Optimization of a phase change material wallboard for building use

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Abstract

In construction, the use of phase change materials (PCM) allows the storage/release of energy from the solar radiation and/or internal loads. The application of such materials for lightweight construction (e.g., a wood house) makes it possible to improve thermal comfort and reduce energy consumption. A wallboard composed of a new PCM material is investigated in this paper to enhance the thermal behavior of a lightweight internal partition wall. The paper focuses on the optimization of phase change material thickness. The in-house software CODYMUR is used to optimize the PCM wallboard by the means of numerical simulations. The results show that an optimal PCM thickness exists. The optimal PCM thickness value is then calculated for use in construction.
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1. Introduction

Because we spend most of our time in enclosed spaces, technology to improve the thermal comfort of buildings has steadily increased, causing a corresponding increase in energy consumption. As a consequence, this has increased the release of polluting agents into the natural environment. Integrating phase change materials (PCM) into building walls is a potential method for reducing energy consumption in passively designed buildings. This tendency is confirmed by numerous papers. For a review, see in [1].

The use of PCM materials for construction has been a subject of considerable interest in the last decade. An interesting feature is that they can store latent heat energy, as well as sensible energy. As the temperature increases, the material changes phase from a solid to a liquid. As this physical reaction is endothermic, the PCM absorbs heat. Similarly, when the temperature decreases, the material changes phase from a liquid to a solid. As this reaction is

exothermic, the PCM releases heat. The main disadvantage of light weight buildings is their low thermal inertia. Obviously, they tend to undergo large temperature fluctuations due to external cooling or heating loads. Using PCM materials in such buildings allows the reduction of temperature fluctuations. This have been proven in several numerical studies [2–5]. The main problem lies in how to include PCM in building walls. A new product, developed by the Dupont de Nemours company is composed of 60% of phase change material included in a polymeric structure. The final product looks like a relatively flexible panel. The innovation, in this case, consists in the encapsulation of a significant quantity of active PCM in a thermoplastic polymer which, after transformation into a relatively thin panel, allows for easy installation in any type of building envelope.

In this paper, the optimal value of the PCM wallboard thickness is investigated. First of all, the optimization assumptions are developed concerning optimal wallboard thickness. In order to calculate the optimal value, the in-house numerical code CODYMUR is used and the results show that an optimal value exists, according to daily external and internal temperature fluctuations.

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Nomenclature

c	specific heat (J/kg K)		ρ	mass density (kg/m^3)
E	energy per square meter (J/m^2)		τ	phase difference (s)
e	thickness (m)		ϕ	function
H	specific enthalpy (J/kg)		Ω	domain (m^3)
h	convection heat transfer coefficient (W/m^2 K)			
q	heat flux (W/m^2)		*Subscripts*	
S	total solar radiation (W/m^2)		e	exterior
T	temperature (K)		eq	equivalent
t	time (s)		i	interior
U	thermal conductance (W/m^2 K)		ins	insulation
x	coordinate (m)		max	maximum
x_i	node coordinate (m)		min	minimum
			opt	optimum
Greek letters			p	plaster
α	solar absorption coefficient (−)		s	stored
Γ	domain boundary (m^2)		wp	wood plate
λ	thermal conductivity (W/m K)			

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2. Optimization assumptions

This section is devoted to a summary of the assumptions used in this paper during the optimization process. First of all, the physical characteristics of the PCM are developed. The second part deals with the configuration retained for the optimization calculation. The last part presents some heuristic arguments of the optimal research.

2.1. Phase change material tested

The new product tested was created by the Dupont de Nemours Society. It is composed of 60% of micro-encapsulated paraffin, which has a melting temperature of about 22 °C. The final form of the PCM material (Fig. 1) is a flexible sheet with a density of $\rho_{PCM} = 1019$ kg/m^3.

The PCM material heat capacity was measured using a differential scanning calorimeter. The thermal analysis was performed in a range of 0–34 °C with heating rates of 2 °C/min. In Fig. 2 shows the measured values of PCM specific heat c. This nearly Gaussian distribution corresponds to a narrow phase change [6].

The thermal conductivity of the PCM material was measured using a guarded hot-plate apparatus. In Fig. 2 shows that under the melting temperature, the thermal conductivity is about 0.22 W/mK and decreases, over the melting temperature to about 0.18 W/mK.

