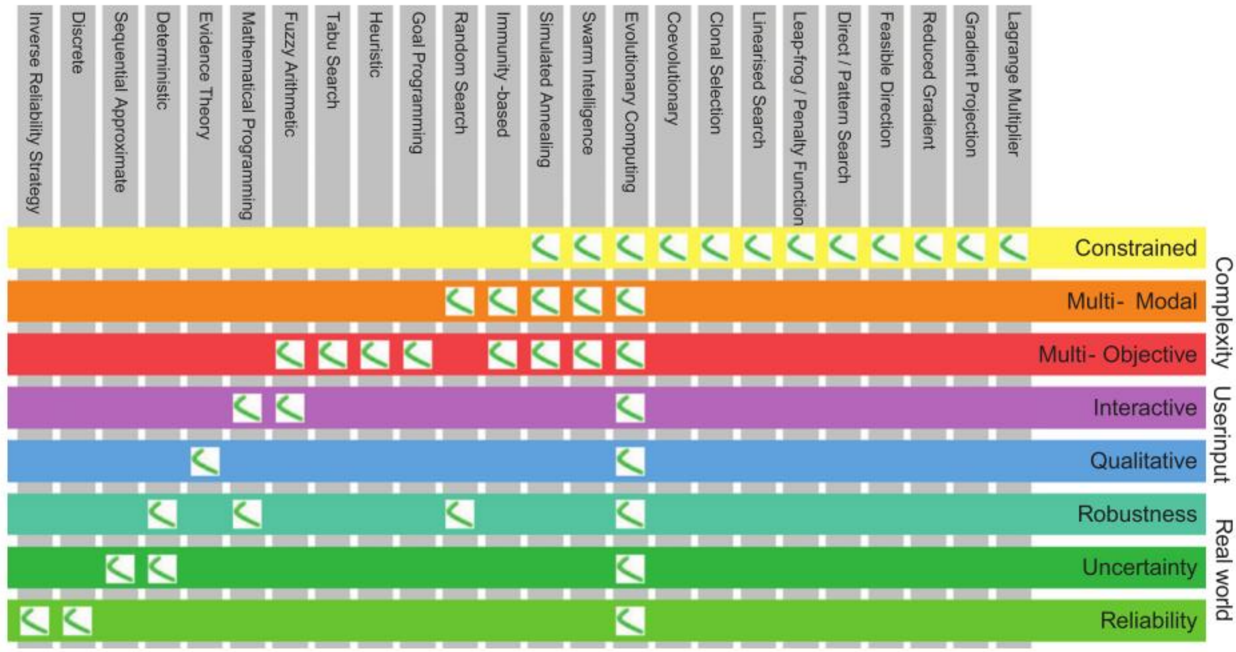

Figure 4. Optimization algorithms and their characteristics, adopted [69].

1.5.2. Optimization stages

Generally, an optimization process could be classified into three phases including: pre-processing phase, optimization phase, and post-processing phase. In simulation-based optimization for building applications the optimization program should interact and exchange data with the simulation program in different stages of pre-processing, optimization, and post-processing (Figure 5).

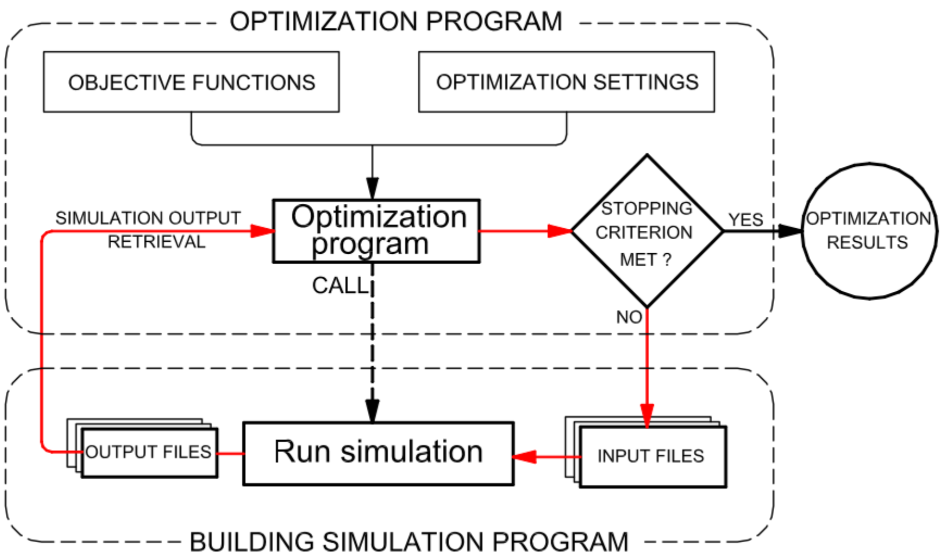

Figure 5. Simulation-based optimization scheme, adopted from [81].

The pre-processing phase plays a significant role in the success of the optimization. In this phase, the most important task is the formulation of the optimization problem. Lying between the frontiers of building science and mathematics, this task is not trivial and requires rich knowledge of mathematical optimization, natures of simulation programs, ranges of design variables and interactions among variables, measure of building performance (objective functions), etc. [81].

In the optimization phase, the most important task of analysts is to monitor convergence of the optimization and to detect errors which may occur during the whole process. In optimization, the ‘‘convergence’’ term is usually used to indicate that the final solution is reached by the algorithm. It is necessary to note that a convergent optimization process does not necessarily mean the global minimum (or minima) has been found. Convergence behaviours of different optimization algorithms are not trivial and are a crucial research area of computational mathematics [81].

In post-processing phase the analysts have to interpret optimization data into charts, diagrams or tables from which useful information of optimal solutions can be derived. The scatter plot is the among mostly-used types while convergence diagrams, tables, solution probability plot, fitness and average fitness plot, parallel coordinate plot, bar charts, etc. are sometimes used. It is always useful to verify whether the solutions found by the optimization are highly reliable or robust [81].

The application of building optimization for real-world design challenges is in its early stage of development [81], but, in recent years, there has been a substantial growth towards the use of optimization techniques for sustainable building design [82]. Single-objective and multi-objective optimization studies are gaining interest and they have been increasingly used for building design applications to optimize for example the energy performance in buildings, among which the building envelope optimization has been prominent [83,84].

Furthermore, a large and growing body of literature has been published on optimization techniques for DSM based on TES and solar PV to reduce energy-related costs of residential buildings and industrial processes [85–87]. Some of these optimization methods are namely, mixed-integer linear programming (MILP) and dynamic programming for a global optimal solution. In addition, metaheuristic methods such as particle swarm optimization and evolutionary algorithms have been implemented by many researchers [88].

2. Objectives

With the advent of computers, mathematical modelling and computer simulation have now become an important economical and fastest way to provide a broad understanding of the practical processes involving PCM [24]. Therefore, numerical simulation and optimization have been gaining interest both in the building and industry sectors to enhance the energy efficiency of the systems and thermal comfort of occupants.

The present thesis is aimed at applying TES materials in the building and industry sectors for energy improvement purposes using simulation and optimization tools. The literature has consistently shown that more research is required regarding the application of TES materials in commercial and residential buildings. There are many issues that should be further clarified and many questions that should be answered. First of all selecting an appropriate numerical simulation tool is an essential step to push forward the research in this field. Further on, controlling the heating and cooling set points have been defined as a crucial issue in residential buildings, especially, when PCM-based passive design is considered.

On the other hand, in many studies, selecting the appropriate PCM melting temperature was pointed out as an important fact to efficiently and effectively apply the passive PCM system in the building envelope.

In addition, protecting the PCM from high thermal stress when it is applied to surfaces with high exposure to solar radiation is another issue that should be investigated further.

Moreover, previous studies related to DSM in industry and building sectors showed that optimization-based simulation can play an important role to improve energy efficiency in the energy sector, however, further research and technology advancement are required for electric load management to address the potential peak load shifting and energy savings considering the new time-of-use tariff structure and elevated electricity prices, high surplus demand charges, and variable solar PV share and its uncertainties in the energy system.

