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A numerical algorithm for carrying out “Whole building hourly analyses” on PCM containing buildings

A. Carbonari, M. De Grassi, A. Giretti

Department of Architecture, Construction and Structures
Polytechnic University of Marche, Engineering Faculty, Ancona, Italy e-mail: alessandro.carbonari@univpm.it; m.degrassi@univpm.it ; a.giretti@univpm.it

A. Bonci

Department of Informatics, Engineering Management and Automation
Polytechnic University of Marche, Engineering Faculty, Ancona, Italy e-mail: a.bonci@diiga.univpm.it .

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Abstract

The adoption of Phase Change Materials (PCM) in building elements constitutes a promising method for solving problems of high energetic consumption, due to the conditioning of buildings in climatic contexts characterized by strong solar radiation. Reliable calculation methods for carrying out “Whole Building Analysis” of buildings with PCM, according to the automated computational methods more generally used and based on transfer function method, were not developed very much.

This contribution illustrates a new technique based on the transfer function method, in order to obtain the heat and temperature values of the extreme surfaces of building envelopes, built with the insertion of PCM. The proposed methodology allows simulating the behavior of walls containing such materials and can be easily integrated in any software for Whole Building analyses, presently on the market, without changing their basic algorithm structure.

The numerical consistency and the reliability of the simulated behaviour results have been demonstrated through a comparison with Finite Element method computation, already validated.

1 Introduction

At present, the forecast of unsteady heat conduction through multi-layered building elements subject to changeable boundary conditions is a relevant problem in the field of buildings’ energetic design. The installation of phase change materials (PCM) layers in the envelopes of buildings has the aim of reducing the thermal gain by conduction through walls, with consequent reduction of the thermal load by conduction, as shown in [1,2]. The use of PCM in construction however is not greatly widespread due also to the fact that design tools useful for the energetic analysis of buildings containing PCM are lacking. Professional software products actually available on the market, for forecasting the energetic consumption of buildings (such as VisualDOE, BLAST..) exploit the Conduction Transfer Function (CTF) method proposed by [3], while guaranteeing a good reliability of the results even with acceptable computational speed. These software products are capable of calculating, under changeable environmental conditions heat flux through multi-layered walls having constant physical and geometric properties, and allow extending the calculation results obtained for the single walls up to the determination of the whole buildings' energetic behavior and the design of heating and cooling systems (with the weighting factors method [3]). However, software products which allow the simulation of the energetic behavior of a building (Whole Building Analysis) capable of using multi-layered walls containing Phase Change Materials (PCM) are not available on the market, because of the difficulty of taking into account the temperature dependent properties of the PCM.

The problem of simulating the energetic behavior of single multi-layer walls containing PCM can now be successfully solved using finite element calculation algorithms, like those based on the algorithms proposed for the first time by [4]. In [5] these numerical algorithms were successfully validated, through their comparison with experimental tests. Other computational methods exist [1]. However other authors [6] have proposed an alternative CTF method suited to inclusion in building simulation software. This approach takes into account the fact that when the phase change occurs, the heat capacity over temperature increases as a step function. Under this assumption they computed heat flux using several sets of CTF coefficients: the number of sets depend on the number of heat capacity steps over temperature. At each simulation time step the algorithm switches between several sets of CTF coefficients according to the temperature of the center of the PCM containing layer. Because the accuracy in the use of CTF method depends on the past values of heat fluxes computed in the previous steps, when the switch is made, a certain degree of inaccuracy is introduced, due to the unknown past values of heat flux relative to the set of CTF coefficients in use. In this paper, a new algorithm based on the CTF theory is proposed for simulating the thermal heat transfer in a multi-layered envelope containing a PCM layer subject to phase change which avoids the switch between different CTF sets of coefficients. This algorithm can be implemented inside software products that carry out Whole Building Analysis, taking into account the presence of PCM, by using their same calculation procedures and basic calculation methods. This paper is organized as follows: Section 2 concerns the description of the characteristics of walls containing PCM; the following section 3 illustrates the proposed calculation method. Section 4 compares the results obtained by the application of the calculation method described in section 3 with the Finite Element one, already validated in [5]. Section 5 concludes.

