

Numerical modeling of phase change materials using simusol software

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HIGHLIGHTS

- Thermophysical modeling of PCM was implemented in Simusol software for first time.
- The whole model is based on experimental test results and theoretical developing.
- A new methodology for latent heat was implemented by a Gauss function.
- Room air temperature ranges within 20–26 °C, with PCM implementation.
- PCM implementation reduces the volumetric air flow for HVAC system up to 87%.

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ABSTRACT

Thermal storage systems with phase change materials offer a high density of energy with a moderate temperature variation as well as the possibility to keep the inner temperature within a comfort range. To achieve this goal, it is necessary to select the most suitable phase change material. In this line, numerical simulations are necessary to predict results and take decisions about the best material that will be implemented on buildings devices for thermal performing. This work aims to study numerically how the inner air temperature of a defined room changes when a double-glazed PCM-filled window is mounted. For this, a new methodology for latent heat was implemented by a temperature-dependent Gauss-function, while an on/off strategy was considered to separate solid from liquid state. Both equations and parameters that involve thermophysical and optical properties were determined experimentally by Modulated Differential Scanning Calorimetry and spectroradiometer techniques, respectively. The resultant numerical model was implemented into the Simusol software for first time. It was found that the inner air temperature can be reduce up to 40% in average, in comparison with empty double-glazed window case, making it possible to reach the expected range of 20–26 °C. Simulation results also revealed that volumetric air flow for HVAC systems could be reduced up to 87% in winter, when PCM is implemented.

1. Introduction

Thermal storage systems (TES) with phase change materials (PCM) offer a high density of energy with a moderate temperature variation [1]. In locations where a PCM storage system has been implemented, the indoor temperature oscillates within a comfort range and less energy is consumed because electrical/gas equipment for acclimatization is replaced [2]. The process of selecting an appropriate PCM is very complicated but crucial for thermal energy storage. The potential PCM should have a suitable melting temperature, desirable heat of fusion, and thermal conductivity depending on the practical application. Thus, the methods of measuring the thermal properties of PCM are very important. Suitable PCM and an appropriate incorporation method into the building material as well as latent heat thermal energy storage

(LHTES) can be economically efficient for heating and cooling buildings. However, several problems need to be tackled before LHTES can be reliably and practically applied.

Simulations of PCM have been improved over several years. By means of different techniques in simulations programs, optical and thermal properties have been implemented and measured on small-scale samples of PCM windows. In this way, different numerical models were developed to run simulations and analyze the thermal performance of PCM systems [1], in particular, double-[3–5] and triple-glazed windows for building applications [6]. Almost all numerical models have been validated by experimental measurements to ensure their simulation results and couple PCM models with programs such as ESP-r [7,8], TRNSYS [9], Energy Plus [10], ANSYS-FLUENT [11] and COMSOL [12,13], among others. Furthermore, finite volume method

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Nomenclature

A_{g1}, A_{g2}	glass solar absorptance, dimensionless
A_p	PCM solar absorptance, dimensionless
C_{eff}	PCM effective heat capacity, J/kg °C
F_{sky}	view factor between the sky dome and the glass 1 surface, dimensionless
g, φ_p	heat generation rate of PCM layer, W/kg
h_o, h_i	air-glass convective heat transfer coefficients, W/m ² °C
h_{pj}	PCM convective heat transfer coefficient, W/m ² °C
HC	PCM heat capacity obtained by MDSC method, J/kg °C
$\dot{H}$	PCM latent heat obtained by MDSC method, W/g
I	solar radiation, W/m ²
m_1, m_2	glass masses, kg
m_p	PCM total mass, kg
n_{air}	refractive index for air, dimensionless
n_g	refractive index for glass, dimensionless
n_{pcm}	compounded refractive index for PCM, dimensionless
N_{uj}	Nusselt number for PCM convection in liquid state, dimensionless
R_{aLj}	Rayleigh number for PCM in liquid state, dimensionless
S_p	transversal area of PCM layer, m ²
t	time, s
T, T_p	PCM temperature, °C
T_m	PCM melting point, °C
T_{ji}	temperature of inner surface of glasses, °C
T_1, T_2	glass temperatures, °C

V_p	PCM total volume, m ³ φ_p is the thermal source term or heat generation
x_{g1}, x_{g2}	glass thicknesses, m
x_p	PCM thickness or gap length, m

Greek symbols

α_i	absorption coefficient, m ⁻¹
β_m	parameter which separates solid from liquid state, dimensionless
β_s	factor that splits the heat exchange with the sky dome between sky and air radiation, dimensionless
Δx_i	thickness of media i, m
Δt	time-step of MDSC test, s
ε	surface emissivity of the glasses, dimensionless
θ_i	angle of solar incidence, °
λ, λ_j	PCM thermal conductivity, Wm/°C
$\lambda_{g1}, \lambda_{g2}$	glass thermal conductivities, Wm/°C
ρ, δ_p	PCM density, kg/m ³
ρ_{i1}	reflectance of the entrance surface of media i, dimensionless
ρ_{i2}	reflectance of the exit surface of media i, dimensionless
σ	Stefan-Boltzmann constant (5.670373 × 10 ⁻⁸ W/sK ⁴)
τ_{pcm}	solar transmittance PCM, dimensionless
τ_{g1}	solar transmittance of the glass 1, dimensionless
v	variable which depends on C_{eff} ,
φ_1, φ_2	heat generation rate of glass layers, W/m ³

has been implemented by Mexican researchers, to study different double pane windows available on the market [14] and coating strategy for reduction of solar energy gain [15]. However, their model only considered the air-gap between glasses.

