Modelling Envelope Components Integrating Phase Change Materials (PCMs) with Whole-Building Energy Simulation Tools: A State of the Art

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Abstract
Building envelope systems that integrate Phase Change Materials (PCMs) are solutions aimed at increasing the thermal energy storage potential of the building envelope while keeping its mass reasonably low. Building envelope components with PCMs can be either opaque or transparent and can be based on different types of PCMs and integration methods. In opposition to conventional building components, these elements present thermal and optical properties that are highly non-linear and depend to a great extent on the boundary conditions. Such a characteristic requires the system development and optimisation process during the design phase to be carried out with particular care in order to achieve the desired performance. In this paper, a review of the existing modelling capabilities of different building energy simulation (BES) tools for PCM-based envelope components is reported, and the main challenges associated with the modelling and simulation of these systems through the most popular BES tools (among them, EnergyPlus, IDA-ICE, TRNSYS, IES-VE, and ESP-r) are highlighted. The aim of this paper is to summarise the evidence found in the literature of the latest development in the successful use of BES to replicate the thermal and optical behaviour of opaque and transparent components integrating PCMs, in order to provide the community of professionals with an overview of the tools available and their limitations.

Keywords
Phase Change Materials, building envelope, modelling, simulation

DOI 10.7480/jfde.2018.3.2572

1 INTRODUCTION

A Phase Change Material (PCM) is a material that presents a change of its phase of aggregation within a desired temperature range and it is used to store and release thermal energy. Latent heat presents higher energy densities compared to sensible heat, thus reducing the amount of required material and volume to store the same amount of energy. The PCM absorbs energy by changing its phase from solid to liquid, and releases that energy by changing its phase from liquid to solid. The use of PCM in building facades aims at reducing the indoor temperature fluctuations, delaying the air temperature peaks, and blocking the incoming radiation when used in transparent components. As a result, thermal comfort is increased, and/or energy consumption is reduced.

1.1 PCM IN OPAQUE COMPONENTS

Different materials and systems can be used to increase the thermal inertia in opaque building envelopes. When related to PCM, the main parameters to consider are as follows: material and thermphysical properties (Cabeza, Castell, Barreneche, de Gracia, & Fernández, 2011); charging/discharging method (Navarro et al. 2016a and b); and integration system (Navarro et al. 2016b).

1.2 PCM IN TRANSPARENT COMPONENTS

An important feature of several PCMs (among them, paraffin wax, salt hydrates) is that they are (partially) transparent to solar radiation. This property makes them suitable for integration not only in opaque components, but also in transparent components (Silva, Vicente, & Rodrigues, 2016; Vigna, Bianco, Goia, & Serra, 2018). When coupled with transparent or semi-transparent components, the PCM becomes an integrated layer with the function of both thermal energy storage and solar shading (Goia, Perino, & Serra, 2014).

1.3 PECULIAR THERMOPHYSICAL AND OPTICAL PHENOMENA OF PCMS

Subcooling

Subcooling (also called supercooling) happens when the PCM solidifies at a lower temperature than the solidification temperature (Bony & Citherlet, 2007). This phenomenon modifies the temperature range where the PCM will store/release the latent energy, and can significantly affect the behaviour and functionality of the PCM. In most simulations of PCM, the effect of subcooling is neglected. This is an acceptable assumption for low rates of subcooling, but it is problematic when subcooling reaches the order of magnitude of the driving temperature gradient between the heat transfer fluid and the storage (Günther, Mehling, & Hiebler, 2007).

Hysteresis

Hysteresis happens when the solidification temperature is different from the melting temperature. Subcooling is then a common cause of hysteresis (Bony & Citherlet, 2007; Mehling & Cabeza, 2008). Hysteresis is also commonly neglected in modelling PCM-based components in software tools for

Building Energy Simulation (BES). Both subcooling and hysteresis are considered to be two main sources of inaccuracy in modelling PCM-based components (Kośny, 2015).