The above aim will be accomplished by fulfilling the following research objectives:

- To carry out a holistic review of the numerical simulation of buildings containing PCM for passive cooling purposes using whole building energy simulation tools to address the methods that have been used to evaluate and analyse the effects of passive PCM-based design on the cooling energy performance in buildings through whole building energy simulation software.
- To evaluate an innovative HVAC operation control based on Fanger thermal comfort model according to BS EN 15251:2007 [52] thermal comfort categories to control the thermostat set points considering the outdoor and indoor boundary conditions. Then, three different types of buildings with different HVAC schedules and PCM layer thicknesses will be analysed. Eventually, the energy savings and payback periods will be reported.
- To implement a single-objective optimization method coupled with an innovative PCM enthalpy-temperature (h-T) function to find out the optimum PCM melting temperature according to the outdoor boundary conditions in both heating dominant and cooling dominant climates.
- To investigate numerically and optimize the benefits of PCM and cool roof when they are used together, mainly to improve the cool roof functionality and durability by reducing the temperature fluctuations of the cool roof exposed to direct solar radiation.
- To investigate the potential for applying optimization-based time-of-use DSM in the industry sector to reduce peak electricity demands and eventually to decrease the annual electricity bill by taking advantage of cold TES (sensible systems, ice or phase change materials) and off-grid solar PV.

3. Thesis structure

The current PhD thesis is based on five journal papers, of which, three of them have been already published in SCI journals, and two of them have been submitted. All the research activities related to the present PhD thesis have been conducted at GREiA Innovació Concurrent at University of Lleida.

With this regard, Chapter I is an introductory section of the present thesis. In this chapter an overview of the energy use in building and industry sector is provided. Further on, literature review has been provided regarding the TES technologies and exclusively the application of PCM for passive design in buildings. In addition, detailed explanations have been provided about the simulation and optimization techniques for energy analysing in buildings.

In Chapter II, the aims and objectives of the present thesis have been presented. In Chapter III a whole scheme of the PhD thesis is provided and classified in two major branches:

1. Study of the use of TES materials in the building sector by utilizing numerical simulation and optimization methods.
2. Implementation of simulation and optimization techniques in industry sector (commercial buildings) for DSM and reduction of the final electricity bills.

In Chapter IV paper 1 is presented. In this paper the methods that have been used to evaluate and analyse the effects of passive PCM-based design on the cooling energy performance in buildings through whole building energy simulation software are addressed. Respectively, an extensive study was done to address the previous, current, and future research trends towards the application of PCM in buildings for passive cooling by means of building energy modelling tools.

In Chapter V the second journal paper is presented. In paper 2, it was intended to fill the gap between the use of passive PCM system in the building envelope and the implementation of an innovative HVAC control system based on Fanger thermal comfort control model. The new thermostat model not only considers the indoor boundary conditions such as indoor air temperature, occupants behaviour, occupants clothing but also takes into account the outdoor boundary conditions as well as the presence of the passive PCM system in the building envelope.

In Chapter VI the third journal paper is presented. Many authors have mentioned the importance of selecting an appropriate PCM melting temperature for passive design in buildings in different climate zones. On the other hand, in many studies, only parametric analysis was carried out to find out the most suitable PCM melting temperature for integrated passive design in buildings which has some limitations. For this reason in this chapter, an innovative enthalpy-temperature algorithm has been applied to determine the optimum PCM melting temperature in cooling dominant climate, heating dominant climates, and in climates with both cooling and heating energy requirements, with the objective of reducing the annual heating, cooling and total energy use.

In Chapter VII the fourth journal paper is presented. Until now, it has been intended to investigate the benefits of PCM system in the building envelope as a passive system to provide thermal comfort and economic benefits. By the way, another innovative solution to reduce energy use in buildings located in hot climates is the use reflective surfaces and cool roof. Cool roof can significantly contribute to reduce energy use and enhance the thermal comfort of occupants in buildings. However, a major problem that exists in such innovative strategies is the extreme thermal fluctuations in cool roof membranes which in long-term decreases the workability of cool roof membranes. In this chapter, a simulation-based optimization methodology is presented to enhance the efficiency of cool roof membrane by applying a PCM layer as a thermal stabilizer for cool roof membrane by reducing its annual thermal fluctuations.

In Chapter VIII the fifth journal paper is presented. In previous papers, the PCM technology was considered as a passive integrated design into the building envelope. In Paper 5, however, a new approach is presented to apply TES with solar PV by assist of simulation-based optimization techniques mainly to reduce peak loads. In this paper optimization-based DSM have been applied to find out the optimum contracted energy demand, and also to find out the optimum combination of TES and solar PV with different capacities. The overall thesis structure is illustrated in Figure 6.

Eventually, Chapter IX outlines conclusions and future studies related to the present PhD thesis.

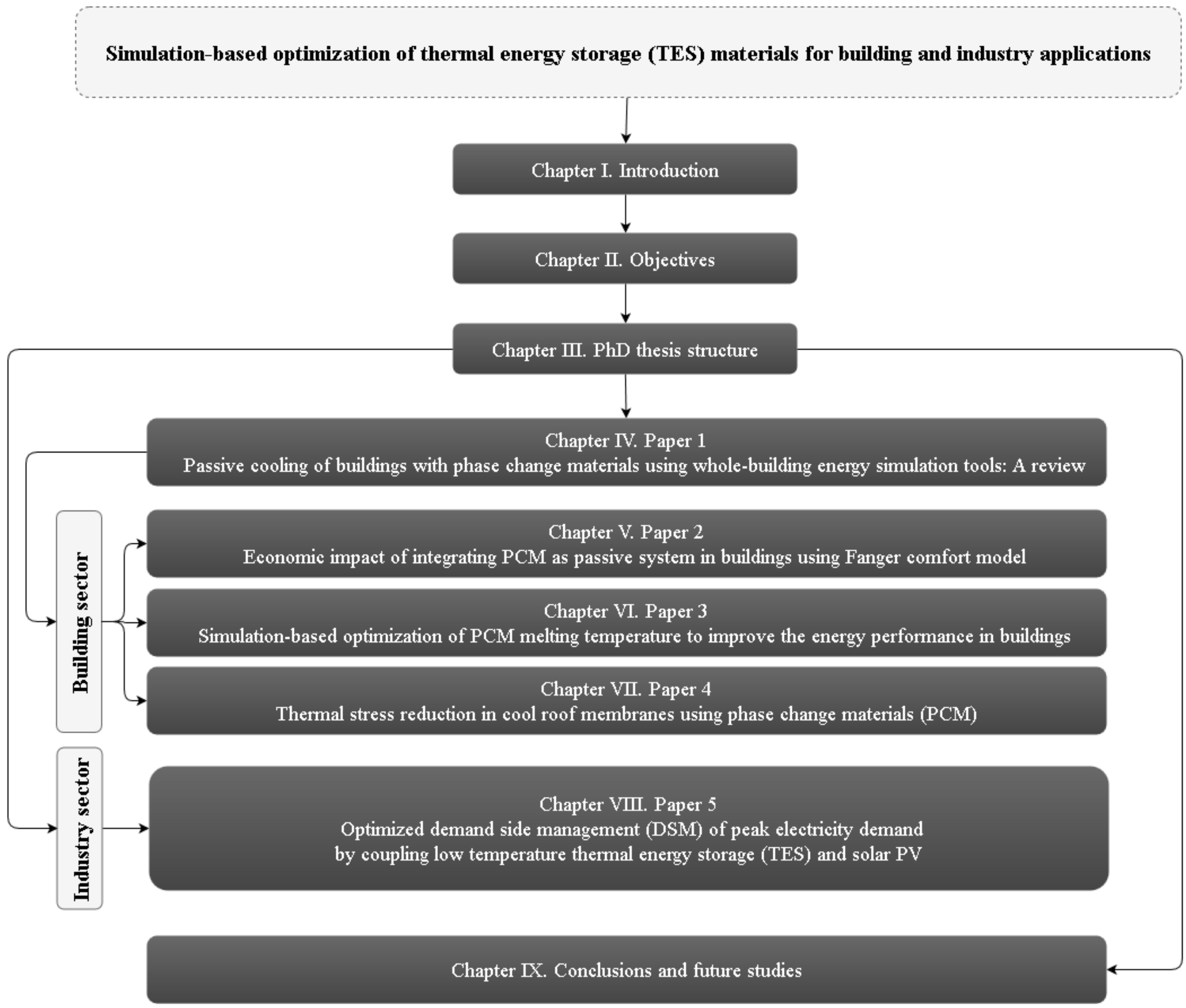

Figure 6. Scheme of the PhD thesis.