Modeling of PCM behavior requires implementing energy balance equations. In order to obtain the flattened shape of the temperature plot while melting or freezing processes are taking place, several authors have proposed different mathematical formulations. Most of them neglect the overcooling effect [16] and the viscosity dissipation due to the low movement of PCM and mushy – liquid state [17]. Liu et al. [5] investigated the thermal and optical performance of a PCM-filled double-glazed unit using a simple model that considers a radiative source term for the PCM layer but not for the glasses. Their results strongly focused on the refractive index and extinction coefficient of PCM and the variation in the temperature of the interior glass surface as well as the transmitted energy. Numerical results were compared with experimental measurements, showing a good correlation between them. A more complex model was developed by Heim and Clarke [8] and implemented on ESP-r software. For the non-linear problem (in the phase change temperature range), the Goodman transform was used to remove the temperature dependence: the effective heat capacity concept was introduced, and thermal balance for a control volume was proposed as shown in Eq. (1).

$$\rho(T)C_{eff}(T)\frac{\partial T}{\partial v}\frac{\partial v}{\partial t} = \nabla \cdot \left[\lambda(T)\left(\frac{\partial T}{\partial v}\nabla v\right) \right] + g(\vec{r}, t) \quad (1)$$

The time dependence on this differential equation makes it possible to obtain the flattened behavior of temperature of PCM at a phase changing process, which means there is no variation in temperature (which is practically constant at melting point). In this range, a constant value of latent heat was considered for the whole process. The model in Eq. (1) was implemented in ESP-r for the first time in order to enhance the program. However, the whole model was improved by Wiprzkowicz [18] with a more detailed C_{eff} concept and an extensive programming routine in FORTRAN [19]. The optical and thermal properties for several types of PCM (pure paraffins with different melting points) were

implemented, and the solar incidence angle dependence of optical properties was also considered. The current version of ESP-r also includes solar lighting performance analysis, and results for a complete year-period can be obtained.

The modeling presented here is promoted by the SOLTREN project from ERANet-LAC, in cooperation with institutes from Poland, Chile, Latvia, and Argentina. The objective of this article is to show a new thermal model for a double-glazed PCM-filled window, which will be mounted in the city of Santiago de Chile for experimental testing and measurements. Like ESP-r and Energy Plus, this model considers the incidence angle dependence as well as optical and physical properties based on experimental measurements. Although Rubitherm® has provided information about heat capacity and latent heat of paraffin samples, the temperatures and heat flows associated with transitions in PCM samples were measured by Modulated Differential Scanning Calorimetry (MDSC) technique. A TA Instruments® DSC Q200 V24.4 device was used. This technique determines the temperature and heat flow associated with material transitions as a function of time and temperature. It also provides quantitative and qualitative data on endothermic (heat absorption) and exothermic (heat evolution) processes of materials during physical transitions that are caused by phase changes, melting, oxidation, and other heat-related changes [20]. Such measurements provide quantitative and qualitative information about physical changes in the heat flow. Latent heat parameter was not considered a constant value, that is, the amount of thermal energy released or absorbed is modeled by a Gauss regression according to the temperature of the sample. Furthermore, solar transmittance measurements were performed using a portable spectro-radiometer LI-1800 model that makes it possible to analyze the solar transmittance in the spectral range from 300 nm to 1100 nm.

The simulation presented here is an improvement of a previous work [21]. This model also considered an automatic solar coating as [15], and the implementation of an air-conditioning system. In this current study, a new model for latent heat was implemented by a temperature-dependent Gauss-function. The energy balance equation of PCM layer and its boundary conditions were modified. Additionally, an

on/of strategy was considered to separate solid from liquid state. The numerical model is conducted on Simusol, an open-access software developed by researchers of Instituto de Investigaciones en Energía No Convencional (INENCO). This software runs on Linux as well as Windows Operative System and can analyze solar-thermal, mechanical, and electrical systems [22,23]. A graphical interface, Dia, is used to assemble diagrams and write equations. The output of the simulation is a function of time, which can be shown as a plot and a spreadsheet. Additional programming in FORTRAN can be added to the main program if a more advanced calculation is needed. For further information, visit www.simusol.org.

2. Experimental setup

Thermophysical and optical properties of PCM must be determined experimentally. The methodology used in the present study is similar to that used by different authors [24,25]: an MDSC technique is performed to obtain heat capacity vs. temperature of PCM, and latent heat value. Moreover, the solar transmittance was measured for different solar incidence angles on both solid and liquid states under real solar gain conditions. The tested paraffins were RT18HC and RT25HC, with a nominal melting point at 25 °C and 18 °C, respectively. However, a first experimental test based on Differential Scanning Calorimetry (DSC) technique was performed, in order to make a first characterization of the two paraffins samples. Fig. 1 shows curves from DSC results, while Table 1 summarizes the thermal information extracted from tests. The latent heats of both samples are calculated by setting a triangle area under the heat capacity curves, while the phase change is taking place.

2.1. Heat capacity (HC) measurement and determination of latent heat ($\dot{H}$)

A TA Instruments® device was used to measure the heat capacity. It was configured to run a MDSC technique. At first, the PCM sample was stabilized at -10 °C, in order to mark an initial process temperature as reference, then heated until 90 °C, and finally cooled until -10 °C again. A ± 10 °C/min ramp was used for all processes. Nitrogen consumption was configured at 10 ml/min. The software tool describes the method as follows:

1. Equilibrate at -10 °C
2. Isothermal for 2 min
3. Mark end of cycle 1
4. Ramp 10.00 °C/min to 90 °C
5. Isothermal for 3 min
6. Mark end of cycle 2
7. Modulate ± 1 °C every 120 s
8. Ramp 10.00 °C/min to 90 °C
9. Isothermal for 2 min
10. Mark end of cycle 3
11. Modulate ± 1 °C every 120 s
12. Ramp 10.00 °C/min to 90 °C
13. Mark end of cycle 4

Fig. 2 shows the heat capacity of the PCM sample resulting from the MDSC measurement. During the phase transition, heat capacity reached 30 J/g°C, which represents a promissory material for building applications. The dashed line corresponds to a Gaussian regression (Eq. (2)) introduced into the simulation model for heat capacity description, with a determination coefficient $R^2 = 0.94$.

$$HC = 1000 \left(a * e^{-\frac{(T(^\circ\text{C})-b)}{2*c^2}} + 2.5 \right) (\text{J/kg } ^\circ\text{C}) \quad (2)$$

where coefficients a, b, and c are equal to 28.5 J/g °C, 25.7 °C, and $2.6 \frac{1}{\sqrt{^\circ\text{C}}}$, respectively. These coefficients were adjusted until the areas under the whole curves (measured and Gaussian) were equal. Note that

coefficient b represents the temperature of paraffin for a maximum peak of heat capacity, and this value was taken as reference to separate solid from liquid phases on the simulation strategy 'flag', instead of the nominal melting point given by the manufacturer. This 'flag' is introduced by the β_m parameter. This operates as an on-off switch varying from 0 to 1, and vice versa, according to the PCM temperature, as displayed in Fig. 3.

