Numerical heat transfer analysis of Phase Change Material (PCM) - enhanced plasters

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Abstract: Heat transfer analysis of novel building materials, such as Phase Change Materials (PCMs), is a challenging task due to their unique thermochemical properties and the complexity of their operation. The aim of this work is to investigate the thermal performance and impact of novel PCM - enhanced plasters via the heat transfer analysis of a building wall under summer dominant conditions. For the implementation of the numerical simulation study, three - dimensional (3D) time - dependent building wall models, incorporating the PCM-enhanced plasters, have been developed in COMSOL Multiphysics. This study will offer fundamental knowledge and important guidance on the conduction of numerical heat transfer modelling incorporating phase change materials, and it will provide significant conclusions on the design optimisation of PCM - enhanced building elements for use in summer- dominant climatic conditions.

Keywords: PCM, plaster, heat transfer, numerical simulation, time-dependent

1. Introduction

Buildings at locations with summer-dominant climatic conditions typically experience large temperature variations between day and night. This causes not only discomfort to the buildings' occupants, but also increased building energy consumption due to the greater demand and use of active temperature control systems.

One effective solution to this problem is passively alleviating those temperature fluctuations with the use and incorporation of latent or sensible heat storage systems within building envelopes. Phase Change Materials (PCMs) are materials that acquire the unique ability to capture and save energy in periods of abundant heat, and release it during periods of necessity. They are heat storage systems that essentially minimise the need for active heating and cooling systems' operation, and achieve significant energy savings by switching electrical consumption from on-peak period to off-peak period [1]. Researchers have already developed and examined a great range of new building elements, including building walls, roofs, floors, and transparent elements that incorporate PCMs through microencapsulation or nanoencapsulation.

Transient heat transfer analysis of novel materials that undergo phase transformation is challenging and complex and must consider the effect from several different influencing parameters. In view of that, state-of-the-art numerical simulation tools have developed features that enable the numerical solution of such problems.

For this work, COMSOL Multiphysics is employed for the numerical investigation of the thermal performance of novel PCM - enhanced plasters for their incorporation in buildings located in summer- dominant environments. The conjugate heat transfer problem is applied to conditions with and without phase change and its numerical simulation results are validated experimentally. The numerical simulation models' validation facilitates the examination of additional building element designs for the optimisation of the PCM - enhanced plasters' operation.

2. Governing Equations

During the solid to liquid phase change, the density of PCMs is modified, resulting in a volume compression. The solid PCM coordinates express all transformations in the initial system, when the solid PCM occupies the domain. Assuming that there is no mixing in the liquid phase, the conduction equation in solid PCM coordinates can be used:

$$\rho C_{eq}\frac{\partial T}{\partial t}+\nabla\cdot\left(-k_{eq}\nabla T\right)=Q$$

Where ρ is the density, C_{eq} is the effective heat capacity at constant pressure, k_{eq} is the effective thermal conductivity, T is temperature, and Q is a heat source.

When the PCM-enhanced plaster reaches its phase change temperature T_{pc}, it is assumed that the phase change take places throughout a period of time. This time interval is defined between $T_{pc}-\Delta T/2$ and $T_{pc}+\Delta T/2$, while the phase of the plaster during this time period is defined by the function, θ. The function, θ, represents the fraction of phase before the phase transition, which is equal to 1 before $T_{pc}-\Delta T/2$ and to 0 after $T_{pc}+\Delta T/2$. Accordingly, the density, ρ, and the specific enthalpy, H, are expressed by [2]:

$$\rho=\theta\rho_{phase1}+(1-\theta)\rho_{phase2}$$
$$\rho H=\theta\rho_{phase1}H_{phase1}+(1-\theta)\rho_{phase2}H_{phase2}$$

where the indices $phase1$ and $phase2$ indicate a material in phase 1 or in phase 2, respectively. The specific heat capacity can then be expressed as follows [2]:

$$C_p=\frac{1}{\rho}(\theta_1\rho_{phase1}C_{p,phase1}+\theta_2\rho_{phase2}C_{p,phase2})+(H_{phase2}-H_{phase1})\frac{da_m}{dT}$$

Where

$$\theta_1=\theta$$
$$\theta_2=1-\theta$$

and the mass fraction

$$a_m=\frac{1}{2}\frac{\theta_2\rho_{phase2}-\theta_1\rho_{phase1}}{\rho}$$

The specific heat capacity is the sum of an equivalent heat capacity, C_{eq} [2]:

$$C_{eq}=\frac{1}{2}\left(\theta_1\rho_{phase1}C_{p,phase1}+\theta_2\rho_{phase2}C_{p,phase2}\right)$$

and the distribution of latent heat C_L [2]:

$$C_L(T)=\left(H_{phase2}-H_{phase1}\right)\frac{da_m}{dT}$$

C_L is then approximated such as the total heat per unit volume released during the phase transformation equals with the latent heat, L [2]:

$$\int_{T_{pc}-\frac{\Delta T}{2}}^{T_{pc}+\frac{\Delta T}{2}}C_L(T)dT=L\int_{T_{pc}-\frac{\Delta T}{2}}^{T_{pc}+\frac{\Delta T}{2}}\frac{da_m}{dT}dT=L$$