2.2. Studied configuration

2.2.1. General assumptions

One important hypothesis used during the optimization implementation is that heat transfer is unidirectional in building walls. This assumption is widely used for the thermal simulations of buildings. The PCM wallboard is used

Fig. 1. DuPont de Nemours material.

in lightweight buildings (or caravans) to reduce room air temperature fluctuations, in particular when overheating occurs [7]. Then, the wall tested is composed, from the outside, of 2 cm of wood, a variable insulating material (like glass wool) with a thickness e_{ins} (for the basic configuration $e_{ins} = 10$ cm), a variable PCM thickness e_{PCM} and 1 cm of plaster. A complete description of this test wall is shown in Fig. 3, and the thermophysical properties of the materials are given in Table 1. The exterior and interior heat transfer coefficients are, respectively $h_e = 25$ W/m^2 K and $h_i = 7$ W/m^2 K. The insulation thickness e_{ins} can vary, but a minimum value is necessary to ensure a correct wall global insulation. In our optimization process, the minimum value
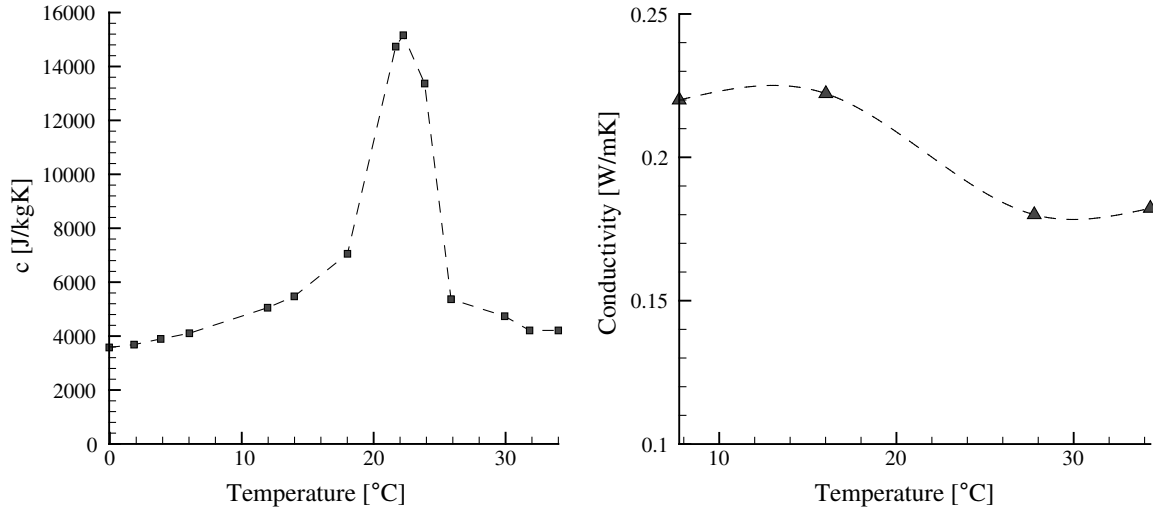
Fig. 2. Experimental specific heat (left) and thermal conductivity (right) of the PCM material.
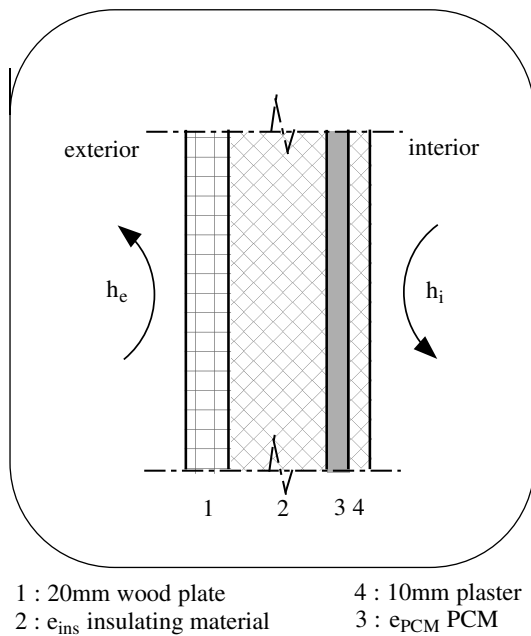

1 : 20mm wood plate
2 : e_{ins} insulating material
4 : 10mm plaster
3 : e_{PCM} PCM

Fig. 3. Test wall composition.

