SIMULATION OF THE BEHAVIOUR OF PHASE CHANGE MATERIALS FOR THE IMPROVEMENT OF THERMAL COMFORT IN LIGHTWEIGHT BUILDINGS

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ABSTRACT

This paper describes the results of a study aimed at assessing the effectiveness of Phase Change Materials (PCM) for the improvement of summer thermal comfort in lightweight buildings. The work is based on simulations on a test room in a real building. By varying the thickness of the PCM panel, installed on the inner side of the internal partitions of the test room, as well as the intensity of the night mechanical ventilation and the ways the panels are installed, some interesting conclusions concerning the effectiveness of PCMs on thermal comfort are obtained. The analysis is supported by new indicators, which help quantify the intensity and the duration of the potential thermal discomfort, as well as the actual duration of PCM activation phase.

INTRODUCTION

The use of PCMs in lightweight buildings, aimed at enhancing thermal inertia and at improving the energy performance, is a quite recent research subject. In fact, (Kuznik et al., 2011) underline that only after 2003 a considerable increase in the number of scientific publications on this topic occurred, witnessing a growing interest in this kind of application. The most active countries in this field are China, United States and France.

Organic PCMs, such as paraffin, fatty acids and polyethylene glycol (PEG), are those mostly used; they show good chemical stability, high latent heat and very limited super-cooling. Unfortunately, they have a low thermal conductivity, which may reduce the penetration of the thermal wave into the bulk of the material and the full exploitation of its latent heat.

The simplest method to use PCM in buildings, and the most used in the past, consists in their impregnation into gypsum, concrete or other porous materials. More recently, micro-encapsulation techniques were developed: they consist in enclosing the PCM in microscopic polymer capsules that form a powder; the powder is then included in a container made up of plastic or aluminum. This product is generally sold as a panel, easy to be handled and installed, from which the PCM cannot leak; the reduced size of the microcapsules enhances the full exploitation of the PCM thus optimizing its effectiveness. More details about these technologies are available in (Tyagi et al., 2011).

MODELLING PCM MATERIALS

The transient one-dimensional heat conduction in a homogeneous single-layered wall may be expressed through the Fourier law as:

$$\lambda \cdot \frac{\partial^2 T(x,\tau)}{\partial x^2} = \rho C \cdot \frac{\partial T(x,\tau)}{\partial \tau} \qquad (1)$$

Here, C is the specific heat capacity of the material. In order to apply Eq. (1) for a PCM undergoing phase change, one can define an *equivalent specific heat capacity* C_{eq}, according to the following definition:

$$C_{eq}(T) = \frac{\partial h}{\partial T} \qquad (2)$$

The evaluation of C_{eq} is performed through laboratory tests, by imposing a periodic temperature variation to a PCM sample and then measuring its enthalpy variation. The most common techniques are the Differential Scanning Calorimetry (DSC) and the microcalorimetry; they mainly distinguish from each other for the speed of variation imposed to the temperature of the sample.

The phase change does not entirely occur at a given temperature: the process is actually completed over a certain temperature range ΔT. According to (Chahwane et al., 2009) and (Virgone et al., 2008), the experimental measurements of the equivalent heat capacity performed through such tests fit a Gaussian curve, like in Eqn. (3), with a maximum heat capacity occurring at the peak melting temperature T_P.

$$C_{eq} = \begin{cases} C_0 + C_1 \cdot e^{-\left(\frac{T_P - T}{\Delta T}\right)^2} & if\ T < T_P \\ C_\infty + C_2 \cdot e^{-\left(\frac{T_P - T}{\Delta T}\right)^2} & if\ T \geq T_P \end{cases} \qquad (3)$$

Here C_0, C_1, C_2 and C_∞ are appropriate constants determined through experimental data.

