Kick-off presentation of the project "*PCMs4Buildings*" - Systems with PCM-filled rectangular cavities for the storage of solar thermal energy for buildings

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Abstract

This paper aims to provide a kick-off presentation of the project "*PCMs4Buildings*" - Systems with PCM-filled rectangular cavities for the storage of solar thermal energy for buildings. The main goal of this project is to develop a CFD methodology for the parametric analysis of the thermal behaviour of new TES systems with rectangular cavities filled with phase change materials (PCMs). These systems are designed to improve the energy performance of buildings. The project also intends to define full-scale prototypes to be numerically and experimentally optimized. "PCMs-4Buildings" is a challenging project involving researchers from different scientific backgrounds, namely civil, mechanical and chemical engineering and two institutions, the Association for the Development of Industrial Aerodynamics (ADAI) and the University of Coimbra (UC). It also involves three research units, the Associate Laboratory of Energy, Transports and Aeronautics (LAETA), the Institute for Sustainability and Innovation in Structural Engineering (ISISE) and the Chemical Process Engineering and Forest Products Research Centre (CIEPQPF),

Keywords: *Buildings applications, Thermal energy storage (TES), Phase change materials (PCMs), Solar thermal energy*

Motivation

The improvement of the energy efficiency of buildings is a worldwide area of research with a market looking for new systems and technologies that could be used to reduce buildings' dependency on fossil fuels, to make use of renewable energy sources, to contribute to a more environmentally efficient energy use, to contribute to match energy supply and demand efficiently (energy storage), and to improve indoor thermal comfort in a more sustainable and cost-effective way.

In this context, Research and Innovation are essential to help Portugal to bring out their leadership in the "green economy" and "sustainable built environment" through the use of new materials, the development of smart technologies and new products with high added value, and the sustainable use of renewable energy sources. This research project intends to contribute to the Strategy for Research and Innovation for a Smart Specialization in the following priority areas: energy; materials and raw materials; and technology of production and industry of product. The project aims to develop new thermal energy storage (TES) systems to take advantage of solar thermal energy for reducing cooling and heating energy demand in the buildings sector. Indeed, these new TES systems are designed to improve the energy efficiency of new/retrofitted buildings. Moreover, phase change materials (PCMs) will be incorporated in the TES systems to allow the storage/release of heat via PCMs' phase change processes. Therefore, new PCM-based systems will be applied to the "traditional" industry of construction and new sustainable innovative products with high added value will be proposed at the end of the project.

These high added value TES systems are aimed to be widely implemented indoors and exported as well. The exportation of these new technologies could be a great opportunity for the Portuguese R&D companies. Moreover, the research carried out in the development of new solar based systems will contribute for the advancement of knowledge of the S&T Portuguese system and to emphasize the research carried out in the national research institutions, mainly in the "Centro" region of Portugal, increasing the competitiveness of the region in research and innovation.

Introduction

The economic panorama and the EU's main legislation concerning the reduction of the energy consumption of buildings have been challenging the national buildings industry and academic community to innovate and to develop new products and technologies for improving the energy efficiency of buildings and to make use of renewable energy sources. Hence, the development of new systems to take advantage of solar thermal energy for reducing cooling and heating demand is crucial considering the challenging energy performance requirements for new buildings and retrofitting. It should be remarked that the concern about the reduction of the energy demand during the operational phase of buildings is no longer just a problem of the western world and the energy-importing countries. The oil-exporting countries have also recognized the importance of reducing the energy consumption of buildings to balance the energy domestic market and exportation.

PCMs are materials that undergo melting/solidification at a nearly constant temperature. Therefore, they are very suitable for thermal management and TES applications. In comparison with the traditional sensible materials used in construction, PCMs provide a large heat capacity over a limited temperature range (due to the latent heat involved in the solid-liquid phase change processes) and they could act like an almost isothermal reservoir of heat. Some PCMs were identified in the literature for integration in different TES systems and several ways of containment (in order to avoid liquid leakage) have been studied and optimized [1,2].

It is known by now that commercial paraffin waxes to be used as PCMs in TES applications have typically low thermal conductivity which can be problematic regarding the efficiency of these elements. The incorporation of fins of high-conductivity material within rectangular macrocapsules containing PCMs has been one of the techniques used for containment and to improve the heat transfer through the PCM-bulk. These capsules can then be integrated in different TES systems such as PCM-enhanced concrete walls, PCM-bricks [3,4], PCM-shutters [5], PCM-window blinds [6-8], PCM-enhanced photovoltaic (PV) panels [9-12], PCM-enhanced solar panels, etc.. For these reasons, solid-liquid phase change in rectangular cavities is of great interest from the theoretical point of view and for the development of new TES systems.