Table 1
Thermophysical properties of the materials

	Density (kg/m³)	Specific heat (J/kg K)	Thermal conductivity (W/m K)
Plaster	825	1000	0.25
Wood plate	500	1600	0.15
Insulating material	15	1030	0.041

of the thickness must fulfill the requirement of the French thermal rules [12] given by the U-value of the wall, $U < 0.47$ W/m² K. The U-value is calculated via

$$\frac{1}{U} = \frac{1}{h_e} + \frac{e_{wp}}{\lambda_{wp}} + \frac{e_{ins}}{\lambda_{ins}} + \frac{e_p}{\lambda_p} + \frac{1}{h_i} \tag{1}$$

Using the given thermophysical properties of Table 1, the minimum thickness of insulation is 8 cm with the wall considered.

2.2.2. External conditions

For the building configuration, outdoor boundary conditions and indoor thermal loads are specified while indoor air temperatures may change in time. The main outdoor conditions are external air temperature and solar radiation. These conditions are taken into account using the equivalent temperature T_{eq} calculated using

$$T_{eq} = T_e + \frac{\alpha S}{h_e} \tag{2}$$

with T_e the exterior air temperature, S the total solar radiations, α the solar absorption coefficient of the surface and h_e the exterior convective heat transfer. In Fig. 4 shows the equivalent temperature calculated for a south vertical wall in Paris in July. From this figure, the assumption of a sinusoidal evolution for exterior equivalent air temperature can be used. Then the optimization process is held using a sinusoidal evolution of the exterior temperature between 15 °C and 35 °C and within a period of 24 h. The impact of external conditions is also studied using a sinusoidal evolution of the exterior temperature between 10 °C and 40 °C.

2.2.3. Internal conditions

The interior air temperature is influenced by outdoor conditions, internal loads and, of course, the building composition. Similarly to the assumption used for exterior temperature, a sinusoidal evolution for the interior air temperature is used. For the interior temperature, the selected sinusoidal evolution is taken between $T_{i,max}$ and $T_{i,min}$, with a phase difference of τ with exterior air temperature. As the PCM melting temperature is around 22 °C, only cases with $T_{i,min} < 22\ °C < T_{i,max}$ are considered. The boundary conditions are summarized in Fig. 5.
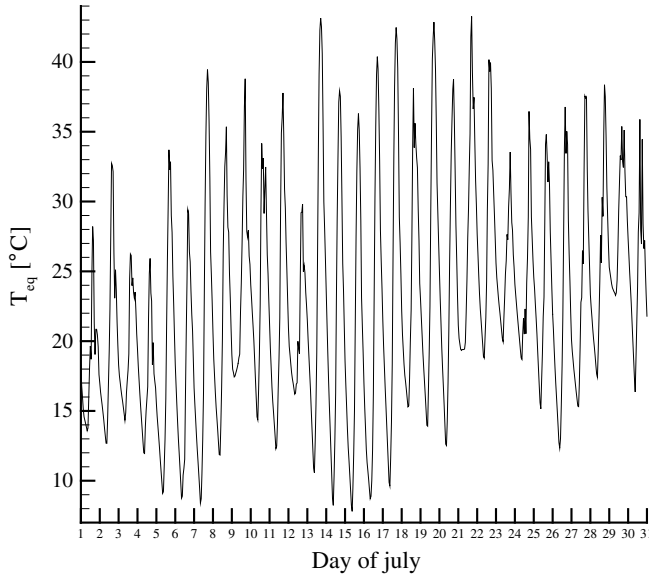
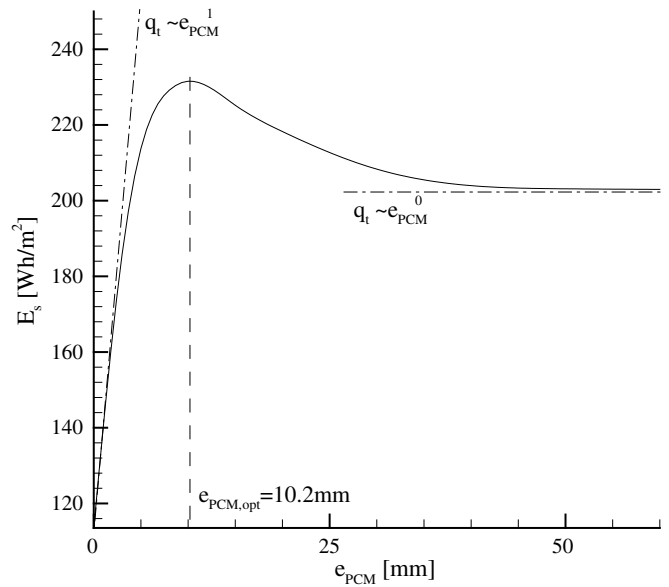Fig. 4. Equivalent temperature: vertical wall in Paris – July.