It is possible to calculate the latent heat in terms of specific thermal power that the PCM can release or absorb. Taking HC values for each time-step, Eq. (3) determines latent heat, and Fig. 4 shows its variations according to the PCM temperature.

$$\dot{H} = HC \cdot \Delta t(\text{min}) \cdot \Delta T(^\circ\text{C}) \cdot 60 (\text{W/g}) \quad (3)$$

In this case, the Gaussian regression is given by Eq. (4) with a determination coefficient of $R^2 = 0.93$. Values for a, b, and c were set at 0.15 W/g, 27 °C, and $3.6 \frac{1}{\sqrt{^\circ\text{C}}}$, respectively. Eq. (4) was also introduced into the Simusol simulation.

$$\dot{H} = 1000 \left(a * e^{-\frac{(T(^\circ\text{C})-b)}{2*c^2}} + 0.02 \right) (\text{W/kg}) \quad (4)$$

2.2. Transmittance measurement

Transmittance was tested on a double-glazed cell with a commercial glass of 4 mm in thickness. The PCM is inside of a glass box, which dimensions are 100 mm $\times$ 100 mm $\times$ 12 mm. The box was placed inside a metallic case painted black, as shown in Fig. 5, to avoid extra solar gain due to reflection on the measurement device surface. Furthermore, measurements of solar gain were carried out for different incidence angles (0, 40, 55, 70, and 80°) and following the sun path.

The device was a Licor 1800 spectroradiometer for 400–1100 nm of wavelength range, and the tested paraffin was RT25HC, in solid as well as liquid states. Results are shown in Fig. 6. Firstly, for each angle, a solar irradiation measurement was taken before solar gain through the PCM-filled cell, to compare both solar gains and calculate the spectral transmittance.

Average transmittance is summarized according to the solar incidence angle in Table 2. As observed for solid state, an average transmittance equal to 0.11 can be obtained for all angles, which simplify numerical simulation and improve timing on calculation.

The melting point was set at $T_m = 25.7$ °C. This value indicates to the simulation when to use the transmittance in the solid or liquid state, as well as the refraction indexes at each state. The simulation proposed here does not take into account a mushy region, as several authors have proposed. However, Eqs. (2) and (4) give a smooth variation in the PCM temperature. The other properties of the materials used in this work are given in Table 3.

3. Problem definition

An east-facing room with a HAVC system was considered. The room

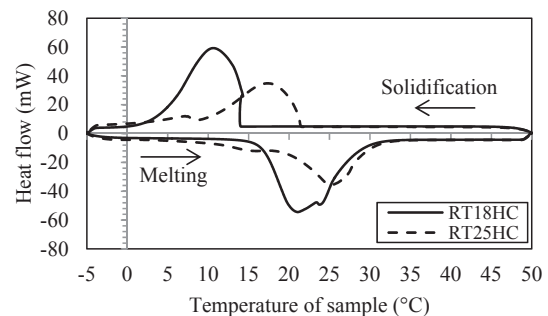


Fig. 1. DSC curves for RT18HC and RT25HC samples.

Table 1
DSC results from measurements.

	Melting		Solidification		Overcooling	Latent heat
	Q_m	T_m	Q_s	T_s		
Sample	mW	°C	mW	°C	°C	J/g
RT18HC	−54.43	21.07	59.25	10.63	10.45	260.6
RT25HC	−35.81	25.19	34.85	17.34	7.86	241.9

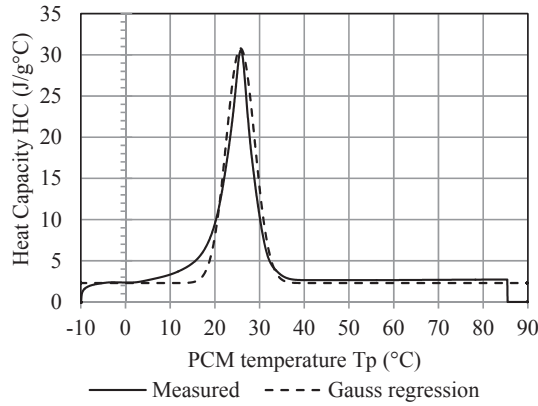


Fig. 2. Heat capacity plot from MDSC test and Gaussian regression.

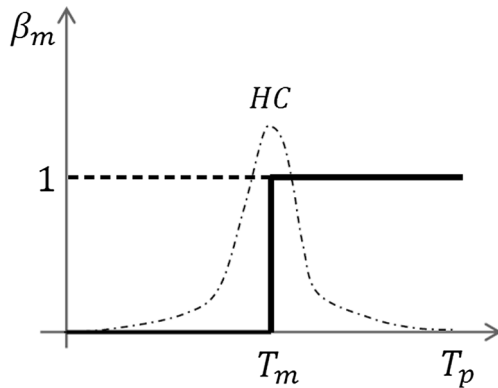


Fig. 3. On-off switching variation of the β_m parameter.

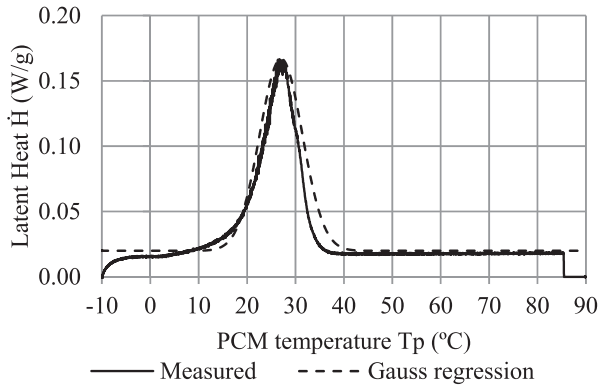


Fig. 4. Latent heat plot from MDSC test and Gaussian regression.



Fig. 5. Experimental setup for measurement device.

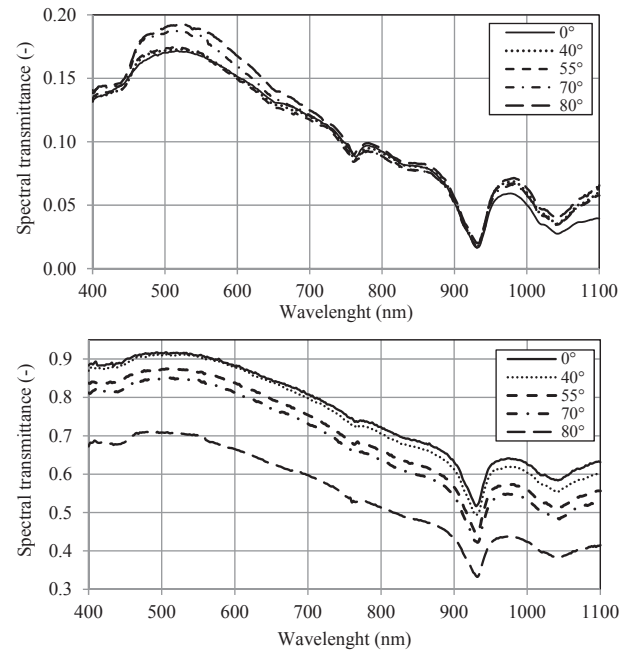


Fig. 6. Transmittance of PCM in solid (a) and liquid state (b).