The honeycomb PCM panel

The PCM panel considered in this study was developed at CSTB (French Scientific and Technical Centre for Building). It consists of an aluminium honeycomb matrix that contains a microencapsulated paraffin with a diameter of approximately 5 µm. Thanks to the high thermal conductivity of the aluminium, heat can be easily transferred through the panel, thus allowing all the PCM included in the structure to work effectively. Two thin aluminium sheaths close the panel, whose overall thickness is 2 cm. More details concerning the honeycomb PCM panel are available in (Fassolette, 2010).

Figure 1 shows the curve describing the equivalent heat capacity according to the experimental tests conducted at CSTB (Rabouille, 2010); the corresponding mathematical formulation is reported in Eqn. (4):

$$C_{eq} = \begin{cases} 1200 + 18800 \cdot e^{-\left(\frac{T_P - T}{1.5}\right)} & if \;\; \mathrm{T} < \mathrm{T_P} \\ 1300 + 18700 \cdot e^{-4 \cdot (T_P - T)^2} & if \;\; \mathrm{T} \geq \mathrm{T_P} \end{cases} \qquad (4)$$

Such equation, obtained through best-fit techniques from the experimental data, does not actually correspond to the general model described in Eqn (3). The melting process starts at around 22°C and ends at 28.5°C; the honeycomb panel has a peak melting temperature T_P = 27.6°C, after which the melting process is completed quite rapidly. The equivalent thermal conductivity of the panel corresponds to 2.8 $W \cdot m^{-1} \cdot K^{-1}$; the volumetric mass is 545 $kg \cdot m^{-3}$.

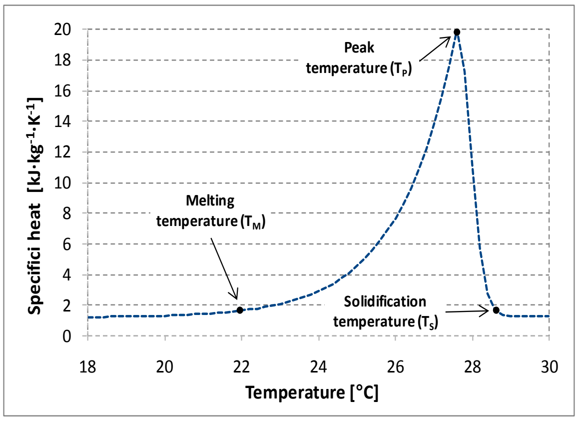

Figure 1 – Specific heat of the honeycomb PCM

PCM modelling on EnergyPlus

In order to simulate the behaviour of a Phase Change Material on EnergyPlus, it is necessary to introduce the curve describing its specific enthalpy as a function of the temperature. If the specific heat capacity is known, see Eqn. (4), the enthalpy can be determined as:

$$h(T) = \int_{T_0}^{T} C_{eq}(T)\, dT \qquad (5)$$

On EnergyPlus, such a continuous function must actually be introduced as a broken line through not more than 16 assigned points. However, such a representation is largely sufficient to describe the function of Eqn. (5), as shown in Figure 2, where the correspondence between the solid line (equation) and the dotted line (broken line introduced on EnergyPlus) is shown to be very high.

Unfortunately, on EnergyPlus it is not possible to include the effect of hysteresis on the heat capacity; actually, according to experimental measurements (Rabouille, 2010), during the solidification phase the curve shown in Figure 1 shifts towards lower temperatures; however, the shift is limited to 0.5°C.

Furthermore, under EnergyPlus the PCMs are simulated using the “Conduction Finite Difference algorithm”, which is able to account for the variation of the thermophysical properties (thermal conductivity, heat capacity) with temperature.

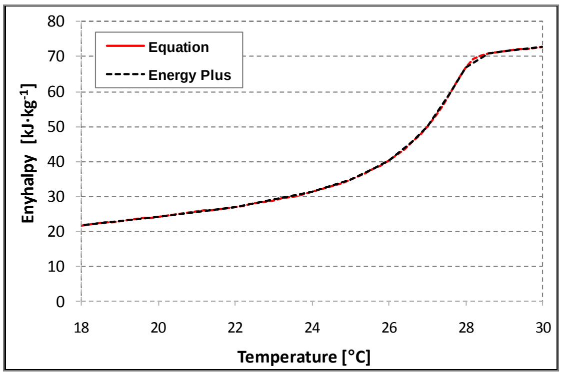

Figure 2 – Enthalpy as a function of temperature

THE CASE STUDY

In order to test the usefulness of PCMs for improving summer thermal comfort in lightweight buildings, a case study is considered. The results of the simulations performed on this case study are used to introduce new indicators for the evaluation of PCM effectiveness.

