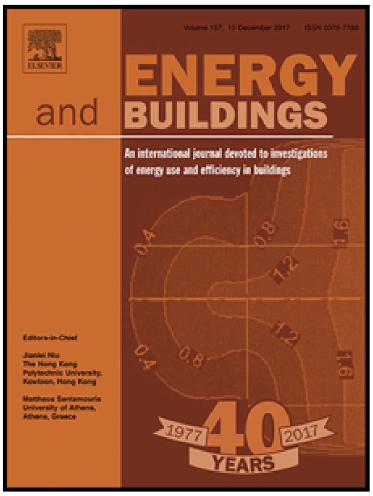

Modeling and experimental validation of an algorithm for simulation of hysteresis effects in phase change materials for building components.

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Highlights

- An algorithm for the simulation of thermal hysteresis in PCM in *EnergyPlus*™ is presented
- The algorithm is validated by comparison with experimental data.
- Simulations and experimental validation with different codes, with and without PCM hysteresis are presented.
- Simulation reliability is sometimes limited, especially for incomplete phase change process
- Conventional characterisation techniques might be insufficient for input data for simulation

Modeling and experimental validation of an algorithm for simulation of hysteresis effects in phase change materials for building components.

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Abstract

The use of Phase Change Materials (PCM) in different building applications is a hot topic in today's R&D activities. Numerical simulations of PCM-based components are often used both for research activities and as a design tool, although present-day codes for building performance simulation (BPS) present some shortcomings that limit their reliability. One of these limitations is the limited possibility of replicating the effects given by thermal hysteresis – a characteristic of several PCMs.

In this paper, an original algorithm that allows hysteresis effects to be accounted for is described and the results from simulations are compared against experimental data. The algorithm is implemented in EnergyPlus™ and makes use of the Energy Management System (EMS) group, one of the high-level control methods available in EnergyPlus™. The algorithm enables the replication of PCM's different heating/cooling enthalpy curves in this BPS tool, which just recently was equipped with an integrated module for the replication of the effects of thermal hysteresis.

A comparison between numerical results from the proposed model and from other methods implemented in BPS tools, and the experimental data provided, shows the impact of the algorithm in the simulation of heat transfer in a PCM layer intent for opaque walls. In general, it is shown that the proposed method presents a better agreement with experimental data than alternative modelling approaches, but it is also seen that all the tested numerical models are not fully able to replicating the behaviour of PCM layers if the PCM does not melt or resolidify completely (i.e. it remains in the phase change) during the charge/discharge cycle. A local sensitivity analysis complements this study and highlights the most relevant parameters that influence the results of a simulation carried out with the proposed model.

Finally, the paper hypothesises that the general discrepancy between simulations and experimental data seen in the case of incomplete melting of the PCM layer can be due to unsuitable data for the thermophysical behaviour of the PCM, which are obtained through conventional characterisation procedures far from the physics of the PCM layer when in real building structures.

Keywords

Building Simulation

Energy Management System (EMS)

EnergyPlus

PCM Hysteresis

PCM Modeling

Phase Change Materials (PCM)

Acronyms

BPS	Building Performance Simulation
DSC	Differential Scanning Calorimetry
EMS	Energy Management System
Erl	EnergyPlus Runtime Language
HVAC	Heating, ventilation, and air conditioning
BCVTB	Building Controls Virtual Test Bed
RT 28 HC	Paraffin wax based PCM with melting area around 28°C
SP 26 E	Salt hydrate based PCM with melting area around 26 °C
PCMH	Phase Change Material- Heating
PCMC	Phase Change Material- Cooling
PC	Poly-Carbonate
DHFMA	Dynamic Heat Flow Meter Apparatus
IC	Influence Coefficient
FVM	Finite Volume Method

FDM	Finite Difference Method

Nomenclature

|Δ|	Absolute value of temperature difference	[°C]
e	Experimental temperature value	[°C]
PRMSE	Percentage root mean square error	[%]
RMSE	Root mean square error	[°C]
s	Numerical (simulated) temperature value	[°C]

EMS code nomenclature

Avg_Temp	EMS Global Variable
C_Wall	EMS Construction Index Variable for Plate Wall_C
Current_Wall	EMS Global Variable
Current_Wall_Status	EMS Output Variable for "Current_Wall"
EMS PCM Code	EMS Program
H_Wall	EMS Construction Index Variable for Plate Wall_H
Hysteresis	EMS Program Calling Manager
Node N	Calculation node inside the PCM layer
Node_PCM	EMS Sensor
PCM_Temp_Trend	EMS Trend Variable to record data of "Node_PCM"
Plate Wall_C	Construction with PCM which has a cooling enthalpy-temperature curve
Plate Wall_H	Construction with PCM which has a heating enthalpy-temperature curve
Wall	EMS Actuator
Wall_PCM	Name of Surface (wall) having PCM

1. Introduction

The interest in the adoption of phase change materials (PCMs) in several building applications, ranging from building components to HVAC systems, is steadily increasing over the last few years in the R&D community. When integrated into building components such as walls, floors, partition walls, glazing systems, these materials have the potential to enhance the heat storage feature of the building fabric. This increased thermal capacity may determine a reduction and delay of the daily peak loads, with a consequent downsizing of the HVAC systems and an increase of occupants' thermal comfort. It is out of the scope of this paper to review the innumerable research activities carried out in the last years on the use of PCM in buildings, and comprehensive recent overviews can be easily found in literature, both at technologies and systems level [1][2][3][4][5], and at materials level [6][7][8][9].

Several studies have shown important benefits related to thermal comfort, energy savings, and HVAC downsizing when these technologies are used in buildings. However, it must be noted that much of these have been limited to laboratory scale testing, or small mock-ups, whilst studies in real buildings have been rather limited. Nonetheless, with advancement in numerical simulation tools, advantages given by the adoption of PCM in full-scale buildings can be studied through building performance simulation codes.

In the last decade, an explosion of studies based on numerical simulations of PCMs in buildings can be observed – in Fig. 1 the number of articles indexed in bibliographic database SCOPUS, which had Phase Change Materials, Simulation, and Building as a keyword or word used in their abstracts, is reported, for the period 2005-2016. Computer simulation tools provide a rapid and low-cost method to assess the performance of different systems, technologies, controls, and in general applications of PCM in full-scale buildings. Nonetheless, it is important to stress that to reach the expected/predicted performance, simulations should be done only when an accurate and validated model has been developed.

Nowadays many building simulation codes are available to assist engineers, architects, designers, researchers, and manufacturing companies to implement PCMs technologies and to evaluate innovative solutions capable of improving the energy and thermal performance of buildings. Most of these building performance simulation (BPS) tools are listed by the U.S. Department of Energy (DOE) web directory [10], and some of them implement modules for the solution of heat transfer and heat storage within PCMs, among which it is possible to list: EnergyPlus, TRNSYS, ESP-r, WUFI Plus, and BSim.

One intrinsic limitation of most of the PCM models which are integrated into a BPS tool is the need to run simulations with a very small-time step (i.e., in order of minutes) to achieve an acceptable level of accuracy. Because of this condition, a one-year thermal performance simulation becomes computationally heavy as iterative methods are used at each time step. Also, the convergence may not be achieved due to numerical instability especially when PCM enters or leaves the phase change region [11]. Currently, none of the whole building simulation programs are using efficient mathematical models that are quick, accurate and numerically stable at a realistic time step.

Furthermore, there are a few shortcomings that affect the full reliability of simulations of PCM in buildings. As highlighted in the literature [12][13][14], sub-cooling and thermal hysteresis are two features recurring in many PCM that are not currently tackled by any BPS tools. The lack of algorithms and strategies to correctly simulate these aspects of the complex dynamic of PCMs can lead to wrong assumptions in designs as well as to not fully reliable findings in research and development.

At the best knowledge of the authors, there is currently no standard versions of BPS tools that is capable of addressing thermal hysteresis effect of PCMs in multilayer constructions, since all the released standard platforms that allow the simulation of PCM-based components offer the modeller the possibility to define just one enthalpy vs. temperature curve as a material property. This approach is in opposition to what is experimentally verified for most of the PCMs, which always show, even if with different extent depending on the nature of the PCM and on the speed of the melting/solidification process, two different peak transition temperature values (one for the melting process and one for the solidification process).

There also exists custom/advanced modules/sub-routines (i.e. for *EnergyPlus*^{TM} [15] and for ESP-r [16]) where hysteresis can be modelled, but the execution of these models usually require full-conversancy in building performance simulation, and actions on the source code are necessary. As a matter of interest, *EnergyPlus*^{TM} integrates in its latest version (v. 8.8), released during the writing of this article, an in-built module for simulation of PCM layers that allows the implementation of thermal properties connected to hysteresis, and based on the custom sub-routing developed by NRGSIM [15]. However, this version only allows the simple simulation of a stand-alone PCM layer, and the simulation of a PCM layer within a multilayer structure is not possible. The future release 8.9 (now in state beta of software development) overcomes this limitation and allows simulation of multi-layered structures that include a PCM layer to be executed[1].

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[1] In the research activity presented in this paper, the beta-version of EnergyPlus^{TM} 8.9, provided by the EnergyPlus Support Team, has been used. More details on this aspect are given in section 1.2.1.

1.1. Research aims

The aims of the research activities presented in this paper are:

- to develop and validate an algorithm in *EnergyPlus*^{TM} that implements the hysteresis effect of PCMs by means of Energy Management System (EMS); and
- to compare the performance of the proposed modelling approach to that of two simulation codes (*EnergyPlus*^{TM} and Wufi®Pro/Plus) which one (*EnergyPlus*^{TM}*)* have recently been implemented in a in-built model for the replication of thermal hysteresis' effects (*EnergyPlus*^{TM} - NRGSIM custom);

The main goal is to provide the community of researchers and practitioners with a more accurate and complete modelling tool for PCM-based building components (such as wall, ceiling, floors), which can be used even without being an expert in software codes for BPS, and therefore without requiring the need to modify and compile the source code of a BPS, if this is a freeware tool.

1.2. Background on PCM modelling in selected BPS tools

Different BPS tools offer the possibility to model PCM-based components. In this research activity, two software tools were selected: *EnergyPlus*™ and *WUFI®Pro/Plus***.** The two BPS tools selected belong to two different categories (freeware and commercial, respectively), and differ in terms of possibilities of simulating hysteresis phenomena (*EnergyPlus*™ implements this possibility, as explained below, though still not in an official release, while *WUFI®Pro/Plus* does not natively allow hysteresis effects to be simulated).

1.2.1. Energy Plus™

Among all the possible BPS tools, the paper presents a strategy and an algorithm that can be directly implemented in *EnergyPlus*™. This software is one of the leading BPS tools and has been developed with financial support of the U.S. Department of Energy. Aside from several features that make this software very powerful for building simulation, it is also worth mentioning that it is freeware and it can thus be used without limitations for both research and professional purpose.

The capability of modelling PCMs was added to *EnergyPlus*™ program version 2.0, released in April 2007, by adding a conduction finite difference (object "*CondFD*") solution algorithm [17]. This algorithm uses a semi-implicit finite difference scheme based on the heat capacity method with an auxiliary enthalpy vs. temperature dataset to account for latent heat evolution [18]. Successful validations of this algorithm in combination with PCM modelling for previous versions of *EnergyPlus*™ were reported by Zhuang [19], Campbell [20], and Chan [21].