2.3. Heuristic arguments

The objective of the optimization process is to increase the storage capacity using as little PCM as possible. Two competing trends exist concerning the use of phase change material wallboards in buildings. When the thickness becomes sufficiently small, the PCM is nearly isothermal. The storage energy process is then only due to temperature changes. In this case, the larger the wallboard, the more important the storage capacity. The storage capacity is then proportional to PCM volume. As the heat transfer is unidirectional, the energy stored by the PCM is proportional to wallboard thickness e_{PCM}. In conclusion, in the $e_{PCM} \rightarrow 0$ limit, the total energy stocked varies in $\sim e_{PCM}^1$. This trend is indicated by the small-e_{PCM} asymptote plotted
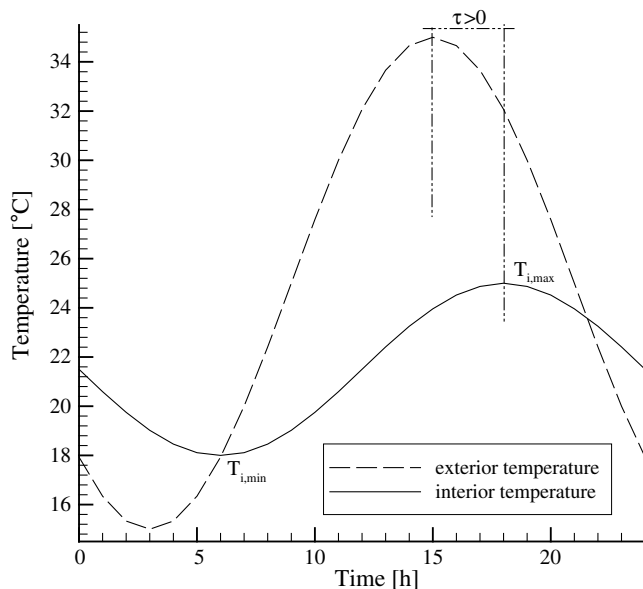

Fig. 5. Air temperature boundary conditions.

Fig. 6. Results concerning the stored energy in a complete day E_s function of PCM thickness e_{PCM}.

in Fig. 6. The penetration time for transient heat conduction t_p can be evaluated by [8]

$$t_p \sim \frac{(e/2)^2}{\alpha} \tag{3}$$

where α is the thermal diffusivity of the medium. When e is large, the time needed for the heat to penetrate the PCM becomes larger than 12 h: and the storage process cannot be complete during a day. Consider next the limit in which e_{PCM} is large enough to consider a semi-infinite material. Increasing e_{PCM} has no effect on the quantity of stocked energy: in the large-e_{PCM} limit, the total energy stocked varies as $\sim e_{PCM}^0$ (constant value). This second asymptote has been added to Fig. 6. The arguments presented below suggest the existence of an optimal thickness, but analytically determining this value is a laborious task. For this reason, numerical simulations are necessary to find the most appropriate value of e_{PCM}.

3. Numerical modeling of phase change materials

The optimization process of the PCM wallboard is performed with the help of numerical simulations. For that purpose, a home made code called CODYMUR is used. This code, developed for thermal simulations of building walls, has been adapted to take into account PCM. The first part of the section is a general presentation of the code, while the second part deals with the needed modifications.

3.1. Presentation of numerical code CODYMUR

CODYMUR allows for the study of the thermal behavior of a wall, supposing unidirectional heat transfer, under

dynamic conditions. It was developed at the Thermal Sciences Center of Lyon in 2002. Considering a wall, external conditions available are climatic data (for various French sites), temperatures, solar radiations etc. CODYMUR carries out calculations for temperatures within a wall as well as thermal flows at the surfaces, as a function of time. The results make it possible to analyze the influence of parameters like the constitution of the wall (thicknesses, materials used for the layers, respective positions of the layers etc.). The studied wall is made of multiple layers associated with a parameter list characterizing heat exchange (absorption of short wavelength radiation and total surface thermal resistances). The initial conditions are either a temperature solution of the stationary problem at the initial moment, or the temperature of the preceding calculation. The boundary conditions are defined by interior and exterior conditions (which correspond obviously to climatic conditions). An environment has two variables: the air temperature and the solar radiative fluxes. A demonstration version of CODYMUR (without the PCM) is freely available [13].