4. Passive cooling of buildings with phase change materials using whole-building energy simulation tools: A review

4.1. Introduction

PCMs can be applied in the building envelopes to decrease the rising cooling energy demands in buildings, however, innovative strategies before being applied to buildings need to be simulated and analysed beforehand. With this regard, the current paper reviews the numerical simulation of buildings containing PCM for passive cooling purposes using whole building energy simulation tools. The present study is an attempt to address the methods that have been used to evaluate and analyse the effects of passive PCM-based design on the cooling energy performance in buildings through whole building energy simulation software. In this regard, an extensive study was done to address the previous, current, and future research trends toward the application of PCM in buildings for passive cooling by means of building energy modelling tools.

4.2. Contribution to the state-of-the-art

Whole-building energy simulation tools are essential for preliminary design and performance analysis of PCM-enhanced buildings. These tools can numerically analyse the dynamic thermal behaviour of the building passively enhanced with PCMs. The current paper overviews the most important simulation tools for building passive cooling design based on the PCM technology. Based on the literature review, EnergyPlus [55], TRNSYS [59], and ESP-r [63] have been extensively used by researchers to study the performance of PCM in buildings.

Various techniques were used by researchers to enhance the building envelope by PCM for cooling energy performance improvement. For example dispersed PCM in drywall, dispersed PCM in gypsum board, pouches filled with PCM, PCM-enhanced insulation and PCM plaster are major methods that have been used. Further on, PCM was applied in different parts of the building such as vertical walls, partitions, floors, ceilings, attic floor and as a component of cool roof. The application of PCM-enhanced wallboards was popular among researchers because of their feasibility of incorporation into the interior surface of walls and ceilings, lower price, and high effectiveness to moderate the indoor temperature and improve the cooling energy performance.

Many authors used simulation techniques to analyse the application of PCM for passive cooling in building under warm temperature climates, however, the current review has shown that in cold climates the melting point temperature of PCM should be optimized in order to achieve higher total annual savings. In addition, literature reviews have shown that there was no detailed analysis of natural ventilation system using sophisticated numerical methods and it was limited to the simple analysis methods.

Moreover, many authors applied parametric method to determine the best PCM solution in their specific design; however, the numerical optimization of PCM-enhanced passive buildings is getting more popular.

4.3. Contribution of the candidate

To carry out this research extensive literature review about the topic was necessary. The candidate studied and analysed numerous journal articles, books, reports, presentations, and webpages to have a closer view towards the studied area and to find out updated information regarding the simulations tools, numerical methods and already available literature on the topic. The most important section of this paper was to compare, contrast, and classify different researchers and findings and to reach to a cohesive and coherent conclusion. Further on, the role of co-authors to comment, revise, and improve the article was of a very significant importance.

4.4. Journal paper

Renewable and Sustainable Energy Reviews 80 (2017) 1239–1255

Contents lists available at ScienceDirect

Renewable and Sustainable Energy Reviews

journal homepage: www.elsevier.com/locate/rser

Passive cooling of buildings with phase change materials using whole-building energy simulation tools: A review

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ARTICLE INFO

Keywords:
Passive cooling
PCM
EnergyPlus
TRNSYS
ESP-r
Natural night ventilation
Whole-building energy simulation

ABSTRACT

Buildings contribute to climate change by consuming a considerable amount of energy to provide thermal comfort for occupants. Cooling energy demands are expected to increase substantially in the world. On this basis, technologies and techniques providing high energy efficiency in buildings such as passive cooling are highly appreciated. Passive cooling by means of phase change materials (PCM) offers high potential to decrease the cooling energy demand and to improve the indoor comfort condition. However, in order to be appropriately characterized and implemented into the building envelope, the PCM use should be numerically analyzed. Whole-building energy simulation tools can enhance the capability of the engineers and designers to analyze the thermal behavior of PCM-enhanced buildings. In this paper, an extensive review has been made, with regard to whole-building energy simulation for passive cooling, addressing the possibilities of applying different PCM-enhanced components into the building envelope and also the feasibility of PCM passive cooling system under different climate conditions. The application of PCM has not always been as energy beneficial as expected, and actually its effectiveness is highly dependent on the climatic condition, on the PCM melting temperature and on the occupants behavior. Therefore, energy simulation of passive PCM systems is found to be a single-objective or multi-objective optimization problem which requires appropriate mathematical models for energy and comfort assessment which should be further investigated. Moreover, further research is required to analyze the influence of natural night ventilation on the cooling performance of PCM.

doi:10.1016/j.rser.2017.05.139.

5. Economic impact of integrating PCM as passive system in buildings using Fanger comfort model

5.1.Introduction

Building energy simulation is a cost-effective and time-efficient solution to estimate the effectiveness of new strategies, designs, and materials applied in buildings. Many authors have been using simulation to investigate the impact of innovative strategies such as PCM to increase the energy efficiency in buildings.

Most of the previous studies investigated the effects of PCM on energy performance and hours out of thermal comfort set point according to a fixed thermostat temperature. However, although a fixed thermostat temperature control could be an option for a specific climate zone and building type, it does not consider the inhibited interactions between outside dry bulb temperature, occupants behaviour, properties of PCM, and thermal comfort acceptability, so that, it does not seem very realistic to set a fixed thermostat operation for indoor thermal comfort level regulation.

In the current chapter, a new methodology using Fanger thermal comfort algorithm is presented to compute the thermostat heating and cooling set points considering the outdoor and indoor boundary conditions (Figure 7).

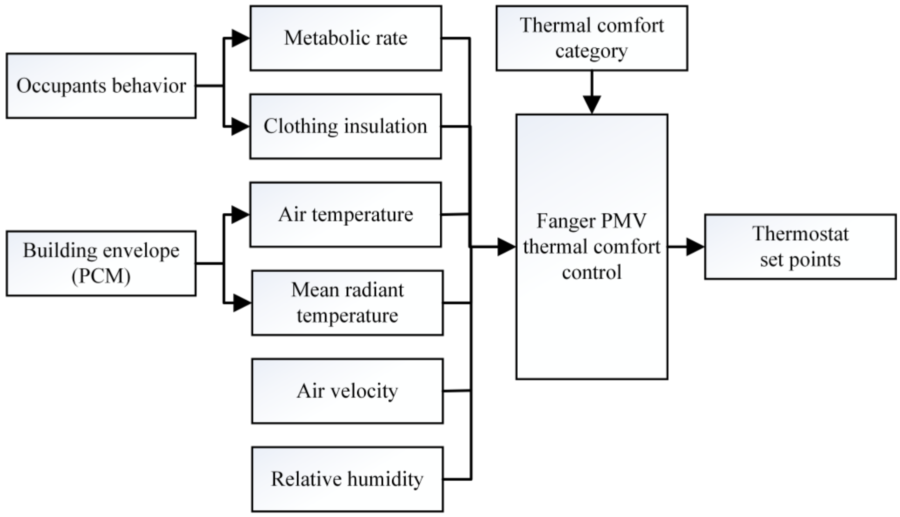

Figure 7. Thermostat set point calculation scheme [89].

5.2. Contribution to the state-of-the-art

A methodology is used to control HVAC operation using Fanger thermal comfort algorithm an based on ISO15251:2006 [52] thermal comfort categories. Three types of building models with different occupancy profiles (24 hour, residential, and office) are considered and also PCM with three different layer thicknesses and melting temperatures are used. Additionally, a payback period analysis was conducted to estimate economic benefits associated to the PCM integration in the building envelope. Moreover, the impact of occupants behaviour on the energy use was investigated.

Integration of PCM under 24 h and residential operational schedules provided energy savings during both winter and summer periods. Additionally, in all thermal comfort categories PCM with 27 °C melting point temperature achieved the highest annual energy savings. In addition, greater energy savings and payback periods were recorded when PCM with 10 mm layer thickness was used. Furthermore, annual energy savings for 24 h schedule were higher than residential schedule.