A custom version of EnergyPlus version 8.1 with a new hysteresis model was developed in part with OSU and NRGSIM inc. The PCM hysteresis modelling methodology used in this custom version has not yet been implemented in the official release of EnergyPlus. It uses an equation based approach for modelling dynamic phase change materials “PCM's” with minimal inputs. The inputs are designed to match the results of differential scanning calorimeter “DSC” testing. The model uses polynomial fitting curves to describe the properties of PCM adapted from the Ginzburg-Landau theory of phase transitions [15]. It uses two hysteresis modelling methods, curve switch and curve track. The former method is used for the partial phase transition whereas the latter is used for the complete phase transition. The custom version of the tool is freely available, but it is not straightforward in its execution, and compiling of the source code is necessary before it can be used. This custom version can be used to simulate multi-layered wall envelope structures where one of the layers is made of a PCM.

In a recent development, the official release of EnergyPlus Version 8.8 integrates the module developed by NRGSIM inc. that allows simulation of hysteresis to be performed. However, in this release, the use of the new module is limited to a mono-layer envelope structure, where the only layer is made of PCM. This is clearly a limitation in terms of simulation possibilities. The future (at the time of the writing of the paper) version of EnergyPlus (release 8.9) is planned to integrate the custom NRGSIM module and to overcome the limitation of mono-layer simulation of version 8.9. Because of the state of development “beta” of the EnergyPlus^{TM} 8.9 used in this paper, and not officially released yet, in the paper such a software tools will be identified as EnergyPlus^{TM} – NRGSIM custom.

In this paper, different modelling approaches using EnergyPlus are used to assess the reliability of different simulation strategies, as explained in Section 3.2.

1.2.2. Wufi®Pro/Plus

WUFI® Pro [22] is a 1D hygrothermal heat and moisture simulation software developed by Fraunhofer IBP, Holzkirken, Germany [23]. The software was chosen for the following test because it represents a very popular tool that allows coupled heat and moisture transfer in transient state to be simulated in wall assemblies by solving the system of equations through the Finite Volume Method (FVM). The calculation method of WUFI® Pro is based on the spatial discretisation of the transport equations and uses the fully implicit scheme for the time discretisation.

More recently WUFI® Plus based on coupling hygrothermal and energetic building simulation was developed by Fraunhofer IBP [24]. In the software, the resulting heat and mass fluxes solved at the building component surfaces are incorporated into zonal models.

Building components containing PCM can be simulated from WUFI® Pro 5.0 version and in WUFI® Plus [25] by assigning a temperature dependent enthalpy data in the hygrothermal function menu of the material/layer data editor. Two main limitations of the software are reported in the literature: the first limitation is represented by the possibility to assign as input data only hourly weather profiles [25], and secondly, the impossibility to implement hysteresis effect.

2. Numerical model

As discussed in the introduction, current releases of BPS tools are unable to model thermal hysteresis effects in PCM due to the limitation that only one enthalpy-temperature curve can be provided as a material property. In this section, the modelling approach adopted to overcome this current limitation in *EnergyPlus™* is presented, together with the explanation of the algorithm and its implementation in the simulation tool.

2.1. The EMS approach

The current version of EnergyPlus™ allows the modelling of a PCM layer to be carried out through the object "*MaterialProperty:PhaseChange*". This object is used to define the enthalpy vs. temperature curve of a given material, whose other thermophysical properties are defined in the object "*Material*", under the same group "*Surface Construction Elements*". A maximum of sixteen pairs of enthalpy-temperature values can be given to describe the non-linear dependence of the internal energy of a PCM on the temperature. The enthalpy corresponding to each temperature point is independent of the direction of the energy storing process – i.e. if the material is cooling or heating. This means, in practice, that only one enthalpy vs. temperature curve can be defined, and it is, therefore, a common practice to provide the values of a "fictitious" curve, calculated as the average between the heating and the cooling enthalpy vs. temperature curves provided in the PCM datasheet. It is important to mention that the simulation of PCM can be only carried out using the algorithm "*ConductionFiniteDifference*" for the solution of the heat balance within the construction element.

Given the present-day fields of the object "*MaterialProperty:PhaseChange*", the strategy to overcome this limitation makes use of the group "*Energy Management System*" (EMS) and its objects [27]. EMS is an advanced feature of *EnergyPlus™*, and it is designed for users to develop customised high-level, supervisory control routines to override selected aspects of *EnergyPlus™* modelling [28]. Conventional use of EMS in simulations are found in advanced HVAC modelling and controls[30][31][32], including faulty HVAC models for Fault Diagnostic Detection [29], real-time building energy simulation [30], co-simulation of several other building energy software codes with Energy Plus using Building Controls Virtual Test Bed (BCVTB) [31][32]. In addition, EMS has also been used as a tool to model occupant behaviour in connection to adaptive comfort theory and occupancy control [33], or other advanced modelling of user's interaction, such as the stochastic use of windows [34]. Furthermore, EMS has also been used for simulation of behaviour and advanced control of dynamic properties in real [35][36] and ideal dynamic window systems [37].

EMS has nonetheless some limitations, and its use requires advanced knowledge of *EnergyPlus*™ and basic computer programming. A simple programming language called EnergyPlus Runtime Language (Erl) is used to describe the control algorithms, which are executed by the *EnergyPlus*™ engine when the simulation is carried out.

In the algorithm to enable the simulation of hysteresis effect of PCM, objects and programs of EMS are used to:

- *Step 1)* Evaluate the state of the heat storage process of the PCM layer at the simulation time-step (whether the PCM layer is cooling down or heating up compared to the previous time-step of the simulation);
- *Step 2)* Select the appropriate enthalpy vs. temperature curve, coherent with the direction of the heat storage process;
- *Step 3)* Instruct *EnergyPlus*™ to carry out the simulation of the time-step with the appropriate construction characterised by the "correct" enthalpy vs. temperature curve, depending on the direction of the heat storage process.

The evaluation of the heat storage process (Step 1), can be easily done through the EMS since the temperature of the internal nodes of a construction element are calculated by "*ConductionFiniteDifference*" algorithm and can be directly acquired by the EMS. A simple way to assess the direction of the heat storage process within the PCM layer is to compare the temperature of a node inside the PCM layer, at the time-step, with the temperature of the same node at the previous time-step: if it is greater, the layer is increasing its internal energy, and a heating (melting) process is taking place; if it is lower than that at the previous time-step, the layer is cooling down (solidifying).

For the execution of Step 2, the EMS selects among two different objects "*Construction*", previously defined by the modeller, the first one related to a wall structure implementing a PCM with an enthalpy vs. temperature curve for heating process and the second one related to a wall structure implementing a PCM with an enthalpy vs. temperature curve for cooling process.

The EMS program is then used, in Step 3, to instruct *EnergyPlus*™ to carry out the simulation with the right "*Construction*" object, previously selected based on the heating or cooling process (Step 1).

2.2. Preliminary settings

Before defining the right program in the EMS environment, it is necessary to set an appropriate space discretisation for the numerical solution of the heat transfer equation. The space discretisation must be so that at least one node falls inside the PCM layer. This node (named **Node N** in these sections) will be recalled in the EMS program. Space discretization is controlled in EnergyPlus™ through a parameter called "*Space Discretisation Constant*" in the object "*HeatBalanceSettings:ConductionFiniteDifference*".

Furthermore, the values used to define the enthalpy vs. temperature curve cannot be directly changed by the EMS, but belong to a specific object in the category "*MaterialProperty:PhaseChange*", it is necessary to define, for each PCM, two objects "*MaterialProperty:PhaseChange*" – one implementing the enthalpy vs. temperature curve for the heating process, and one implementing the enthalpy vs. temperature curve for cooling process. Moreover, each object "*MaterialProperty:PhaseChange*" needs to be connected to a main object "*Material*", where the other thermophysical and optical properties of a construction material are given, two objects "*Material*" need to be defined – one for the PCM during the heating process and one for the PCM during the cooling process. If the PCM is not the only layer of a construction element (as usually happens), it is then necessary to define two different "*Construction"* objects, where the two different "*Material*" objects are coupled with other layers to form the construction element. For the sake of this explanation, the two "Constructions" objects are called **Plate Wall_H** (corresponding to the PCM with the enthalpy vs. temperature curve for the heating process), and **Plate Wall_C** (corresponding to the PCM with the enthalpy vs. temperature curve for the cooling process).

Once these two pre-settings are implemented, it is possible to move to the EMS group and define the objects and program necessary to execute the simulation.

2.3. Working algorithm code

The EMS objects and how they can be used in *EnergyPlus*™ to make the algorithm for the hysteresis modelling are discussed in detail in ***Appendix A***.

3. Validation

The performance of *EnergyPlus*'s and WUFI's PCM module was first compared with the experimental data without considering the hysteresis effects. Furthermore, the performance of the EMS code described in the above section was validated against experimental data from measurements in a Dynamic Heat Flow Meter Apparatus (DHFMA). In this section, after introducing the experimental procedure to acquire empirical data, the impact of the

EMS code on the simulation of the PCM's layer temperature evolution is shown and it is highlighted that the proposed approach allows for a better agreement between experimental data and numerical simulations to be achieved.

3.1. The HFM experimental analysis

Laboratory measurements were performed by means of DHFMA [25][38], evaluating the response of PCM under sinusoidal periodic solicitations as reported in [39][40]. Tests were performed by using two different solicitations, aimed at on one hand to reach a complete phase transition (Test 1) and on the other hand to reach only a partial phase transition (Test 2).

3.1.1. Specimens

For this study, two different types of PCMs were used, one characterised by a moderate thermal hysteresis (PCM-a) and one characterised by a much more relevant thermal hysteresis (PCM-b).

The first PCM-a is a paraffin-based PCM product named "RT 28 HC" by RUBITHERM GmbH [41]. The thermal properties of this PCM, derived from the technical data sheet, are given in Table 1. Data to calculate the specific heat vs. temperature and the enthalpy vs. temperature curves were also obtained from the technical datasheet.

The second PCM-b is a salt hydrate product named "SP 26 E" by RUBITHERM GmbH [42], whose thermophysical properties are reported in Table 1. This type of PCM usually shows much higher energy storage density (i.e. narrower melting/congealing range) than paraffin-based PCM. Hysteresis effects in salt hydrates are also more relevant than in paraffin because of the combination of the thermophysical properties of these materials (higher thermal conductivity, higher density, higher energy storage density). This characteristic can be well understood comparing the enthalpy vs. temperature curves of the PCM–a (Fig. 2) with those of the PCM–b (Fig. 3). The area between the curve for the heating process and the one for the cooling process gives the impact of the hysteresis effect: the larger the area, the higher the effect on the thermal behaviour of the PCM due to the hysteresis. This area is at least 10 times larger in Fig. 3.b (PCM-b) than in Fig. 2.b (PCM-a).

The two PCMs were chosen for their easy availability and because of their wide diffusion for their use in buildings, and they represent two different levels of impact of hysteresis on the overall performance of the PCM.

The two PCM specimens were built by filling a hollow polycarbonate panel 10 mm thick; these methods were already tested in [43][44] and represent a fast and easy way to enclose PCM in a stabilised shape that allows performing measurements by using a DHFM apparatus.

The polycarbonate panel filled with PCM was sandwiched between two gypsum board panels (thickness 12.5 mm) in order to avoid the direct contact between the PCM filled polycarbonate and the instrument plates: this solution allows the temperature in the upper and lower interface of PCM to be measured, and to therefore use such temperature readings for the validation process.

The physical characteristics of each layer are illustrated in Table 2. Moreover, the enthalpy/temperature curves of the two PCM are illustrated in Figure 2 & 3.

