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Impact of the enthalpy function on the simulation of a building with phase change material wall

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ABSTRACT

Recent studies concerning phase change material (PCM) characterization show that important errors occur if differential scanning calorimetry (DSC) experiments are misinterpreted. Therefore, it is important to know the influence of such misinterpretation on system modeling. The present work deals with phase change materials integrated in building structure to reduce overheating. The objective is to evaluate the discrepancies consequences (temperatures, heat fluxes), due to the use of the misinterpreted DSC experiments at different heating rates to determine the enthalpy, in comparison with those determined with the actual value of the enthalpy of the PCM determined by a proven inverse method. A numerical model of a single-family house with a phase change material mortar is developed to evaluate the thermal comfort in the building. The results show that for free-running temperature, none of the enthalpy curve deduced directly from DSC can predict correctly the thermal behavior of the house and the thermal comfort. Moreover, the more the DSC heating rate and the more the discrepancy with the results from the reference inverse method.

1. Introduction

What is the impact of a bad assumption on the modeling of a good concept? Of course, this is a very important question to solve before considering the assessment or the design of the concept with numerical modeling. This question is even more important for complex systems where a lot of physical phenomena interact. Building is a complex system[1] and simulation of heat transfers, and related energy issues, always require modeling. Among solutions designed to reduce building energy consumption or increase comfort, an interesting concept is the integration of phase change materials (PCM) in building structure [1,2] taking advantage of the high value of the latent heat of solid/liquid transformation.

The concept of phase change material in building walls comes from the 70s [3,4]. When the indoor temperature increases, the material is changing phase from solid to liquid. The energy required for the phase change is taken from the inside of the building. Similarly, when the indoor temperature is decreasing, the material is changing phase from liquid to solid. The energy of this phase change is released inside the building. The storage/release of thermal energy during the phase change can be used to decrease heating consumption [5–8] or to increase thermal comfort in summer [9–11].

Modeling the complexity of the building requires to take into account all the physical phenomena. This detailed approach consists in solving the room energy balance (air volume) taking into account conduction, convection and radiative heat transfers. Moreover, internal gains such as occupants or equipments have to be considered. Dealing with the modeling of PCM in building structure, different approaches exist in the literature with different methods [12–24]. In most of the case, these numerical models solve the phase change process using the heat capacity method [17,25,26]. For such modeling, the phase change process is taken into account considering the evolution of the apparent heat capacity with temperature: it is then necessary to evaluate this curve using material characterization.

The apparent heat capacity consists in considering that the differential scanning calorimetry (DSC) thermogram represents only

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[1] In buildings, heat transfers are conduction, convection, radiation and heat transfer due to mass transfer. Moreover, in buildings, occupants induce also complexity.

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Nomenclature

List of symbols

C	specific heat capacity ($J\,kg^{-1}\,K^{-1}$)
h	specific enthalpy ($J\,kg^{-1}$)
m	DSC sample mass (kg)
T	temperature (°C)
t	time (s)
U	transmission coefficient ($W\,m^{-2}\,K^{-1}$)
w	weight (kg)

Greek letters

β	heating rate ($K\,min^{-1}$)
ϵ	emissivity
λ	thermal conductivity ($W\,m^{-1}\,K^{-1}$)
ρ	density ($kg\,m^{-3}$)
Φ	heat flux (W)

Subscript

app	apparent
DSC	differential scanning calorimetry
op	operative
s	surface
w	window
0	reference

a variation of the specific heat and that its extra-variation (peak) at the melting is an extra-variation of the specific heat versus the scanned temperature.

