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# Multiple bi-phase interfaces in a PCM layer subject to periodic boundary conditions characteristic of building external walls

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#### Abstract

The thermal fields, which form in a PCM layer subject to external and internal loadings that operate on the external wall of buildings, are determined by a physical model that describes conduction in the solid phase and the liquid phase and the phase change of the melting temperature with a thermal balance equation at the bi-phase interface. The system of equations is resolved with a finite difference numerical model that uses a resolution algorithm that provides for the contemporaneous presence of one or more bi-phase interfaces in the layer. The thermal analysis in steady periodic regime conditions by a layer situated in Turin has highlighted that layer behaviour varies monthly in relation to the number and position of the bi-phase interfaces that form in the layer.

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#### 1. Introduction

The phase change in a PCM layer situated within the external wall of an air-conditioned building modifies the trend of the temperature and of the heat flux with consequent reduction of the peaks of thermal power and of the energy transferred in the wall. The use of this technology for the reduction of energy requirements has led to studies and research on the thermal behaviour of PCMs that have produced models of different complexity, which, in almost all cases, have been solved numerically. The mathematical formulation of the thermal exchange in a PCM layer is known as the Stefan Problem the solution of which is only available for semi-finite or finite monodirectional geometries and surrounding temperature or heat flux constant in time [1]. The analytical solution of the Stefan problem in a finite

layer subject to periodic boundary conditions was instead given recently by Mazzeo et al. [2]. The complexity of the resolution is due to the discontinuity of the heat flux at the bi-phase interface whose position is variable in time, with a consequent variation of the domain of the solid and liquid phase.Several authors, through numerical models used to solve the Stefan Problem and through experimental investigations, have addressed the problem of the thermal behaviour of a PCM layer in a steady periodic regime [3-4]. In the building walls, the boundary conditions that characterise the outdoor environment and the air conditioned indoor environment that generally give rise to several bi-phase interfaces in the layer thus rendering the problem yet more complex. The presence of multiple interfaces in materials subject to phase change has been highlighted in the literature by Choi et al. [5-6].In numerical models, the thermal transfer in a PCM layer is resolved by methods that describe the phase change through a modification of the specific heat capacity or the enthalpy in a range around the melting temperature in an equivalent monophase layer with variable thermophysical properties that are variable with the temperature. Such methods [1], known as the apparent heat capacity methods, the effective capacity method, and the enthalpy method, allow for the numerical resolution of the thermal exchange problem without explicitly determining la position of the eventual bi-phase interfaces and consequently the configuration of the phases in the layer. In this work, we address the problem of the determination of the thermal field in a PCM layer subject to periodic boundary conditions. Steady periodic regime is representative of the behaviour of walls, especially during the summer period. The finite difference model and the resolution algorithm, obtained by modifying those proposed by Halford [7], are used to evaluate the position of the eventual bi-phase interfaces of solidification and of melting which originate in the layer, the field of temperature and of the heat flux in the solid phase and in the liquid phase, the heat fluxes entering and exiting the layer. Such heat fluxes are used for the calculation of the energy transferred and the energy stored in a latent form while the surface temperatures are used for the calculation of the attenuation of the maximum excursion. The evaluations were conducted considering a phase change material subject to boundary conditions that are typical of building walls.

#### 2. Calculation model

The equations describing the thermal exchange in a layer subject to phase change are the general equation of thermal conduction in the solid phase and in the liquid phase, Eq. (1), and the balance equation at the bi-phase interface at the melting temperature, Eqs. (2) and (3):

$$\frac{\partial^2 T}{\partial x^2} - \frac{1}{\alpha} \frac{\partial T}{\partial t} = 0 \quad (1) \qquad \left[ k_l \frac{\partial T_l}{\partial x} - k_s \frac{\partial T_s}{\partial x} \right]_{x = X_M} = \rho H \frac{dX_M}{dt} (2) \qquad T_l(X_M, t) = T_s(X_M, t) = T_M(3)$$

with H fusion latent heat,  $T_M$  melting temperature and  $X_M$  position of the bi-phase interface.