Table 2

Average solar transmittance for RT25HC paraffin sample.

Incidence angle	0°	40°	55°	70°	80°
Solid	0.10	0.10	0.10	0.11	0.11
Liquid	0.76	0.74	0.70	0.68	0.55

Table 3

Properties assumed for materials.

Property	RT25HC	Glass	Glass wool	Gypsum
Conductivity λ ($W m^{-2} K^{-1}$)	0.21	0.8	0.03	0.3
Density ρ ($kg m^{-3}$)	870	2500	14	2330
Absorptivity α (%)	2	5	–	–
Refraction index n (solid)	1.52	1.52	–	–
Refraction index n (liquid)	1.43	–	–	–

is located in the city of Santiago de Chile (Latitude: -33.44 , Longitude: -70.65 , altitude: 572 m.a.s.l.). All walls are isolated by a glass wool-gypsum configuration, as shown in Fig. 7. The solar irradiation impinges only on the east-facing wall and passes through the window. It was assumed that there were no thermal gains/losses through the lateral walls or the wall opposite the window. Thermal exchange between

indoor and environmental temperature nodes is only possible through the window and east-facing wall (where the window is situated).

The simulation was carried out for the most representative Julian days of the year, with ± 2 days, as specified in Table 4. For these days, climatic data were obtained from a typical meteorological year (TMY) database, where global horizontal solar irradiation (GHSI), environmental temperature (ET), and wind speed (WS) were considered to be

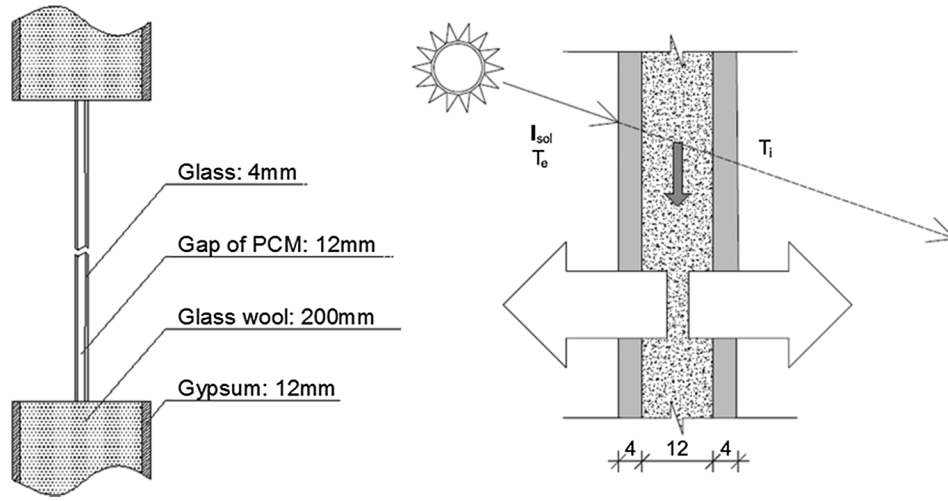


Fig. 7. Wall configuration (left) and PCM-filled double-glazed window scheme (right).

Table 4

Configurations of days to run the simulation.

	March(Autumn)	June(Winter)	September(Spring)	December(Summer)
Julian day	75	162	258	344
Added days	73,74 – 76, 77	16, 161 – 163, 164	256, 257 – 259, 260	342, 344 – 345, 346

external conditions. In the case of GHSI, it was necessary to apply the Liu-Jordan method [19] to obtain the hourly solar irradiation on the east-facing wall (Fig. 8).

The HVAC system was configured according to the schedule shown in Fig. 9, where the values of the air flow are given in $\text{m}^3 \text{h}^{-1}$. Each value for each time range was set in order to keep the inner temperature within a range of 20–26 °C as the comfort zone. The low values correspond to the natural infiltrations into the room. From 6:00 to 7:00 a.m., higher ventilation is necessary to refresh the air inside the room, before the workday starts. Then, from 8:00 a.m. to 4:00p.m., constant ventilation is configured.

The external geometry of the room is $2.4 \times 2.6 \times 4.4 \text{ m}^3$ and the PCM-filled window is $1.1 \times 1.1 \text{ m}^2$. This window is in the center of the east-facing wall, as shown in Fig. 10.

As stated for HVAC, a schedule for internal heat gains (IHG) was assumed to be the heat source of the indoor temperature node (air room). As shown in Fig. 11, the value of 480 W corresponds to 260 W generated by two workers from 8:00 a.m. to 4:00 p.m. and 220 W produced by the electrical equipment in the same period.

4. Physical and mathematical model

Simulations of phase change processes in applications where conduction is the dominant heat transfer model have provided a more accurate prediction of the temperature and heat flow in the material as well as indoor thermal conditions during thermal cycling [16]. Climatological variables, such as wind speed, solar radiation, and environmental temperature were considered into boundary conditions. Their variation is hourly, as was obtained from the meteorological database. Regarding to convective coefficients, they were calculated based on methodology described in [26]. Fig. 12 shows the physical model implemented in the present simulation. When solar energy reaches the unit surface, one part of it is absorbed by the double-glazed unit, and the other part is transmitted and reflected. The boundary conditions on the exterior and the interior surfaces include the effect of thermal radiation and convection. In the PCM and glass layers, solar energy undergoes reflections many times between inner and outer surfaces. The heat transfer in the double-glazed unit filled with PCM is divided into

three parts: the outer glass layer (glass 1), the PCM layer, and the inner glass layer (glass 2).