In office operational schedule remarkable cooling energy savings were observed in all cases with PCM, however, during the heating period, the energy use increased when PCM was applied to the reference model. Moreover, for this building profile the best annual energy savings corresponded to the models with 5 mm layer of 27 °C melting point PCM.

In addition, the effect of occupants clothing on the annual energy savings was investigated. Energy savings and economic benefits were improved further when the occupants wore warmer clothes in the evening and at night-time in winter.

5.3. Contribution of the candidate

All the results obtained in this article are based on numerical simulations using EnergyPlus and ConFD PCM model in this whole building energy simulation tool. It was of interest to see how the incorporation of passive PCM technology in building envelopes can regulate the thermostat set points calculated based on thermal comfort model. Additionally, the impact of occupants' behaviour on the final energy benefits when PCM is applied in the building was analysed. The candidate prepared all reference prototypes and then applied new strategies such as Fanger HVAC control model and PCM components into the models. Numerous simulations were performed to obtain the results. Afterwards, the simulation results were analysed and final results were written, compared and contrasted. Moreover, the co-authors of the present paper played an important role to improve it and to increase the academic quality of the study with their valuable comments and revisions.

5.4. Journal paper

Energy and Buildings 112 (2016) 159–172

Contents lists available at ScienceDirect

Energy and Buildings

journal homepage: www.elsevier.com/locate/enbuild

Economic impact of integrating PCM as passive system in buildings using Fanger comfort model

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ARTICLE INFO

Article history:
Received 29 June 2015
Received in revised form 27 November 2015
Accepted 4 December 2015
Available online 10 December 2015

Keywords:
PCM in building envelopes
Fanger thermal comfort
EnergyPlus simulation
Payback period

ABSTRACT

In buildings, HVAC systems consume a high amount of energy to provide thermal comfort for occupants. A methodology is presented in this paper to control thermostat operation of the buildings considering the effects of indoor and outdoor boundary conditions and phase change material (PCM) characteristics. EnergyPlus v8.1 building energy simulation software was used to analyze the energy performance of the PCM incorporated building models and to implement Fanger model to control HVAC thermostat operation according to BS EN 15251:2007 thermal comfort categories. Three types of building HVAC schedule, PCM with different melting points and layer thicknesses were studied for Madrid climate zone. Moreover, the impact of occupants clothing on the energy consumption was investigated. Furthermore, payback analysis was conducted to find out the economic benefits of PCM integration into the building envelopes. Application of PCM improved the cooling and heating energy performances except for the office model in winter (heating period). Additionally, higher energy savings and lower payback periods were observed when PCM with higher melting point was applied to the buildings. Eventually, energy savings in PCM incorporated models were found to improve further when occupants changed their clothing behavior in winter.

doi: 10.1016/j.enbuild.2015.12.006.

6. Simulation-based optimization of PCM melting temperature to improve the energy performance in buildings

6.1. Introduction

It is well known that when, the selection of PCM melting temperature during the design phase of a passive PCM system in building envelopes is critical. Moreover, this selection have to consider the use of the building and the different climate conditions, as it is a determining factor to improve the energy performance and/or thermal comfort in naturally [90] and mechanically [91] ventilated buildings. However, in available literature, little discussion has been made on the energy optimization of PCM-enhanced passive buildings addressing the appropriate melting temperature of PCM taking into account various climate conditions.

The objective of the present paper is to use a single-objective optimization method coupled with an innovative PCM enthalpy-temperature (h-T) function to find out the optimum PCM melting temperature according to the outdoor boundary conditions. Moreover, it is intended to show that using optimized PCM can yield energy savings while still ensuring indoor thermal comfort, in both heating and cooling dominant climates.

6.2. Contribution to the state-of-the-art

In the present paper, simulation-based optimizations were performed using EnergyPlus whole-building energy simulation coupled with a generic optimization program (GenOpt). In order to optimize the PCM melting temperature in each climate zone a new methodology is presented to iteratively select PCM h-T curve which reduces the time-consuming process of h-T curve introduction to EnergyPlus at the beginning of each simulation with different PCM peak melting points, hence, simulation and optimization are continued until the optimum h-T curve is found (Figure 8). This process increases the simulation and optimization speed and also enhances the precision of finding the optimum PCM melting temperature.

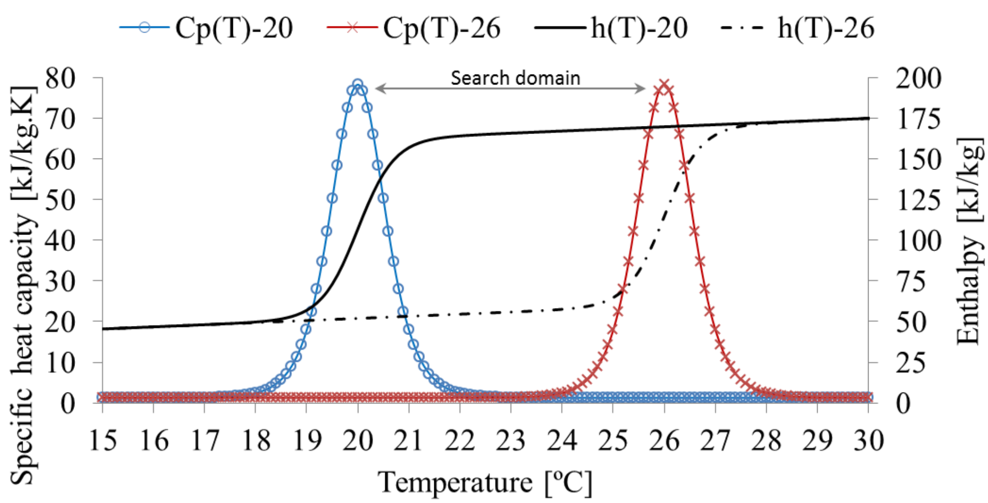

Figure 8. The iterative PCM melting temperature selection scheme [92].

To apply this method, the h-T values were written in the form of a series of continuous functions and were implemented into the pre-processing stage of the optimization (Eq. 4). A continuous function is referred to a function for which sufficiently small changes in the independent variables result in arbitrarily small changes in the objective function:

$$\mathrm{T} \triangleq \left\{ T_{opt} \in \mathbb{R}^{n} \,\middle|\, T_{\min}{}^{i} \leq T_{opt}{}^{i} \leq T_{\max}{}^{i}, i \in \{1,\dots,n\} \right\}, \tag{4}$$

where $20 \leq T_{\min} < T_{\max} \leq 26$, and $T_{opt} = T_{ref} \pm \mathbb{R}$

where T is a set of optimum PCM peak melting temperatures T_{opt}, T_{min} and T_{max} are the minimum and maximum allowed temperatures for the PCM peak melting point. In order to classify different climate conditions, the updated Köppen-Geiger [93] main climates classification is used as a reference to the general climate of the regions of the world.

In Figure 9, the worldwide distribution of optimum PCM melting temperature in different climates according to Köppen-Geiger classification is shown. For example, it can be seen that different optimum PCM peak melting temperatures were obtained to enhance the annual total heating and cooling energy performance in Madrid and Seville, both of which with warm temperate classification (C). This could be because of other influencing factors such as the altitude, the humidity ratio, intensity of solar irradiance on the exterior surfaces, and wind characteristics of these regions. Additionally, it can be perceived that in high latitude regions such as Stockholm, a high amount of energy use for heating could be saved. However, an important issue that should be taken into account in designing PCM-enhanced passive buildings is the proper optimization of PCM melting temperature considering the overall annual benefits. Also, another achievement that is noteworthy is that the PCM-enhanced gypsum technology can lead to notable energy savings in many regions in the world, for both heating and cooling dominant climate zones.