Since the temperatures on the surrounding surfaces of the PCM layer can fluctuate around the melting temperature, the calculation algorithm considers the eventual contemporaneous presence of more solidification or fusion bi-phase interfaces. On the external surface of the PCM layer, we considered convective and radiative short and long wavelength thermal exchanges; for internal surfaces we considered thermal exchanges through unitary surface heat transfer coefficient. The numerical discretization of Eqs. (1), (2) and (3) leads to relations for the calculation of the temperatures in nodes non subject to phase change and of the fractions of liquid  $\lambda$  present in the subvolumes of the nodes at the melting temperature. The relations obtained, for the calculation of the temperature and of the liquid fraction  $\lambda$  of liquid in surface node 1 in contact with external air, in internal nodes j and in node N in contact with the internal air, are reported, respectively, in (4-9).In the preceding relations, the thermal resistances and the heat capacity, which are different in the liquid phase and in the solid phase, are

updated at each instant taking into consideration the positions of the fusion or solidification bi-phase interfaces. The k-th bi-phase interface, positioned in subvolume  $j_k$ , is calculated by summing the thicknesses of the subvolumes previous to subvolume $j_k$  to the portion of the subvolume  $j_k$  in the liquid phase if the interface is a fusion bi-phase interface  $[X_{M,k} = (\sum_{i=1}^{j_k-1} \Delta x_i) + \Delta x_{j_k} \lambda_{j_k}]$ , and to the portion in the solid phase if the interface is a solidification bi-phase interface  $[X_{M,k} = (\sum_{i=1}^{j_k-1} \Delta x_i) + \Delta x_{j_k} \lambda_{j_k}] + \Delta x_{j_k} (1 - \lambda_{j_k})]$ . Figure 1 reports the calculation algorithm created that consists of three subprogrammes to determine at different instants the temperature and liquid fraction present in the node, which can be entirely in a solid phase, a liquid phase or in a phase change .Each subprogramme uses values of temperature and liquid fraction in one node in the two preceding temporal instants to determine correctly the thermodynamic state and the temporal instants. The model and algorithm created differ from those used by Halford and Boehm.



Fig. 1. Algorithm flowchart

In their model they adopt some simplifications considering a uniform spatial discretization of the layer, identical thermophysical properties for the liquid and solid phase, and thermal resistances, which are constant in time in the nodes interested in the phase change. Furthermore, the algorithm evaluates the thermodynamic state in the nodes in the successive instant as a function of just the temperature and liquid fraction values in the nodes in the preceding instant. The algorithm does not contemplate the contemporaneous presence of more bi-phase interfaces of fusion and of solidification in the layer.

#### 3. Thermodynamic configurations and thermal behaviour of the layer

The calculation model created was used for thermal analysis in steady periodic regime conditions. We considered a PCM layer of a thickness equal to 0.06 m with k = 0.43 W/(m K),  $\rho = 1510$  kg/m<sup>3</sup>,  $c_p = 1900$  kJ/(kg K), latent heat of fusion H = 160 kJ/kg and melting temperature of 15°C. The hourly data of the