For glasses 1 and 2 respectively, the mathematical boundary conditions for the calculation domain are given as:

$$\lambda_{g1} \frac{\partial T_1}{\partial x_{g1}} = F_{sky} \beta_s \varepsilon \sigma (T_{io}^4 - T_{sky}^4) + \varepsilon \sigma F_{sky} (1 - \beta_s) (T_{io}^4 - T_c^4) + h_o (T_{io} - T_c) + m_1 \varphi_1 \quad (5)$$

$$\lambda_{g2} \frac{\partial T_2}{\partial x_{g2}} = h_i (T_{2o} - T_a) + \varepsilon \sigma (T_{2o}^4 - T_a^4) + \sum \sigma \varepsilon F_j (T_{2o}^4 - T_j^4) + m_2 \varphi_2 \quad (6)$$

According to Liu et al. [4,5]:

$$\beta_s = \sqrt{0.5(1 + \cos \theta_i)} \quad (7)$$

$$F_{sky} = 0.5(1 + \cos \theta_i) \quad (8)$$

$$T_{sky} = 0.0552 T_e^{1.5} \quad (9)$$

The Σ term in Eq. (6) represents the radiative interaction between the inner glass surface of the window and all inner wall surfaces at their T_j temperatures. For the PCM layer, the energy balance is given by Eq. (10) and the temperature of the PCM node is given by solving Eq. (11). The effect of convection must be considered when describing the melting process [4,9,27,28]. In those cases, solid and liquid parts must

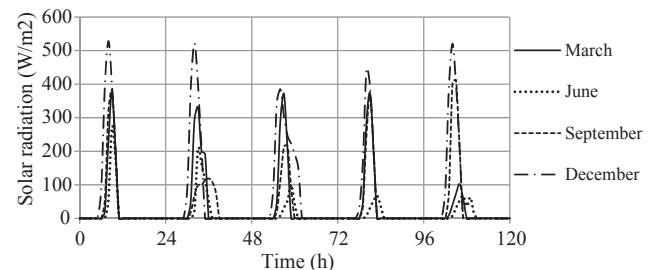


Fig. 8. Solar radiation impinging on eastern wall.

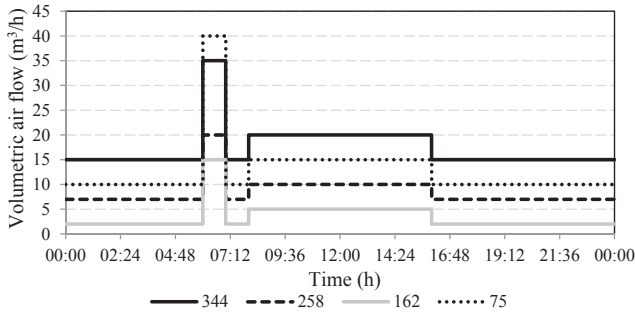


Fig. 9. HVAC – volumetric air flow configuration.

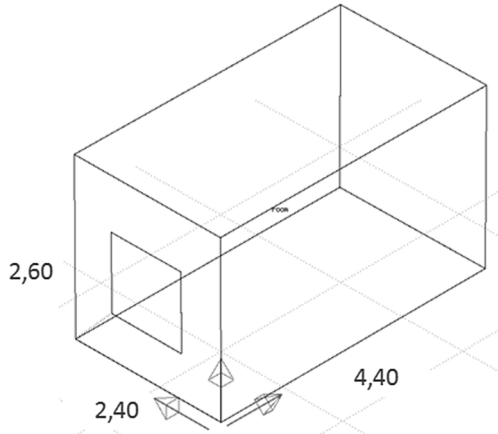


Fig. 10. Geometry of the simulated room.

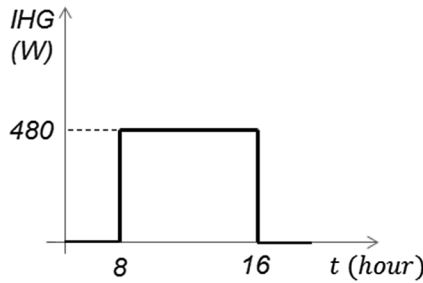


Fig. 11. Internal heat gain schedule.

be identified in all directions. In the other hand, Durakovic and Torlak [29] have found out a good matching between computational and experimental results, while convection effect was neglected in their 2D-PCM model. The Simusol program is for 1D problem in scale construction, where solid and liquid fraction is calculated based on the

temperature and the latent heat stored [30]. The internal convection is introduced in this model (Eqs. (12) and (13)) [31].

$$\sum_{j=1}^{j=2} \lambda_j (1 - \beta_m) \frac{\partial T_p}{\partial x_p} + \sum_{j=1}^{j=2} h_{pj} \beta_m S_p (T_p - T_{ji})$$

$$= m_p H C \frac{\partial T_p}{\partial t} + m_p \dot{H} \beta_m + \delta_p V_p \varphi_p \quad (10)$$

$$\rightarrow \frac{\partial T_p}{\partial t}$$

$$= \left(\sum_{j=1}^{j=2} \lambda_j (1 - \beta_m) \frac{\partial T_p}{\partial x_p} + \sum_{j=1}^{j=2} h_{pj} S_p (T_p - T_{ji}) \beta_m - m_p \dot{H} \beta_m - \delta_p V_p \varphi_p \right) \frac{1}{m_p H C} \quad (11)$$

$$h_{pj} = N_{uj} \frac{\lambda_j}{x_p} \quad (12)$$

$$N_{uj} = 0.046 (Ra_{l,j})^{1/3}, \quad 10^6 \leq Ra_{l,j} \leq 10^9 \quad (13)$$

In Eq. (11), while sensible heating or cooling is taking place, the β_m factor is zero and the $\partial T_p / \partial t$ term varies linearly with heat gain by conduction and by the volumetric radiative source term φ_p . When the PCM temperature reaches the melting or freezing point, the β_m factor is switched-on into 1 while $\partial T_p / \partial t = 0$, so that the PCM temperature remains invariable. As a result, the latent heat $\dot{H}$, convective flux and thermal source φ_p provide the thermal gain to the PCM layer. Eq. (11) is solved by Simusol because it is defined as a linear differential equation. It is, therefore, necessary to define initial conditions for all temperatures of nodes that involve mass.