This research project aims at experimentally and numerically investigating the heat transfer through a vertical stack of rectangular cavities filled with PCMs (in terms of both melting and solidification processes) for new TES applications for buildings. The problems to be studied lie in the mainstream area of the:

- characterization of the heat transfer through rectangular cavities filled with PCMs;
- characterization of the thermophysical properties of PCMs;
- computational fluid dynamics (CFD) simulations considering phase-change processes:
- experimental evaluation of the overall transient heat transfer through both small- and full-scale, non-homogeneous TES building structures.

It is believed that the proposed work will give new and relevant contributions to the present knowledge in these fields. The particular goals are:

- to evaluate alternative methods for the thermophysical characterization of PCMs;
- to develop a CFD methodology for the detailed parametric analysis of the thermal behaviour of TES systems with rectangular cavities filled with different kinds of PCMs;
- to develop an experimental methodology to provide a large set of benchmarking results for numerical validation purposes and for the assessment of the thermal performance of some prototypes;
- to define full-scale prototypes to be numerically and experimentally optimized and to be used in the design of new TES systems for buildings.

Literature review

The incorporation of PCMs in TES applications for buildings has been subject of great interest and much work has been developed worldwide, as reviewed by several authors [13-15]. The research topics range from the most general to very specific ones, covering issues such as the use of simple PCM-wallboards for reducing heating and cooling energy demand of lightweight buildings [16], and the use of more complex systems with cavities filled with PCMs to take advantage of solar thermal energy [3-8].

Soares et al. [17] developed an experimental setup to evaluate the heat transfer through a vertical stack of rectangular cavities filled with PCMs (small TES unit) in terms of both melting and solidification processes. Two types of PCMs were used: a free-form PCM and a microencapsulated PCM. The term "free" means that the metallic container is the only way of containment in order to avoid liquid-leakages and that the molten PCM can freely move inside the enclosure due to buoyancy forces. The experimental results provided data for benchmarking and validation of numerical models. Important findings concerning the influence of natural convection and subcooling during charging and discharging were also discussed. The authors concluded that natural convection in the free-form PCM must be considered in every simulations to well describe the charging process. During discharging, subcooling must also be considered in the case of free-form PCMs. It was also concluded that natural convection and subcooling can be neglected when modelling cavities filled with microencapsulated PCMs. In a different work, the same authors have evaluated the influence of the cavities' aspect ratio and the influence of the imposed boundary conditions during the charging and discharging experiments [18]. More work must be developed to better understand the heat transfer with solid-liquid phase-change through rectangular cavities filled with different PCMs with horizontal fins emerging from vertical heated/cooled surfaces. Moreover, some efforts should be directed to adapt the experimental-setup to evaluate the effect of the inclination-angle on the convection-driven melting of free-form PCMs in rectangular enclosures. These results are very important to optimize the design of TES units for the thermal management of PV panels.

Other findings concerning the heat transfer through rectangular cavities filled with commercial free-form paraffin waxes are pointed out in the literature related with the thermal management of PCM-enhanced PV panels [9-12]. This is an active area of research and several studies were recently reviewed in refs. [19] and [20]. It has been claimed that the performance of these systems can be improved by placing a TES unit with PCMs on the panels back to reduce high operating temperatures. Results showed that the aspect ratio of the cavities; the number, dimension and shape of the fins, the natural convection and subcooling play an important role in the thermal regulation period. Despite the research carried out, there is still a lack of reliable experimental and numerical approaches to be used in the optimization of these systems.

Some of the most promising TES systems for buildings are those related with harnessing solar energy for heating during winter and those optimized to reduce overheating during summer [18]. The design of portable, rotary and movable PCM-systems associated with the glazed façade can also be used to reduce heating and cooling energy demand. These systems can integrate a vertical stack of rectangular cavities filled with PCMs, which is the case of the exterior PCM-shutter proposed by Soares et al. [5]. This system was designed to take advantage of solar energy for winter night time indoor heating. A two-dimensional phase-change heat diffusion model based on the enthalpy formulation was used to evaluate the performance of the TES system. The results were promising but the influence of natural convection, hysteresis and subcooling phenomena were not considered in the numerical model.

An interior PCM-window-blinds system was proposed by Soares et al. [6] in the 1st edition of the 'Prémio Ramos Catarino Inovação' innovation award. It is composed by a set of rotary vertical or horizontal wall segments, which can rotate around their vertical or horizontal shafts. Moreover, all segments can be assembled together and collected within the wall. Each segment section consists of an aluminium cavity to be filled with PCMs. The enclosures are coupled with an insulation layer, which is essential to control the direction of the heat flux, especially during discharging. The first prototype of this system was evaluated by Silva et al. [7] considering the blinds installed in an outdoors full-scale lightweight test cell. The results showed that the system can be used to reduce overheating in lightweight construction with big windows facing south. This TES system was further evaluated by some authors [2].

