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IMPACT OF MODELLING THE HYSTERESIS PHENOMENON OF PHASE CHANGE MATERIALS ON THE BUILDING PERFORMANCE SIMULATION

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Abstract

The hysteresis of phase change materials (PCMs) is a temperature delay of the enthalpy curves between the melting and solidification. This work assesses the impact of modelling the PCM hysteresis on the building performance simulation. To this end, a series of PCM models, considering and not the hysteresis phenomenon, are implemented in EnergyPlus for a PCM with 3 °C of temperature delay. A commercial building located in Frankfurt is used to perform the annual building energy simulations for the different PCM models. The results reveal important conclusions about the accuracy of the current PCM hysteresis model in EnergyPlus.

Introduction

Energy storage materials accumulate the excess heat in indoor air and can be used for the free cooling of buildings. In particular, phase change materials (PCMs) have attracted great attention from the construction sector to improve the energy efficiency of buildings in the last decade (Cabeza and Chàfer, 2020). While undergoing their phase transition, PCMs can store and release large amounts of energy and get a stabilizing thermal effect inside buildings (Cascone et al., 2018).

Several efforts have been made to develop and implement numerical models of PCMs to predict their complex phenomena in different applications. In particular, there is a great interest in properly evaluating the performance of PCMs in buildings to exploit their benefits. This is highly needed because, despite their enormous energy-saving potential, the successful use of passive PCM-based systems in buildings is not implicitly guaranteed, since their performance directly depends on the interplay with daily thermal cycles (Saffari et al., 2017). Moreover, exist a specific phenomenon of PCMs, the so-called PCM hysteresis, which is strongly related to heat transfer and makes the behaviour of PCMs even more complex.

Within this context, Klimeš et al. (2020) performed a comprehensive review of the current efforts in computer modelling and experimental investigation of phase change hysteresis of PCMs. That article presents a critical discussion of the current modelling approaches for the PCM hysteresis phenomena. This also includes some information about the implementations of the PCM models in whole building energy simulation software. However, a discussion about the hysteresis model implemented in EnergyPlus is not addressed. Furthermore, in the current bibliography, no works are reporting the quantitative impact of considering the hysteresis phenomenon of PCMs in the building performance simulation.

The current work aims to assess the impact of modelling the hysteresis phenomenon of PCMs on the building performance simulation. In particular, the work is focused on properly describing and evaluating the PCM models implemented in EnergyPlus. To this end, a series of PCM models, including the single and the dual curve approach, for a PCM with 3°C of delay between melting and solidification curves are implemented in EnergyPlus. A commercial building located in Frankfurt is employed as a case study to perform the annual building simulations for the different PCM models.

Methods

Case study building

The medium office of the reference building models of the US Department of Energy (DOE) is chosen as a case study building (Deru et al. 2010). This is a commercial building with three floors (bottom, medium, and top), see Figure 1a. Each floor comprises four perimeter thermal zones and one large core thermal zone, resulting in a total building area of 4982.19 m2.

The original equipment for air-conditioning of the occupied thermal zones is removed and replaced by ideal HVAC systems, whose thermostat control is set to 20 °C for heating and 24 °C for cooling. The rest configuration of the model (internal loads, occupant, schedules, etc.) is kept as the original. See supplementary research data for further information about the detailed configuration of the EnergyPlus models.

The case study is assumed to be in Frankfurt, Germany. Thus, all the results are obtained for annual hourly simulations using Frankfurt's recent typical meteorological year (TMYx.2004-2018) (Crawley and Lawrie, 2022).

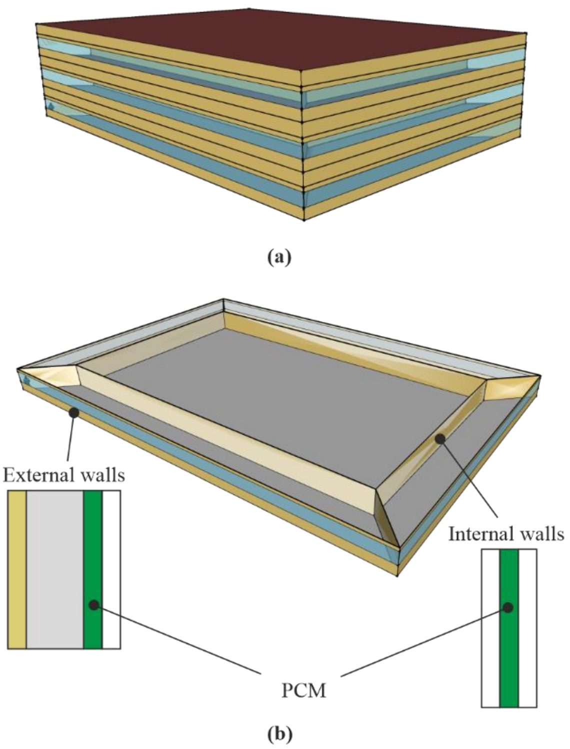

Figure 1: Case study building. (a) Medium-office prototype building model from DOE. (b) PCM configuration in external and internal walls.

