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Modeling aspects in simulation of phase change materials used for thermal regulation of buildings

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Abstract

Phase change materials applications involve a wide variety of fields starting from building engineering through the development of new types of material for thermal regulation of buildings [1], going to the development of hi-tech material for thermal comfort in apparel [2]. Improving civil engineering solutions and develop new materials for more efficient building leads to very significant opportunities to decrease the energy demand for civil purpose, as well as to reduce global energy consumption and greenhouse gas emissions at the buildings' level [1]. The set-up of a modelling tool able to simulate the thermal evolution over model sample of a phase change material allows to investigate on the role played by materials' thermo-physical properties as well as on geometric characteristic of the material system composed by the phase change material encapsulated on a classical building material matrix. On the other hand, the set-up of such virtual tool is not trivial because it requires the coupling of phenomena of different nature: phase change material droplet dispersion simulation; the heat transfer within the system composed by different domines and its mutual coupling. In this work, the modelling aspects related to the simulation of a transient thermal evolution through a material model developed by programming tools are presented. Particularly, the study was devoted to analysing the insulating performances of a building material made by cellular concrete added with 1% of glycerine. The simulation was performed for 90min with a wall temperature of 25°C and an initial temperature 2°C.

Keywords: modeling; insulation; phase change materials; building

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Public Interest Statement

While many of the advances in materials science have been driven by breakthroughs in material design and fabrication, understanding the changes that occur in a material during its utilization or operation in devices is of immense importance for its successful integration. Considering these aspects and the continued growth in materials research, there is a clear need for new topical journals which can serve researchers to understand the phase transitions and exploit the phenomena to current, state-of-the-art research in the field of materials science, moreover with full accessibility.

1. Introduction

Greenhouse gases emissions is a long term emerging environmental issue [1], and it represents an even bigger problem if considered in conjunction with the growth of oil prices. As a response to this scenario it is important to develop the utilization of different energy sources.

Many fields of research are intended to: develop policies to cut energy demands, find methods to reach a sufficient supplies stability and avoid fluctuations, make important advances to intensify the efficiency of the overall technology related to energy generation, find alternative energy sources in place of the common fossil sources [2], [3].

The improvement of efficiency in energy fields can be fostered by the development of new storage devices with the aim of reducing the existent supply-demand disparities while diminishing peaks in the loads; the energy that can be stored by these devices are either electrical, thermal and mechanical;

in particular, the ability to store latent heat is centred on the ability of a material to absorb and release energy whenever it undertakes a phase change, either from liquid to solid, gas to liquid and vice versa. The storage of latent heat is principally interesting because it offers a good energy storage density and is capable of functioning with a very little temperature change or even without any temperature change, more specifically this process takes place at the phase transition temperature for a particular material [4]–[6].

All the above justifies how PCMs are observed as a concrete key for dropping energy demands in edifices: their ability to store and release heat in a small temperature range increases the thermal inertia of the buildings and steadies the climate of the interiors.

In the following Table1, an overview of the main known PCMs is presented [7]–[9].

Table 1:Overview of the main PCMs used in the construction fields [7].

Organic compounds	Paraffins	Inorganic compounds	(Inorganic) Eutectics
Polyglycol E 400	Paraffin C_{14}	H_2O	58.7%Mg(NO)3·6H2O
Polyglycol E 600	Paraffin C_{15}–C_{16}	$LiClO_3·3H_2O$	+ 41.3%MgCl2·6H2O
Polyglycol E 6000	Paraffin C_{16}–C_{18}	$Mn(NO_3)_2·6H_2O$	
Dodecanol	Paraffin C_{13}–C_{24}	$LiNO_3·3H_2O$	66.6% $CaCl_2·6H_2O$
Tetradodocanol	Paraffin C_{16}–C_{28}	$Zn(NO_3)_2·6H_2O$	+ 33.3% $MgCl_2·6H_2O$
Biphenyl	Paraffin C_{18}	$Na_2CO_3·10H_2O$	
HDPE	ParaffinC_{20}–C_{33}	$CaBr_2·6H_2O$	48%$CaCl_2$+4.3%NaCl
Trans-1,4-polybutadiene	ParaffinC_{22}–C_{45}	$Na_2HPO_4·12H_2O$	+ 0.4%KCl+ 47.3 H_2O
	Paraffin C_{23}–C_{50}	$Na_2S2O_3·5H_2O$	
Propianide	Paraffin wax	$Na(CH_3COO)·3H_2O$	47% $Ca(NO_3)_2·4H_2O$
Naphtalene	Octadecane	$Na_2P2O_7·10H_2O$	+ 53% $Mg(NO_3)_2·6H_2O$
Erythitol		$Ba(OH)_2·8H_2O$	
Dimethyl-sulfoxide		$Mg(NO_3)_2·6H_2O$	60%Na(CH2COO)·3H_2O