Accordingly, the apparent heat capacity, C_p, the effective thermal conductivity, k, and the effective density, ρ, are then defined as [2]:

$$C_p=\frac{1}{\rho}(\theta_1\rho_{phase1}C_{p,phase1}+\theta_2\rho_{phase2}C_{p,phase2})+C_L$$
$$k=\theta_1k_{phase1}+\theta_2k_{phase2}$$
$$\rho=\theta_1\rho_{phase1}+\theta_2\rho_{phase2}$$

3. Methods

The methodology followed in this work targeted the modelling of the PCM-enhanced plasters' behaviour in summer-dominant conditions to predict their impact on the heat transfer analysis of a building element. For this purpose, four different model designs were developed in COMSOL Multiphysics:

- A reference building element, incorporating conventional lime plaster (REFPLASTER)
- A building element, incorporating a lime plaster enhanced by the addition of 5% by weight PCM (PCMPLASTER5)
- A building element, incorporating a lime plaster enhanced by the addition of 10% by weight PCM (PCMPLASTER10)
- A building element, incorporating a lime plaster enhanced by the addition of 20% by weight PCM (PCMPLASTER20)

The results of the numerical simulation studies of the reference building element and the building element incorporating 5% by weight PCM-enhanced plaster have also been experimentally validated. The verification of the models enabled the establishment of the thermal performance of the rest of the PCM-enhanced plaster model designs and the identification of the benefits that arise from different PCM concentrations with reference to the effect of the diurnal variability in the interior of the building.

4. Theory

A number of numerical simulation studies have been conducted for the solution of heat transfer problems that incorporate phase change. Based on the results of a network analysis, the recent trends in this field have been identified.

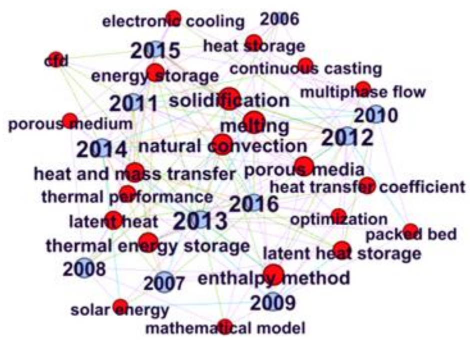

Figure 1. Network analysis for literature on numerical simulation of heat transfer with phase change

The focus of several studies found in the literature is the investigation of the natural convection mechanisms of liquid PCM and of methods to enhance the melting rate inside PCM enclosures [3]. The objective of the numerical simulations conducted in Ziaei et al. [4] was the identification of the geometric features that lead to the fastest melting process for the PCM in a cylinder. Also, Fan et al. [5] investigated the influence of fin height in a circumferentially finned spherical capsule on melting heat transfer and TES performance of the PCM system.

Research is also particularly interested in the solidification and melting processes of different PCMs. In Kant et al. [6], the performance of five different fatty acids (capric acid, lauric acid, myristic acid, palmitic acid and stearic acid), when used with aluminum containers were investigated, while Bondareva, and Sheremet, [7] carried out mathematical simulation of natural convection with phase transition inside an enclosure with a local heat source for the identification of melting and solidification problems for industrial application. In addition, the aim of Arena et al. [8] was to simulate the melting and solidification processes in containing boxes and heat transfer devices of different geometrical features which may constitute an element of a more complex TES system.

Multiphase flows, thermal flows and thermal multiphase flows with phase change was the focus of the work of Li et al. [9], which provided a comprehensive review of the Lattice Boltzmann (LB) method for thermofluids and energy applications. The review revealed certain inconsistencies, defects, and common features of multiphase and thermal LB models, while recent developments in improving the thermodynamic and hydrodynamic consistency, reducing spurious currents and enhancing the numerical stability were also highlighted.

Other recent trends identified in numerical simulation studies incorporating phase change included the definition of heat transfer coefficients and the implementation of the enthalpy method. Sun et al. [10] employed numerical simulation for the definition of the effective thermal conductivity coefficients of expanded graphite/paraffin phase change composites. Also, the heat transfer behavior of micro-foam impregnated with PCM was investigated by Hu et al. [11]. Three phase change models, including the apparent specific capacity method, the enthalpy method assuming a pure body and the enthalpy method assuming a binary mixture, which are used to predict the energy behaviour of a PCM cement mortar sample were assessed by Tittelein et al. [12].