Silva et al. [3] proposed a PCM-brick, which was further studied by Vicente et al. [4]. The system is composed by a hollow clay brick enhanced with an aluminum macrocapsule filled with a free-form PCM. The experimental results were promising regarding the attenuation and time delay of the indoors air temperature fluctuation when testing this kind of wall. However, the authors did not carry out any optimization of the rectangular cavity to ensure that the PCM volume was optimized.

The study of natural convection in enclosures filled with free-form PCMs is also an active area of research in the thermal management of electronic devices. Different PCM-based heat sinks with vertical fins emerging from top and bottom heated surfaces have been recently studied [21-26]. These units are different from those used in vertical systems mainly concerning the orientation of both the enclosure and fins. Since the heat transfer mechanisms during phase change depend on the configuration and orientation of both system and fins, the main findings regarding the influence of natural convection within these heat sinks can only be carefully applied to vertical building applications.

To sum up, the study of natural convection in rectangular cavities filled with free-form PCMs is not new and several experimental [10,27-29], numerical [30-32] and both experimental and numerical [11] studies can be found in literature. Results showed that the aspect ratio of the cavities, the number, dimension and shape of the fins, the natural convection and subcooling play an important role in the melting and solidification cycles. Despite the research carried out, there is still a lack of reliable experimental and numerical approaches that can be used for the optimization of new TES systems with rectangular cavities filled with free-form PCMs. The results of this project will improve the fundamental understanding of the convection-driven melting process in rectangular enclosures.

Plan and methods

The research team has been working on three main research areas: (*i*) the dynamic simulation of energy in buildings with PCMs [16]; (*ii*) the numerical and experimental assessment of integrating PCMs in TES systems [3,5,17,18]; and (*iii*) the thermophysical characterization of PCMs [17]. With this project, the team aims to merge efforts to develop a holistic methodology (*i*) to evaluate unconventional methods for measuring the main thermophysical properties of free-form and microencapsulated PCMs; (*ii*) to evaluate and characterize the overall transient heat transfer through small and full-scale TES systems; (*iii*) to develop a validated CFD strategy for the parametric analysis and optimization of different TES units and prototypes, and (iv) to propose and optimize new TES prototypes.

This project aims to create an active multidisciplinary lab provided with the skills and equipments necessary to study new TES systems incorporating vertical stacks of rectangular cavities filled with PCMs in their structure. With this organization scheme, the team will be better positioned within the peers as all the research steps, from the thermophysical characterization of the materials to the final evaluation of the thermal performance of prototypes, will be covered by the research project. Indeed, the team will be better positioned to participate in worldwide interlaboratory studies and to join a network of scientists that today exchange not only samples to be characterized, but also researchers to potentiate the research carried out. The team will put great efforts in the development and validation of new ideas to provide new TES systems to the construction sector and, simultaneously, in the publication and dissemination of the research carried out. The scientific potential of the project is huge and it is believed that it will give new and relevant contributions to the present knowledge in all the covered research fields.

To attain their goals, the team proposes a research plan composed by six main tasks:

1. thermophysical characterization of PCMs;
2. numerical modelling and CFD evaluation;
3. tests in the small-scale experimental setup;
4. tests in the Guarded Hot Box Apparatus;
5. definition of full-scale prototypes;
6. technical seminar and workshop.

TASK 1 refers to the evaluation of alternative methods for the thermophysical characterization of PCMs. TASK 2 involves the numerical modelling of the heat transfer with solid-liquid phase change and the development of a CFD methodology for a detailed parametric analysis of the thermal behaviour of TES systems. TASK 3 involves developing an experimental methodology to provide benchmarking data for numerical validation purposes considering an existing setup designed to measure the transient heat transfer with phase-change through small-scale TES units. TASK 4 involves adapting the existing Guarded Hot Box Apparatus to evaluate the thermal performance of full-scale prototypes in a transient mode and to provide experimental data for validating more complex CFD models. TASK 5 involves the design of full-scale prototypes to be numerically and experimentally optimized. TASK 6 involves organizing a technical seminar and a final workshop to disclose the achieved results.

The efforts are primarily directed to the optimization of a small experimental setup developed in the Mechanical Engineering Department of the University of Coimbra and described in refs. [17] and [18]. The setup was designed to evaluate the transient heat transfer through a small non-homogeneous TES unit with horizontal metallic fins emerging from vertical heated/cooled surfaces. Task 3 keeps on studying the problem defined in refs. [17] and [18] and more experimental data for benchmarking and validation of numerical models will be provided concerning the thermal performance of different TES units with different cavity aspect ratios and the test of different boundary conditions during the experiments. These data will be used to validate the numerical model developed during the first part of Task 2.