PCM modelling

Materials with variable thermal capacity as PCMs can be modelled in EnergyPlus. The specific thermal capacity property of the materials is iteratively calculated at each time step as:

$$cp(T) = \frac{h_i^j - h_i^{j-1}}{T_i^j - T_i^{j-1}}, \qquad \textbf{(1)}$$

where h is the enthalpy (J/kg), T is the temperature (°C), i indicates the material node, and j and j-1 indicate the current and previous time steps, respectively.

Two main models for representing PCMs are available in EnergyPlus: *i)* a single curve, and *ii)* a dual curve. In the first one, *MaterialProperty:PhaseChange*, a single curve for the enthalpy as a function of the temperature should be provided. Then, this curve is employed to calculate the variable thermal capacitance using Equation (1).

The option for modelling materials with hysteresis, *MaterialProperty:PhaseChangeHysteresis*, is a dual curve model. In the EnergyPlus manuals, this model is not reported in detail. However, according to the EnergyPlus Engineering Reference, this second model also evaluates the previous state of the material temperature to capture the hysteresis physics present between melting and solidification processes. The model employs the enthalpy curve of melting or solidification depending on whether the material is heating or cooling, respectively. Other thermophysical properties are employed depending on whether the material is liquid, solid, or in transition.

Moreover, by inspecting the EnergyPlus source code, it was found that the hysteresis model employs the parametric equations proposed by Egolf and Manz (1994) to generate each enthalpy curve for melting and solidification. This asymmetrical model defines the enthalpy curve as a function of the latent heat during the entire phase change process (Δh), the peak melting temperature (T_m), and the temperature distances (τ_1 *and* τ_2) defining the mushy regions regarding the peak melting temperature, see Figure 2.

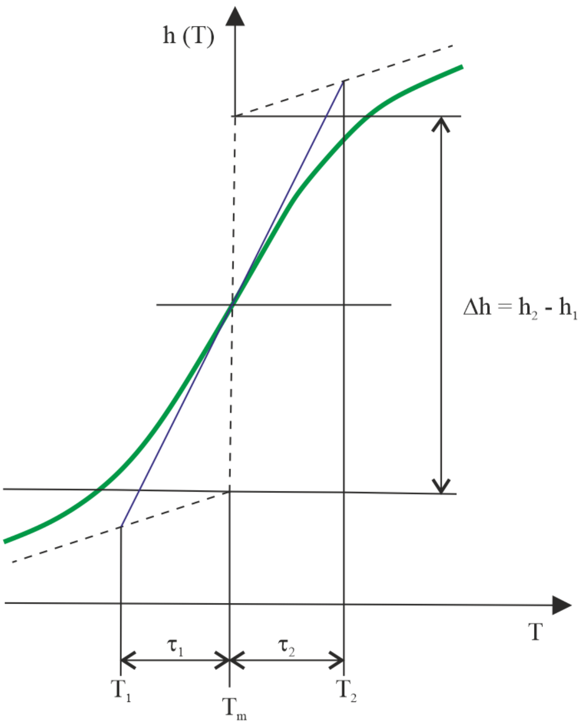

Figure 2: Discontinuous and continuous models for specific enthalpy, Egolf and Manz (1994).

The Egolf and Manz parametric model is defined as:

$$h(T) = cp_1 T + \eta_1 \qquad T \leq T_m \tag{2}$$

$$h(T) = cp_1 T_m + \Delta h + cp_2 (T - T_m) + \eta_2 \qquad T > T_m \tag{3}$$

with

$$\eta_n = \frac{\Delta h}{2} e^{-2\frac{T-T_m}{\tau_n}} \qquad \tau_n \in [1,2] \tag{4}$$

PCM case studies

The Nextek-D24 is employed as a reference PCM, see Figure 3. This PCM is proper for the current research because it has a hysteresis delay, and its melting/solidification temperatures are within the range of the thermostat control (20-24 °C). The enthalpy curves for melting and solidification were obtained by differential scanning calorimetry (DSC) measurements using heating/cooling rates of 0.5 K/min.