The building simulated on EnergyPlus is shown in Figure 3. It corresponds to a part of a real office building situated in Grenoble (France), on which honeycomb PCM panels will be installed in the framework of the French project SIRTERI.

The main façade of the building faces west; every room measures 5 × 3.5 m^2, with a height of 2.6 m. Floors and ceilings are made by a concrete slab as thick as 200 mm; the internal walls are composed by 7-cm thick gypsum boards. The façade has an internal 100-mm layer of concrete, insulated on the external side by a 7-cm layer of glass wool. The windows are provided with a wood frame and double-glazing (6 mm glass plus 15 mm air gap). Internal venetian blinds are also available; in the simulation, they are normally open, unless the solar radiation incident on the external glazing rises over 200 W·m^{-2}.

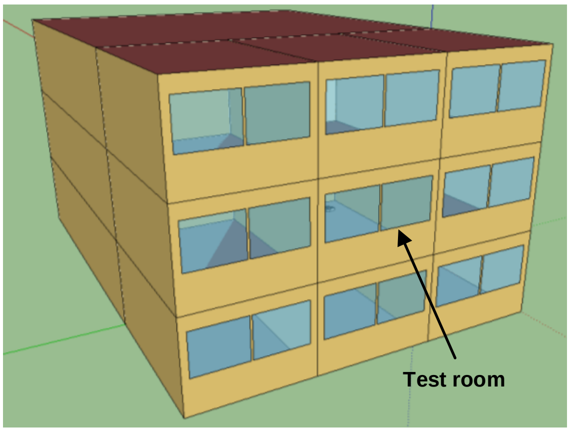

Figure 3 – Model of the simulated building

The space behind the offices at each floor is occupied by a large corridor and by a series of identical offices facing east. The honeycomb PCM panels are placed on the inner sides of the internal walls only in the central room (test room); more details concerning dimensional data for the test room are reported in Table 1.

As far as ventilation is concerned, a constant rate corresponding to 0.5 ACH is considered for hygienical purposes. However, in order to test the effect of night ventilation on PCM performance, an additional mechanical ventilation rate is also introduced between 21:00 and 06:00; different simulations are performed by varying such an air flow rate between 2 and 8 ACH.

The simulations are performed on EnergyPlus over the summer period (June - September), by using the weather data of Lyon (France). The "Conduction Finite Difference" algorithm has been chosen; the calculation time step is 3 minutes.

Table 1
Relevant dimensional data for the test room

Floor surface	17.5 m^2
Window surface	3.6 m^2
Surfaces covered with PCM	31.2 m^2
Room volume	45.5 m^3

RESULTS: COMFORT EVALUATION

When assessing the effectiveness of PCMs for improving summer building thermal comfort, one usually looks at the indoor temperature profile, and evaluates the reduction yielded by the use of PCM in comparison with the case without PCM.

As an example, (Virgone et al., 2009) show that a reduction of the peak operative temperature between 1°C and 2°C can be achieved during a representative summer day in an office room in southern France, depending on the extension of the surface covered by a 0.5 cm thick PCM. (Voelker et al., 2008) studied the effect of adding microencapsulated paraffin to a 3-cm gypsum plaster in a test room; the simulations, carried out over one representative week, showed a potential reduction of 2°C of the peak indoor air temperature.

According to the same approach, the results obtained through the simulations for the test room of Figure 3 during a representative day are reported in Figure 4.