2 Thermal behavior of a wall containing PCM

The main characteristic of PCM [2] is that it has changeable physical properties, and does not respond in the same way to the same temperature input, in particular, its behavior depends on their internal temperature. It behaves like a standard high thermal capacity material if it is solid or liquid, while it behaves like a heat absorber/generator during the phase change, which produces a thermal energy absorption during the fusion phase and a heat discharge during the solidification phase. The insertion of PCM in the building envelopes aims at solving the overheating problem of walls when strongly irradiated, as for instance, during summer periods. Thanks to the high thermal storage capacity of PCM, if it is inserted inside dry assembled lightweight walls (Fig. 1), it is possible to confer high thermal inertia to the wall in a pre-established temperature range, even if with a modest weight increase, thus determining the lowering of the thermal load peaks and their shifting in time.

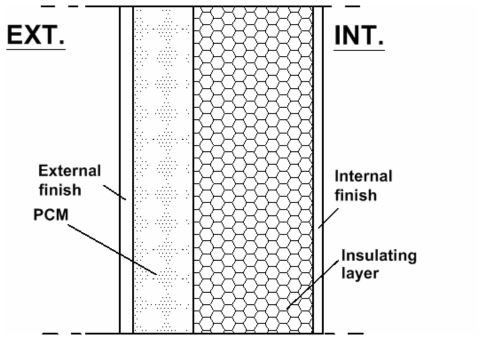


Figure 1: Example of standard PCM containing stratification for standard dry assembled envelopes

Assuming as constant the internal air temperature at a pre-established value using a system, when the external wall is hit by solar radiation, inward flux starts from the exterior towards the interior. The heat flux caused by external irradiation causes an increase in the temperatures within the wall and increases the gradient over temperature between the exterior and the interior. When the PCM reaches its melting temperature, it absorbs the thermal flux coming from the exterior completely, establishing a constant gradient between it and the internal part of the wall, hence the incoming flux penetrating the internal environment remains constant up until temperature variations at the PCM level are had, avoiding overheating. At this point, before the end of the external irradiation of the wall, two situations can take place: the PCM layer melts completely and, from a certain moment on, it is no longer capable of absorbing heat or the PCM layer never melts completely in all its thickness, hence, when the external surface starts cooling it is capable of absorbing other heat. In both cases a certain period of time is needed (generally longer than the one needed for fusion) in order to allow the PCM's solidification.

3 The numerical model

In this section, the computation of the temperature and the heat flux in any interface within a wall will be summarized and then used for the simulation of PCM containing walls. By considering a multi layer wall having an interface of interest and supposing that the exterior layer is formed by *n* layers and the interior one is formed by *m* layers. By identifying with a subscript *o* the variables referred to the portion facing the exterior (*outside*), with a subscript *i* the variables referred to the portion facing the interior (*inside*), with *s* the Laplace variable, then the temperature T_o and the heat flux φ_o on the external surface of the wall, known temperature T_i and flux φ_i on the internal surface, can be described by the following equation [7]:

$$\begin{bmatrix} T_o \\ \varphi_o \end{bmatrix} = H(s)\begin{bmatrix} T_i \\ \varphi_i \end{bmatrix} = H_o(s)H_i(s)\begin{bmatrix} T_i \\ \varphi_i \end{bmatrix} = \prod_{j=1}^{n}\begin{bmatrix} A_{oj}(s) & B_{oj}(s) \\ C_{oj}(s) & D_{oj}(s) \end{bmatrix}\prod_{k=1}^{m}\begin{bmatrix} A_{ik}(s) & B_{ik}(s) \\ C_{ik}(s) & D_{ik}(s) \end{bmatrix}\begin{bmatrix} T_i \\ \varphi_i \end{bmatrix} \tag{1}$$

where the generic h^{th} $H_h(s)$ matrix can be expressed as follows:

$$H_h(s) = \begin{bmatrix} A_h(s) & B_h(s) \\ C_h(s) & D_h(s) \end{bmatrix} = \begin{bmatrix} \cosh\left(L_h\sqrt{\frac{s}{\alpha_h}}\right) & \frac{\sinh\left(L_h\sqrt{\frac{s}{\alpha_h}}\right)}{k\sqrt{\frac{s}{\alpha_h}}} \\ -k_h^2 \cdot \sqrt{\frac{s}{\alpha_h}} \cdot \sinh\left(L_h\sqrt{\frac{s}{\alpha_h}}\right) & \cosh\left(L_h\sqrt{\frac{s}{\alpha_h}}\right) \end{bmatrix} \tag{2}$$

and where L_h is the thickness of the h^{th} layer, α_h represents the layer's diffusivity having the form $\alpha_h=k_h/(\rho_h c_h)$ where k_h, ρ_h and c_h are respectively the h^{th} layer's conductivity, density and specific heat. By defining the temperature and the heat flux in a generic wall interface as $[T^*,\varphi^*]^T$ it is possible to split the system in two subsystems as shown in equations (3) and (4):