Capric acid		$(NH_4)Al(SO_4)\cdot 6H_2O$	+ 40%$CO(NH_2)_2$
Capricinic acid		$MgCl_2\cdot 6H_2O$	
Laurinic acid		$NaNO_3$	66.6%Urea + 33.4%NH_4Br
Miristic acid		KNO_3	
Lakisol		KOH	
Palmitic acid		$MgCl_2$	
Stearic acid		NaCl	
Acetamid		Na_2CO_3	
Propionamid		KF	
		K_2CO_3	

As a natural consequence, the application of PCMs in any specific application urges the need for an investigation that is able to determine how and how much the PCMs application is able to improve the thermal performances of the considered system (walls, ceilings etc.), this to validate any additional costs for the implementation of the above mentioned PCM based systems [10].

For this reason, a precise modeling of the energy storage capability of the chosen systems is necessary to come to an optimum in the design and in materials choice for any given system [11]–[14].

In this particular study, a precise model is set up on Comsol Multiphysics (Comsol AB, Sweden), regarding a cylindrical sample of cellular concrete with 1% glycerine, thus resulting in an in-deep study of the insulating performances of the system.

2. Model implementation

A mathematical model [15], [16] of heat transfer in the analysed phase change material (PCM), was implemented. Equations, boundary conditions and numerical aspects are briefly discussed in the following subsections.

2.1. Transport equations

The heat transfer phenomena that take places during thermal evolution over PCM model sample are described by the classical unsteady state heat transfer equation by conduction into the cellular concrete matrix [17]:

$$\rho\, C_p \frac{\partial T}{\partial t} = \nabla \cdot k\nabla T \qquad (1)$$

and by the same heat transfer equation added by the convective term into the PCM material component composed by 1% of glycerine:

$$\rho\, C_p \frac{\partial T}{\partial t} = \rho\, C_{p\mathbf{u}}\, \nabla T + \nabla \cdot k\nabla T \qquad (2)$$

where T is the temperature within the sample, t is the process time, k is the thermal conductivity, ρ is the density, Cp is the mass heat capacity and **u** the fluid velocity into the

PCM material in the liquid phase. The eq.2 will have a null heat conduction term when is in the solid state.

During the PCM material phase change a fictitious specific heat could be defined as:

$$\boldsymbol{C_p = \frac{1}{\rho}\left(\theta_1\,\rho_1\,C_{p,1} + \theta_2\,\rho_2\,C_{p,2}\right) + L_{1-2}\,\frac{\partial \alpha_m}{\partial T}} \qquad (3)$$

Where $\boldsymbol{\theta_1}$ is the mass fraction of the PCM phase 1 (solid) and $\boldsymbol{\theta_2}$ refers to the phase 2 (liquid), ρ_1 and $C_{p,1}$ refers respectively to density and specific heat of phase 1, ρ is the medium density defined as $\rho = \boldsymbol{\theta_1}\,\rho_1 + \boldsymbol{\theta_2}\,\rho_2$, $\mathbf{L_{1-2}}$ is the latent heat from phase 1 to phase 2 and

$$\boldsymbol{\alpha_m = \frac{1}{2}\,\frac{\theta_2\,\rho_2 - \theta_1\,\rho_1}{\theta_1\,\rho_1 + \theta_2\,\rho_2}} \qquad (4)$$

While the physical properties depend on temperature, Eqs. (1) and (2) are dependent on each other and the problem must be solved in a coupled form.

3. Geometry and material

The material geometry was composed by disk of cellular concrete material with a defined thickness. The PCM material dispersed inside the external matrix was simulated implementing a developer method code into Comsol Multiphysics software (Comsol AB, Sweden), adding randomly placed spheres of random diameter between a minimum and maximum value. The code add spheres until the desired concentration of PCM was reached. The cellular concrete by the Comsol library material was used and two custom materials were created respectively for the Glycerine liquid and solid phase. The material geometry at 1% of glycerine is reported in figure 1.