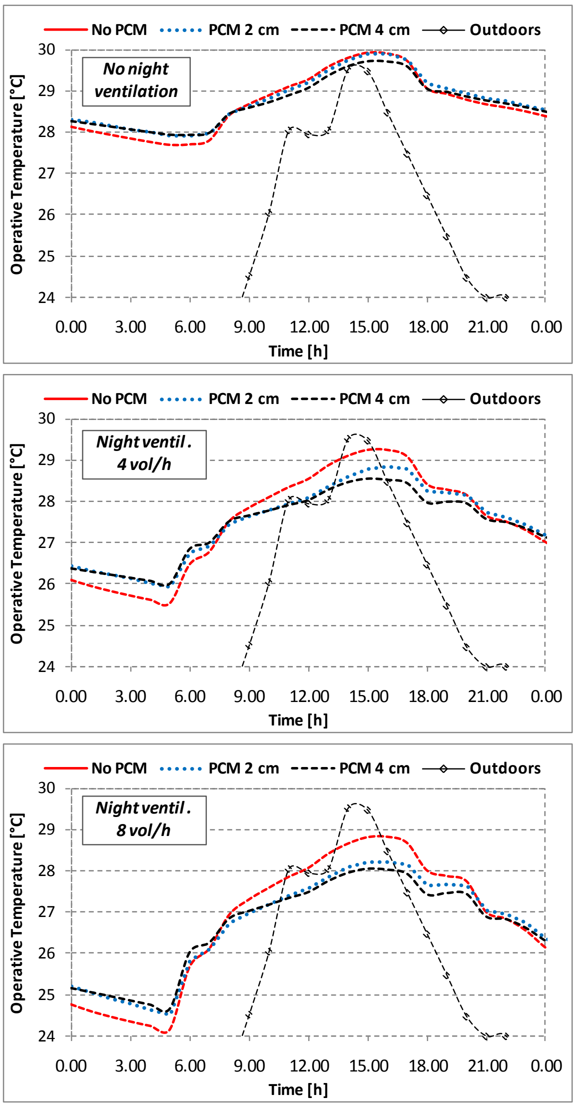

Figure 4 – Operative temperature profile (2nd of July)

The operative temperature profiles show that the effectiveness of the PCM is highly connected to the night ventilation rate: if no ventilation is performed, no relevant effects of the PCM emerge if compared to the case without PCM. On the other hand, if night ventilation is activated it is possible to observe a reduction of the peak operative temperature as high as 0.5 °C at 4 ACH and 0.8°C at 8 ACH. The use of a thicker panel (4 cm) does not imply relevant improvements if compared to the 2-cm panel.

Nevertheless, the authors believe that such a common approach is not sufficient for a thorough description of the PCM effectiveness. As remarked also by (Kuznik et al., 2011), even if several studies concerning the use of PCMs in buildings have been recently published, there is a lack of indicators allowing the evaluation of the real effectiveness of the proposed solutions on a more comprehensive basis. As a first remark, the behaviour of the PCM should be evaluated over a longer time lapse; in fact, the PCM could not work properly during particularly hot and sunny days, when solidification is not effectively performed, or it could result useless during fresh and cloudy day, when melting is not produced. To this aim, it may be interesting to look at the monthly average of the maximum daily values of the operative temperature; as an example, Figure 5 reports the values of this parameter for the present case study as far as the hottest months are concerned.

However, no information is provided concerning the duration of the discomfort sensation, the capability of the occupants to adapt and react to the discomfort as well as the actual activation of the melting phase in the PCM. For this reason, new interesting parameters are introduced in the following.