$$\begin{bmatrix} T_o \\ \varphi_o \end{bmatrix} = \begin{bmatrix} A_o(s) & B_o(s) \\ C_o(s) & D_o(s) \end{bmatrix} \begin{bmatrix} T^* \\ \varphi^* \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} T^* \\ \varphi^* \end{bmatrix} = \begin{bmatrix} A_o(s) & B_o(s) \\ C_o(s) & D_o(s) \end{bmatrix} \begin{bmatrix} T_i \\ \varphi_i \end{bmatrix} \tag{3,4}$$

These equations relate the interface temperature and heat flux variables with respect to the same variables on the extreme wall surfaces. The systems (3) and (4) can be solved in regards to $[T^*,\varphi^*]^T$ by known $[T_o,T_i]^T$ as suggested by Mitalas [8]. The following result is obtained:

$$\begin{bmatrix} T^* \\ \phi^* \end{bmatrix} = \frac{1}{B(s)} \cdot \begin{bmatrix} B_i(s) & B_o(s) \\ D_i(s) & -A_o(s) \end{bmatrix} \cdot \begin{bmatrix} T_o \\ T_i \end{bmatrix} \tag{5}$$

where $B(s) = A_o(s)B_i(s) + B_o(s)D_i(s)$, represents the term $H_h(1;2)$ of the matrix $H_h(s)$ expressed in (2) and referred to the system formed by the whole wall. For the purpose of this contribution, the evaluation of the phase of PCM will be monitored by using equation (5). The classical application purposes of an hourly simulation software is to compute the incoming and outgoing heat fluxes having the extreme surface temperatures as input data. Rearranging system (1), the following one is obtained:

$$\begin{bmatrix} \varphi_o \\ \varphi_i \end{bmatrix} = \begin{bmatrix} \dfrac{D(s)}{B(s)} & \dfrac{-1}{B(s)} \\ \dfrac{1}{B(s)} & \dfrac{-A(s)}{B(s)} \end{bmatrix} \cdot \begin{bmatrix} T_o \\ T_i \end{bmatrix} \tag{6}$$

In this way, a standard software can compute the unknown boundary fluxes (or heat gain), given extreme surface temperatures as boundary conditions; hence a hourly simulation program is able to compute both thermal loads and system consumption of a building, with the conventional procedure. The time domain solution of the heat fluxes φ_o and φ_i can be computed by referring to a generic ramp input $T(0;t) = g(t) = t$, having Laplace transform $g(s) = 1/s^2$. These solutions require the computation of their response factor $Y_r(t)$, that is the anti-transform of the following relation:

$$Y_r(s) = \frac{D(s)}{B(s)} \cdot \frac{1}{s^2} \tag{7}$$

where the subscript r means that we are discussing a ramp impulse. Now it is possible to apply the complex inversion theorem and calculate $Y_r(t)$ as in [9]:

$$Y_r(t) = L^{-1}\left[\frac{D(s)}{B(s)} \cdot \frac{1}{s^2}\right] = t\left[\frac{D(s)}{B(s)}\right]_{s=0} + \frac{d}{ds}\left[\frac{D(s)}{B(s)}\right]_{s=0} + \sum_{k=1}^{\infty} \frac{1}{\beta_k^2} \cdot \frac{D(s)}{B'(s)}_{s=-\beta_k} \cdot e^{-\beta_k t} \tag{8}$$

Where β_k is the roots of $Y_r(s)$ on the negative semi axis of the complex plane and $Y_r(s)$ is given by:

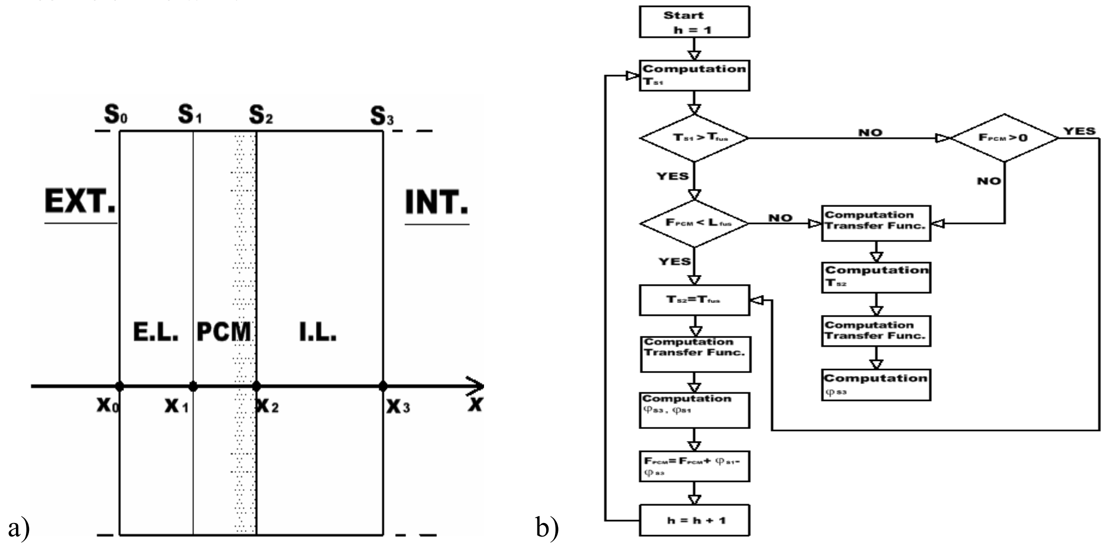
$$Y_r(s) = \frac{1}{s^2}\left[\frac{D(s)}{B(s)}\right]_{s=0} = t\left[\frac{D(s)}{B(s)}\right]_{s=0} + \frac{1}{s}\frac{d}{ds}\left[\frac{D(s)}{B(s)}\right]_{s=0} + \sum_{k=1}^{\infty} \frac{c_i}{s+\beta_k} \tag{9}$$

The need to sample the response factors at hourly intervals and to implements a computer algorithm for computing $Y_r(t)$ entails the need to use the Z-Transform, in place of the s-Transform. Defining Δ the sampling time interval (usually 1 hour); the Z-Transform of (9) is given by the expression [9]:

$$Y_r(t) = \frac{\Delta}{z(1-z^{-1})^2}\left[\frac{B_{in}(s)}{B(s)}\right]_{s=0} + \frac{d}{ds}\left[\frac{B_{in}(s)}{B(s)}\right]_{s=0} + \frac{1}{(1-z^{-1})} + \sum_{k=1}^{\infty} \frac{c_i}{1-e^{-\beta_i \Delta z^{-1}}} \tag{10}$$

In the same way the other response factors of the $X_r(t)$ and $Z_r(t)$ type as in [9] can be calculated. These expressions can be used for computing the wall thermal variables $\varphi_o(n\Delta)$, $\varphi_i(n\Delta)$, $T_o(n\Delta)$ and $T_i(n\Delta)$ for $n = 1,2, \ldots$ sampling time interval.

The calculation of the thermal parameters of the PCM containing walls using the transfer functions is generally carried out on an hourly basis; the capability of monitoring simultaneously with the same hourly rate the temperature and the heat flux values within a wall by means of equation (5) allows us to understand whether or not the PCM is in its melting condition. From this information it is possible to understand if the PCM will act as a heat flux absorber or emitter, which keeps its temperature fixed on melting values or whether it behaves as a normal layer with known physical properties. Given a generic PCM containing wall as in Fig. 2-a, the following terms will be used to represent its built-in elements: *EL* identifies the generic layer or multi-layered placed externally as compared to the PCM; *IL* identifies the generic layer or multi-layered placed internally as compared to the PCM; *GS* identifies the entire wall.



a) b)

Figure 2: PCM containing stratification (a); algorithm used for computing the incoming flux (b)

Fig. 2-a shows the layer stratification, the reference system on which the interfaces are evaluated and the symbols which will be used here on. The calculation of the buildings' thermal gain depends on the amount of incoming flux through the entire stratification hour by hour and on the PCM state. The proposed method for calculating the heat flux takes into account the PCM's state by computing the temperature on interface S_2 between PCM and *IL* layer at every hour iteration, by means of the aforementioned transfer function method proposed, and then carrying out the incoming heat flux calculation by using the boundary conditions given by the temperatures in S_2 and S_3. In this way, the incoming flux will be determined with respect to the two known boundary conditions, the first of which derives, as previously stated, from the hourly calculation of the temperature whereas the second is a consequence of indoor environment.