3.1.2. Experimental setup

The experimental test was carried out by means of a Lasercomp FOX600 single sample heat flow meter apparatus. Temperatures were measured by means of type-E thermocouples (measurement accuracy ±0.25 °C), connected to an external data logger. Thermocouples were placed in the PCM core, and at the upper and lower boundaries of the polycarbonate PCM filled panel.

The dimensions of the specimens cover all the area of the instrument plates (600 x 600 mm). Both the plates surfaces are heated/cooled (homogenous temperature field) while the measurement area is strictly in the middle of the specimen (254 x 254 mm). Since the thickness of the specimen (10 mm) is more than eight times lower than the external side of the HFM (ratio suggested by EN 12667:2002 standard) lateral heat losses can be considered negligible.

The Heat Flow Meter Apparatus generally used for steady state thermal conductivity measurement was adjusted to perform dynamic experiments, i.e. imposing a sinusoidal temperature solicitation (periodic cycle of 24 h) in the upper plate and maintaining a constant temperature the lower plate. The experiments were considered concluded after two sinusoidal cycles (test duration = 48 h). Nevertheless, the first 24 h cycle were used only as initialisation period and were afterwards discarded. In this way, only the last 24 h cycle was used for the validation process. As mentioned, the tests were carried out on the two PCMs imposing a lower plate temperature equal to the nominal melting temperature of the PCM, and an upper temperature solicitation with different amplitudes of ±12°C and of ±6 °C, for testing the complete phase transition (Test 1) and to test partial phase transition (Test 2), respectively. The test conditions are summarised in Table 3.

3.2. Simulation of a virtual heat flux meter apparatus in BPS tool

The heat flux meter apparatus experiments were replicated virtually using EnergyPlus™ v. 8.4, WUFI® Pro, and the beta version of EnergyPlus™ v. 8.9 (not officially released to the public at the time of the writing of the article). An overview of the different simulation approaches tested in this paper is given in Table 4.

The temperature values of the upper plate (sinusoidal) and the lower plate (constant) were forced as the surface temperature of the wall imposing a surface convection coefficient h_c infinitely high. The settings of the simulation in EnergyPlus™ were set as it follows. The heat balance algorithm was set to Conduction Finite Difference Method, and Crank Nicholson Second Order "Difference Scheme" was used for calculations. "*Space Discretisation Constant*" was set to 0.5 whereas "*Relaxation Factor*" was set to 0.01. "*Inside Face Surface Temperature Convergence Criteria*" was set to the minimum possible value, i.e. 10^{-7}. Impendence of the results from the spatial and time discretisation was verified by varying the space discretisation constant (the variable that can be controlled in EnergyPlus related to the spatial discretisation) and the simulation time-step (in the range 1 to 3 min., which is the maximum time-step allowed by EnergyPlus in case of Conduction Finite Difference Method).

Simulations were carried out using the same boundary conditions imposed in the experiments. Simulation runs were long enough so that a periodically stabilised response was achieved. Four runs were carried out to test the effect of the algorithm for hysteresis with different features of the PCM layer:

- EP_COOL: the wall sample was simulated using the conventional approach in EnergyPlus™ and using as the only enthalpy vs. temperature curve, the curve related to the cooling process in Fig. 3;
- EP_HEAT: the wall sample was simulated using the conventional approach in EnergyPlus™ and using as the only enthalpy vs. temperature curve, the curve related to the heating process in Fig. 3;
- EP_AVG: the wall sample was simulated using the conventional approach in EnergyPlus™ and using as the only enthalpy vs. temperature curve, the fictitious curve obtained as the average of the heating and cooling curves, shown in Fig. 3;
- EP_EMS (only in *EnergyPlus*™): the wall sample was simulated using the EMS approach presented in this paper to account for thermal hysteresis effects (and thus with both the two enthalpy vs. temperature curves for heating and cooling process illustrated in Fig. 3).

Computational times for the three simulations were identical, considering possible small changes due to a different use of the CPU. It is possible to affirm that the use of the EMS (in the algorithm for the simulation of hysteresis effects, EP_EMS) does not increase the computational load of the simulation, and thus does not have any drawback from a functional point of view.

Additionally, three simulation runs (WUFI_HEAT, WUFI_COOL, and WUFI_AVG) were also carried out on WUFI® Pro v. 6.1. The settings of the simulation were arranged as it follows. In *WUFI® Pro* (based on the finite volume method), space was discretised by using the option coarse grid (100 elements) with adaptive mesh refinement at the boundary of each layer, while the time discretisation was equal to the DHFM measurement output (666 seconds). Moreover, in the numeric window, the options *increased accuracy* and *adapted convergence* where flagged, while the *moisture transport calculation* was excluded.

The beta version of EnergyPlus 8.9, which integrates the custom version developed by NRGSIM, was also tested for all the four cases. For Test 1, where the complete phase transition is seen, the Curve Track option is selected for the hysteresis modelling methodology whereas, for Test 2 where incomplete phase change happens, Curve Shift is used. In the graphs shown in later sections and Appendix B, the simulation result from this model is shown with the name "EP_NRGSIM".

3.3. Results

Experimental data and numerical data from the four rounds of simulation (two different PCMs, with complete and incomplete phase transition) with all the different approaches (see Table 4) were compared both quantitatively and qualitatively. Values of internal temperature nodes were used to carry out the verification of the modelling approach and to assess its performance. For all the results presented in Tables 5–7, Figs 5–7 and Figs. B1–B4, the temperature datum shown is that of the Node T_{PCM} is, both for experimental and simulations. In the simulations, the datum for the Node T_{PCM} is taken from the mid node in the PCM layer, as different numbers of nodes are obtained with different combinations of Spatial and Time discretisation.

Quantitative estimation of the matching between numerical and experimental results was carried out using the following indices:

- Percentage root mean square error (PRMSE, [%]), calculated according to the Eq. (1):

$$PRMSE = \sqrt{\frac{1}{n} \cdot \sum_{j=1}^{n} (\frac{s_j - e_j}{e_j})^2} \quad (1)$$

, where n is the total number of readings over a certain period, and e_j and s_j are the experimental and simulated values, respectively.

- Root mean square error (RMSE [°C]), calculated according to the Eq. (2):

$$RMSE = \sqrt{\frac{1}{n} \cdot \sum_{j=1}^{n} (s_j - e_j)^2} \quad (2)$$

- The average value of the absolute difference between simulated and measured values $|\Delta|$ [°C] Eq.(3):

$$|\Delta| = \frac{1}{n} \cdot \sum_{j=1}^{n} \left| s_j - e_j \right| \tag{3}$$

In Table 4 the values of PRMSE, RMSE and |Δ| for the four PCMs for the four different runs are reported. These error values are with simulation done on EnergyPlus™ Version 8.4.

Qualitative validation was carried out comparing the time profiles for the stabilised period of the simulated and experimental temperature values. The temperature evolution inside the PCM layer of the sandwich sample is shown in Fig. 5 and in Fig. 6 for the wall with the PCM-a “SP 26 E” and the wall with the PCM-b “RT 28 HC”, respectively. Fig.5 and Fig.6 show all the four cases of experiments. In all the four graphs, the simulation result of EP_EMS and EP_NRGSIM model is compared with EP_AVG and WUFI_AVG (where an average of heating and cooling curves is used). Individual graphs of each individual software with experimental and EP_EMS is shown in Appendix B for the sake of completeness.

When the PCMs only show a partial phase transition, the reliability of all the simulation tools is lower, and higher errors are recorded when simulations are compared to experimental results. The possible explanation for this behaviour is that the physics involved in partial phase change is much more complicated in full transition, as the material is continuously in the phase change range. Furthermore, it is possible that experimental results are more sensitive to the sub-cooling phenomena, which is not accounted in simulation software packages. Moreover, another possible explanation can be the uncertainty in the input data of the PCM and other materials used in the experiments.

Results highlight that both EnergyPlus and WUFI are sufficiently accurate only to simulate PCM characterised by low hysteresis during their complete phase transitions. The main differences among the results of the two software packages are due to lack of accurate synchronisation in WUFI: in fact, as highlighted in [25], one of the limitations of this software is that only hourly time profile interpolated for smaller time steps can be assigned as the boundary condition.

The comparison between the output of the simulations and the experimental data demonstrates the reliability of the proposed approach for the simulation of PCM-based components in EnergyPlus™. Quantitatively, a slightly better match (lower PRMSE and RMSE) between experimental data and simulation is recorded when the new algorithm, i.e. EP_EMS is adopted compared to other approaches. Furthermore, using the EMS_EP, higher improvement in the results was seen in incomplete melting conditions (tests 2).

Qualitatively, the effect of the algorithm accounting for the hysteresis effects is identifiable in Figure 7. There, it is possible to see that by using EP_EMS, the obtained numerical solution from the algorithm are closer to experimental data, both during the heating and cooling process, if compared to the other simulation methods that do not account hysteresis, as expected this is particularly important for the salt hydrate PCM-a. When the comparison is carried out with the numerical simulation that made use of the averaged enthalpy vs. temperature curve (EP_AVG), the difference between the simulation with the proposed method and the conventional approach is less evident, yet still present.

The simulation results of EP_NRGSIM model compared with experimental and EP_EMS simulation results can be seen in Appendix B. While this approach obtained closer numerical solution while cooling, it obtained significant error in the heating phase. After trying both available methods of PCM hysteresis modelling strategies, none of these give acceptable results when compared to experimental data. Whereas in usability terms, the major flaw in using this version is that the while official version of EP uses Enthalpy-Temperature curve data to model PCM, this EP_NRGSIM model uses polynomial fitting curves to describe the properties of PCM. This poses a challenge to modellers as by using polynomial fitting curves method, they might not be able to represent Enthalpy-Temperature curve accurately which may further lead to inaccuracies in the result. Furthermore, the compiled version of this tool is not available and hence it requires extra work before it can be actually used.

Results on PCM-a demonstrate that both Energy Plus and WUFI can be used for PCM characterised by low hysteresis (PCM-a). Nevertheless, all the models are not totally accurate when were applied to simulate incomplete phase transition of the PCMs (Test 2).

4. Local Sensitivity Analysis on the proposed model for EnergyPlus using EMS

To highlight the parameters and inputs that are particularly influential (sensitive) to the final error difference between the simulation results and experimental results, a local sensitivity analysis was applied on the EP simulation model which uses the EMS algorithm discussed in the above sections (EP_EMS). All the properties of the materials used in the sandwich specimen were used as the parameters for this sensitivity analysis.

4.1. Methodology

In the following sensitivity analysis, 14 parameters were chosen which represented the thermo-physical properties of the materials used in the specimens which were then applied a perturbation of ± 5% to their nominal value. The output of each simulation was $|\Delta|$ (degree) which is an average of the difference between the temperature of each time step of experimental and simulated values. The influence of each parameter is calculated from Equation (4) that represents the dimensionless "Influence Coefficient" (*IC*) [45], which is the percentage of changing in the output due to a percentage of perturbation in the input.

$$IC = \frac{\Delta\mathrm{OP} \div \Delta\mathrm{OP}_{BC}}{\Delta\mathrm{IP} \div \Delta\mathrm{IP}_{BC}} \tag{4}$$

Where ΔOP and ΔIP represent the changes in output and input, respectively; and $\Delta\mathrm{OP}_{\mathrm{BC}}$ and $\Delta\mathrm{IP}_{\mathrm{BC}}$ are the output and the input base case values.