external air, the apparent sky temperature and of solar irradiation are relative to average monthly days of the city of Turin. Indoors, the air temperature is constant and is equal to 20°C during the heating period. 26°C during the cooling period, and 23 °C in intermediate months. The heat transfer coefficient on the two faces considered are  $h_{(c,r),i}=7.7 \text{ W/(m^2 K)}$ ,  $h_{c,e}=20 \text{ W/(m^2 K)}$  and  $h_{r,e}=5.35 \text{ W/(m^2 K)}$  while the solar absorption coefficient is  $\alpha$ =0.6. The layer, oriented to the South, was modelled with 19 nodes and a temporal step  $\Delta t = 5$  s was used for the integration. Figure 2 shows, upon variation of time in a period P = 24 hours, some thermal configurations obtained in the layer and identified with (a), (b), (c), (d) and (e). For each configuration, we report as a function of time, above, the temperature trends of the external air  $T_{ea}$ , of the sky  $T_{sky}$ , of the absorbed solar radiation  $\alpha \Phi_s$ ; the trends of the equivalent external temperature  $T_{eq}$  [8], of the internal air  $T_{ai}$ , of melting  $T_M$ , and of the temperature in the nodes are also reported. Instead, below, the data referring to the heat flux on the external surface  $\Phi_1$ , in the different nodes of the layer and on the internal surface  $\Phi_{int}$ ; are reported, while in the centre the corresponding trends of the biphase interface positions  $x_M$  and of the respective latent heat energy stored per unit time are shown. Whatever the thermodynamic configuration of the layer, the mean temperature value, corresponding to stationary conditions, varies linearly in the layer and the relative heat flux is constant. Figure 2a relates to a layer in which the temperature at each instant is less than the melting temperature: the layer is not subject to phase change and is always in a solid phase. In figure 2b, the layer is not subject to phase change and is always in a solid phase. In figure 2b, the temperature in the layer is always greater than the melting temperature and the layer is always in a solid phase. In both cases, the maximum excursion of temperature fluctuations is reduced from the outside towards the inside and the relative maximum and minimum peaks undergo a time lag. The heat flux presents a similar behaviour. Figure 2c is relative to a layer in which a bi-phase interface is present, which has one portion in a solid phase and the other in a liquid phase. If the temperature on one of the faces surrounding the layer, at a given instant of the period, become equal to the melting temperature, the bi-phase interface which enters the layer originates; it then inverts the direction and reconstitutes the initial monophase layer. Only a part of the layer undergoes a phase change. The figure shows that the solid-liquid phase change interests a part of the volume of surface node 19 in contact with the internal air. The temperature in the node remains constant during the phase change with a variation in slope at the beginning and the end of the process (fig. 2c, on the left). Figure 2c, in the centre, shows the volume affected by the phase change and the portions in solid and liquid phase at the different temporal instants. In the same image, the trend of the latent energy stored per unit time, which is proportional to the advancement speed of the bi-phase interface (Eq. 2) are shown. The first increases and reaches a maximum value; it decreases successively until it cancels itself in the instant in which the bi-phase interface inverts the direction and the solidification process begins. During such a process, the energy released per unit time always grows and reaches the maximum value in the instant in which the phase change ceases and the volume is entirely in a solid phase. The latent storage modifies the heat exchanges in surface node 19, which is subject to phase change and, consequently, also those in the other nodes. During such a process, the energy released per unit time always increases and reaches a maximum value in the instant in which the phase change ceases and the volume is entirely in a solid phase. In particular, fig. 2C below, during the fusion process, the convective-radiative heat flux exchanged with the indoor environment is constant, since the different in temperature between the surface node at the melting temperature and the indoor environment is constant. It follows that the variation in latent energy storedper unit time determines the reduction of the conductive heat flux between surface node 19 and adjacent node 18 and successively in the other nodes of the layer, attenuating proceeding towards the outside. In the instant in which the process fusion stops, the conductive heat flux exiting the node becomes equal to the convective-radiative heat flux entering the node. In the successive solidification process, the latent energy released per unit time determines the increase of the heat flux exiting the surface node towards the inside, while the convective-radiative heat flux remains constant.