Liu et al. [5] have implemented equations to calculate the volumetric radiative source terms φ_1 , φ_2 and φ_p , as follows:

$$\varphi_1 = \frac{\tau_{g1} A_{g1} I \cos \theta_i}{\Delta x_{g1}} \quad (14)$$

$$\varphi_2 = \frac{\tau_{g1} \tau_{pcm} A_{g2} I \cos \theta_i}{\Delta x_{g2}} \quad (15)$$

$$\varphi_p = \frac{\tau_{pcm} A_p I \cos \theta_i}{\Delta x_p} \quad (16)$$

Each absorptance is calculated following Li et al. [32] for glass 1, PCM, and glass 2, respectively:

$$A_{g1} = 1 - \rho_{11} - \frac{(1 - \rho_{11}) \rho_{12} \text{EXP}(-2\alpha_1 \Delta x_{g1})}{1 - \rho_{11} \rho_{12} \text{EXP}(-2\alpha_1 \Delta x_{g1})} \quad (17)$$

$$A_p = 1 - \rho_{p1} - \frac{(1 - \rho_{p1}) \rho_{p2} \text{EXP}(-2\alpha_p \Delta x_p)}{1 - \rho_{p1} \rho_{p2} \text{EXP}(-2\alpha_p \Delta x_p)} \quad (18)$$

$$A_{g2} = 1 - \rho_{21} - \frac{(1 - \rho_{21}) \rho_{22} \text{EXP}(-2\alpha_2 \Delta x_{g2})}{1 - \rho_{21} \rho_{22} \text{EXP}(-2\alpha_2 \Delta x_{g2})} \quad (19)$$

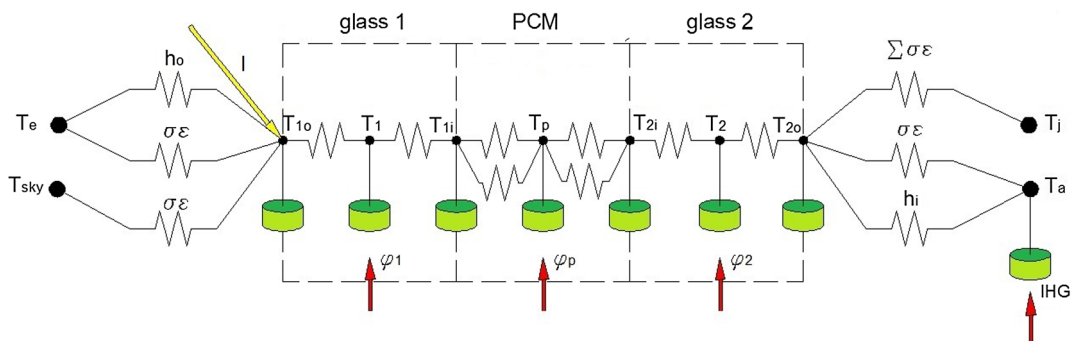


Fig. 12. Scheme of the double-glazed unit filled with PCM.

The interface reflectance is calculated based on Fresnel's relations [33] as follows:

$$\rho_{11} = (n_{\text{air}} - n_g)^2 / (n_{\text{air}} + n_g)^2 \quad (20)$$

$$\rho_{12} = \rho_{p1} = (n_g - n_{\text{pcm}})^2 / (n_g + n_{\text{pcm}})^2 \quad (21)$$

$$\rho_{p2} = \rho_{p2} = (n_{\text{pcm}} - n_g)^2 / (n_{\text{pcm}} + n_g)^2 \quad (22)$$

$$\rho_{21} = (n_{\text{pcm}} - n_g)^2 / (n_{\text{pcm}} + n_g)^2 \quad (23)$$

$$\rho_{22} = (n_g - n_{\text{air}})^2 / (n_g + n_{\text{air}})^2 \quad (24)$$

For n_{pcm} , the β_m factor was also applied (Eq. (25)), in order to split the solid and liquid phases of the paraffin.

$$n_{\text{pcm}} = (1 - \beta_m)n_{\text{pcm-sol}} + \beta_m n_{\text{pcm-liq}} \quad (25)$$

5. Simulation outputs

Simusol runs and generates a spreadsheet with a 7-s time-step for each parameter. If any parameter is asked to plot, Simusol generates graphs for all thermal nodes. The values of the room and PCM node temperature were saved at each time-step. To aid the analysis, the histories of these parameters were presented for all five days for the most representative months. Simulations were carried out for different scenarios: no-PCM – no-HVAC, no-PCM – HVAC, PCM – no-HVAC, and finally PCM – HVAC. For no-PCM cases, the gap between glasses was considered as filled with air.

Fig. 13a–d shows a comparison of the indoor room temperature for all scenarios. The overheating was produced in both PCM and no-PCM cases without the HVAC system. It was necessary to implement a ventilation system to have a temperature variation within a range of 20–26 °C as the comfort zone. The HVAC air volumetric flow coefficients were introduced above, in Fig. 8. By implementing PCM-filled double-glazed windows, the overheating was highly reduced in no-HVAC cases by an average of 23 °C, as seen in Fig. 13a–d. This represents a reduction about 40% on temperature peak.

Fig. 14 shows the variation in the temperature of the PCM node, for the HVAC case. The temperatures reach values below the melting point, but the paraffin does not completely melt. This behavior can be related to the east orientation of the façade, where the solar gain is not enough to melt the paraffin.

The worst scenarios occur in winter and autumn, where the PCM is solid practically all the time and the environmental temperature is lower than in the other months, so solar transmittance corresponds to the solid state of the paraffin (Fig. 15). This could represent an inconvenience from the point of view of indoor lighting, so more luminaries would be necessary.

Simulations with an RT18HC paraffin type were also carried out to compare results and thermal performance; in particular, PCM node temperature, solar transmittance, and room air temperature. For this case, the MDSC test and transmittance measurements were also performed. Results of experimental tests are summarized in Table 5.

The HVAC coefficients shown in Fig. 9 were also used in this case. Therefore, the volumetric air flow decrease is the same as that shown in Fig. 18. The main difference in simulation results is that the PCM node temperature can reach the melting point (Fig. 16a) more easily than RT25HC paraffin, and it represents an advantage in solar transmittance value (Fig. 16b), particularly in autumn and summer.

The indoor room temperature remains within the defined range of 20–26 °C, as shown in Fig. 17, for all cases where the double-glazed windows are filled with RT18HC paraffin and the HVAC is switched-on.

The implementation of a HVAC system depends on the requirements of building acclimatization. The simulations carried out in this work have considered four scenarios: no-PCM – no-HVAC, no-PCM – HVAC, PCM – no-HVAC, and PCM – HVAC. It is important to analyze how the

implementation of PCM in a double-glazed window affects to the HVAC performance. In other words, the modification on volumetric air flow is studied in this work by comparison between no-PCM – HVAC and PCM – HVAC cases. For HVAC scenarios with PCM, an important reduction in volumetric air flows is achieved, in contrast to the no-PCM base-case. As shown in Fig. 18, the maximum reductions are 87% in winter, 78% in spring, 70% in autumn, and 69% in summer, for working hours. It also can be observed that the highest reduction takes place in winter, followed by spring season. In other words, this reduction means an important decrease in the size of the HVAC equipment and in electrical consumption and capital costs.