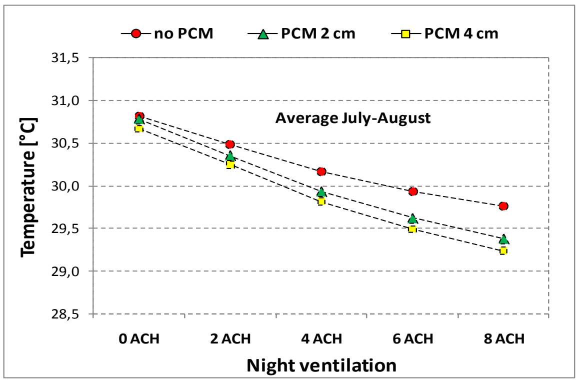

Figure 5 – Average of the daily maximum operative temperature

New parameters

One way to quantify the intensity of an uncomfortable thermal sensation due to overheating in a living space is the evaluation of the difference between the room operative temperature and a threshold value; moreover, the duration of the overheating is also important. On these basis, the authors propose a new indicator called *Intensity of Thermal Discomfort* (ITD): it can be defined as the time integral of the difference between the current operative temperature and the upper threshold for comfort (T_{lim}), and its calculation is carried out according to Eqn. (6) (Evola et al., 2011):

$$ITD_{over} = \int_P \Delta T^+(\tau) \cdot d\tau$$

$$\text{with } \Delta T^+(\tau) = \begin{cases} T_{op}(\tau) - T_{lim} & \text{if } T_{op}(\tau) \geq T_{lim} \\ 0 & \text{if } T_{op}(\tau) < T_{lim} \end{cases} \quad (6)$$

Here, P is the period over which the integration is performed; in case of buildings that are not used all day long (offices, schools), P should correspond to the actual time of occupancy, since the temperature measured out of this interval is not significant for the evaluation of thermal comfort. The definition of the threshold value T_{lim} is linked to the choice of a specific thermal comfort theory. As an example, Fanger's model, implemented in the ASHRAE Standard 55 (Ashrae, 2004), allows the definition of an optimal value for the operative temperature as a function of several parameters related to the indoor environment (air velocity, humidity) and to the occupants (activity and clothing), without any correlation with the external environmental conditions.

On the other hand, according to the *adaptive approach* developed by Humpreys and Nicol, recently included in (EN standard 15251, 2007), people can react to changes in the environment by taking appropriate actions or by changing their attitudes, in order to restore a comfortable condition. As a consequence, the authors of the *adaptive approach* argue that the comfort operative temperature can be calculated as a function of the running mean outdoor air temperature (Nicol and Humphreys, 2010). Three categories of comfort are also introduced: category I holds over a range of four degrees centered around the comfort operative temperature, and corresponds to a high level of expectation. In this work, the threshold value T_{lim} corresponds to the upper limit of category I.

It is also possible to introduce a further indicator, called *Frequency of Thermal Comfort* (FTC), as the percentage of time within a given period during which the indoor thermal comfort conditions are accomplished, i.e. when the indoor operative temperature falls within the limits of category I defined in the adaptive thermal comfort theory.

Figure 6 shows the comparison amongst the different proposed solutions, based on the use of the ITD parameter calculated on a seasonal basis. First of all, the effectiveness of PCMs on the ITD is significant only if combined with ventilation, otherwise the ITD reduction is negligible (around 5%). Furthermore, the effectiveness of the PCM is strictly related to the night mechanical ventilation rate, since the ITD decreases linearly by increasing it even if an asymptotic behaviour seems to emerge at 8 ACH. At 8 ACH the seasonal ITD obtained with a 2-cm PCM panel installed on the internal faces of the test room is 27% lower than that observed in the case without PCM. Such a data is far more interesting and significative than the results shown in Figure 4, as it refers to a longer period of time and accounts for both the intensity and the duration of the discomfort sensation. Furthermore, one can notice that, for a given ventilation intensity, the use of a 4-cm PCM panel may further reduce the ITD of only the 5%, despite using twice as much material as for the 2-cm panel.