4.2. Results

The complete bar diagram of the "Influence Coefficient" for 14 analysed parameters is reported in Figure 8. From the results, it is possible to see that the most influential parameters on the algorithm are the density of PCM and, surprisingly, the thickness and conductivity of gypsum board. These results can partially justify the difference between predicted and measured temperatures since the measurement uncertainty for each influential parameter are not well known, especially for data retrieved from literature (measurement uncertainty is not provided). This highlights that the measuring uncertainty of the highest sensitive parameters must be carefully evaluated when experimental data is used to validate the code.

5. Discussion

In the presented study, the reliability of two different building simulation software (Energy Plus and WUFI), and different simulation approaches were tested for the simulations of different type of bulk PCMs under different sinusoidal temperature conditions (complete and incomplete phase transition). Results reveal that both software packages are adequate to simulate PCM characterised by low hysteresis during their complete phase transitions indicating not a significant mismatch in the temperature profile (synchronisation). On the contrary, high inaccuracies occur when they are used to simulate incomplete phase transitions and PCM characterised by significant hysteresis. Such a disagreement is seen regardless of the modelling approach adopter (e.g. EP_EMS or EP_NRGSIM).

This newly developed approach for the modelling of thermal hysteresis features in PCM has been tested to prove that it is a robust and reliable algorithm that can be executed in *EnergyPlus*™ without increasing the computational load. Numerical results obtained through this method are coherent with the physical phenomena, and it has been shown that other, simplified simulation approaches that neglect hysteresis can lead to significant over-/under-estimation of the temperature evolution inside a wall that contains a PCM layer. However, it is important to stress that the proposed approach does not lead to significant improvements compared to alternative methods (such as EP_NRGSIM), even if the input data required by the proposed method are more user-friendly than those required by alternative approaches (i.e. the EP_EMS methods directly implements the enthalpy-temperature curves characterised through DSC analyses). For this sake, an IDF file for *EnergyPlus*™ Version 8.4 is attached to this paper as Supplementary material, and it can be used to replicate the simulations presented in Section 3. By changing the values of the enthalpy vs. temperature curves in the objects “*MaterialProperty:PhaseChange*” researchers can test different types of PCMs.

This paper opens up the question whether simulation tools replicating PCM behaviour are accurate enough, in case of the incomplete melting of the PCM layer. In particular, it is important to stress that the incomplete melting of PCM is often the desired condition for optimal operation, as once the PCM has completed the phase change, its ability to store thermal energy is limited.

One observation that can be made is that simulation of PCM’s behaviour is based (directly or indirectly) on the enthalpy-temperature curve, which describes the relationship between thermal energy stored in the bulk material and its increase in temperature. However, such a characteristic is measured through dedicated thermophysical analysis on small quantities of the bulk material, usually in the order of mg. Such an analysis characterises the material under very particular conditions, which are very far from those when the material is applied in real building structures. In such a situations, the thermophysical behaviour of the material might be more complex than that of the small sample that is characterised (e.g. in terms of penetration of the heat wave). Furthermore, the conventional characterisation of the enthalpy-temperature curve of a PCM is always carried out with a complete cycle of melting/resolidification process. Very seldom, if almost never, the incomplete melting/resolidification process is investigated, and how an incomplete phase change process impacts on the following phase change process is not investigate.

The main take-home lesson that this research activity wants to share is therefore the need to improve the characterisation methods for PCM that are planned to be used in building construction. In this context, the reference is not only to the problem, that has been well-known for many decades (for example [46]), that the of the speed of the heating/cooling rate in DSC analysis and its influence on the resulting enthalpy-temperature curve, but rather if DSC analyses alone are sufficient input data to the simulation tools. These analysis do not consider complex mechanisms in heat transfers through full-scale PCM layer, which instead are seen under real applications. Phase changes are usually characterised by non-negligible kinetic dependency and non-equilibrium characteristics that may become even more evident when complex heat transfer phenomena comes into place (something that is relatively missing in DSC analyses).

An example of the different results that can be obtained in characterising the enthalpy-temperature curve between diverse standardised and not standardised procedures (including DSC) can be seen in a recent investigation on of granular PCM composites [47], showing how it is hard to define a single valid methodology in characterising the phase change behaviour.

In this paper, dynamic measurements carried out with a DHFMA have been carried out to provide experimental data for model validation. In a previous research activity [48] carried out with the same device, attempts have been made to derive enthalpy-temperature curve through inverse modelling. The results from this activity presented in this paper highlight how further investigation on the determination of the material's properties when adopted in full-scale structures are still very necessary, in order to improve the reliability of simulations.

6. Conclusions

The lack of suitable models to account the effect of thermal hysteresis of PCMs is nowadays a major shortcoming of BPS tools, well acknowledged in the scientific literature. In this paper, a new modelling approach that includes the hysteresis phenomenon that can be applied to different versions of *EnergyPlus*™ is presented.

The novel algorithm makes use of the EMS group in *EnergyPlus*™ and allows the implementation of two "enthalpy vs. temperature" curves to correctly model both the melting and the congealing process of PCMs. The full set of code scripts for the EMS group is given in the paper so that it can be easily adopted by researchers and professionals that make use of this software for building performance simulation. Thought the modelling strategy presented in this paper is functioning for *EnergyPlus*™, the approach behind it can be replicated for other BPS tools using their own features and programming languages. The solution presented in this paper just requires the code available in Appendix A to be copied and pasted, with some minor changes according to the parameters of IDF (Input Data File, the compiled file that contains data to be processed by the EnergyPlus™ engine for simulation) where the PCM component is to be modelled.

The validation of the code against experimental data demonstrated the reliability of the modelling approach and showed coherence between the achieved numerical results and the expected behaviour of the code. Computational load due to the use of EMS is not increased compared to conventional modelling strategy in *EnergyPlus*™ that does not account for hysteresis effects. The presented algorithm is therefore robust, reliable, and computationally efficient (at least compared to other available codes). However, it is important to highlight that the numerical results obtained with the proposed model are just significantly better than those with more conventional models, and that in general, in case of incomplete melting/resolidification process of the PCM, the agreement between simulation and measurement is quite questionable. .

This paper thus demonstrates how more or less advanced simulation tools can replicate PCM's behaviour up to a certain extent. The hypothesis developed at the end of this activity is that the mismatch between experimental and numerical data might be due to the procedure used to characterise the bulk PCM. In this respect, this research activity shows the need to invest in more research activities leading to more significant input data for building performance simulation tools.

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Appendix A: EMS objects and program

The temperature of ***Node N*** is acquired by EMS using the object “Sensor”, compiled according to the strings here below, where the field “*Output:Variable*” is “*CondFD Surface Temperature Node N*” and the “*Index key name*” is the name of the surface that is made of the construction containing the PCM layer (for the sake of explanation, this surface is called ***Wall_PCM***). This sensor is named, in these sections, ***Node_PCM***, and will be recalled later in the EMS program. Using the nomenclature describe here above, the following lines can be entered in IDF file to create this sensor.

```
EnergyManagementSystem: Sensor,
Node_PCM,         ! − Name
Wall_PCM,         ! − Output: Variable or Output: Meter Index Key Name
CondFD Surface Temperature Node N;  ! − Output: Variable or Output: Meter Name
```

The object “Actuator” is then used, in conjunction with the input object called “*EnergyManagementSystem:ConstructionIndexVariable*” (see below) to link different constructions and allow the swap between the construction with the heating and that with the cooling enthalpy vs. temperature curve. In this object, the “Actuated Component Type” field is “*Surface*”, and the “Actuated Component Control Type”, which gives the control type, is “*Construction State*”. The following lines can be entered in IDF file to create this actuator.

```
EnergyManagementSystem: Actuator,
Wall,                 ! − Name
Wall_PCM,         ! − Actuated Component Unique Name
Surface,            ! − Actuated Component Type
Construction State;     ! − Actuated Component Control Type
```

Few variables need to be defined in the EMS to allow a smooth execution of the program to be carried out.

First, using the object “*ConstructionIndexVariable*”, two variables, named ***H_Wall*** and ***C_Wall***, in this example, need to be defined, identifying the construction with the PCM in heating mode and in cooling mode, respectively (identified by the names ***Plate Wall_H*** and ***Plate Wall_C***). The following lines can be entered in IDF file to create these variables.

EnergyManagementSystem: *ConstructionIndexVariable*,
H_Wall,   ! − *Name*
Plate Wall_H;   ! − *Construction Object Name*

EnergyManagementSystem: *ConstructionIndexVariable*,
C_Wall,   ! − *Name*
Plate Wall_C;   ! − *Construction Object Name*

Second, using the object "*GlobalVariable*", to additional variables, named ***Avg_Temp*** and ***Current_Wall*** are created and will be called in the EMS program for checking the state of the heat storage process (heating vs. cooling). The following lines can be entered in IDF file to create this variable.

EnergyManagementSystem: *GlobalVariable*,
Avg_Temp,   ! − *Erl Variable* 1 *Name*
Current_Wall;   ! − *Erl Variable* 2 *Name*

Third, a trend variable (named ***PCM_Temp_Trend*** in this example) needs to be created by using the object "*EnergyManagementSystem:TrendVariable*". A trend variable is a log of historical values for Erl variables. A trend log is an array that goes back in time, and for this example, the trend variable includes the values of the previous 20 time-steps. The aim of this trend variable, used in combination with the "*@TrendAverage*" function in the EMS program, is to calculate, at the time step *t-1*, the value of the temperature of the PCM node (**Node_PCM**) as the average value of a given number of previous time steps (the given number is called directly in the EMS program and will be described later). This strategy is adopted to obtain a smoother history of temperature values for the PCM node (node ***N***), since when close to a change between the heating and cooling process (and vice-versa), the numerical solutions of the heat transfer equation can lead to a temperature value that is oscillating around a stable value, for several time-steps. This averaged temperature value will be then used, in the main EMS program, to assess whether the PCM layer is melting or solidifying. The following lines can be entered in IDF file to create the trend variable.

```
EnergyManagementSystem:TrendVariable,
PCM_Temp_Trend,            !- Name
Node_PCM,    !- EMS Variable Name
 20;                 !- Number of Timesteps to be Logged
```

Fourth, an optional output variable (herewith named ***Current_Wall_Status***) can be created to record the current wall construction status and return this characteristic at every time-step for control purpose. Through this variable, it is possible to check that the program is actually swapping from one wall construction to another (and this means from the enthalpy vs. temperature curve for the heating process to the one for the cooling process). The following lines can be entered in IDF file to create the output variable.

```
EnergyManagementSystem:OutputVariable,
Current_Wall_Status,       !- Name
Current_Wall,              !- EMS Variable Name
Averaged,                  !- Type of Data in Variable
ZoneTimestep;              !- Update Frequency
```

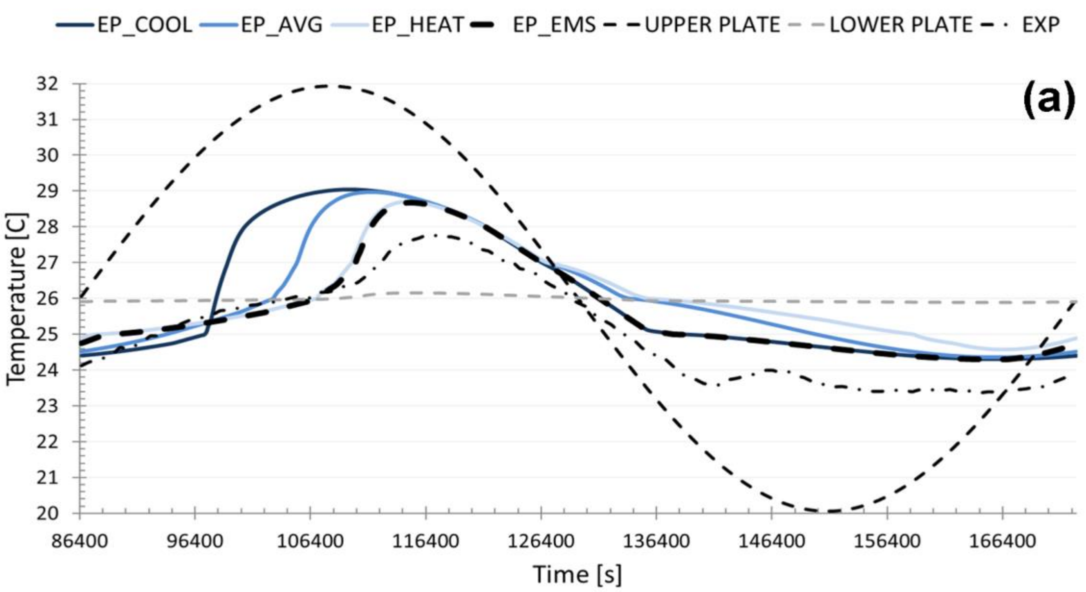
After variables initializations, the focus can be moved to the EMS program (herewith called **EMS PCM Code**) which is first introduced through the object "*ProgramCallingManager*". Through this object, the execution of the program is set to occur after EMS calling point called "*BeginTimestepBeforePredictor*". This point occurs close to the beginning of each time-step, but before the predictor executes. The term "*Predictor*" refers to the step in *EnergyPlus*™ simulation when all the calculations happen for Zone HVAC. The following lines can be entered in IDF file to define the program calling manager object.