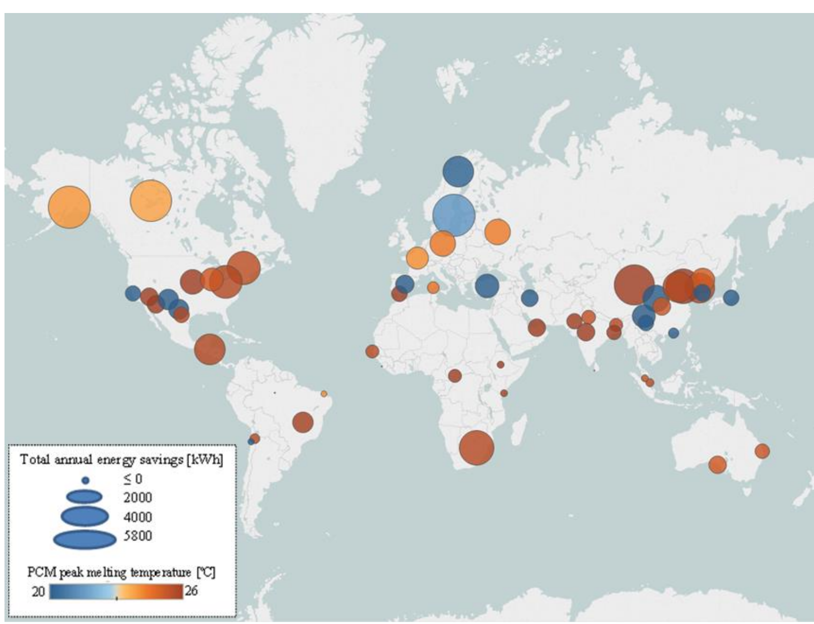

Figure 9. Global energy savings due to use of PCM passive system in building envelopes [92].

In addition, the present study found that, generally, in cooling dominant climates (climates with high CDD) PCM melting at about 26 ºC (with melting range of 24 ºC-28 ºC) leads to higher energy savings such as Brisbane, while, in heating dominant climates (climates with high HDD) the best melting point for the PCM is close to 20 ºC (with melting range of 18 ºC-22 ºC) such as Stockholm. Furthermore, in climates with both heating and cooling energy demand (climates with high HDD and CDD) the optimum PCM melting point could be between the maximum and minimum peak melting temperatures such as Seville.

6.3. Contribution of the candidate

A great effort was devoted by the candidate to prepare the simulation and optimization models. In the present study EnergyPlus PCM model was used for PCM simulation in the building envelope. Further on, the new PCM enthalpy-temperature functions were implemented into the GenOpt pre-processing step. This function permits the optimization of PCM melting temperature in a continuous way since the peak melting temperature of PCM changes by the change of optimization variable with lower and upper bound limits. We used the cluster facility of the University of Lleida to carry out the simulations and optimizations. The simulations and optimization for all climate zones required more than a week to be finished. Eventually, the simulation and optimization results were analysed by the candidate and the final results and discussions were made according to the objectives of the paper. Moreover, the co-authors of the present paper played an important role to improve it and to increase the academic quality of the study with their valuable comments and revisions.

6.4.Journal paper

Applied Energy 202 (2017) 420–434

Contents lists available at ScienceDirect

Applied Energy

journal homepage: www.elsevier.com/locate/apenergy

Simulation-based optimization of PCM melting temperature to improve the energy performance in buildings

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HIGHLIGHTS

- A novel PCM h-T function is implemented for PCM melting temperature optimization.
- Optimization is applied to find the optimum PCM melting in different climates.
- High energy savings are achieved in buildings with PCM-enhanced gypsum technology.
- In cooling dominant climates PCM melting at 26 °C achieves higher energy savings.
- In heating dominant climates PCM melting at 20 °C achieves higher energy savings.

ARTICLE INFO

Article history:
Received 18 February 2017
Received in revised form 8 May 2017
Accepted 13 May 2017

Keywords:
Passive cooling
GenOpt
Building energy simulation
PCM optimum melting

ABSTRACT

Globally, a considerable amount of energy is consumed by the building sector. The building envelope can highly influence the energy consumption in buildings. In this regard, innovative technologies such as thermal energy storage (TES) can help to boost the energy efficiency and to reduce the CO_2 emissions in this sector. The use of phase change materials (PCM), due to its high heat capacity, has been the centre of attention of many researchers. A considerable number of papers have been published on the application of PCM as passive system in building envelopes. Researches have shown that choosing the PCM melting temperature in different climate conditions is a key factor to improve the energy performance in buildings. In the present paper, a simulation-based optimization methodology will be presented by coupling EnergyPlus and GenOpt with an innovative enthalpy-temperature (h-T) function to define the optimum PCM peak melting temperature to enhance the cooling, heating, and the annual total heating and cooling energy performance of a residential building in various climate conditions based on Köppen-Geiger classification. Results show that in a cooling dominant climate the best PCM melting temperature to reduce the annual energy consumption is close to the maximum of 26 °C (melting range of 24–28 °C), whereas in heating dominant climates PCM with lower melting temperature of 20 °C (melting range of 18–22 °C) yields higher annual energy benefits. Moreover, it was found that the proper selection of PCM melting temperature in each climate zone can lead to notable energy savings for cooling energy consumption, heating energy consumption, and total annual energy consumption.

doi:10.1016/j.apenergy.2017.05.107

7. Thermal stress reduction in cool roof membranes using phase change materials (PCM)

7.1. Introduction

In the last years the Southern European countries such as Italy and Spain have been experiencing an increasing level of cooling energy use, which is likely to increase in next decades [46].

Cool roof materials can be effective and low cost solutions for building energy performance improvement in summer and UHI mitigation, when considered as both building skins and urban applications [94]. From the results presented by other authors [95], it can be seen that cool roofs can effectively contribute to increase the thermal-energy performance during cooling season in buildings. However, their effectiveness along the whole year can be affected by building features and other boundary conditions.

An existing problem in cool roof membranes is the extreme temperature fluctuations on the cool roof surface due to solar radiation absorption. TES materials can offer a unique solution to decrease these high temperature fluctuations. Within this context, combination of cool roof and PCM represents a promising application [96].

The objectives of this chapter are to reduce the thermal stress of the polyurethane membrane due to thermal fluctuations which imposes damages on the cool roof membrane, and to decrease the annual energy use.

7.2. Contribution to the state-of-the-art

To implement the new cool roof and PCM passive strategies, a multi-family residential apartment was selected from ASHRAE Standard 90.1- 2013 prototype building models and slightly modified [97]. However, since almost all zones of this building prototype are identical, in the present study, only one zone of the building prototype was considered to reduce the simulation and optimization cost (Figure 10).

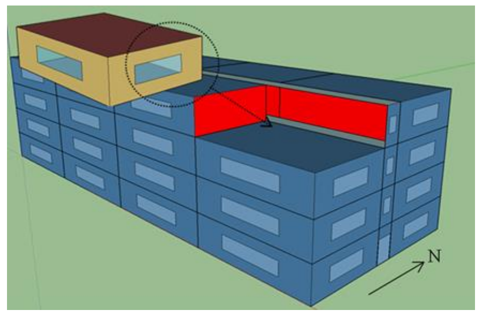

Figure 10. Reference building prototype.

Then, PCM and cool roof membrane were integrated into the building roof construction. The properties of the cool roof membrane were derived from the experimental study already performed by Pisello et al. [98]. The white cool roof membrane has 30% optimized white paste and presents a high solar reflectance value of above 85% (300-2500 nm). Further on, the physical properties of Rubitherm CSM containing RT50 PCM was used in the simulation program [99].

In the current study, EnergyPlus building simulation coupled with GenOpt optimization tool using a hybrid optimization algorithm based on Hooke and Jeeves [70] and Particle Swarm Optimization [78].

Two different optimization scenarios were taken into account. The first objective (Scenario 1) is to optimize the PCM peak melting temperature to reduce the annual sum of mean daily temperature of the cool roof membrane external surface which was implemented into the EnergyPlus subroutine using EnergyPlus Runtime Language and EMS. Eventually, the optimization algorithm minimizes the heat stress function.

And the second objective (Scenario 2) is to find an optimum PCM peak melting point to minimize the total annual electricity consumption of the heat pump. It should be said that simulation-based optimization were carried out under different climate conditions according to Köppen Geiger classification [100].