It is worth mentioning that the curves (and their slopes), obtained through dynamic DSCs, are always affected by the selected heating/cooling rates. However, the adoption of a 0.5 K/min rate in constructions and building applications represents a good compromise between well-experimentally measured heat storage data and low heating/cooling rate errors.

Therefore, given the uncertainties of PCM hysteresis and its impact on the building performance simulation, four PCM case studies are proposed. In the first three cases, the enthalpy curve for melting, solidification, and a mean curve of both (melting and solidification), are employed via the single curve model of EnergyPlus. In the remaining case, the melting and solidification curves are employed to set the hysteresis model of EnergyPlus and evaluate its impact on the building energy performance.

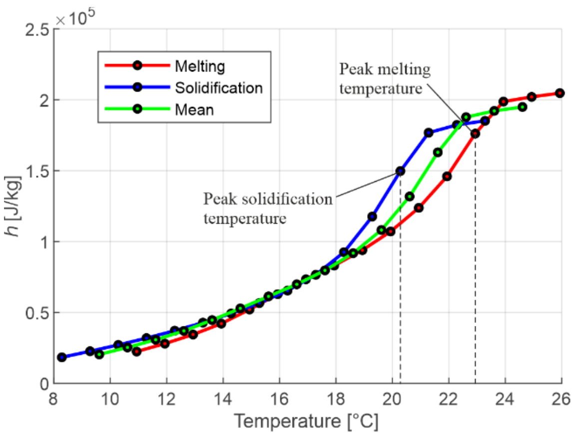

Figure 3: Enthalpy curves for the Nextek-D24 PCM. Melting and solidification curve were obtained by DSC measurements. The "mean" curve was obtained as an average of melting and solidification curves for the research purpose.

Table 1 summarizes the configuration of the hysteresis PCM model in EnergyPlus.

Therefore, a PCM layer of 10 mm is added to the existing constructions for external and internal walls, as shown in Figure 1b.

To simulate PCMs in EnergyPlus, the conduction finite-difference solution algorithm (CondFD) is employed along with 30 time steps per hour to guarantee accurate results (Tabares-Velasco et al. 2012).

Table 1: Setting of the hysteresis PCM model in EnergyPlus.

Property	**Solid-state**	**Liquid-state**
Thermal conductivity [W/m-K]	0.2	0.2
Density [kg/m³]	880	770
Specific Heat [J/kg-K]	2000	2000
Property	**Melting curve**	**Freezing curve**
Δh [J/Kg]	240300	
Peak Temperature [°C]	22.935	20.283
τ_1 [°C]	12	12
τ_2 [°C]	1.5	2

Results and discussion

Simulation results

Figure 4 shows the monthly loads for heating and cooling obtained for the four PCM case studies and the Baseline model (building without PCM) in Frankfurt city.

Regarding heating loads, the cases using the single PCM curve model have larger loads during the winter months compared to the Baseline model. These cases have a slightly better performance compared to the Baseline model during the moderate temperature seasons (spring/autumn). Conversely, the case that employs the dual curve (hysteresis model) presents a significant reduction in the heating loads for all the seasons.

Regarding cooling loads, the cases using the single curve model of PCM reduce loads for all the months except for the winter ones, which present a similar performance to the Baseline model. The case that employs the PCM hysteresis model presents a significant reduction of the cooling loads in the summer months, but its performance is similar or worsens in the resting months.

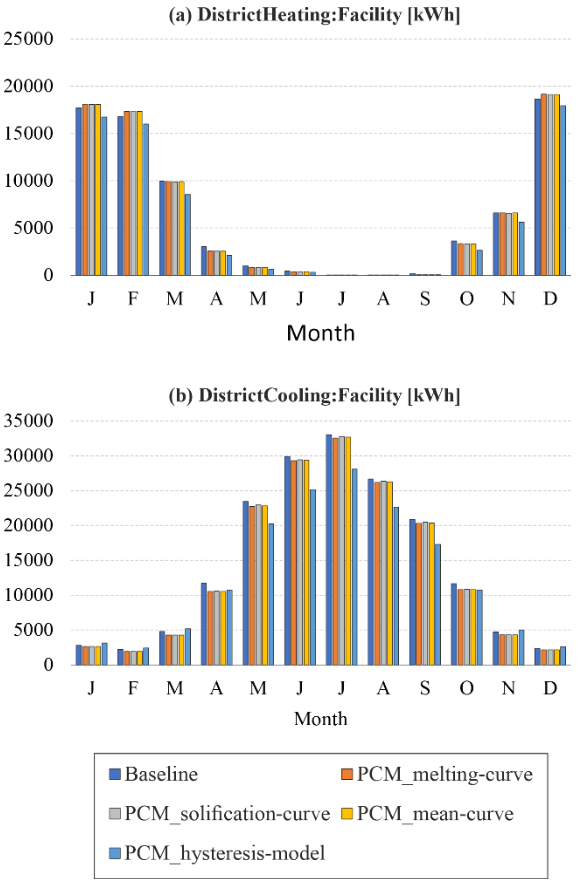

Figure 4: Monthly heating and cooling loads obtained for the case studies.