Numerical simulation has also been established as an effective tool for the optimization of PCM applications in buildings. The key objective of the work undertaken in Jayalath et al. [13] was the optimisation of PCMs' operation for the improvement of buildings' thermal performance in Melbourne. Similarly, Soares et al. [14] focused on the optimization of new small thermal energy storage (TES) systems for buildings

The numerical investigation of phase change materials with porous structures is also a dominant subject among current research. Gopalan and Eswaran [15] performed simulations to assess the impact of such media as thermal conductivity enhancers, while Bottarelli, et al. [16] used fluid flow and heat transfer in porous media to perform a yearly simulation for the definition of the thermal performance of a drainage trench filled with encapsulated PCMs as granular filler.

5. Numerical model

To perform the thermal performance of the defined building element, 3D geometry was employed, while a time-dependent study was chosen to satisfy the non-steady nature of the problem. The study also employed the Conjugate Heat Transfer module and the Heat Transfer with Phase Change feature to enable the examination of the transient temperature transfer in the PCM-enhanced plaster incorporated in the building element. Appropriate boundary conditions were also used to represent the climatic conditions in a summer-dominant environment.

5.1 Geometry and materials

Figure 2 represents the three-dimensional (3D) geometry that was employed in COMSOL Multiphysics for the simulation of the operation performance of the building elements under investigation. The building element is 0.4 m wide, 0.22 m deep and 0.2 m high, and is comprised of a 2 cm thickness layer of plaster applied on a concrete block. The concrete block has a hollow core, with a single bone of 0.04 m thickness cutting across its centre, as shown in Figure 2. Table 1 outlines the thermophysical properties of the above materials.

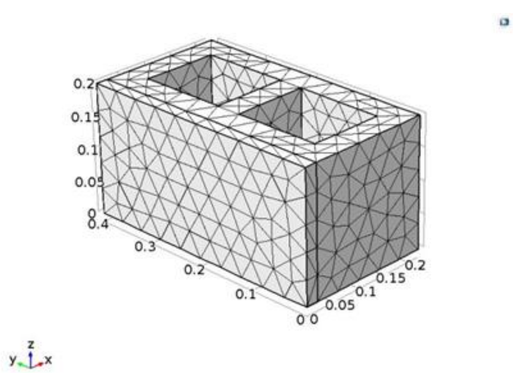

Figure 2. Geometry and mesh of three-dimensional (3D) numerical models developed in COMSOL Multiphysics.

Table 1: Thermophysical properties of building materials employed for the numerical simulation study

Materials	ρ [kg/m^3]	C_p [J/(kgK)]	k [W/(mK)]
Concrete block	1100	900	0,900
Plaster	1739	834	0,687
PCM-enhanced plaster (5%)	1533	935	0,570
PCM-enhanced plaster (10%)	1379	1022	0,398
PCM-enhanced plaster (20%)	1289	1076	0,309

The choice of PCM was based on its melting temperature for its suitability of operation in summer-dominant conditions. Accordingly for the particular study, Micronal DS 5038X by BASF having a melting temperature of 26 ºC was employed. The PCM was incorporated in the plaster at 5%, 10%, and 20% by weight to develop the PCM-enhanced plasters under investigation, the thermophysical properties of which are also provided in Table 1. The product information of Micronal DS 5038X is summarised in Table 2.

Table 2: Micronal DS 5038X product information

Product type	Powder
Melting point [˚C]	26
Overall storage capacity [kJ/kg]	145
Latent heat capacity [kJ/kg]	110
Apparent density [kg/m^3]	250-350

5.2 Boundary conditions

For the numerical simulations, transient modelling for conjugate heat transfer in solids and liquids was adopted, in addition to the phase change feature of the Heat Transfer module of COMSOL Multiphysics. The PCM-enhanced plaster was set to change phases throughout the simulation according to the product properties given in Table 2.

The initial temperature of the building element, T_{in} and the exterior boundary conditions, T_{ext} were defined according to actual measured temperatures averaged per hour. The exterior boundary conditions, which the external plaster layer was exposed to, were inserted as an interpolation in the simulation study and are illustrated in Figure 3.

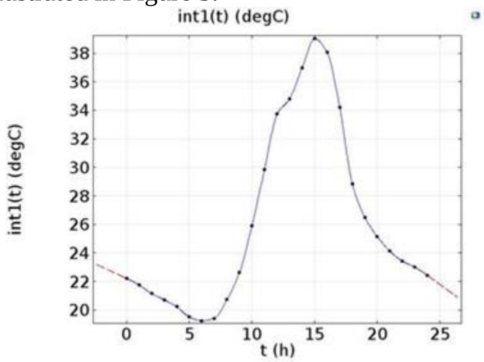

Figure 3. Exterior boundary conditions employed for the simulation study.