From the results of the Scenario 1 it can be generalized that in all studied climate zones the utilization of PCM together with cool roof membrane can effectively reduce the annual average thermal stress of the cool roof membrane. From the results 18% to about 30% reductions in the annual average thermal stress of the cool roof membrane surface could be observed. Additionally, it can be seen that the optimum PCM peak melting temperature to reduce the annual thermal stress of the cool roof membrane ranges from 10 ºC to 30 ºC.

However, from the results obtained in Scenario 2 (Table 2) it can be seen that in all climates the annual total electric energy could be reduced by applying macro-encapsulated PCM into the roof construction together with cool roof. These savings range from below 1% to above 6%.

For instance, in Ceduna, Brisbane, and Seville annual energy savings of 4.50% (973 kWh), 6.4% (416 kWh), and about 4% (852 kWh) could be achieved by using PCM with peak melting temperatures at 13.8 ºC, 13.8 ºC, and 10 ºC, respectively.

Another interesting fact that could be seen from these results is that, despite of optimizing the annual energy use, in all cities annual thermal stress from 16% to 27% could be achieved. These reductions despite of being, in general, lower that the results presented in the last section in terms of optimizing the thermal stress reduction of the cool roof membrane, but still offer considerable benefits.

Table 2. Optimum PCM melting temperatures to reduce the annual heat pump electricity consumption.

Köppen Geiger climate zone	City	$\overline{\Delta T}_{annual}$ (K)		$\overline{\Delta T}_{annual}$ reductions (%)	T_{peak} PCM (ºC)	E_{tot} savings (kWh)	E_{tot} savings (%)
		Reference	CR+PCM				
BSk	Albuquerque	18	14.3	19.4	10.0	2202	1.59
BSk	Midland	18	14.3	18.5	10.0	1736	3.35
BSk	Ceduna	16	11.4	27.2	13.8	973	4.49
BSh	Del Rio	12	10.4	16.7	11.3	1254	1.89
BWh	Abu Dhabi	17	13.5	21.1	20.0	2075	0.59
BWh	Phoenix	18	14.8	17.4	10.0	1384	2.16
BWk	Las Vegas	16	13.4	18.2	10.0	1479	2.35
Cfa	Brisbane	14	10.3	26.2	13.8	416	6.42
Cfa	Madrid	16	12.4	23.2	10.0	1605	2.72
Cfa	Tokyo	14	10.8	20.5	10.0	2517	1.93
Cfa	Perugia	11	8.1	24.0	12.5	2466	0.26
Cfa	Milan	14	10.9	24.0	10.0	2792	1.39
Cfb	Berlin	9	7.1	24.3	13.8	4814	0.43
Cfb	Johannesburg	15	10.3	33.4	15.0	968	3.91
Cfb	Paris	10	7.8	24.3	12.5	3466	0.93
Csb	Ankara	16	12.4	20.5	20.0	4062	1.39
Csa	Tehran	14	11.8	17.4	10.0	1695	1.43
Csa	Seville	17	13.4	22.8	10.0	852	4.15
Csa	Barcelona	12	8.8	23.9	10.0	1139	2.44
Csa	Cagliari	12	9.0	22.3	10.0	1108	2.18
Csa	Palermo	9	7.0	21.2	12.5	709	2.12
Csa	Nice	10	7.7	20.4	11.3	1152	1.77
Csa	Adelaide	13	9.3	28.2	13.8	1006	3.55
Cwa	Hong Kong	7	6.0	19.8	15.0	911	0.82

7.3.Contribution of the candidate

In the present study, the author had to select the reference building prototype and modify it slightly to integrate the cool roof membrane and PCM layers. Afterwards, to analyse the annual average heat stress reduction by PCM, a function was written ~~applied~~ by author using EnergyPlus Runtime Language and Energy Management System in EnergyPlus. This function gets the minimum and maximum daily temperature of the cool roof membrane surface with intervals of one minute then calculates a mean temperature difference value for the whole analysis period (one year). Then, simulation models coupled with GenOpt optimization tool using a hybrid optimization algorithm with Hooke and Jeeves and PSO methods. Applying this hybrid optimization technique achieves the optimum result faster in comparison to when these algorithms are used independently. Further on, the new PCM enthalpy-temperature functions were implemented into the GenOpt pre-processing step. Simulation-based optimization was performed to analyse the influence of PCM on the heat stress reduction of cool roof, and on the other hand, to reduce annual total electricity consumption of the heat pump. Finally, the simulation and optimization results analysed by the candidate and the final results and discussions were made according to the objectives of the paper. The results presented in this research provide further understanding on the application of PCM to protect building materials. In the current study, the objective was to reduce the thermal stress in the cool roof membrane; however, this methodology can be used with other building construction materials. Moreover, the co-authors of the present study effectively contributed to improve its scientific quality.

7.4.Journal paper

Energy and Buildings 158 (2018) 1097–1105

Contents lists available at ScienceDirect

Energy and Buildings

journal homepage: www.elsevier.com/locate/enbuild

Thermal stress reduction in cool roof membranes using phase change materials (PCM)

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ARTICLE INFO

Article history:
Received 24 August 2017
Received in revised form 20 October 2017
Accepted 21 October 2017

Keywords:
Cool roof
PCM
Optimization
Simulation
Thermal stress

ABSTRACT

A considerable amount of energy is used in the building sector for air conditioning purposes. Additionally, the building sector contributes to the urban heat island (UHI) phenomenon which causes temperature rise in urban areas. Cool roof is an emerging passive cooling technology that can contribute to reduce the cooling energy use in buildings and to mitigate the UHI effects in the urban area. Cool roofs and reflective coatings, despite of being effective in terms of reducing the cooling thermal loads in buildings and decrease the UHI, can suffer from extreme thermal stress which negatively influences their lifespan and performance. Thermal energy storage (TES) is a promising technology which can be applied together with cool roof technology to decrease the extreme thermal stress due to solar radiation as well as providing thermal inertia to the building. In this study, simulation-based optimization will be used to optimize the PCM melting temperature when integrated into a polyurethane-based cool roof membrane to reduce the thermal stress of the cool roof and also to improve the annual energy performance of the building. The optimization results showed that the application of PCM and cool roof technologies together can reduce the severe thermal stress of the cool roof membrane when the optimization objective is the annual thermal stress of the cool roof. On the other hand, when PCM melting temperature is optimized to reduce the annual energy needs, higher annual energy savings could be achieved with acceptable reductions in the cool roof membrane thermal stress.

https://doi.org/10.1016/j.enbuild.2017.10.068

8. Optimized demand side management (DSM) by coupling cold thermal energy storage (TES) and solar PV for on-peak electricity demand reduction in industry

8.1.Introduction

For a proper operation, the electricity system needs to be in balance. This means that the power supply and demand in the electricity network has to match at all times. A major issue for electricity suppliers is the peak demand which increases the electricity price because at peak-hours expensive and inefficient generators have to work for electricity generation. Reducing some of this peak demand would benefit the whole energy system including suppliers and consumers.

Using flexible resources in the power system such as solar PV, storage, and demand management can offer a unique solution to increase the security and satiability of the whole energy system, to bring economic benefits, and to make low-carbon transition achievement possible [101].

DSM is a proactive way to increase the energy efficiency among customers in the long-term, and can reduce both the electricity peak power demand (kW) and the electricity consumption (kWh) [102], especially when it is coupled with TES and solar PV.

The principal objectives are, first, to reduce contracted power demands and to shift electrical chiller peak loads from on-peak hours to off-peak hours, by taking advantage of cold TES and off-grid solar PV; and second, to determine the optimum combinations of contracted power at different tariff periods by integrating TES and solar PV technologies with different capacities, taking into account the solar PV variations and surplus charges of power demand.

8.2.Contribution to the state-of-the-art

First of all to estimate the annual energy bill for an industrial consumer it was assumed that for running the industrial processes of an industrial unit, a conventional energy system with no demand management facilities, neither solar PV nor TES system has been considered. The industrial processes of the analysed case study take place from 8:00 to 17:00 all days except Saturdays and Sundays, requiring 450 kW of electric demand for cooling processes. To calculate the electricity consumption, the Spanish electricity tariff structure (6.1A time-of-use tariff structure) was considered.