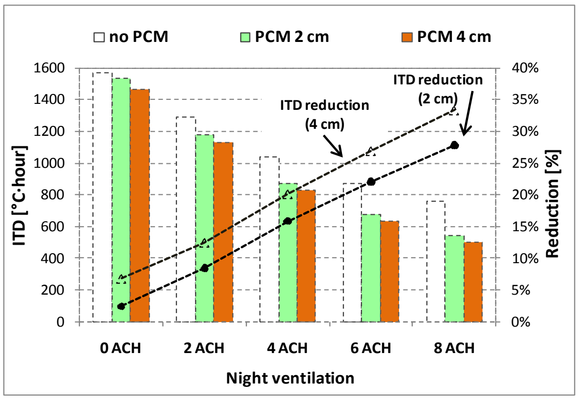

Figure 6 – Comparison based on the ITD parameter.

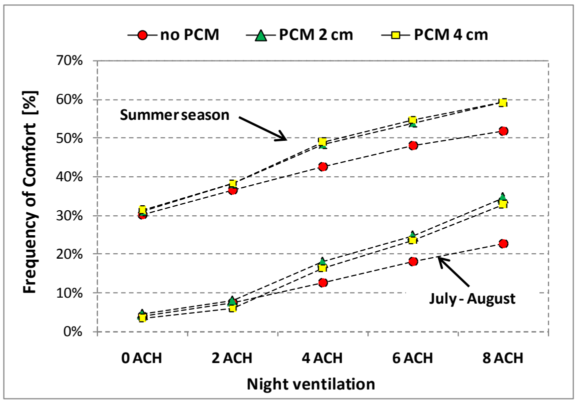

Figure 7 – Comparison based on the FTC parameter.

In Figure 7 the same comparison is done by looking at the FTC indicator. One can learn that during the whole summer season (June – September) the adaptive thermal comfort is assured for up to the 60% of the occupancy at 8 ACH (10% more than the case without PCMs), no matter which is the thickness of the installed PCM; anyway, 4 ACH are sufficient to provide comfort for the 50% of the occupancy, while under 2 ACH no significant increase of FTC occurs. However, the FTC drastically reduces if looking only at the two hottest months (July, August): as an example, FTC = 18% at 4 ACH if installing the PCM panels. In both cases, the role of the mechanical ventilation to activate the PCM panels appears to be major.

RESULTS: SURFACE TEMPERATURE

Another way to evaluate the effectiveness of a PCM for the improvement of building thermal comfort is the analysis of the internal surface temperatures. As shown in Figure 8 for the simulation of a typical hot summer day, the installation of a 2-cm honeycomb PCM panel on the internal walls of the test room can reduce the peak surface temperature of about 0.5°C – 1°C if compared with the absence of PCM. This contributes to the reduction of the mean radiant temperature and therefore of the operative temperature.

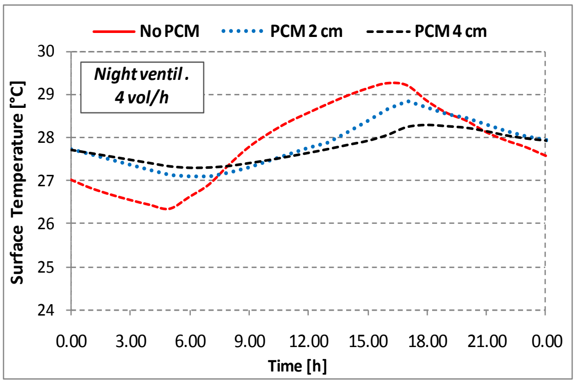

Figure 8 – Daily profile of the surface temperature.

Furthermore, the daily fluctuation of the surface temperature is limited to around 2°C, or even to 1°C with 4-cm PCM panels. However, this piece of information is not sufficient to give a comprehensive description of the PCM effectiveness: it refers to a very limited period, and does not provide significant understanding of the actual activation of the PCM, which should ideally keep as long as possible in the transition phase to better exploit its latent heat.

New parameters

In order to improve the description of the behaviour of the PCM panels, the authors propose to introduce an indicator called *Frequency of Activation* (FA). This indicator corresponds to the percentage of time within a given period during which the PCM is actually activated, i.e. it undergoes phase-change. In this case, it is more interesting to consider the whole warm period as the period of integration, since this new indicator would give important information about the correct design of PCM panels by looking at its behaviour over a long-lasting period.