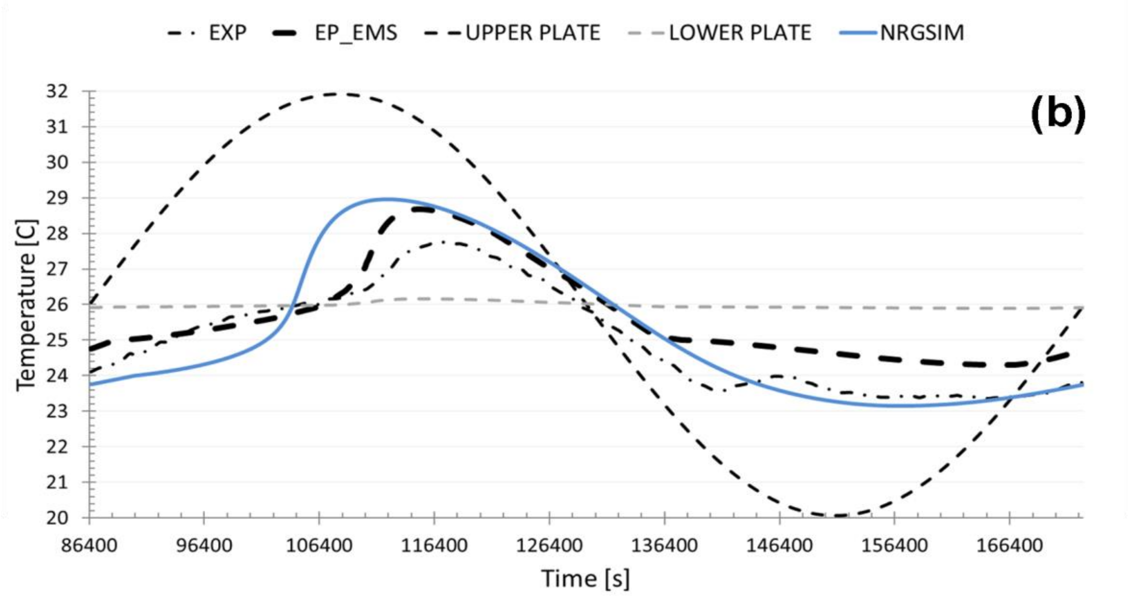
```
EnergyManagementSystem:ProgramCallingManager,
Hysteresis,                          !- Name
BeginTimestepBeforePredictor,        !- EnergyPlus Model Calling Point
EMS_PCM_Code;                         !- Program Name 1
```

Finally, the actual EMS program containing the conditional expressions to select the right enthalpy curve (through the selection of the correspondent "*Construction*") is defined. It is possible to see that the program makes use of the function "*@TrendAverage*", as previously described, to average the value of the temperature of the PCM node (Node N), based on the information stored in the trend variable ***PCM_Temp_Trend***. The "*@TrendAverage*" function is called, in this example, with an index of *12*, meaning that it will return the running average of values of the temperature in the previous last 12 time-steps. This number is arbitrary and depends on several aspects (e.g. time-step of the simulation, heat transfer conditions), so every modeller is free to choose a value that fits best with its specific simulation. The following lines can be entered in IDF file to implement the EMS program.

```
EnergyManagementSystem: Program,
EMS_PCM_Code,                                   ! −  Name
SET Avg_Temp  =  @TrendAverage PCM_Temp_Trend 12,        ! −  Program Line 1
IF Node_PCM  >  Avg_Temp,              ! −  A5
SET Wall  =  H_Wall,                   ! −  A6
ELSEIF Node_PCM  <  Avg_Temp,     ! −  A7
SET Wall  =  C_Wall,                   ! −  A8
ENDIF,                                   ! −  A9
SET Current_Wall  =  Wall;             ! −  A10
```

Appendix B: Inter-software comparison





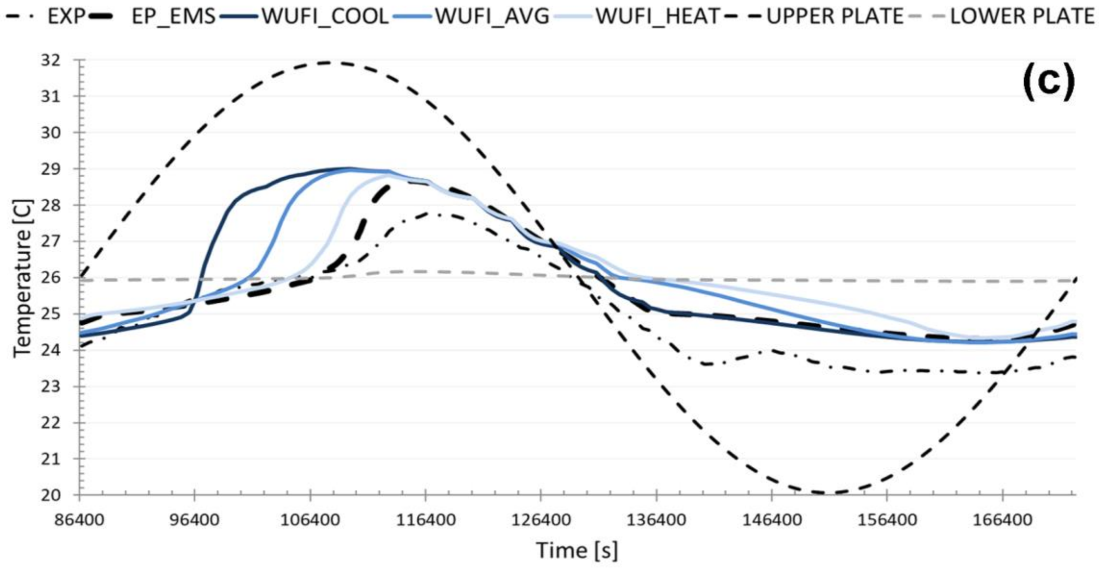


Figure B.1: *Temperature evolution of* ***SP26E*** *for Node* T_{PCM} *under a stabilized periodic cycle with sinusoidal amplitude of ±6.*