Even in this case, such a modification is propagated within the internal nodes of the layer, attenuating proceeding towards the outside. In figure 2d, the layer is affected by two fusion/solidification bi-phase interfaces generated by the external surface temperature oscillation around the melting temperature. Starting from a completely liquid phase layer, on the external face, a first solidification bi-phase interface is generated, which penetrates the layer and affects node 1 volume and affects, in part, the volume node 2. Such an interface, once maximum depth is reached, inverts direction and is transformed into a fusion interface. Successively, again starting from the external face, a second fusion interface originates which, after having determined the phase variation in the volume of node 1, reaches the first interface in node 2 and restores the starting liquid phase in the entire layer (fig. 2d, centre). In the same image, the trend of the latent energy stored per unit time associated with the formation of the first and second bi-phase interface is reported. During the solidification process, the energy released per unit time before increases; it reaches a maximum value and then decreases until it annuls itself in the instant in which the bi-phase interface changes direction. In this instant, the fusion process starts with an accumulation of energy that increases at first and, successively constant following the formation of the second bi-phase interface. The second fusion interface gives rise to a trend of stored energy per unit time that grows linearly and which annuls itself in the instant in which the interface reaches the first fusion interface. It is necessary to highlight that the spatial discretization of a layer subject to phase change requires a dense spatial discretization in order to render the advance of the bi-phase interface continuous in the passage from the volume of one node to the successive one. In such a way, once the phase change in a node has finished, the time necessary for the second node to reach the melting temperature is reduced, thus avoiding arrest and the successive reboot of the bi-phase interface. In such a transient, the latent energy stored per unit time annuls itself, generating a perturbation that is extinguished asymptotically once the melting temperature has been reached in the successive node. Such a perturbation, present on the first solidification interface and on the second fusion interface in the passage between node 1 and node 2, is highlighted by the trend of the heat fluxes in the layer shown in figure 2d, bottom. The analysis of this figure highlights that the formation of the solid-liquid interface on the external face of the wall, with the release of the stored latent heat, determines the increase in the heat flux lost by surface node 1 towards the outside and a reduction in the heat fluxes towards the other nodes within the layer. The phase change in node 2 gives rise to an increase in the heat flux exiting node 2 which becomes very approximate to the heat flux lost by node 1, while the heat flux in the other nodes is almost constant. In the successive instants, the heat fluxes exiting from node 1 and 2 towards the outside are reduced following a reduction in the velocity of the bi-phase interface until they become equal, in the instant in which the process is inverted, to the heat flux in the successive nodes. When the second fusion interface forms on the external surface, with the first interface also being a fusion interface involving the second node, the heat flux from the outdoor environment in the node 1 is used entirely for the advancement of the second fusion interface while the first fusion interface, which has an opposite direction, only uses the internal conductive heat flux. In such conditions, the conductive heat flux in node 2, coming from the adjacent nodes, is almost nil, that of node 1 is equal to the stored latent energy per unit time, and the heat flux in the successive nodes is equal to the energy stored per unit time of the first interface. When the phase change is completed, the heat flux coming from the outside penetrates the layer and successively decrements and shifts. Figure 2e regards a layer in which three bi-phase interfaces form, one close to the internal surface and the other two on the external surface. The temperature field is reported at the top, the position of the bi-phase interface and the relative stored energies per unit time in the centre, and the heat flux field at the bottom. On the internal face, the solid-liquid bi-phase interface involves the volumes of nodes 16, 17 and 18, while surface node 19 is always in a liquid phase. On the external face, the second fusion bi-phase interface and the successive third solidification interface involve both the volumes of nodes 1, 2 and in part the volume of node 3.In this node, the restoration of the solid phase occurs.



Fig. 2. Temperature field, external and internal loadings and melting temperature (top images), position of the bi-phase interfaces and latent heat stored (images in the centre) and heat flux field (bottom images) as a function of time in a PCM always solid (a) and always liquid (b), in presence of one (c), two (b) and three (c) bi-phase interface.

With reference to the first interface, during the solidification face, the yielding of stored latent heat per unit time increases, reaching a maximum and annuls itself in correspondence with the inversion of the biphase interface with the start of the fusion process. During the fusion process, the latent heat trend is similar to the preceding one and, in the instant in which it is annulled the bi-phase interface arrests and inverts the process. During the solidification process with the interface in node 16, the heat flux in node 17 and in the successive nodes is constant in that both the temperature of the indoor environment and the temperature of node 16 are constant. A similar behaviour is found in temporal instants the interface in node 17 and 18 for the temperatures and for the heat flux in the successive nodes. For this reason, the heat flux exiting the indoor environment and the conductive one between nodes 19 and 18 is constant. Considering the external face, the trend of the stored energy per unit time from the second fusion interface at first increases; it reaches a maximum and then decreases and annuls itself in the instant in which the third solidification interface originates on the external surface. The energy released through the solidification process increases in time and is annulled in the instant in which the third interface reaches the second. The heat flux, in the time interval during which the second fusion interface moves towards the inside, it reduces in the nodes successive to the interface, since the heat flux entering from the external surface is used for the phase change. In the nodes, which precede the interface, the heat flux increases by a quantity equal to the corresponding latent energy stored per unit time. In the time interval in which also the third solidification interface is operating in the nodes that precede the interface, the heat flux exiting towards the outdoor environment increases by a quantity equal to the energy released per unit time during the solidification process, while it is annulled in all the successive nodes in a liquid phase, included between the third interface and the second interface. Table 1 reports the number and type, starting from the outside towards the inside, of the interfaces that form within the layer for all the months of the year. Furthermore, in order to characterise the layer dynamically, we report the values that some typical parameters assume, defined by means of the energy in transit in the layer in a semi-period and of the fluctuating component of the heat flux.