Table 2 summarizes the annual loads for heating and cooling obtained for the case studies. Compared to the Baseline model (without PCM), the case with the single curve PCM model and using the melting enthalpy curve reduces 2.39% of total loads. Of this total reduction, the performance of the building slightly worsens for heating (-0.38%) while improving by 3.63% for cooling. Similar pattern results are found using the solidification enthalpy curve, but 2.13% of total loads are saved compared to the Baseline model. The case that uses the mean enthalpy curve presents an average performance of previous models, reducing 2.29% of the total annual loads.

The case that employs the hysteresis model reduces 11.22% of total annual loads, and these are for both heating (9.51%) and cooling (11.99%).

Table 2: Summary of the annual ideal loads obtained for the case studies.

Case	**Heating $[kWh/(m^2.y)]$**	**Cooling $[kWh/(m^2.y)]$**	**Total $[kWh/(m^2.y)]$**	**Heat. saving [%]**	**Cool. Saving [%]**	**Total saving [%]**
Baseline model	15.67	34.96	50.63	-	-	-
PCM-melting curve	15.73	33.69	49.42	-0.38	3.63	2.39
PCM-solidif. curve	15.69	33.86	49.55	-0.13	3.15	2.13
PCM-mean curve	15.7	33.77	49.47	-0.19	3.40	2.29
PCM-hysteresis model	14.18	30.77	44.95	**9.51**	**11.99**	**11.22**

Discussion

The differences observed between the cases that employ the single curve model are mainly because of the delay in the melting temperature of the curves. Although these differences can seem small because of the relative impact compared to the Baseline model, the uncertainty between using one curve, or another, is not minor. This means that the choice between using the melting or solidification curve can be reflected in up to 11% of the relative difference in the building performance. Furthermore, this uncertainty will depend on the delay between the melting and solidification curves, as well as the accuracy of the experiments to obtain the enthalpy curve data of PCMs.

Regarding the building performance by using the PCM hysteresis model, it increases considerably (over four times) compared to the ones employing the single curve model. Because of this large difference, several hourly analyses similar to the shown in Figure 5 were performed trying to understand the physical reason that drives them. However, no clear conclusion can be drawn from these analyses, demonstrating the real reasons why the hysteresis phenomenon significantly improves building performance.

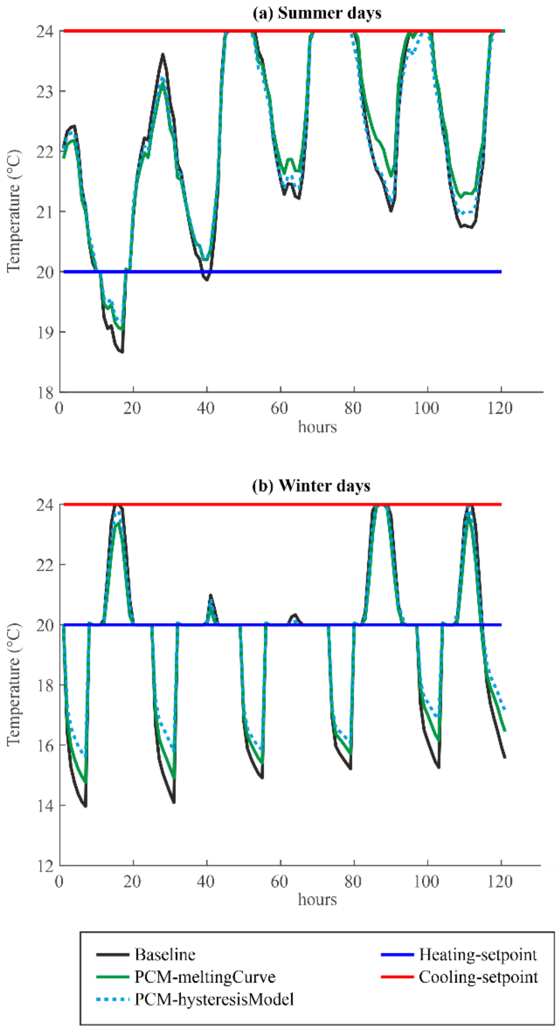

Figure 5:Hourly indoor temperature comparison in the perimeter zone 1 (Bottom). (a) Summer days – June. (b) Winter days – January.