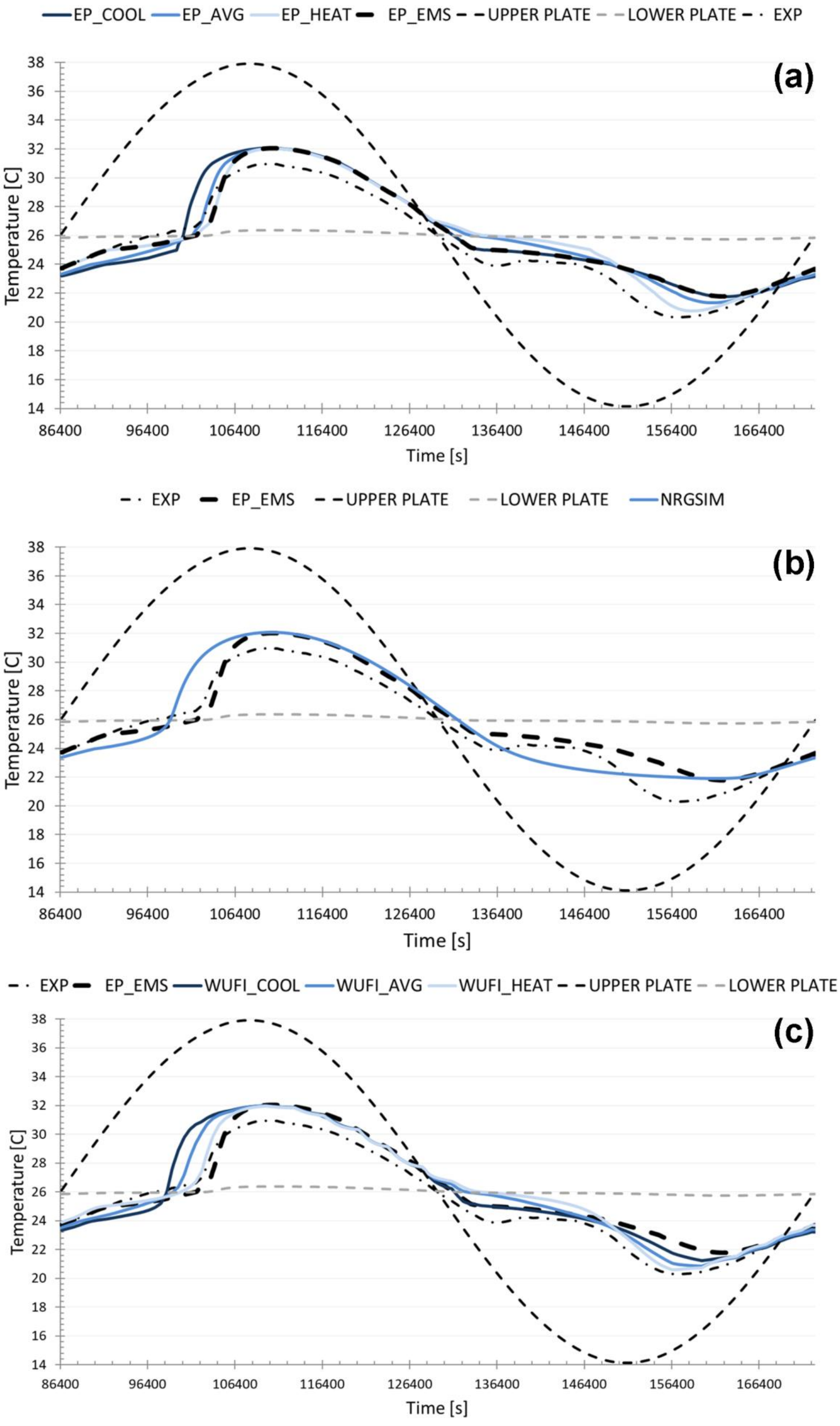
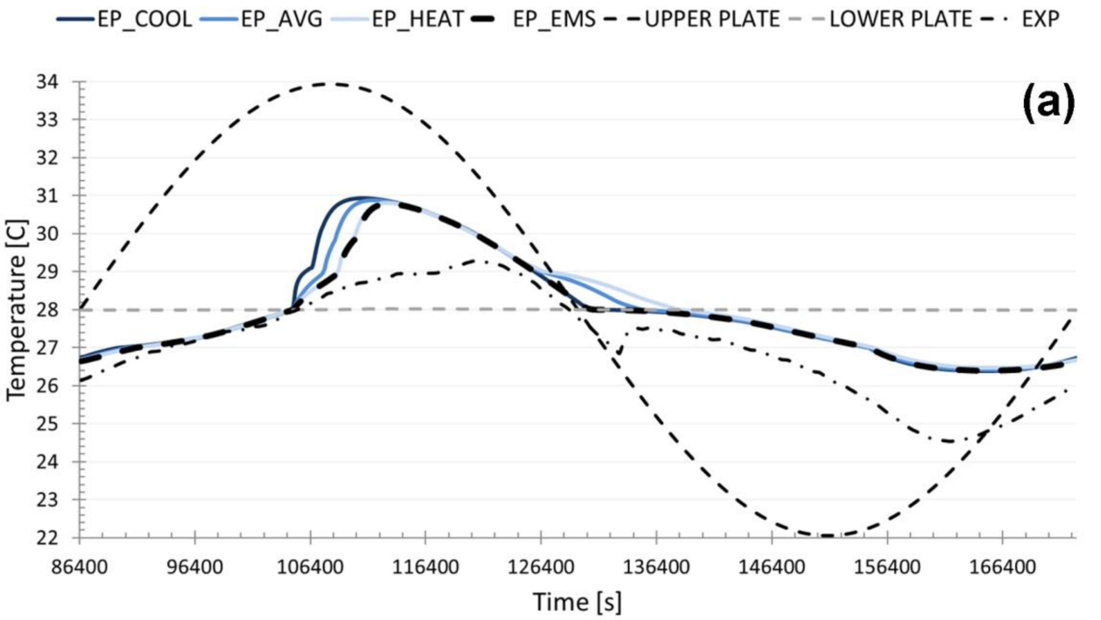
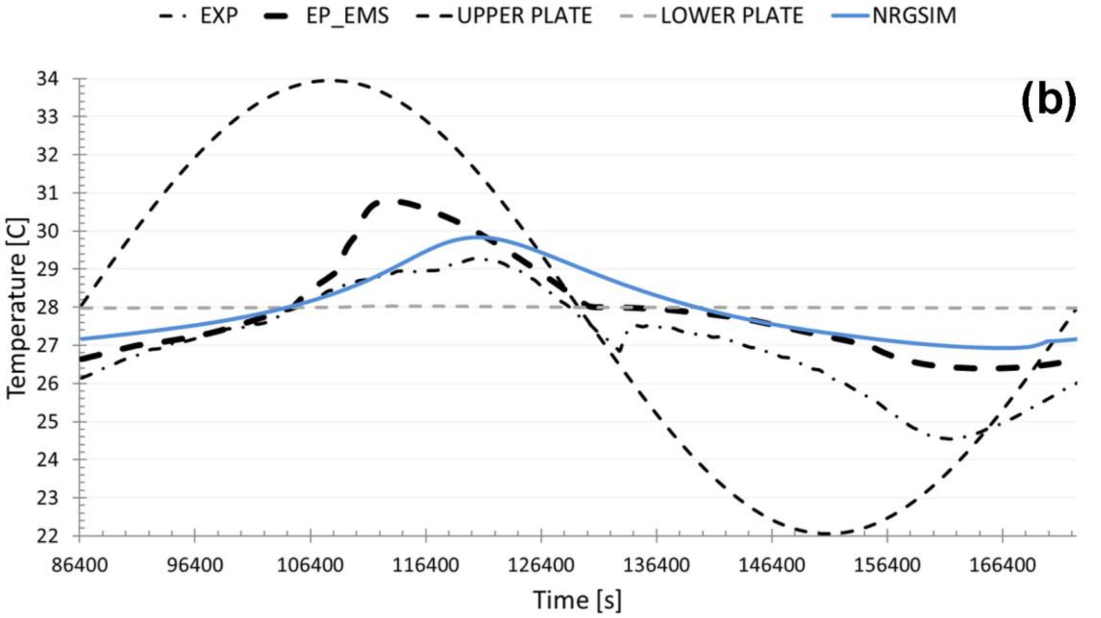

EP_COOL
EP_AVG
EP_HEAT
EP_EMS
UPPER PLATE
LOWER PLATE
EXP
(a)
Temperature [C]
Time [s]
EXP
EP_EMS
UPPER PLATE
LOWER PLATE
NRGSIM
(b)
Temperature [C]
Time [s]
EXP
EP_EMS
WUFI_COOL
WUFI_AVG
WUFI_HEAT
UPPER PLATE
LOWER PLATE
(c)
Temperature [C]
Time [s]
38
36
34
32
30
28
26
24
22
20
18
16
14
86400
96400
106400
116400
126400
136400
146400
156400
166400

Figure B.2: *Temperature evolution of* ***SP26E*** *for Node* T_{PCM} *under a stabilized periodic cycle with sinusoidal amplitude of ±12.*


EP_COOL
EP_AVG
EP_HEAT
EP_EMS
UPPER PLATE
LOWER PLATE
EXP
(a)
Temperature [C]
34
33
32
31
30
29
28
27
26
25
24
23
22
86400
96400
106400
116400
126400
136400
146400
156400
166400
Time [s]


EXP
EP_EMS
UPPER PLATE
LOWER PLATE
NRGSIM
(b)
Temperature [C]
34
33
32
31
30
29
28
27
26
25
24
23
22
86400
96400
106400
116400
126400
136400
146400
156400
166400
Time [s]

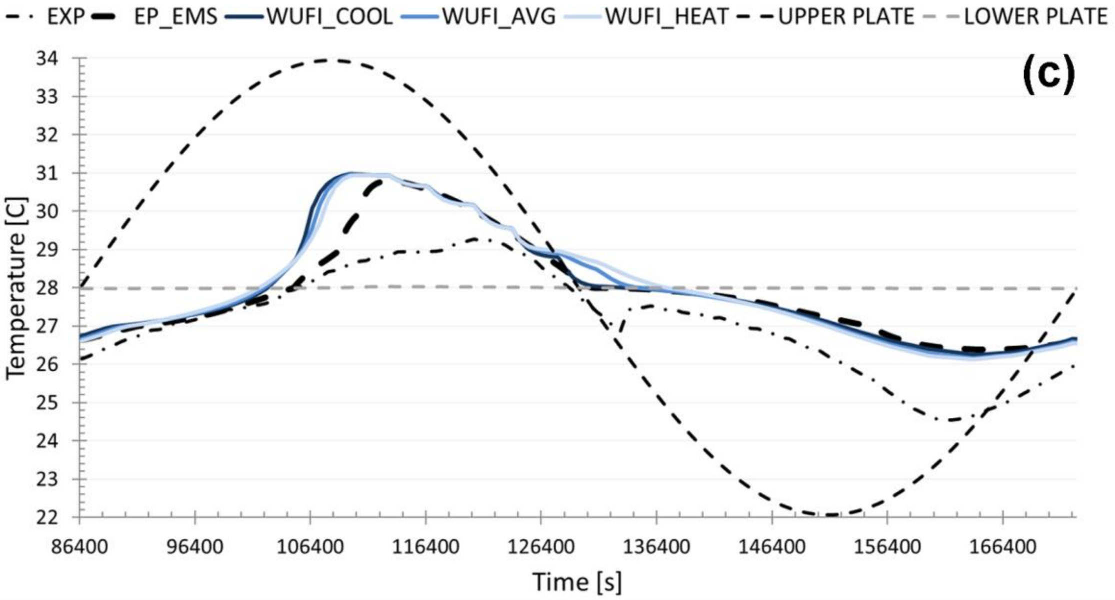

EXP
EP_EMS
WUFI_COOL
WUFI_AVG
WUFI_HEAT
UPPER PLATE
LOWER PLATE
(c)
Temperature [C]
34
33
32
31
30
29
28
27
26
25
24
23
22
86400
96400
106400
116400
126400
136400
146400
156400
166400
Time [s]

Figure B.3: *Temperature evolution of* ***RT28HC*** *for Node* T_{PCM} *under a stabilized periodic cycle with sinusoidal amplitude of ±6.*

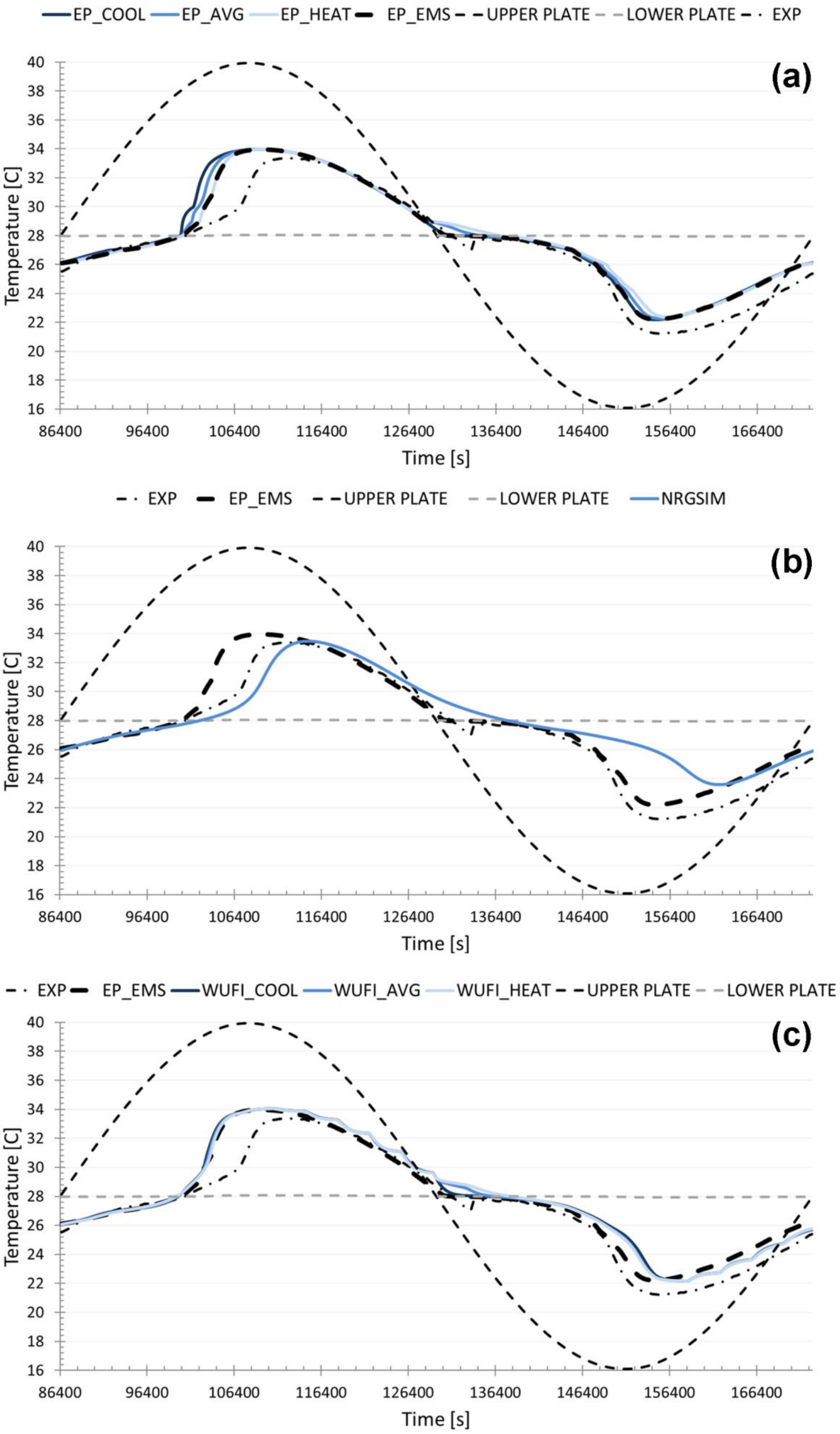

EP_COOL
EP_AVG
EP_HEAT
EP_EMS
UPPER PLATE
LOWER PLATE
EXP
(a)
Temperature [C]
40
38
36
34
32
30
28
26
24
22
20
18
16
86400
96400
106400
116400
126400
136400
146400
156400
166400
Time [s]
EXP
EP_EMS
UPPER PLATE
LOWER PLATE
NRGSIM
(b)
Temperature [C]
40
38
36
34
32
30
28
26
24
22
20
18
16
86400
96400
106400
116400
126400
136400
146400
156400
166400
Time [s]
EXP
EP_EMS
WUFI_COOL
WUFI_AVG
WUFI_HEAT
UPPER PLATE
LOWER PLATE
(c)
Temperature [C]
40
38
36
34
32
30
28
26
24
22
20
18
16
86400
96400
106400
116400
126400
136400
146400
156400
166400
Time [s]