In fact, if its value is too low, and thus the PCM keeps in its liquid or solid phase for a too long time, it means that it is not used in a correct way and its latent heat capacity is not exploited. An ideal PCM should have *FA* = 100%; anyway this is not easy to accomplish, as the activation of the PCM is highly linked to the climatic conditions. As an example, in a fresh and cloudy day, the PCM will hardly undergo melting, and it will behave like an additional layer of solid lining.

In order to calculate the *FA* indicator, the PCM is considered to be "activated" if its surface temperature, provided by EnergyPlus as an output, falls between its melting temperature point and its solidification temperature, which correspond for the honeycomb panel to 22°C and 28.5°C respectively (see Figure 1). As an example, from the results shown in Figure 9, which refers to the months of July and August, it is possible to say that the 2-cm panel works quite well with 4 ACH, since it is activated on average for more than the 50% of the time. We can also see that, during the rest of the time, the PCM tends to remain molten, probably because night ventilation is not sufficient to induce solidification after a too hot or sunny day.

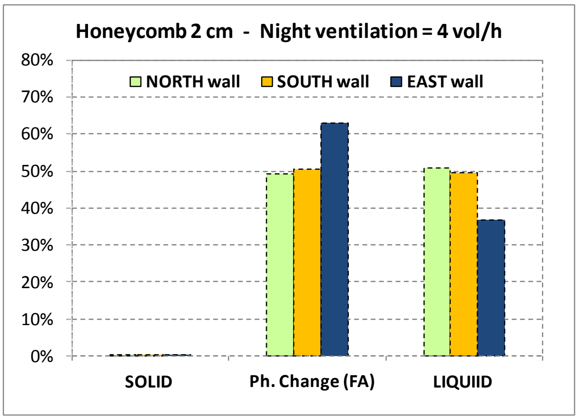

Figure 9 – Frequency of Activation for the honeycomb PCM (July-August)

Furthermore, by using such an indicator we can make a distinction between the three partition walls, and understand that, for the case study, the better behaviour competes to the panel installed on the east wall – the one facing the window. This probably occurs because it is the farthest from the window and consequently less solicited by the incoming solar radiation, which may cause a rapid melting.

This new indicator is useful not only to set an optimised thickness for a given PCM panel but also to compare different types of materials and to make the best choice amongst them.

In Figure 10 the specific heat of two different PCM panels is shown. One corresponds to the honeycomb panel developed at the CSTB (black line), the other one to the Energain® (red line) commercialised by the company DuPont de Nemours, whose performance is described in (Kuznik et al., 2008). The main characteristics of these PCMs are reported in Table 2. As one can see in Figure 11, for the case study, the choice of the PCM implies very different values of the frequency of activation.

In particular, the Energain would result to be totally inappropriate since it would keep its liquid phase for most of the time. This is quite reasonable since its peak melting temperature is too low if compared with the actual indoor temperatures.

Table 2
Properties of Honeycomb PCM and Energain®

PCM	**λ** $[W{\cdot}m^{-1}{\cdot}K^{-1}]$	**Ρ** $[kg{\cdot}m^{-3}]$	**L** $[Wh{\cdot}m^{-2}]$
Honeycomb	2.8	545	125.9
Energain®	0.18 – 0.22	1019	77.7