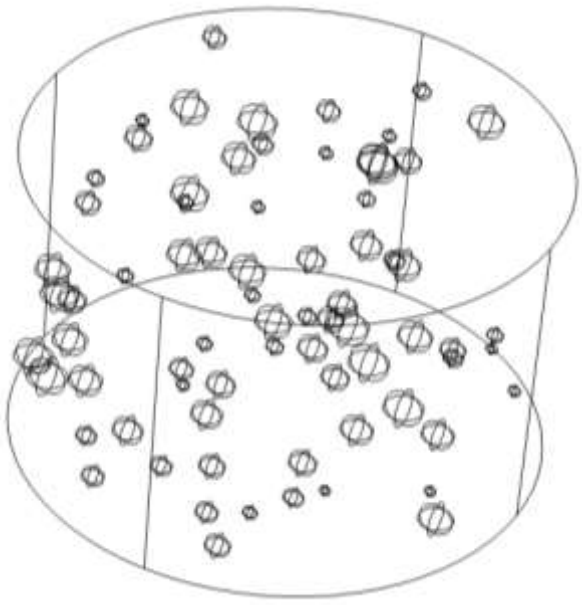

Figure 1: Material geometry from the developer method created in Comsol composed randomly placed spheres. PCM % = 1% v/v

The cellular concrete material is characterized by $\rho = 600.0\, Kg/m^3$, $C_p = 850.0\, J/(kg\, K)$ and $k = 0.1400\, W/(m\, K)$; the glycerine on the solid phase by $\rho = 1260\, Kg/m^3$, $C_p = 543.5\, J/(kg\, K)$ and $k = 0.2950\, W/(m\, K)$; the glycerine on the liquid phase by $\rho = 1260\, Kg/m^3$, $C_p = 2412\, J/(kg\, K)$ and $k = 0.2950\, W/(m\, K)$; the glycerine phase change temperature is equal to $T_{trans} = 18°C$.

4. Initial and boundary conditions

It is assumed that the entire material sample is at uniform initial temperature T_0=2°C (275.15 K). As boundary conditions for the heat transfer equation, continuous domains were considered assuming ideal conductive transport in the interfaces between cellular concrete and the dispersed PCM material domains. For the external surfaces different considerations were made. The external lower face of the material disk was considered at fixed uniform temperature T=25°C imposed at initial time as a step function from 2 to 25°C at t = 0. The upper face was considered as convective heat wall in the free air with a heat flux equal to:

$$\boldsymbol{q_{eq} = h\,(T_{air} - T)} \qquad (5)$$

where h was considered equal to 5 $W/\,m^2K$ and $T_{air} = \mathrm{T}_0$.

The lateral disk walls were considered thermally insulated assuming that the heat transfer is not negligible only in face-to-face z direction.

5. Numerical solution solver implementation

The implemented model was solved by the Comsol Multiphysics software [18]. Numerical tests were performed with different mesh parameters to evaluate the simulation results and to find the best mesh settings. The meshed geometry was reported in figure 2. The set providing the best spatial resolution for the considered domain and for which the solution was found to be independent of the grid size, was composed of 106773 tetrahedrons, 10854 triangles boundary elements, 2418 edge elements, 456 vertex elements with 122325 degrees of freedom. The numerical solution was attained on a server equipped with a motherboard Supermicro X11DAi-N, 2 x CPU Intel Xeon Silver 4214 @ 3.2 GHz, 24 cores, 48 thread; equipped with a RAM of 128 Gb DDR4 2400 MHz. The server run under Windows 10 operating system at Department of Computer Engineering, Modeling, Electronics and Systems (D.I.M.E.S.), University of Calabria, Italy.

6. Results and discussion

The numerical solution of the proposed model allows to acquire the transient spatial temperature distribution. Figure 3 shows a temperature distribution on y-z plane of the material model after 90 min. The considered system, heaven if non-homogeneous, reveals a quite uniform temperature distribution along y direction in a large portion of the investigated domain. The major temperature gradient, as expected, is observable in z direction.