During Task 2, the team starts to improve the two-dimensional phase-change heat diffusion model based on the enthalpy formulation described in ref. [5]. The numerical model follows the control-volume method with a fully-implicit formulation and allows the alternating melting and solidification of a pure PCM. This first version of the model neglects the advection terms in the general equation for conservation of energy. To well describe the laminar flow with phase-change, the team will improve the model considering the advections terms in the energy conservation and will therefore include the coupled solution of the continuity and the momentum equations. Moreover, the homemade open-source code will be enhanced to simulate non-pure PCMs, taking into account the influence of natural convection, subcooling and hysteresis phenomena. Once the numerical model is validated, it will be used to define more complex CFD simulations using the commercial code CFX from ANSYS®. The team will start to evaluate a PCM module in the CFD tool (based on the previous open-source code). The numerical results will be validated using full-scale experimental results from Task 4. Once validated, the CFD model will be used as an advanced solver technology to achieve reliable and accurate solutions in a quick and robust way. This model will be used for the numerical optimization of the configuration of several prototypes defined during the implementation of the project (Task 5).

For measuring the thermal performance of full-scale prototypes incorporating rectangular cavities filled with PCMs, the Guarded Hot Box Apparatus developed in the Civil Engineering Department of the University of Coimbra will be used during Task 4. The experimental setup will be instrumented accordingly with international standards, allowing to accurately measure the heat transfer in each prototype. After instrumentation, several calibration and exploratory tests will be carried out in order to ensure the reliability of the measurements. The big challenge of this task is to adapt the Guarded Hot Box Apparatus for measuring the transient heat transfer through elements considering solid-liquid phase change processes. This task is linked to the second part of Task 2. The preliminary numerical results will be used to help the adaptation of the experimental setup and then, experimental data will be used for validating the CFD model.

The efforts of the team are also directed to the thermophysical characterization of commercial PCMs. It should be remarked that the product datasheet of the majority of PCMs does not specify the thermophysical properties in both solid and liquid phases, which is crucial for modelling. When an effort is carried out to match experimental and numerical results many uncertainties related to the measurements and several numerical errors have to be considered. This is not easy to do in standard thermal analyses, but it is even harder to do when a material changes its phase in time with the variation of temperature. Therefore, the characterization of PCMs is essential to provide reliable data for modelling. This is a challenging task considering conventional equipments and methods, which are commonly designed to test solid or liquid materials. Moreover, the majority of techniques are designed to test pure substances which exhibit no subcooling, no hysteresis, no significant variation of the thermal conductivity with temperature, and no temperature change during its solid-liquid phase change. Most of the commercial PCMs to be used in construction elements are not pure as the pure substances are very expensive. Therefore, the uncertainty of the measurements for characterizing the PCMs is an active area of research. Cabeza *et al*. [33] reviewed the conventional and unconventional technologies available for the thermophysical characterization of PCMs, describing different equipments and techniques to analyze the thermophysical properties of PCMs, such as the specific heat, the latent heat and melting temperature, and the thermal conductivity and diffusivity. During Task 1, the team aims to evaluate alternative methods to provide the main thermophysical properties of the PCMs used in the experiments, which are necessary for the numerical modelling task.

Conclusion

This paper presented an overview of the 3-year funded research project "*PCMs-4Buildings*" - Systems with PCM-filled rectangular cavities for the storage of solar thermal energy for buildings. The main goal of this project is to develop a combined experimental/CFD methodology for the parametric analysis of the thermal behaviour of new TES systems with rectangular cavities filled with different kinds of PCMs: free-form and microencapsulated PCMs. These TES systems are intended to be used to improve the energy performance of buildings by reducing the energy demand for heating and cooling, and by taking advantage of solar thermal energy. At the end of the second year, the research team aims to organize a scientific meeting in Coimbra, comprising a school and a technical seminar on the theme "Thermal storage with PCMs to take advantage of solar energy". At the end of the project, the team also intends to organize a workshop to present the main results. These events will be strongly supported by the University of Coimbra through the Energy for Sustainability (EfS) initiative.

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Acknowledgements

This project has been financed by FEDER - Fundo Europeu de Desenvolvimento Regional funds through the COMPETE 2020 - Operational Programme for Competitiveness and Internationalisation (POCI), and by Portuguese funds through FCT - Fundação para a Ciência e a Tecnologia in the framework of the project POCI-01-0145-FEDER-016750 | PTDC/EMS-ENE/6079/2014.