5.3 Meshing

It was determined that the most appropriate mesh for this model was a free tetrahedral meshing. The mesh type was set to physics-controlled and its size was set to normal. There were 2385 elements used for the simulation of 3 days of transient heat transfer.

6. Results and Discussion

6.1 Experimental validation

The simulation results for the REFPLASTER and the PCMPLASTER5 are presented in Figure 4. This figure also illustrates the experimental results for validation purposes. The simulation results for both cases are found in good agreement with the experimental results. Referring to Figure 4, the temperature peaks and troughs of the REFPLASTER vary by less than 1 ˚C and 0.5 ˚C, respectively, while the deviations in the peak and trough of the temperature profiles of the PCMPLASTER5 are slightly higher – a difference of 1.5 ˚C for the peak value, and 1 ˚C for the trough value. Furthermore, the timing of the temperature peaks and troughs between the actual and simulated values are found in line.

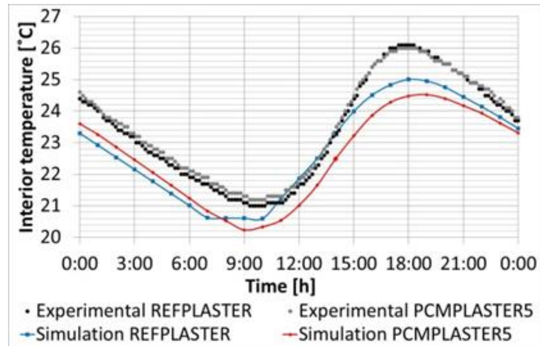

Figure 4. Simulation and experimental temperature results of interior surfaces for REFPLASTER and PCMPLASTER5

6.2 Additional model designs

Figure 5 illustrates the simulation temperature results of the interior surfaces of the building element model designs under examination. The temperature fluctuations experienced by the PCM-enhanced plasters due to their exposure to the external weather conditions allow the PCM to change phase twice - from solid to liquid to solid - within a time period of 24 hours.

The simulation results indicate that the reference building element is presented with the greatest diurnal variability, while the more the percentage weight of the PCM in the PCM-enhanced plaster, the smaller the range of the diurnal fluctuation. Accordingly, the case of the model design PCMPLASTER20 is illustrated with the lowest peak temperatures and the higher trough temperature values. This difference in the diurnal variation of the PCM-enhanced building elements is a result of the incorporated PCM's operation. Another evident effect from the PCM operation is that the time required for the interior temperatures of the PCM-enhanced building elements to rise and drop at their maximum and minimum values is longer in comparison to the conventional plaster case.

Excerpt from the Proceedings of the 2016 COMSOL Conference in Munich

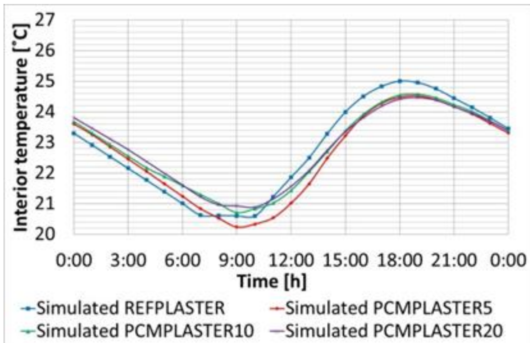

Figure 5. Simulation temperature results of interior surfaces for REFPLASTER, PCMPLASTER5, PCMPLASTER10, and PCMPLASTER20

7. Conclusions

This work indicated that the physical processes occurring during time-dependent phase change heat transfer in PCMs and PCM-incorporated element can be numerically modeled using COMSOL Multiphysics. In particular, the accuracy and validity of the numerical simulation models developed for the characterization of the thermal performance of novel PCM-enhanced building elements has been verified by data acquired from experimental work. The numerical simulation results of the interior spaces are found to be in good agreement with the experimental results, in terms of both temperature peaks and their timing.

The numerical analysis also showed that all three PCM-enhanced building elements, incorporating 5% by weight PCM, 10% by weight PCM, and 20% by weight PCM, achieved reductions in the impact of the diurnal temperature variation in the interior spaces of the building elements in comparison to the reference plaster building element. The decrease is a contribution of both the PCM-enhanced plaster composition itself, i.e. lower thermal conductivity and density, and higher heat capacity than the reference case, as well as of the operation of the PCM. The findings validated that that there is a positive correlation between the percentage weight of PCM within the PCM-enhanced plaster, and the effectiveness of the building wall in alleviating the impact of diurnal variability within the interior of buildings. Based on the findings of this work, the design optimisation of PCM-enhanced plasters for their application in buildings located in summer-dominant climatic conditions is defined, such as the desired results on thermal comfort and building energy consumption can be realised.

8. References

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