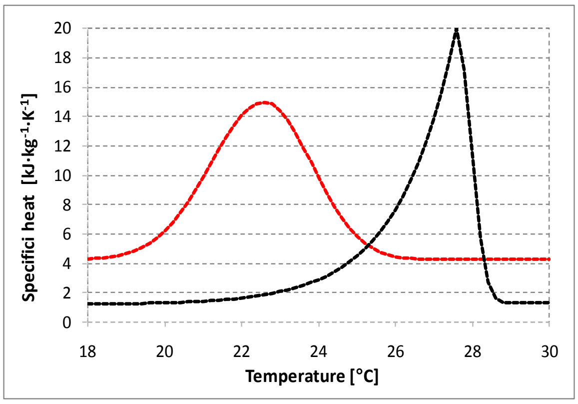

Figure 10 – Comparison honeycomb / Energain®

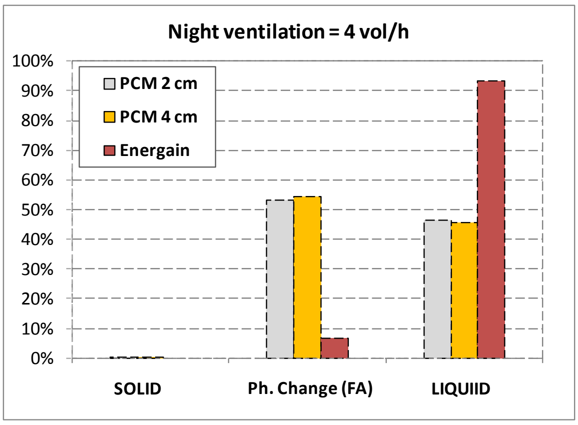

Figure 11 – Comparison based on the frequency of activation

POSSIBLE IMPROVEMENTS

One of the limit of the proposed solutions is the low efficacy of the heat exchange between the PCM-panel and the indoor air. Even with an intense night ventilation, the ITD reduced weakly (approx. 20% with 4 ACH whatever the thickness, see Figure 12) since the convective heat exchange occurs only on one side of the PCM-panel and with a limited air velocity.

As one can see in Figure 12, a significant reduction of the *ITD* may occur by ventilating the PCM-panels on both sides by means of a ventilated air gap that enhance the regeneration of the PCM panels at night and consequently their effectiveness. Such a system is under development in the framework of the ongoing project SIRTERI.

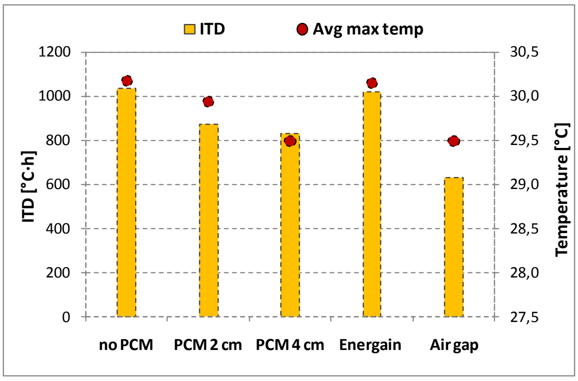

Figure 12 – ITD comparison for different PCMs and strategies

CONCLUSION

In this paper new indicators were defined that allow to better manage the use of PCMs in buildings for thermal comfort purposes. On the one hand, the *intensity of thermal discomfort (ITD)* and the *frequency of thermal comfort (FTC)* are able to effectively describe the effect of different PCM solutions and strategies (including night ventilation) on the indoor thermal comfort of a building. On the other hand, the *frequency of activation (FA)* is more strictly related to the performance of the PCM, since it accounts for its actual time of activation; for this reason, it can be useful for choosing the type of material in the view of maximizing its effectiveness in long-lasting applications.

The results presented in this paper show the primary importance of an intense night ventilation to better exploit the latent heat of the PCMs. Furthermore, the choice of the type of PCM is of major importance and should be done carefully to avoid inappropriate uses. Further investigations are ongoing in order to increase the heat exchange and consequently the effectiveness of the PCMs for thermal comfort purposes, whose results will be presented in following papers.

All the presented indicators can be easily used since they are based on simple outputs normally provided by the most common software for energy building simulation.

ACKNOWLEDGEMENT

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NOMENCLATURE

C	specific heat capacity, J·kg^{-1}·K^{-1}
FA	frequency of activation, %
FTC	frequency of thermal comfort, %
h	specific enthalpy, J·kg^{-1}
ITD	intensity of thermal discomfort, °C·h
L	latent heat, Wh·m^{-2}
T_M	melting temperature, °C
T_P	peak temperature, °C
T_S	solidification temperature, °C

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