3.2. Modifications of CODYMUR

3.2.1. General concepts

The preceding version of CODYMUR [9,10] supposed that all thermophysical properties of the materials were constant. That made it possible to carry out integration in time by an implicit method. In our case, the density remains constant (equal to $1019 \, \text{kg/m}^3$). On the other hand, conductivity and specific heat are variable with the temperature of PCM. Also, it was necessary to carry out the following modifications:

- enter conductivity and specific heat varying with temperature,
- modify the integration in time method: use of an explicit method with automatic time step modification.

3.2.2. Formulation of the thermal problem

The unidirectional heat transfer problem is given by

- heat conduction equation

$$\rho \frac{\mathrm{d}H}{\mathrm{d}t} = \mathrm{div}(-\vec{q}) \text{ with } \vec{q} = -\vec{\nabla}T \tag{4}$$

- initial conditions

$$T(x, t = 0) = T_0(x) \tag{5}$$

- boundary conditions

$$\begin{cases} -\vec{q} \cdot \vec{n}|_e = -h_e(T(x = 0, t) - T_e(t)) \\ -\vec{q} \cdot \vec{n}|_i = -h_i(T(x = e, t) - T_i(t)) \end{cases} \tag{6}$$

with H enthalpy, λ the thermal conductivity and q the heat flux.

The enthalpy is linked to the temperature via

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \frac{\mathrm{d}H}{\mathrm{d}T} \cdot \frac{\mathrm{d}T}{\mathrm{d}t} \tag{7}$$

and

$$C(T) = \frac{\mathrm{d}H}{\mathrm{d}T} \tag{8}$$

Then, Eq. (4) becomes [11,4]

$$\rho C(T) \frac{\mathrm{d}T}{\mathrm{d}t} = \mathrm{div}(-\vec{q}) \tag{9}$$

A weak formulation of the problem in the calculation domain Ω which boundary is Γ gives

$$\int_\Omega \rho C(T) \phi_i \frac{\mathrm{d}T}{\mathrm{d}t} = \int_\Omega \phi_i \mathrm{div}(-\vec{q}) \mathrm{d}\Omega \forall \phi_i \text{ continuous in } \Omega$$

$$= \int_\Omega [\mathrm{div}(-\phi_i \vec{q}) - \lambda(T) \vec{\nabla}\phi_i \vec{\nabla}T] \mathrm{d}\Omega \tag{10}$$

$$= -\int_\Gamma \phi_i \vec{q} \vec{n}|_\Gamma \mathrm{d}\Gamma - \int_\Omega \lambda(T) \vec{\nabla}\phi_i \vec{\nabla}T \mathrm{d}\Omega$$

With $T(x, t) = \sum T_j(t)\phi_j(x)$, Eq. (10) is

$$\sum_j \frac{\mathrm{d}T_j}{\mathrm{d}t} \cdot \int_\Omega \rho C(T)\phi_i\phi_j \mathrm{d}\Omega$$

$$= -\int_\Gamma \phi_i \vec{q}\vec{n}|_\Gamma \mathrm{d}\Gamma - \sum_j T_j \left[\int_\Omega \lambda(T)\vec{\nabla}\phi_i\vec{\nabla}\phi_j \mathrm{d}\Omega \right] \tag{11}$$

If the functions are linear on the interval $[x_i, x_{i+1}]$, the quantity $\vec{\nabla}\phi_i \vec{\nabla}\phi_j$ is constant and the gradient is also constant. In this interval, $\int_\Omega \lambda(T)\mathrm{d}\Omega$ is

$$\int_\Omega \lambda(T)\mathrm{d}\Omega = \int_{x_i}^{x_{i+1}} \lambda(T)\mathrm{d}x = \frac{\mathrm{d}x}{\mathrm{d}t} \int_{T(x_i)}^{T(x_{i+1})} \lambda(T)\mathrm{d}T \tag{12}$$

Integration over time in this system is carried out by an explicit Euler scheme, with an automatic time step calculation: indeed, the characteristic time of this system can become very small and it is necessary to adapt the time step according to the stiffness of the system ([7]). The mass matrix, via the heat-storage capacity, is a function of time: it is thus recomputed at each time step.