Three different optimization scenarios were considered to apply optimization and to analyse the possibility of shifting on-peak loads from daytime to nighttime by adopting DSM system on the basis of time-of-use tariffs and compare them with the reference model (Figure 11 a): Scenario 1. time-of-use tariff DSM coupled with only cold TES system (Figure 11 b), Scenario 2. time-of-use tariff DSM coupled with only off-grid solar PV (Figure 11 c), and Scenario 3. time-of use tariff DSM coupled with both cold TES and off-grid solar PV systems (Figure 11 d).

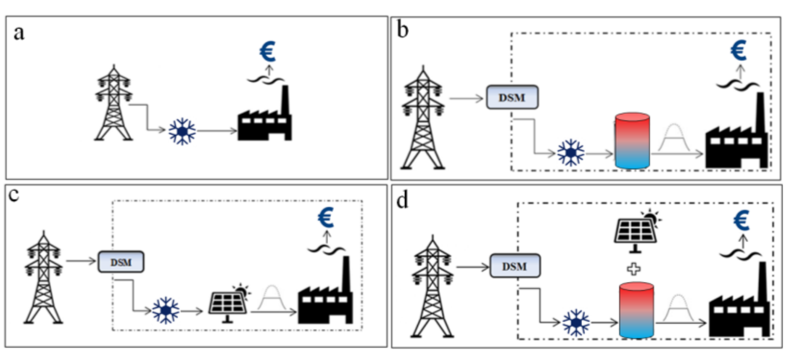

Figure 11. Schematic view of the methodology.

An important achievement in the present research that should be highlighted is that the application of TES can substantially reduce the peak demand costs for industrial processes. More importantly, in line with global energy policies, it was shown that using only off-grid solar PV can have little influence on peak load shifting, however, the integration of TES with solar PV technology can improve the performance of the PV system by reducing the its intermittency due to solar radiation variations.

It is notable to add that, when cold TES and solar PV are coupled together, further economic benefits could be achieved in comparison with using these two technologies independently. These improvements are shown in percentage in Figure 12, in case of Denver.

Improvements due to coupling PV+TES [%]				
TES [kWh]	PV 25 kW	PV 50 kW	PV 80 kW	PV 100 kW
75	6	5	3	3
150	7	6	4	4
225	8	7	5	5
300	8	7	6	6
600	8	8	7	7
900	7	8	7	8
1200	6	8	8	8
1500	5	7	8	8
3000	3	5	7	7
4500	2	4	5	6
6000	2	3	4	5
7500	1	3	3	4
9000	1	2	3	3

Figure 12. Economic benefits by using DSM coupled with cold TES and solar PV, Denver.

From the presented results it can be concluded that integration of TES and PV technologies can bring economic benefits for industrial consumers with high electric demands and also to help the grid to reduce its constraints.

The proposed method can be readily applied in dairy factories, beverage and food processing factories, cold-storage facilities, supermarkets, and any industrial processes with substantial cooling demand.

8.3.Contribution of the candidate

This paper was carried out in different stages. First of all, in the preliminary stage simulations and control strategies were applied without optimization to have a general understanding of the problem and solution. Afterwards, optimization methods were used for DSM to optimize the combination of electricity contract powers, using TES and solar PV with different capacities. Additionally, the influence of PV intermittency and surplus charges were considered in the case study.

8.4.Journal paper

Applied Energy 211 (2018) 604–616

ELSEVIER

Contents lists available at ScienceDirect

Applied Energy

journal homepage: www.elsevier.com/locate/apenergy

Optimized demand side management (DSM) of peak electricity demand by coupling low temperature thermal energy storage (TES) and solar PV

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H I G H L I G H T S

- Constraint integer programming was used for optimization of electricity tariffs.
- Demand side management was used with PV and TES for peak electric load shifting.
- Higher demand can be reduced by low temperature TES compared with solar PV system.
- Coupling TES and solar PV technologies can improve the overall system performance.

A R T I C L E I N F O

Keywords:
Thermal energy storage (TES)
Solar PV
Demand side management (DSM)
Optimization
Energy management

A B S T R A C T

Cooling in the industry sector contributes significantly to the peak demand placed on an electrical utility grid. New electricity tariff structures include high charges for electricity consumption in peak hours which leads to elevated annual electricity costs for high-demanding consumers. Demand side management (DSM) is a promising solution to increase the energy efficiency among customers by reducing their electricity peak demand and consumption. In recent years, researchers have shown an increased interest in utilizing DSM techniques with thermal energy storage (TES) and solar PV technologies for peak demand reduction in industrial and commercial sectors. The main objective of the present study is to address the potential for applying optimization-based time-of-use DSM in the industry sector by using cold thermal energy storage and off-grid solar PV to decrease and shift peak electricity demands and to reduce the annual electricity consumption costs. The results show that when cold thermal energy storage and solar PV are coupled together higher annual electricity cost savings can be achieved compared to using these two technologies independently. Additionally, considerable reductions can be seen in electricity power demands in different tariff periods by coupling thermal energy storage with off-grid solar PV.

https://doi.org/10.1016/j.apenergy.2017.11.0

9. Conclusions and future work

Globally, a considerable energy is needed to provide heating and cooling in building and industry sectors. In residential and commercial buildings a considerable amount of energy is used for air conditioning and in the industry sector cooling and refrigeration plants require a huge amount of electricity to run their processes. Today, energy matters, and energy efficiency is crucial for all habitants in the world.

On one hand, the energy sector emits a great amount of CO_2 which causes global warming and damages life on earth. On the other hand, energy suppliers have increased the electricity prices to encourage all consumers to reduce their consumptions and to adopt renewable strategies and use more renewable energies in their system.

Thermal energy storage (TES) offers a unique opportunity for energy conservation in energy systems. Thermal energy storage materials can effectively reduce the energy use in building and industry sectors by storing a high amount of energy in small temperature ranges and release it when it is necessary. However, such innovative and revolutionary materials must be optimally designed and integrated into the building envelope or energy system, or must be efficiently controlled when coupled with renewable systems such as solar PV in order to work efficiently and effectively.

For this sake, energy simulation and optimization is of a high importance for preliminary design and analysis of innovative and renewable systems.

The present thesis makes several noteworthy contributions to the application of simulation and optimization to promote and advance the usage of thermal energy storage materials in building and industry sector.

With this regard, five papers have been published based on simulation and optimization with innovative methodologies to further increase the understanding of students, engineers, stakeholders and all energy and building related sectors about TES applications and benefits.

- Generally, the main findings that could be highlighted in the present doctoral dissertation are that simulation and optimization techniques can push forward the application of TES in both building and industry sectors towards a more efficient design. More specifically, using simulation and optimization techniques is an essential step in early design and evaluation of both passive and active systems based on TES. For the passive application, which is particularly dedicated to the building sector, the importance of numerical simulation and optimization techniques were highlighted for different purposes. For instance, passive TES methods using PCM incorporated into building envelopes can improve the thermostat function; increase the energy savings for both heating and cooling by optimized PCM melting temperature, and protect other of building materials. For the active application, however, the benefit of TES was highlighted to shift industrial peak loads and to increase the economic benefits of using solar PV system.
- In particular, from the first paper entitled "Passive cooling of buildings with phase change materials using whole-building energy simulation tools: A review" it can be said that simulation-based optimization is getting more popular among researchers to analyse the cooling energy performance and comfort benefits yielding from TES materials for building applications. However, it is not feasible to recommend a unique passive PCM solution for all climates, and additionally parametric studies may partially achieve the optimum design parameters to get the optimum energy benefits. It was seen that in spite of having validated simulation tools, the lack of optimization techniques and the proper design in many researchers led to negligible energy improvement due to the use of PCM technology. Accordingly, simulation-based optimization techniques should be used to have clearer design guidelines towards using PCM for both heating and cooling dominant climates.

- The second paper which is entitled “Economic impact of integrating PCM as passive system in buildings using Fanger comfort model” highlights the influence of passive PCM system on reducing or increasing heating and cooling thermostat set points in winter and summer seasons, respectively; in buildings with high thermal comfort expectancy. Further on, it was seen that if occupants adopt themselves with slightly higher or lower temperatures through changing their clothing habits more benefits can be obtained from the PCM passive system.
- In the third paper which is entitled “Simulation-based optimization of PCM melting temperature to improve the energy performance in buildings” valuable design guidelines were provided for building construction materials, engineers, and architects to use PCM-enhanced gypsum boards with optimized melting temperature for a specific climate zone as a passive strategy in buildings envelopes to provide both cooling and heating energy benefits for different climates. The design guidelines provided in the present thesis can be already used by both building engineers and architects.