Figure B.4: *Temperature evolution of* ***RT28HC*** *for Node* T_{PCM} *under a stabilized periodic cycle with sinusoidal amplitude of ±12.*

Figure

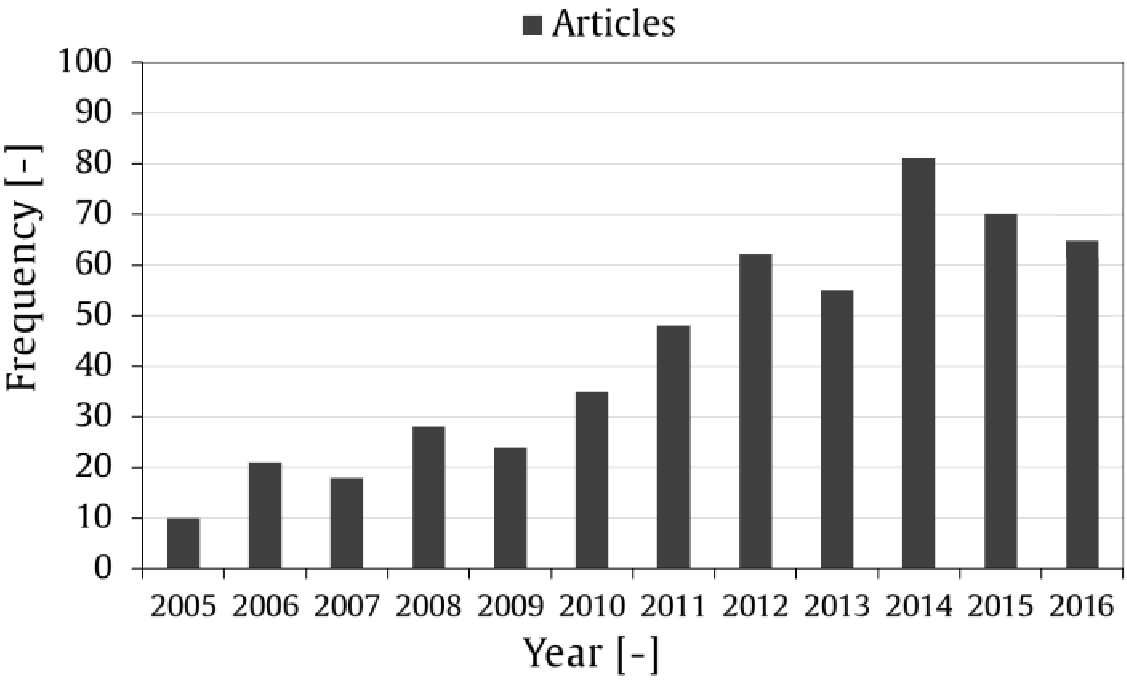


Figure 1. *Number of articles listed in the bibliographic database SCOPUS, which had Phase Change Materials, Simulation, and Building as a keyword or word used in their abstracts, is reported, for the period 2005-2016.*

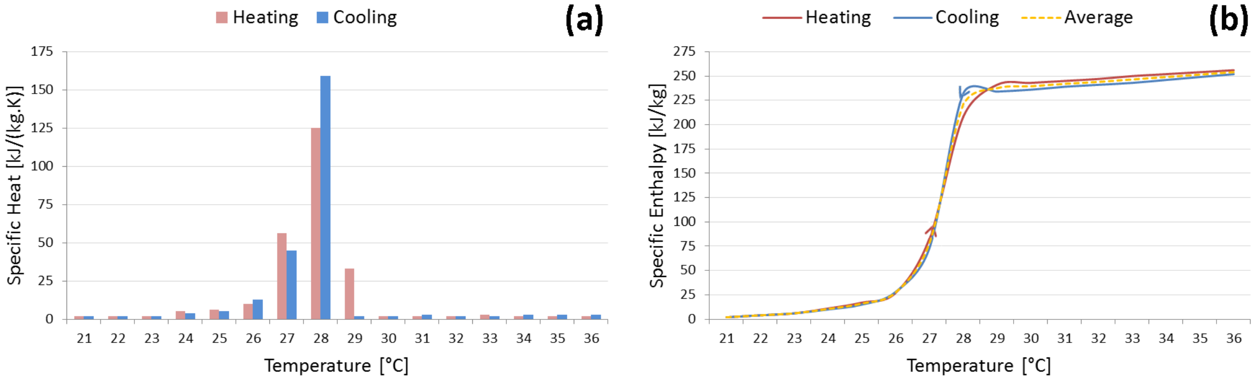


Figure 2. *Specific heat vs. temperature (a) and enthalpy vs. temperature (b) for heating and cooling process of the PCM-a (paraffin wax)*

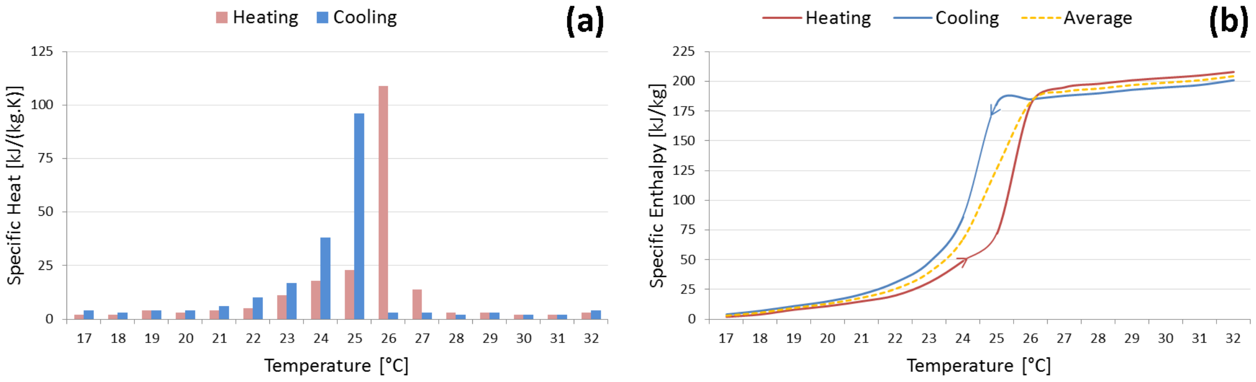


Figure 3. *Specific heat vs. temperature (a) and enthalpy vs. temperature (b) for heating and cooling process of the PCM-b (salt hydrate)*

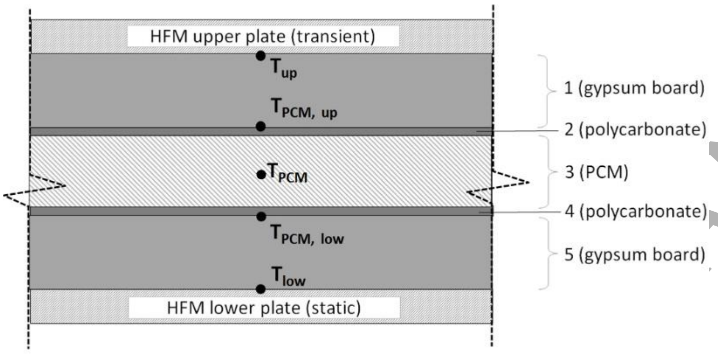


Figure 4. *Layout of the measured specimen*

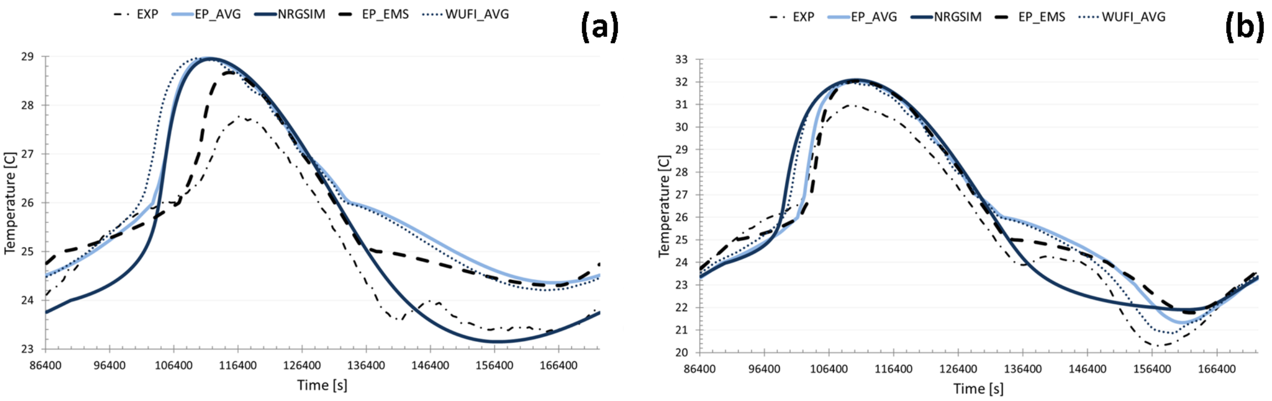


Figure 5. *Temperature evolution of SP26E for Node T_{PCM} under a stabilized periodic cycle. (a) Comparison between experimental data and simulations with sinusoidal amplitude of ±6(20°C -32°C); (b) Comparison between experimental data and simulations with sinusoidal amplitude of ±12(14°C -38°C).*