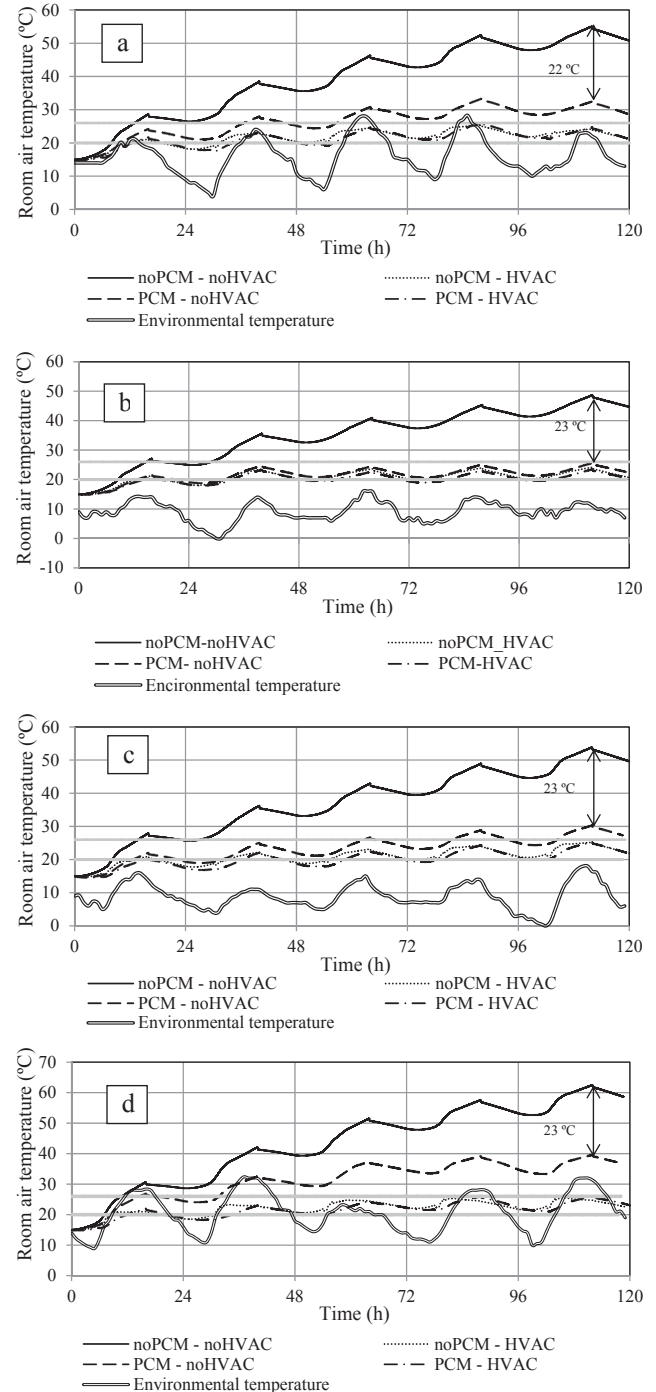


Fig. 13. Air room temperature for a) $n = 75$ (autumn), b) $n = 162$ (winter), c) $n = 258$ (spring), and d) $n = 344$ (summer).

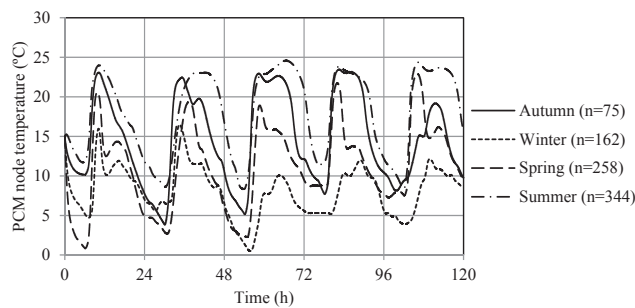


Fig. 14. PCM node temperatures for most representative days.

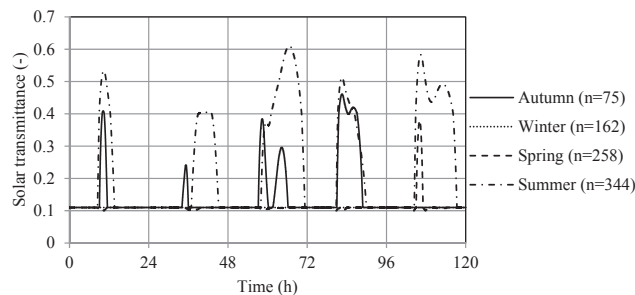


Fig. 15. Solar transmittance of PCM-filled window, for HVAC case.

Table 5

Results of transmittance measurements and MDSC test of RT18HC sample.

Average solar transmittance					
Incidence angle	0°	40°	55°	70°	80°
Solid	0.13	0.12	0.11	0.09	0.09
Liquid	0.75	0.73	0.69	0.63	0.33
Heat capacity coefficients (Eq. (2))	a = 50.2 J/g°C b = 18.7 °C c = 1.7 °C ^{-0.5}				
Latent heat coefficients (Eq. (4))	a = 0.24 W/g b = 21 °C c = 2.4 °C ^{-0.5}				

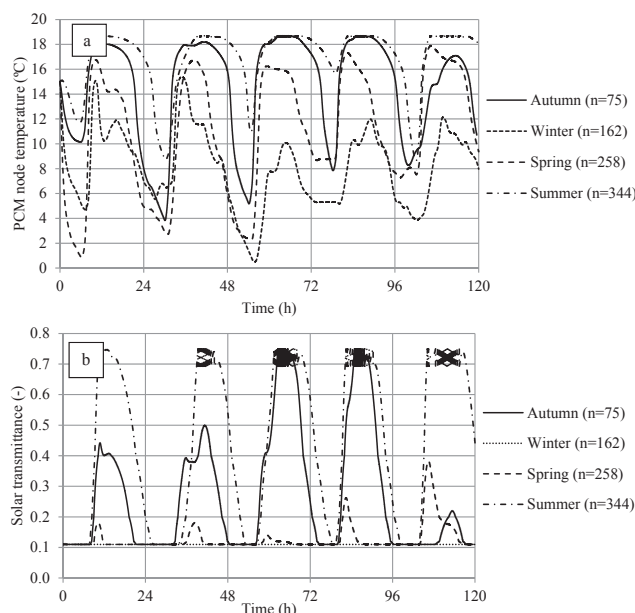


Fig. 16. Results of simulation for RT18HC paraffin. a) PCM node temperature, b) solar transmittance.