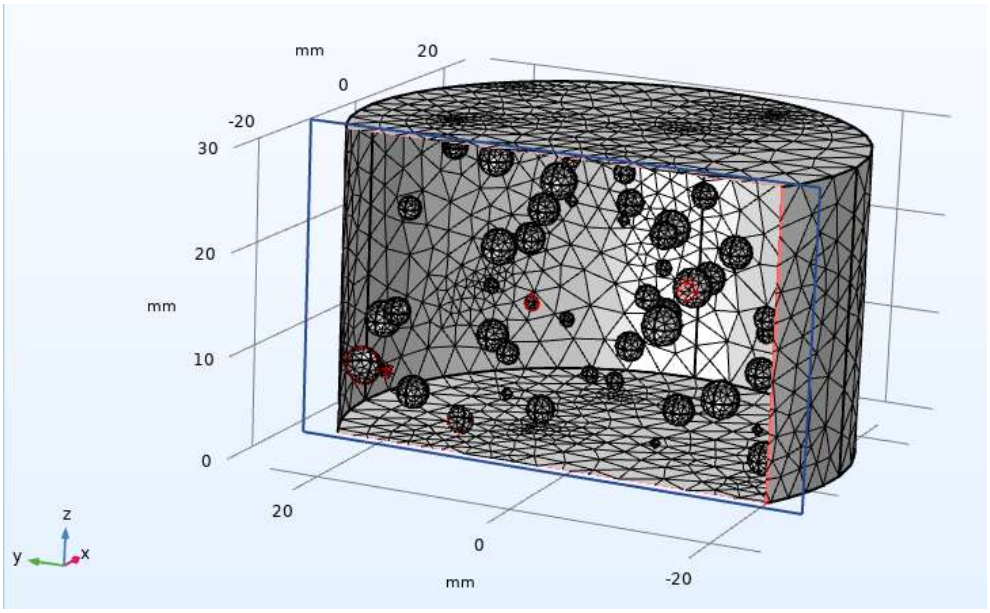

Figure 2: Geometry mesh of the PCM material model

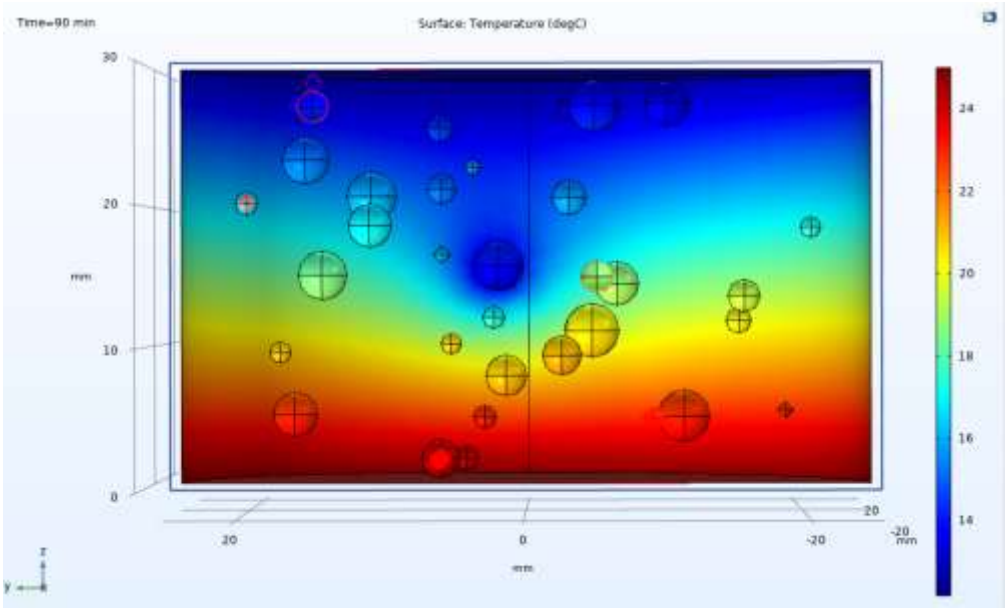

Figure 3: Temperature distribution on a y-z plane section of the material model. t=90min

Figure 4 shows the external wall average temperature evolution. After a response time of 3 minutes the model shows a temperature rising on the analysed surface that will settle on a steady state at more than 60 minutes. The major advantage of the presence of PCM material droplets is the lengthen the transition heating time. This effect is better represented in figure 5 where a single PCM sphere temperature evolution is reported. Around its melting point, the PCM material induces a delay on temperature rising evolution that could be modified changing the PCM concentration.