More precisely, the apparent heat capacity is issued from the differential scanning calorimetry measurements via:

$$C_{app}^{DSC\,\beta}(T) = \frac{\Phi_{DSC}}{m \times \beta} \quad (1)$$

where Φ_{DSC} is the heat flux measured by DSC, β the DSC heating rate and m the DSC sample mass. Similarly, an apparent specific enthalpy can be deduced from the apparent heat capacity via:

$$h_{app}^{DSC\,\beta}(T) = \int_{T_0}^{T} c_{app}(T)dT \quad (2)$$

where T_0 is a reference temperature. It is important to note that, in the previous equations, the temperature is the DSC programmed temperature whereas it has been demonstrated that the temperature field inside the sample is not homogeneous [27], inducing errors in the apparent quantities calculation.

The main problem is that the thermogram shape depends on the heating rate β and on the sample weight of the PCM m [27]. The previous well-known remark is one explanation considering the differences existing among the literature values [28,29]. The studies of [30,31] show that the reliable measurement of PCM using DSC requires low heating and cooling rates which does not comply with the typical standards used in DSC analysis of polymers or similar materials [32].

In [33], high measurement discrepancies are highlighted if no precautions are taken. Also, the DSC measurement must be used carefully to avoid mistakes in the results interpretation [34]. The authors also show that the DSC apparent heat capacity is not representative of the thermodynamic behavior leading to high discrepancies in the evaluation of temperature fields and/or heat flux fields. A similar conclusion is presented in [35] in the case of a mortar layer with PCM.

In a previous work, we have already presented our method to determine the actual value of the specific enthalpy during the melting of a pure substance or a binary solution. It consists in using an inverse method and details of it can be found in [36].

The objective of the present study is to evaluate the effect of the enthalpy function evaluation on the simulation of a building with PCM mortar. The mortar layer is placed on the floor to reduce the temperature in summer.[2] Two different approaches are compared: (1) the use of $h(T)$, the enthalpy deduced from an inverse method presented in detail in [34–36]; this later method being considered as the reference and (2) the use of the apparent enthalpy functions $h_{app}^{DSC\,\beta}(T)$, deduced from DSC curves at different heating rates β: $1\,K\,min^{-1}$, $2\,K\,min^{-1}$ and $5\,K\,min^{-1}$.

2. Method

The objective of the study is to numerically evaluate the discrepancy, for a whole building, between the actual enthalpy function deduced from an inverse method and the apparent enthalpy functions deduced from DSC. The building considered in our work is a single-family house located in Lyon (France). The modeling of this building is presented in Section 2.1. The enthalpy method is used to model the phase change in the PCM mortar. This model is detailed in Section 2.2.

2.1. House modeling

The thermal behavior of a low-energy house is modeled using the simulation environment Modelica [37]. The house view and plan are presented in Fig. 1. This house is a single-storey building with a living area of $110\,m^2$. The interior of the house is considered as a single thermal zone. No internal loads are considered in the house model. The ventilation air change per hour is $0.6\,h^{-1}$.

The house walls composition, from inside to outside, is detailed in Table 1. The conduction in the walls is modeled using unidirectional heat equation. A finite-volume discretization scheme is used to approximate the partial differential equation, so that thermal mass is taken into account. The combined convective and radiative[3] heat transfer coefficients for the walls are $7.7\,W\,m^{-2}\,K^{-1}$ inside and $25\,W\,m^{-2}\,K^{-1}$ outside for verticals walls. Low-emissivity double glazing are used for windows with a transmission coefficient of $U_w = 1.1\,W\,m^{-2}\,K^{-1}$ and $\epsilon = 0.2$.

From the winter season modeling, the energy consumption and the heating requirements calculated by the numerical modeling correspond to a low-energy house average values [38].

2.2. PCM modeling

The PCM mortar is designed to be added as a material layer on the internal surface of the floor to replace the screed. Such integration is optimal for heat transfers [1]. The main assumptions of the model are:

(i) Unidirectional heat transfer by conduction is assumed in the PCM mortar layer.
(ii) Convection in the PCM is neglected.
(iii) The density and conductivity of building materials are considered independent of temperature.

[2] For European summer, because of the beam solar radiation incidence angle, the solar flux is reaching mainly the building floor.

[3] Longwave radiation only.