4. Determination of the PCM optimal thickness

This section is devoted to the determination of optimal PCM thickness. The first part shows the existence of the optimum and its calculation for a specific case. The following parts are concerned with the estimation of the impact of some parameters: insulation thickness, outdoor condition, phase difference and indoor condition. Finally, the optimal value is commented.

4.1. Existence of the optimum: case of $\tau = 0$ h, $T_{i,min} = 18\,°C$, $T_{i,max} = 25\,°C$ and $e_{ins} = 10$ cm

In order to find the optimal thickness, a set of numerical experiments is held using the modified version of

CODYMUR presented in Section 3 and for the test case described in Section 2. For each thickness e_{PCM}, the heat density fluxes at the interior and exterior surfaces are computed. Then the stored energy E_s per square meter of wall is calculated for a complete day. Obviously, the released energy is equal to the stored one for a repetitive day.

Fig. 6 shows that the stored energy is optimal for a PCM thickness of around 1 cm. Layers in which the thickness is higher than this value are less interesting concerning energy storage: for a temperature swing with a period less than 24 h, only a maximum of 1 cm of PCM is really affected by heat loads. The value of $e_{PCM} = 0$ mm corresponds to the storage capacity of the wall without PCM. The inertia of the light weight wall is double with 1 cm of phase change material wallboard whereas the total wall thickness and weight only increase, respectively by 4% and 20%. An interesting phenomenon concerns the presence of a peak Fig. 6. When $e_{PCM} > e_{PCM,opt}$, not all the PCM wallboard is affected by the thermal flow. Nevertheless, the global resistance of the wall increases because of the insulating effect of

PCM. Then the thermal flow which passes through the wall decreases, and decreases the storable energy capacity. When e_{PCM} is large enough, the thermal flow cannot pass through the wallboard and then the PCM acts like semi-infinite material: it is a horizontal asymptote.

4.2. Impact of the insulation thickness

Fig. 7a shows the curves obtained for four insulating material thicknesses: $e_{ins} = 8$ cm, $e_{ins} = 10$ cm, $e_{ins} = 15$ cm and $e_{ins} = 20$ cm, and other parameters corresponding to the reference case of part 4.1. From this figure, the insulation thickness doesn't affect the optimum PCM thickness value. This is due to the low exterior heat flux which can pass from the exterior through the insulating material.

4.3. Impact of outdoor air swing

The impact of the outdoor air condition is evaluated using two different swings: a sinusoidal evolution of the