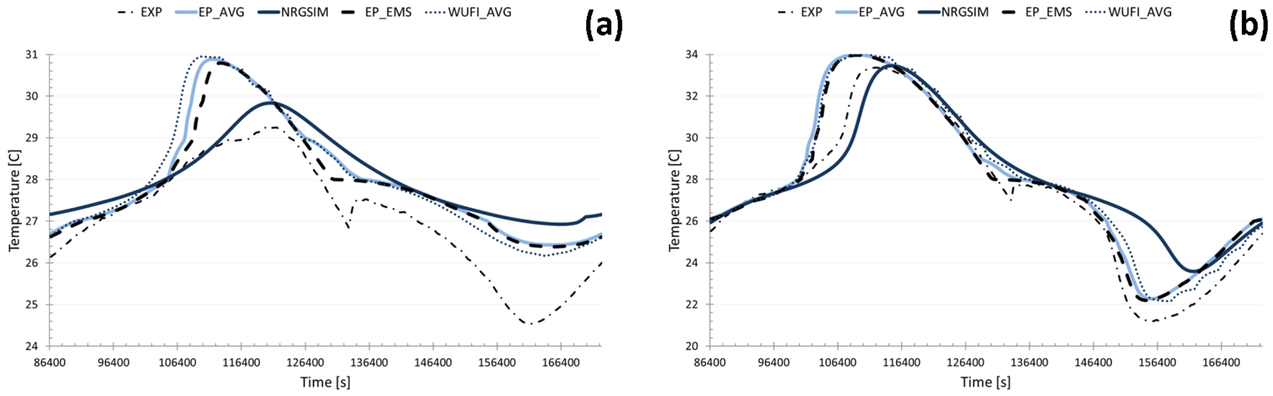


Figure 6. *Temperature evolution of RT28HC under a stabilized periodic cycle. (a) Comparison between experimental data and simulations with sinusoidal amplitude of ±6(22°C -34°C); (b) Comparison between experimental data and simulations with sinusoidal amplitude of ±12(16°C -40°C)*

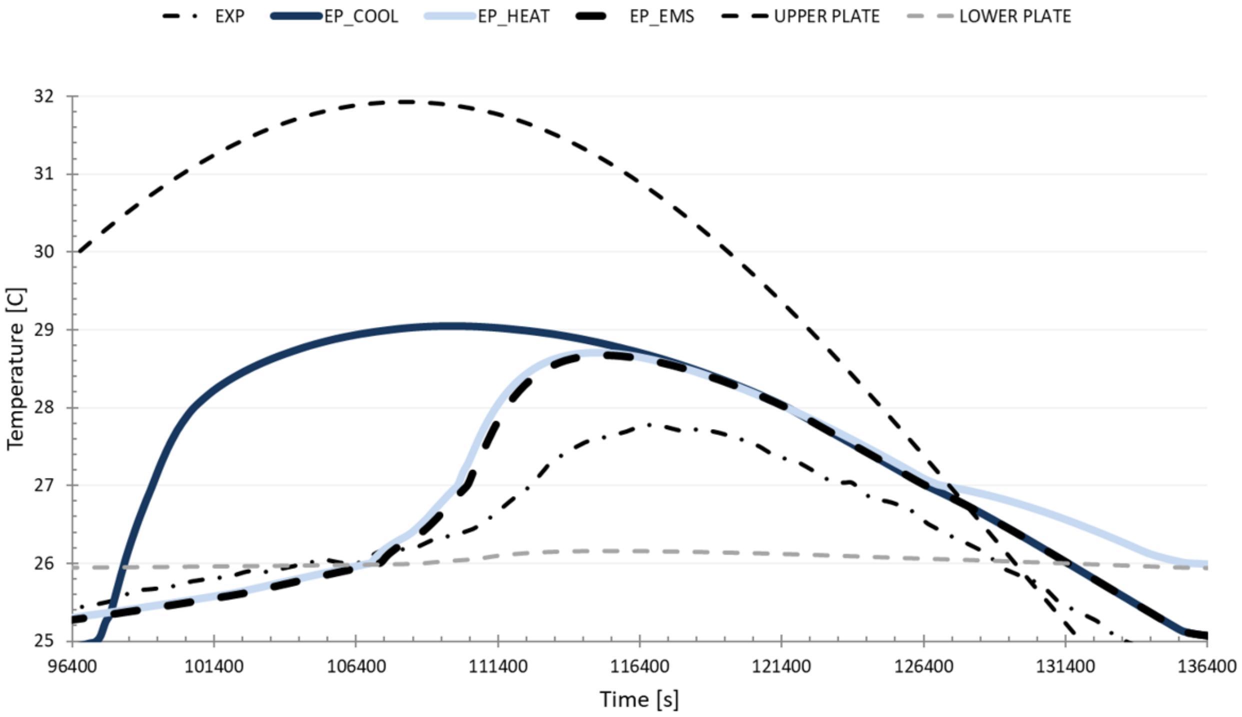


Figure 7. *Temperature evolution of SP26E for Node* T_{PCM} *under a stabilized periodic cycle. with a sinusoidal amplitude of ±6.*

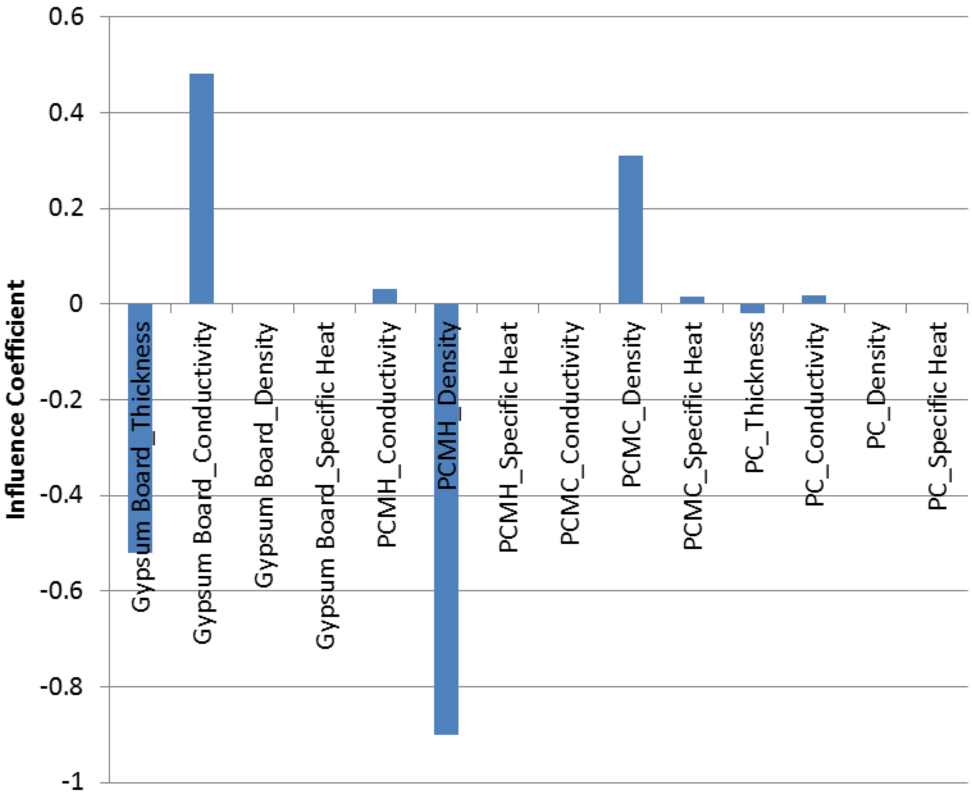


Figure 8. *Influence coefficient of selected 14 parameters.*

Table 1. *Thermophysical properties of the two PCMs.*

Name	**Material Class**	**Melting range** [°C]	**Congealing range** [°C]	**Specific heat capacity** [kJ/kg·K]	**Density (solid)** [kg/l]	**Density (liquid)** [kg/l]	**Conductivity** [W/(m·K)]
PCM-a	Paraffin Wax	27-29	29-27	2.0	0.88	0.77	0.2 (both phases)
PCM-b	Salt Hydrate	25-27	25-24	2.0	1.50	1.40	0.6 (both phases)

Table 2*. Physical properties of each material that constitute the specimen. * (Average value between solid and liquid phase).*

`	Name	d [mm]	ρ [kg/m^3]	c [J/kg/K]	λ [W/mK]
1	Gypsum board	12.5	720	1090	0.19
2	Poly-carbonate	0.5	1200	1200	0.20
3	PCM-a	9.0	825*	2000	0.20
	PCM-b		1450*	2000	0.6
4	Poly-carbonate	0.5	1200	1200	0.20
5	Gypsum board	12.5	720	1090	0.19

Table 3. Test conditions

Specimen	Test condition	Upper plate temperature [°C]	Amplitude [°C]	Lower plate temperature [°C]
PCM-a	Test 1	16 - 40	±12	28
	Test 2	22 - 34	±6	28
PCM-b	Test 1	14 - 28	±12	26
	Test 2	20 - 32	±6	26

Table 4. Key features of the different simulation approaches analysed in this paper.

Short name	Main Simulation Environment	Hysteresis effect simulation	Enthalpy-Temperature curve used	Notes
EP_COOL	EnergyPlus 8.4	No	Cooling curve	
EP_HEAT	EnergyPlus 8.4	No	Heating curve	
EP_AVG	EnergyPlus 8.4	No	Average between cooling and hearing curve	
EP_NRGSIM	EnergyPlus 8.9	Yes	Polynomial fitting	Module integrated in beta version of

			curve based on heating and cooling curves	EnergyPlus 8.9 Experimental data from heating and cooling curves require processing before use in the BPS, which uses polynomial fitting curve
EP_EMS	EnergyPlus 8.4	Yes	Both heating and cooling curve	Suitable for any release of EnergyPlus with EMS
WUFI_COOL	Wufi Pro 6.1	No	Cooling curve	
WUFI_HEAT	Wufi Pro 6.1	No	Heating curve	
WUFI_AVG	Wufi Pro 6.1	No	Average between cooling and hearing curve	

Table 5. Different error indices for different simulation runs on EnergyPlus for all PCMs.

Method	PCM	PRMSE [%]	RMSE [°C]	|Δ| [°C]
EMS	RT28_6	3.7%	0.99	0.80
	RT28_12	4.0%	1.05	0.69
	SP26_6	3.2%	0.78	0.70
	SP26_12	4.3%	0.99	0.82
AVG	RT28_6	4.1%	1.09	0.90
	RT28_12	4.5%	1.20	0.80
	SP26_6	4.8%	1.20	1.01
	SP26_12	4.4%	1.07	0.96
COOL	RT28_6	4.1%	1.10	0.90
	RT28_12	4.7%	1.28	0.81
	SP26_6	5.0%	1.27	1.04
	SP26_12	4.9%	1.20	1.05
HEAT	RT28_6	4.1%	1.08	0.90

	RT28_12	11.1%	2.59	1.98
	SP26_6	5.0%	1.20	1.03
	SP26_12	4.0%	1.00	0.85

Table 6. Different error indices for different simulation runs on WUFI for all PCMs.

Method	PCM	PRMSE [%]	RMSE [°C]	|Δ| [°C]
AVG	RT28_6	4.0%	1.08	0.91
	RT28_12	4.4%	1.15	0.80
	SP26_6	4.8%	1.20	0.99
	SP26_12	3.8%	0.99	0.83
COOL	RT28_6	4.1%	1.10	0.91
	RT28_12	4.5%	1.19	0.80
	SP26_6	5.0%	1.27	1.03
	SP26_12	4.6%	1.17	0.93
HEAT	RT28_6	3.9%	1.06	0.91
	RT28_12	4.3%	1.14	0.81
	SP26_6	4.8%	1.18	1.01
	SP26_12	3.5%	0.89	0.75

Table 7. Different error indices for simulation runs on

EP_NRGSIM version of EP for all PCMs.

Method	PCM	PRMSE [%]	RMSE [°C]	|Δ| [°C]
NRGSIM	RT28_6	4.4%	1.13	0.92
	RT28_12	7.1%	1.60	1.06
	SP26_6	3.4%	0.89	0.69
	SP26_12	4.6%	1.18	1.03