The new proposed procedure computes the incoming heat flux through the S_3 surface starting from the temperature values on the S_2 and S_3 interfaces, where the temperature value on S_2 depends on the S_0 and S_3 temperatures, on the PCM temperature and on its level of fusion. Therefore, the possibility to calculate the temperature at which the PCM is found at every hourly iteration is of great importance. Fig. 2-b summarizes the procedure used for the calculation of the thermal gain (incoming heat flux), where the symbols used are the following: T_s identifies the temperature on the generic *S* surface; T_{fus} identifies the PCM melting temperature; F_{PCM} is the variable storing the cumulative thermal energy absorbed by the PCM during the melting process at each iteration; L_{fus} identifies the latent heat of fusion per surface unit of PCM; φ_s is the generic heat flux, on the generic S surface; *h* is the number of iterations carried out, and therefore is incremented by one hour.

In the algorithm procedure shown in Figure 2-b, the first step is based on the check of the PCM's temperature: if it is lower than the melting one another check on the variable storing the thermal energy F_{PCM} absorbed by PCM up until that iteration is carried out. On the basis of the value taken on by F_{PCM}, two possibilities can occur:

- if $F_{PCM} > 0$ it means that the PCM is not completely melted and the temperature of the wall at the PCM level is kept equal to that of the PCM fusion ($T_{S2} = T_{fus}$) up until it has finished solidifying;
- if $F_{PCM} = 0$ then it means that the PCM is completely in the solid state and the wall is considered as in the ordinary case: therefore the temperature value T_{S2} is calculated and it is possible to proceed with the calculation of the flux incoming through the wall using the two boundary conditions given by the same T_{S2} and T_{S3};

If, from the first check, it is found that the PCM's temperature is higher than the fusion one ($T_{S1} > T_{fus}$), the algorithm checks whether it has already absorbed all the latent heat of fusion L_{fus}, or if there is still some solid PCM for storing more thermal energy. In practice, the following two cases can occur:

- if the PCM is completely melted ($F_{PCM} = L_{fus}$) the wall is considered as in the ordinary case and the value of the temperature between the PCM and *IL* (T_{S2}) is calculated before computing the incoming flux using as boundary conditions the afore mentioned temperature T_{S2} and T_{S3};
- If the PCM is not completely melted ($F_{PCM} < L_{fus}$) the temperature of the layer at the PCM's level is kept equal to the fusion one and then the value of the incoming flux is calculated on the basis of this temperature; at each iteration the value of the incoming flux entering the PCM is stored in F_{PCM}; its temperature will be allowed to rise once the layer is completely melted.

4 Experimental validation

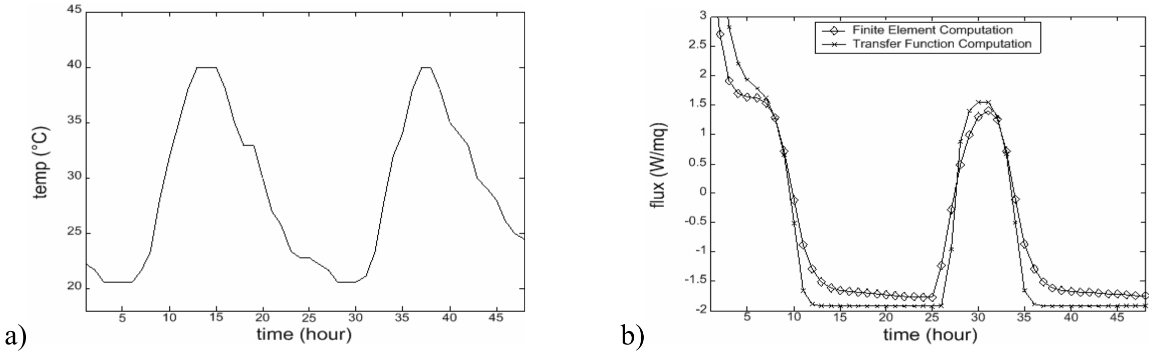
The procedure described in Section 3 is now tested on a stratification which will allow verifying the efficiency of the algorithm proposed for the simulation of PCM inserted in the wall. We presume to have a stratification for external envelopes made up of 4 layers, as in Table 1. The wall is assumed to be equipped with a *3 cm* thick PCM layer, melting at *32°C* . The boundary conditions applied are:

1. temperature of the internal air $T_{ai} = 26$ °C, with adduction coefficient equal to *7.7 W/(m·K)*;
2. on the external surface of the wall S_0, the temperature course T_{ae} is equal to Fig. 3-a.