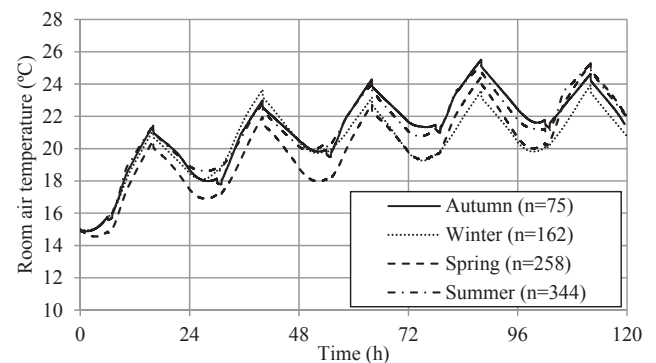


Fig. 17. Room air temperature with RT18HC paraffin, and HVAC switched-on.

6. Conclusions

In this paper, a thermal model of a PCM-filled double-glazed window was developed based on optical and thermal properties obtained from experimental measurements. Modeling based on the predominance of conduction as the heat transfer mechanism, along with the effect of latent heat storage on the thermal behavior, made it possible to obtain reasonable numerical results and determine the most suitable materials for building applications. The novelty of this work is that latent heat was not considered a constant value (i.e.: 240 J/g). Eqs. (3) and (4) give the latent heat as a package of thermal energy which is released or absorbed at each time-step while melting or freezing processes are taking place. The importance of energy variation with temperature during phase change and its direct effect on the solution dynamics are portrayed. This method is not a lever rule, like those implemented by several authors, but it is as simple as theirs.

Solar transmittance, room air temperature, PCM node temperature, and possible savings in electrical/gas consumptions are reported in this paper. Numerical results indicate that RT18HC paraffin is more suitable than RT25HC from the point of view of solar transmittance and lighting performance inside the room. For both paraffins, the temperature of the room reaches the expected range of 20–26 °C, but an HVAC system is necessary to avoid overheating. Results also show that the room air temperature fluctuation is in a smaller magnitude when PCM is implemented, compared to the base case. Similar results can be observed in Zhao et al. [34], who determined a comfort range of temperature between 24.5 °C and 25.3 °C, for a cavity with floor radiation heating system and integrated PCM. Vaz Sá et al. [35] have obtained the same comfort range of inner temperature (24–26 °C) for summer days, by a three-dimension finite elements method (FEM) for simulation. By simply implementing PCM materials in double-glazed windows, an important decrease in indoor temperature can be achieved. In the present case study, indoor room temperature decreased by 23 °C, in comparison with the no-PCM case (air between glasses).

This study is a contribution to the integration of latent heat storage materials within buildings. The model, implemented in Simusol to calculate the effect of phase change, performed as expected but further refinements are required. However, to design the appropriate material properties for passive heating during winter and cooling during summer (i.e., long-term heat storage systems), a more comprehensive analysis using multicriterion optimization is required. Although PCM behaved as expected, macro-scale experiments are necessary to validate the model. Additionally, a more accurate description of the PCM structure with variable density and conductivity, along with the overcooling effect, will be done in future models.

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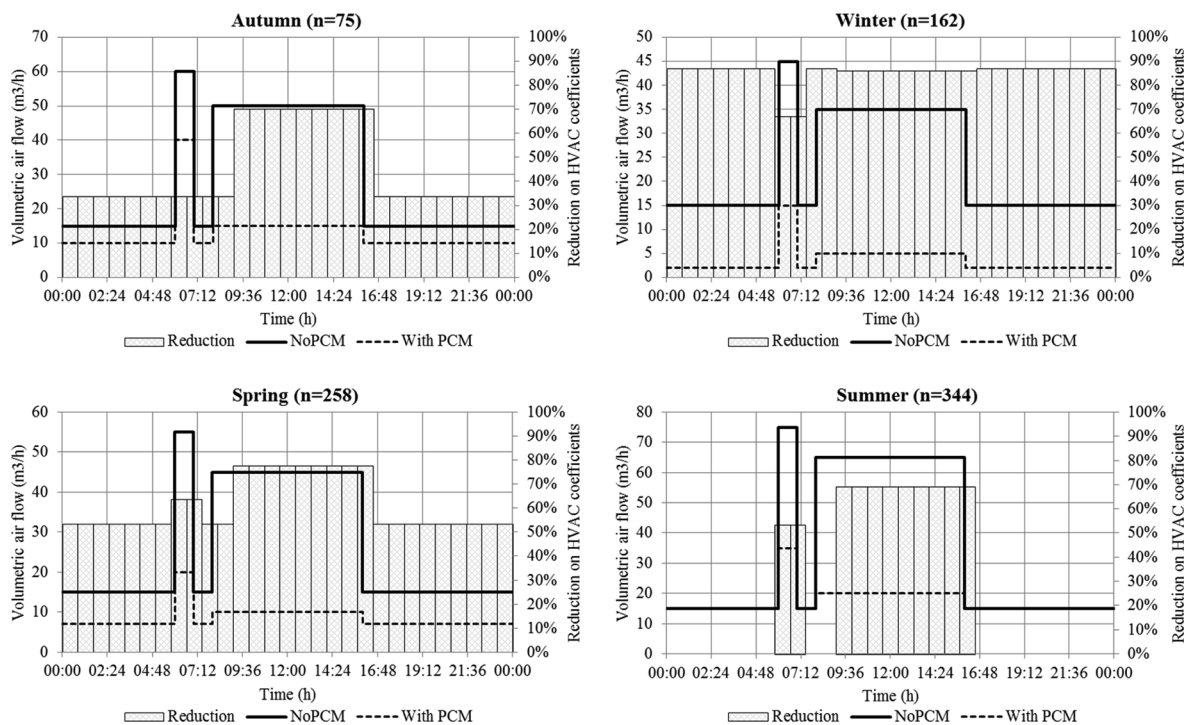


Fig. 18. HVAC volumetric air flow reduction, for both scenarios: NoPCM and with PCM.

component for thermal energy storage in buildings). The authors wish to acknowledge researchers from Institute of Physical Energetics – Energy Resources Laboratory, and Pontificia Universidad Católica de Chile, for providing support on numerical modeling.

Declaration of Competing Interest

The authors declared that there is no conflict of interest.

Appendix A. Supplementary material

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.applthermaleng.2019.114772>.

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