- In the fourth paper which is entitled “Enhancing cool roof durability using phase change material (PCM)” it was observed that the passive PCM technology, in addition to provide energy saving benefits can protect the building materials from excessive thermal shock, if properly optimized for this purpose. This can improve the durability and workability of such materials and increase their lifespan. Examples of such materials are cool roof membranes which have high influence on the reduction of cooling loads in buildings. This finding is a step forward towards using effective integration of two technologies to achieve low-carbon future.
- From the fifth paper which is entitled “Optimized demand side management (DSM) by coupling cold thermal energy storage (TES) and solar PV for on-peak electricity demand reduction in industry” it could be understood that TES applied as an active system in the industry sector can contribute to specific cost

savings by reducing and shifting the peak loads thanks optimization-based DSM techniques. Also, the application of TES can improve the performance of solar PV system, especially in energy systems with high integration of PV generation. The research results presented herein adds to the body of knowledge that how the integration of two renewable solutions can lead to better performance and improvement of the whole energy system in the industry sector. These valuable achievements promise a future with more renewable energies integration.

Several noteworthy results have been obtained in the current thesis regarding the use of TES materials in buildings whether integrated in the building envelope or in the refrigeration system for peak load shifting. By the advent of technology and appearance of new materials and technologies, newer and more advanced strategies are required for the application of TES materials in buildings and their integration in the renewable energy systems.

Today, the energy policies are shifting towards integration of renewable technologies and control systems. Accordingly, the future research and studies will considerably put shed on this area.

Particularly, the application of solar PV and TES for electricity peak-load shifting and for dispatching the energy system from the grid at expensive hours, in building and industry sectors will be studied using optimization and advance control techniques.

Further studies will be carried out using single- and multi-objective optimization to implement TES materials in buildings.

Additionally, simulation and optimization studies will be carried out to analyse the impact of natural ventilation with TES materials in buildings for passive cooling.

Besides, machine learning techniques will be used to create analytical models out of large building simulation results to predict energy use of buildings.

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Appendix 1. Additional research activities

Appendix 1.1. Other journal publications (2 published papers) (h-index 3)

The author of the present thesis also participated in other research activities in close collaboration with recognized international universities and research centres. The following journal papers contribute to above-mentioned scientific and academic collaborations:

- P. Marin, **M. Saffari**, A. de Gracia, X. Zhu, M.M. Farid, L.F. Cabeza, S. Ushak, Energy savings due to the use of PCM for relocatable lightweight buildings passive heating and cooling in different weather conditions, Energy and Buildings. 129 (2016) 274–283. doi:10.1016/j.enbuild.2016.08.007.
- Piselli, **M. Saffari**, A. de Gracia, A.L. Pisello, F. Cotana, L.F. Cabeza, Optimization of roof solar reflectance under different climate conditions, occupancy, building configuration and energy systems, Energy and Buildings. 151 (2017) 81–97. doi:10.1016/j.enbuild.2017.06.045.

Appendix 1.2. Contributions to conferences (10 international conferences)

The author of the present thesis also participated in other research activities in close collaboration with recognized international universities and research centres. The following conference papers contribute to above-mentioned scientific and academic collaborations:

- P. Marín, **M. Saffari**, A. de Gracia, L.F. Cabeza, S. Ushak, Simulation and Thermal Evaluation of Containers Using PCM in Different Weather Conditions of Chile: Energy Savings in Lightweight Constructions, in: ICSEB 2016 : 18th International Conference on Solar Energy and Buildings, International Journal of Energy and Power Engineering Vol:3, No:7, London, UK, 2016.

- **M. Saffari**, A. de Gracia, C. Fernández, D. Boer, L.F. Cabeza, Thermal energy storage (TES) coupled with pv to reduce on-peak demand, in: 11th ISES EuroSun Conference - International Conference on Solar Energy for Buildings and Industry, International Solar Energy Society, Palma de Mallorca, Spain, 2016.

- C. Piselli, A.L. Pisello, A. de Gracia, **M. Saffari**, F. Cotana, L.F. Cabeza, Optimization of Coupled Building Roof Solar Reflectance Capability and Insulation Level for Annual Energy Saving under Italian Climate Zones, in: 17th CIRIAF National Congress - Sustainable Development, Human Health and Environmental Protection, Perugia, Italy, 2017.

- **M. Saffari**, A. de Gracia, C. Fernández, M. Belusko, D. Boer, L.F. Cabeza, Optimization-based demand side management using thermal energy storage and solar PV for peak electricity demand reduction, in: 10o Congreso Nacional Ingeniería Termodinámica (CNIT), Lleida, Spain, 2017.

- **M. Saffari**, A. de Gracia, C. Fernández, L.F. Cabeza, PCM optimization for passive cooling and heating, in: 10º Congreso Nacional Ingeniería Termodinámica (CNIT), Lleida, Spain, 2017.

- **M. Saffari**, A. de Gracia, C. Fernández, G. Zsembinszki, L.F. Cabeza, Study on the optimum PCM melting temperature for energy savings in residential buildings worldwide, in: 3rd International Conference "Innovative Materials, Structure and Technologies" , (IMST 2017), Riga, Latvia, 2017.

- **M. Saffari**, A. de Gracia, C. Fernández, J.R. Castro, L.F. Cabeza, PCM melting temperature optimization for passive cooling and heating, in: 12th Conference on Advanced Building Skins, Bern, Switzerland, 2017.

- **M. Saffari**, A. de Gracia, C. Fernández, M. Belusko, D. Boer, L.F. Cabeza, Price-Based Demand Side Management (DSM) Coupled with Cold Thermal Energy Storage (TES) and Solar PV for Peak-Load Reduction, in: Solar World Congress (SWC 2017), Abu Dhabi, UAE, 2017.

- C. Piselli, A. L. Pisello, A. de Gracia, **M. Saffari**, F. Cotana, L. F. Cabeza, Optimization of Coupled Building Roof Solar Reflectance and Thermal Insulation Level for Annual Energy Saving Under Different Climate Zones, in: Solar World Congress (SWC 2017), Abu Dhabi, UAE, 2017.

- **M. Saffari**, M. Belusko, A. Tiruneh, L. Cirocco, A. de Gracia, L. F. Cabeza, Optimum control of thermal energy storage system (TES) coupled with solar photovoltaic (PV) for commercial refrigeration application, 14th International Conference on Energy Storage , Adana, Turkey, 2018.

Appendix 1.3. Research stay abroad

In the third year and last year of my PhD study, I had the opportunity to join the research group of Dr. Martin Belusko from Barbara Hardy Institute at University of South Australia (UniSA), Adelaide, South Australia under INNOSTORAGE international project scholarship. During four months of my research stay, I could participate in a research project about the optimum control of TES and solar PV systems and I have been carrying out this research since then.

As an early-stage researcher it was an absolutely great chance to meet new students and researchers over there and to have a generalized idea about their research lines. Further on, I could experience the Southern Australian academic and research facilities and environment specifically, at Mawson Lakes campus at UniSA.

University of South Australia

Appendix 1.4. Participation in projects

- Identificación de barreras y oportunidades sostenibles en los materiales y aplicaciones del almacenamiento de energía térmica. Ministerio de economía, industria y competitividad ENE2015-64117-C5-1-R (MINECO/FEDER), 2016-2018.

- Use of innovative thermal energy storage for marked energy savings and significant lowering of CO2 emissions (INNOSTORAGE). European Commission Seventh Framework Programme (FP/2007-2013), Nº PIRSES-GA-2013-610692, 2013-2017.

- PhD on Innovation Pathways for TES (INPATH-TES), European Union's Horizon 2020 research and innovation programme, Nº 657466, 2015-2018.

- Grup de recerca en energia en maquinària agroindustrial. AGAUR, Modalitat grup de recerca consolidat Nº 2014 SGR 123, 2014-2016