Table 1: Typology and physical properties of the stratification used for testing

Layer ID	**Layer name**	**Physical properties**				
		Conductivity (*W/(m·K)*)	Spec. heat (*J/(kg·K)*)	Density (*kg/(m³)*)	Thickness (*m*)	Latent heat (*J/kg*)
1	**External plaster finish**	1.2	1000	900	0.015	-
2	**PCM layer**	0.6	3600	1450	0.03	190000
3	**Insulating layer**	0.04	1000	20	0.12	-
4	**Internal plaster finish**	1.2	1000	900	0.015	-

The values of temperature on the external surface were obtained by a calculation of the sun-air temperature [8] which reasonably could take place on a wall of the type described in Table 1, placed in a Mediterranean climate at a latitude of approximately *40°C*. On the basis of the afore mentioned boundary conditions two simulations were carried out: the first using an algorithm built in accordance with the procedure described in Section 3 and implemented in MatLab 6.5 environment; the second, acting as validation tool, obtained using a finite element algorithm, which faithfully forecasts the systems' response, which comes from the calculation of the finite elements which, as demonstrated by [5], gives excellent reliability guarantees: a direct comparison with the experimental data demonstrated that the shift between the theoretical values and those deriving from laboratory tests have an average value inferior to 0.4%. The finite element calculation is therefore taken as reference, and in relation to it, the error committed with the transfer function method is evaluated.



a) b)

Figure 3: Temperature assigned on the external surface of the wall (a); comparison between the results obtained with finite element and transfer function calculations (b).

The diagram in Fig. 3-b compares the incoming fluxes computed through the transfer function method, with the one obtained using the finite elements method, relative to the same experimental situation, whose simulation takes up a period of 48 hours: the flux is considered negative if directed towards the interior and positive if directed towards the exterior. The qualitative course between the two cases results to be practically coinciding. By observing the shift the following conclusions can be drawn:

1. during the phase change which occurs when the PCM reaches *32°C*, the incoming flux remains constant, and equal to $2\ W/m^2$, that is very low for lightweight walls of the kind under consideration located in warm climates like in this case;
2. the difference between the two fluxes in correspondence of the "step" never tops the $0.3\ W/(m^2\cdot K)$ value, that is, less than 19% of the real value;
3. the transfer function method overestimates the time needed for the fusion and solidification by approximately one hour for this particular case.

In this case, the sun-air temperature assigned on the surface was not sufficiently high to determine the PCM complete fusion. Finally, Fig. 4 illustrates the results obtained if a *1 cm* thick PCM layer is positioned in the wall, with the same boundary conditions described for the previous case.

From the qualitative point of view we can note how the PCM's fusion and then solidification phases can be well observed - with a maximum peak for the incoming heat that tops twice the one obtained by the diagram of Fig. 2-b because the PCM's layer is too thin and not capable of absorbing all the heat that passes from the exterior towards the interior of the wall. During night time the heat flux absorbed by the PCM is completely released allowing for solidification.

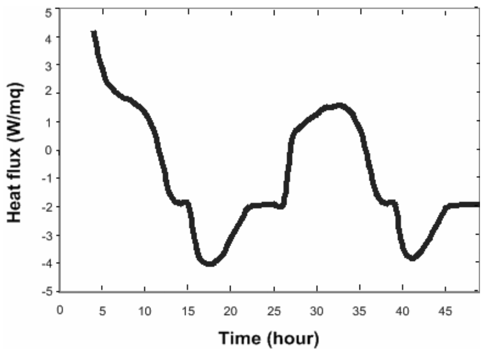


Figure 4: Incoming heat flux for a wall with a 1 cm thick PCM layer.

5 Conclusions

The software programs presently on the market for carrying out whole building analysis do not foresee the possibility of inserting layers made up of PCM within walls. The algorithm presented in this contribution, which in the validation situation provides satisfactory results, suggests a possible approach to the forecasting of the behavior of walls containing PCM, at present really useful because PCMs are object of a growing interest in the field of construction. The principal advantage of this method consists in the fact that it can be integrated within existing software packages for whole building analysis, without requiring structural changes to the overall algorithm which they avail themselves of. Moreover, it can be used to: design the opportune characteristics of the PCM layer to be inserted in the wall, given the particular design and climatic context under consideration; estimate the achievable internal thermal gains and energetic savings, in support of the feasibility study during building design. In this way, architects have a powerful design tool in their hands, capable of estimating the improvements deriving from the insertion of PCM in buildings, favoring a worldwide spread of this sustainable technique, aimed at the reduction of energetic consumption and comfort improvements of buildings, based on PCM.

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