One common behaviour observed is several incomplete daily cycles for the PCMs. This means that the PCMs start the melting/solidification process, but the daily variation temperature is not enough to complete the process. This behaviour, which is common for passive use of PCMs in building, and the numerical phenomenon described below, could explain the large improvements achieved by the hysteresis model.

As mentioned before, the hysteresis model employs the enthalpy curve of melting or solidification depending on whether the material is heating or cooling, respectively. This approach allows considering two different shapes of curves for melting and solidification processes, and also the delay between them because of the hysteresis phenomenon. However, “virtual numerical energy” can be generated because of this approach when incomplete cycles occur.

Figure 6 shows a schematic graph describing this situation. The thermal capacity is employed to be clear. For some days, the PCMs store energy from the indoor air by using the melting curve. If the storing process is complete, the PCMs can store their full capacity. This is the energy below the melting curve, see the orange area in Figure 6. When these PCMs are cooling, they switch to the solidification curve to model the hysteresis process. If the cooling process is incomplete, e.g., the PCMs´ temperatures only decrease until an incomplete value (Ti), these PCMs can partially release the energy they have storage. At this point, if the PCMs heat again, they start to store energy using the melting curve. In this situation, although the storage capacity of the PCMs could be full, they accumulate extra energy because of the numerical implementation. In this situation, with incomplete cycles of storage/release of energy in PCMs, which is common in buildings, the numerical implementation generates an amount of fictitious extra energy that can drive large heating/cooling load reductions. The impact of this numerical phenomenon will depend on the temperature delay between the enthalpy curves, the number of partial energy storage/release cycles, and the amount of PCMs installed in the building.

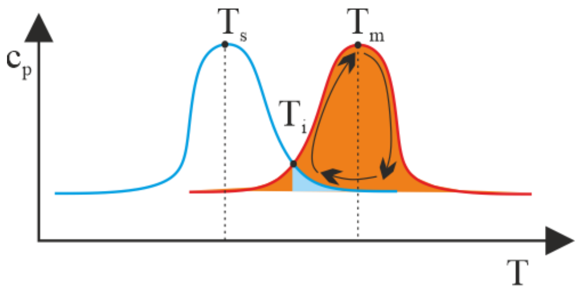

Figure 6: Scheme of the “virtual numerical energy” in the hysteresis modelling of PCMs.

Conclusion

A detailed study was presented regarding the impact of modelling the PCM hysteresis on the building performance simulation. To this end, a series of PCM models, considering and not the hysteresis phenomenon, were implemented in EnergyPlus for a PCM with 3 °C of temperature delay. The medium office of the reference building models of the US department of energy (DOE) was employed as a case study building. Annual simulations for the different PCM modelling approaches were performed using the typical meteorological year in Frankfurt, Germany.

On one hand, for the cases considering the single curve PCM model, the simulation results indicated that the inclusion of the PCM into the building can reduce the annual total loads by 3.29% and 2.13% compared to the Baseline model, by using the melting and solidification PCM enthalpy curve, respectively.

Furthermore, it was found that these improvements in total loads are because of a reduction in the cooling loads since, in both cases, the annual heating loads increased by incorporating PCM into the building. Moreover, the differences observed in the building energy performance regarding using the melting or the solidification enthalpy curve are because of the temperature delay between them. This was also validated through a third PCM case study, which achieved an average energy performance by using a mean enthalpy curve of both (melting and solidification).

On the other hand, the simulation results for the case study employing the PCM hysteresis model of EnergyPlus showed a large total load reduction of 11.22% compared to the Baseline model. This total improvement results from important load reductions for heating (9.51%) and cooling (11.99%). Several hourly analyses were carried out to find the reason for these large improvements. However, it was not possible to demonstrate the physical reason driving such load reductions.

Finally, a discussion about the numerical implementation of the hysteresis model was carried out. From this, a potential reason for the large differences was found, since the numerical implementation of the PCM hysteresis model can generate an amount of fictitious extra energy if partially melting/solidification cycles occur. Although some efforts for properly switching between the melting/solidification curves seem to be currently implemented in EnergyPlus, there is not a physical reason that justifies the large differences found. So, it is not recommended to employ this model until further validations.

Future works should focus on performing a deep description and validation of the hysteresis model of PCMs in EnergyPlus.

Research data

For closer analysis (or their reproduction), all the EnergyPlus models developed in this work can be found at http://dx.doi.org/10.5281/zenodo.6572513

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