(a) impact of insulation thickness

(b) impact of outdoor air swing

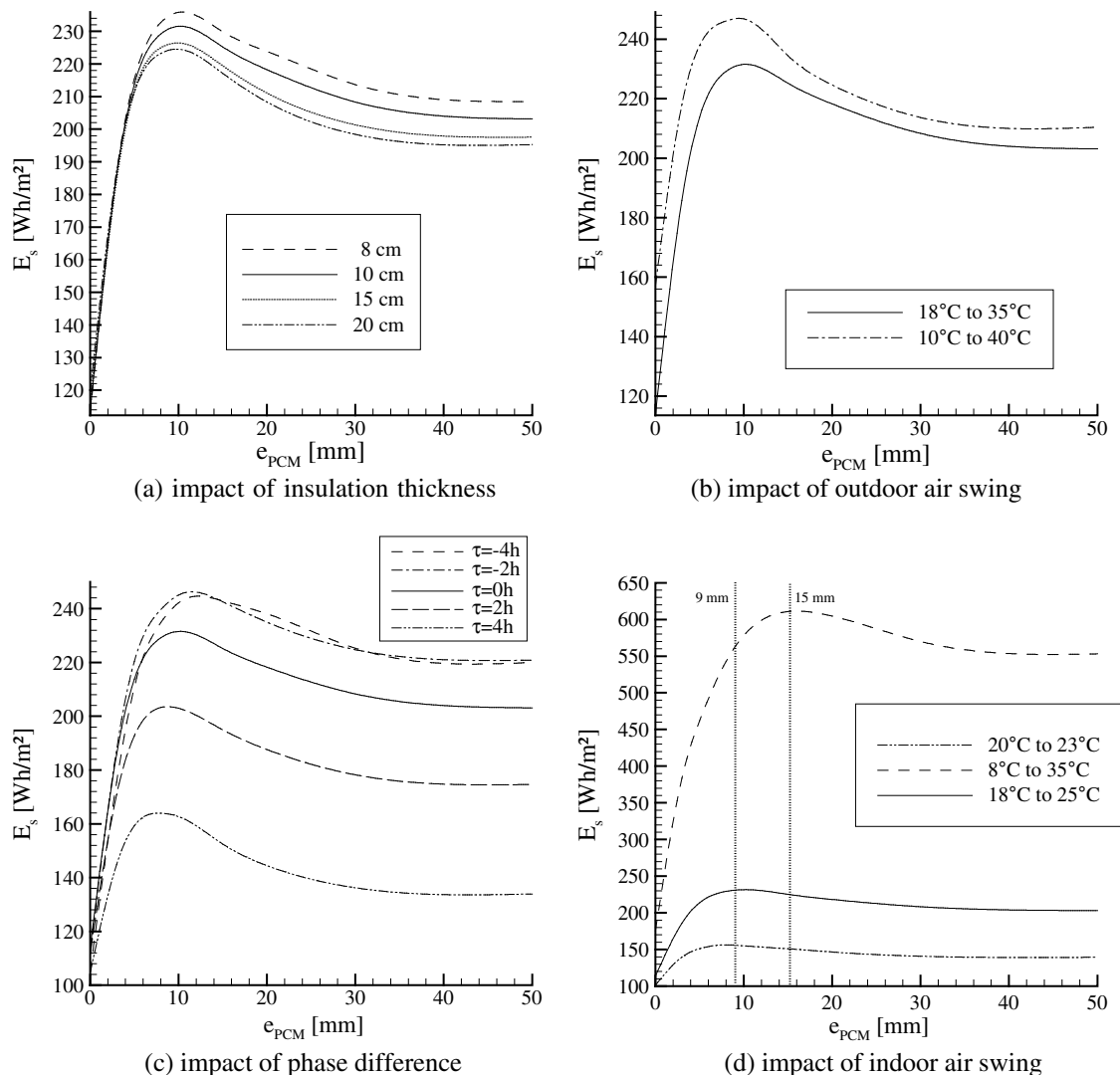(c) impact of phase difference

(d) impact of indoor air swing

Fig. 7. Impact of various parameters on optimal PCM thickness.

exterior temperature between 15 °C and 35 °C and the same evolution excepting the minimal and maximal temperatures which are, respectively 10 °C and 40 °C. The other parameters are those of the reference case of part 4.1. In Fig. 7b shows the results obtained for the optimum value. The external condition does not much affect the optimal PCM thickness value. Once again, this is due to the insulating material.

4.4. Impact of phase difference

Fig. 7c shows the curves obtained for four phase differences τ: $\tau = -4h$, $\tau = -2h$, $\tau = 0h$, $\tau = +2h$ and $\tau = +4h$, the other parameters corresponding to the reference case of part 4.1. The optimal value varies between 9 mm and 11.5 mm.

4.5. Impact of indoor air swing

The indoor air temperature swing is a very important parameter of the problem. To evaluate its impact, three cases are tested: the reference case, a few fluctuations case with $T_{i,min} = 20$ °C and $T_{i,max} = 23$ °C and a hard fluctuation case with $T_{i,min} = 8$ °C and $T_{i,max} = 35$ °C. The other parameters correspond to the reference case.

Fig. 7d shows the impact of indoor air swings. The optimum value varies between 9 mm and 15 mm. However, the higher value correspond to a non-realistic case because the purpose of the PCM is to reduce significantly the indoor air temperature swing.