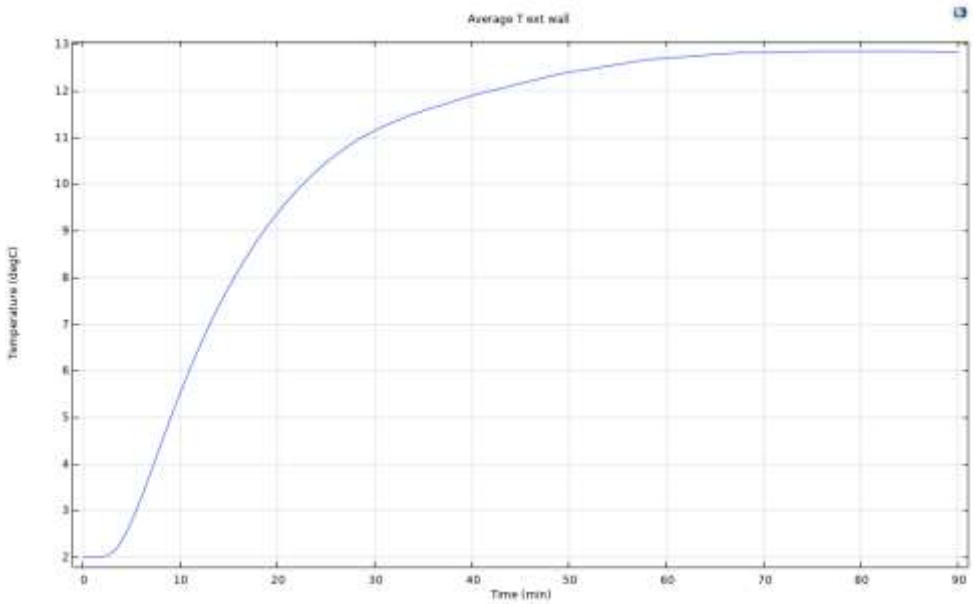

Figure 4: External wall average temperature evolution vs time

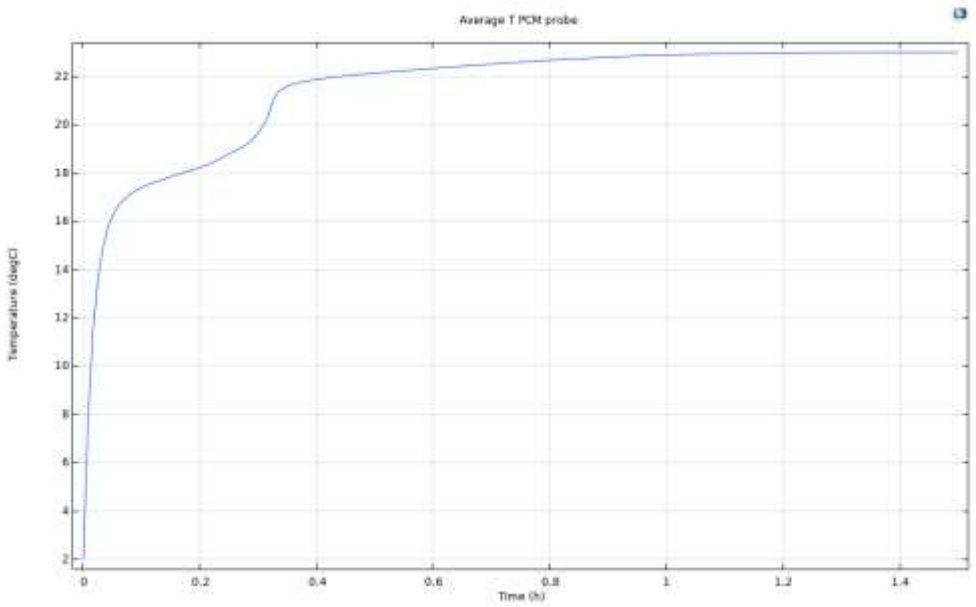

Figure 5: Single PCM sphere average temperature evolution. Centre of the sphere: x=-7.79mm, y=-19.45mm, z=5.67mm

7. Conclusions

In this work, a thermal evolution model within a PCM added building material was presented. A programming geometry to simulate the random presence of PCM particles with randomly distributed dimensions was also developed implementing a developer method in Comsol multiphysics software. The investigated material was composed by building cellular concrete modified by 1% dispersed particles of Glycerine as PCM enhancer material. A time dependent study was performed on 90min of thermal evolution and a steady state was observed at more than 1 hour. The temperature rising is significantly delayed by the presence of PCM material, and the modelling techniques could predict it.

The presented model, that would be a starting tool for PCM material development, could be developed and implemented in different PCM studies. Moreover, it represents a powerful approach to optimize the PCM concentration, to study different matrix dispersions, to analyze the presence of other PCM materials without prohibitive economic and computational efforts.

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