Table 1. Number and type of the bi-phase interfaces	s, decrement factor f	in terms of	f fluctuating	energy,	fraction	of latent	energy		
stored $\Delta H/\Delta U$ and decrement factor $f_T$ in terms surface temperatures for all the months of the year.									

	JAN	FEB	MAR	APR	MAY	JUN	JUL	AUG	SEP	OCT	NOV	DEC
N° interface	0	1	3	3	2	0	0	0	1	2	2	1
Phases configuration in the layer	Always solid phase	s-l	s-1 1-s s-1	s-1 1-s s-1	1-s s-1	Always liquid phase	Always liquid phase	Always liquid phase	s-l	1-s s-1	1-s s-1	s-l
$\mathbf{f}_{\mathrm{E}}$	0.332	0.313	0.015	0.006	0.237	0.401	0.398	0.379	0.359	0.016	0.119	0.317
ΔΗ/ΔU	0.000	0.210	0.823	0.856	0.430	0.000	0.000	0.000	0.016	0.937	0.472	0.110
$f_{T}$	0.408	0.311	0.044	0.035	0.419	0.427	0.427	0.434	0.444	0.110	0.218	0.336

The ratio  $f_E$  between the energy entering the indoor environment and the energy entering the layer characterises the transfer of energy in the layer, while the ratio  $\Delta H/\Delta U$  between the latent stored energy and the total stored energy characterises the latent storage. Lastly, the ratio  $f_T$  between the maximum excursion of the internal surface temperature and the corresponding swing on the external surface defines the decrement factor of the temperature fluctuation. In the presence of a phase change,  $\Delta H/\Delta U$  depends on the number and on the advancement velocity of the bi-phase interfaces that determine the volumes involved in the phase change. In particular, with an interface, such a fraction is variable between 1.6% and 21%; with two between 43% and 93.7%; and with three between 82.3% and 85.6%. Concerning  $f_E$ , in the absence of phase changes it is equal to 0.33 if the phase is solid, and approximately 0.39 if the phase

is liquid. In the presence of a bi-phase interface, such a ratio varies between 0.31 and 0.36; with two interfaces, it is between 0.016 and 0.24; and with three interfaces, it is between 0.006 and 0.015.  $f_T$  varies between 0.43, in the absence of phase change, and 0.035 in the presence of three bi-phase interfaces.

#### 4. Conclusions

The analysis in steady periodic regime conditions of a PCM layer, with reference to Turin climatic data and with a constant temperature within the indoor environment, has highlighted that the thermodynamic state of the layer is variable over the course of the year. It is possible for the layer to not present phase changes, or it can even be the location of one, two or three interfaces of fusion or of solidification. The energy stored or released in the unit of time following the phase change is directly proportional to the advancement speed of the bi-phase interface, which is determined by the external and internal loadings and by the presence of other interfaces that may be present in the layer. The storage-release phenomena of latent heat at the melting temperature modify the dynamic behaviour of the layer and it depends on the fraction of latent energy stored. With an increase in the number and speed of the bi-phase interface, the fraction increases and determines a drastic reduction of the decrement factors, both in terms of energy and temperature. The dynamic properties of the PCM layer depend on the trend of the internal and external surface temperatures compared to the melting temperature, which determine the number of bi-phase interfaces. The variation speed of the loadings determines the speed of advancement of the interfaces.

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#### **Biography**

Domenico Mazzeo is a PhD student in the Department of Mechanical, Energy and Management Engineering at the University of Calabria (UNICAL). He has completed his undergraduate studies at the UNICAL in 2012. His research interests include the energy efficiency in buildings, the thermal energy storage and the renewable energy technologies.