4.6. Conclusions concerning the optimum

The reference test case shows an optimum of about 10 mm. Even if the optimal thickness value of PCM depends mainly on the indoor air swing, the value of 10 mm corresponds to a good compromise considering the realty of the swings considered. In order to illustrate the effect of 10 mm of PCM compared to other materials, Fig. 8 summarizes the maximum stockable energy between 18 °C and 26 °C for 10 mm of material and for 24 h.
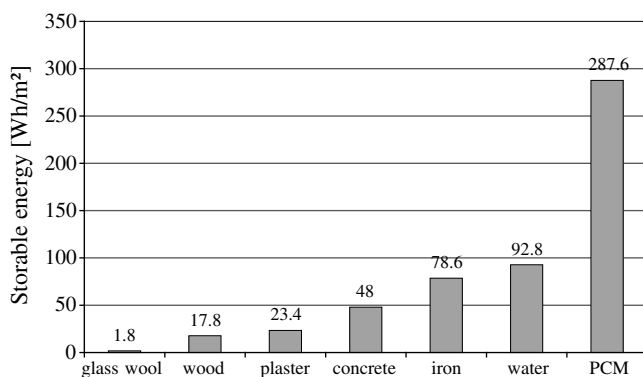

Fig. 8. Maximum storable energy between 18 °C and 26 °C for 10 mm of material and for 24 h.

5. Conclusions

The use of phase change material wallboards allows the enhancement of the thermal inertia of buildings. In order for its use with an optimal storage effect during a complete day, the PCM thickness must be optimized. An optimization process was performed using a test case of a lightweight wall and interior/exterior temperature evolutions within a period of 24 h. Numerical simulations were held using a homemade software modified to take into account phase change materials. The results concerning stored energy in a complete day function of PCM thickness showed that the optimal thickness is 1 cm. This 1 cm wallboard allows a doubling of the thermal inertia of the building. This stored energy prevents building rooms from overheating during hot days, and during the night, the released energy increases the minimum air temperature. On the whole, PCM allows a decrease in temperature fluctuations inside rooms.

Given that the software analyzes only the behavior of a single wall, it is not possible to have a direct coupling between this wall and the temperature of the room: it would therefore be necessary to treat the entire room, to take into account solar radiation and air treatment systems. However, the analysis of flows exchanged with a room's interior side of a wall enabled us to quantify the energy stored and released by the wall with a probable assumption of interior temperature changes. This allowed us to calculate the optimal thickness of PCM to be included in room walls.

References

[1] V.V. Tyagi, D. Buddhi, PCM thermal storage in buildings: a state of art, Renewable and Sustainable Energy Reviews 11 (2007) 1146–1166.

[2] D. Heim, J.A. Clarke, Numerical modeling and thermal simulation of phase change material with ESP-R, in: Proceeding of the Eight International IBPSA Conference, Eindhoven, August 11–14, 2003, pp. 459–466.

[3] E.F. Helmut, C. Stetiu, Thermal performance of phase change wallboard for residential cooling application, Report of Energy and Environment Division, University of California, USA, 1997, p. 24.

[4] H. Manz, P.W. Egolf, Simulation of addition induced melting and solidification in the bulk of a translucent building façade, in: Proceeding of the Fifth International IBPSA Conference, Madison, August 14–16, 1995, pp. 252–258.

[5] M. Ibanez, A. Lazaro, B. Zalba, L.F. Cabeza, An approach to the simulation of PCMs in building applications using TRNSYS, Applied Thermal Engineering 25 (2005) 1796–1807.

[6] K. Darkwa, P.W. O'Callaghan, Simulation of phase change drywalls in a passive solar building, Applied Thermal Engineering 26 (2006) 853–858.

[7] F. Kuznik, J. Virgone, J.J. Roux, Energetic efficiency of room wall containing PCM wallboard: a full-scale experimental investigation, Energy and Buildings 40 (2008) 148–156.

[8] A. Bejan, Convection Heat Transfer, third ed., John Wiley and Sons, 1994.

[9] J. Virgone, J. Noel, ARCHICUBE et CODYMUR, logiciels de simulation des ponts thermiques et du comportement thermique

d'une paroi en régime variable, in: CIFQ Proceeding, Québec, Canada, 2003.

[10] J. Virgone, J.J. Roux, Y. Gao, J.J. Noel, Développement d'outils d'études dynamiques en thermique du bâtiment, in: CLIMAMED Proceeding, Lisbonne, Portugal, 16–17 April, 2004, p. 20.

[11] Feustel, H.E. Stetiu, C. Thermal performance of phase change wallboard for residential cooling application, Report LBL-38320, Lawrence Berkeley National Laboratory, 1997.

[12] RT 2005, Arrêté d'application du 24 mai 2006, Journal Officiel de la République Franaise, Texte 14, 2006.

[13] http://www.jnlog.com/codymur1.htm.