Convective heat exchange

Heat transfer by convection with PCM is different from ordinary convection. PCM can transport significant amounts of latent heat in the melting temperature range with comparatively little fluid movement and the density changes that drive convection are much stronger. In most simulations, the effect of natural convection is neglected, and is often included (both experimentally and numerically) (Fantucci, Goia, Perino, & Serra. 2018) in the conductive heat transport – i.e. an equivalent conductivity, which also accounts for the contribution of convection in liquid phase, can be used.

PCM optical properties

When a PCM is integrated in a transparent system, its optical properties become driving elements in the thermophysical behaviour of the system. The optical properties of PCM layers are highly dependent on the state of aggregation of the PCM: in solid/musky state, the PCM layer behaves like a highly diffusive material characterised by high scattering phenomena; in a fully liquid state, the behaviour shifts to that of a conventional transparent component, with dominating direct-to-direct transmission mode (Goia, Zinzi, Carnielo, & Serra, 2015). This dynamic feature leads to more complex information to be experimentally collected in order to describe the performance of these glazing systems.

1.4 AIM OF THE PAPER

The aim of this paper is to compare the available BES models capable of simulating PCM in building envelopes, as well as to summarise the evidence found in the literature of the latest development in the successful use of BES to replicate the thermal and optical behaviour of opaque and transparent components integrating PCMs. The paper targets, in particular, the design professionals' community, as well as graduate students and researchers who are currently approaching the modelling and simulation of PCM-based solutions with a limited background in the field.

It is not an intention of this paper to deepen the reasons for adopting PCMs in building, nor to report evidence of the effect of such implementations. Readers interested in these topics can easily find innumerable literature review papers addressing these questions. On the contrary, this paper focuses on the overview of the BES tools available for modelling and simulating PCM-based envelopes, along with their potentials and limitations.

2 SIMULATION REQUIREMENTS

Phase Change Materials integrated in building components affect its thermal performance. Thus, accurate modelling of PCM must be linked and performed in conjunction with the thermal simulation of buildings.

The dynamics of melting and solidification involve a moving boundary that separates the two different phases with drastically different transport properties. Moreover, the PCM behaviour is highly non-linear when changing phase, since its enthalpy (energy storage capacity) changes dramatically with temperature. Therefore, numerical methods are required, and simplified techniques such as conduction transfer functions (CTF) are unsuitable (Cabeza, 2015).

Some numerical models attempt to approximate the solution to simplified Stefan problems. These so-called 'strong formulations' determine the moving solid-liquid boundary and the temperature profiles, and can be based on either fixed or variable grid methods (Hu & Argyropoulos, 1996). However, these models require too much computational effort for practical applications. Therefore, the so-called "weak formulations" are commonly used to simulate the behaviour of a PCM system and to represent the absorption and release of energy. Some of these formulations are the effective heat capacity method, heat integration method, source-based method, and the enthalpy method. Nowadays, the effective heat capacity method and the enthalpy method are the most extended ones (Voller, 1997).

These methods (both weak and strong formulation) can be, and have been, applied to both PCM in opaque and in transparent/translucent building envelope systems. Though it is reasonable to expect that the performance of these methods is independent from the application in an opaque or in a transparent/translucent system, it must be observed that dedicated investigations that compare them in the setting of a transparent/translucent building system have not yet been carried out. All the above-mentioned approaches have also been adopted for modelling PCM layers in the transparent building envelope.

PCM simulation requires short time steps and fine discretisation of the physical domain in order to avoid numerical errors and/or phase-change jumping. Moreover, special attention must be paid in the determination of the temperature-enthalpy curve. Other physical phenomena can also be included in the models, such as convection heat transfer inside the PCM, subcooling of the PCM, and enthalpy hysteresis.

When integrated in transparent or semi-transparent components exposed to solar radiation, non-linearity is also seen in the optical properties of the PCM layer, which becomes an important variable in the simulation as they determine the interaction with the solar radiation – and ultimately most of solar energy intercepted by the layer. In general, the optical behaviour of these systems can be modelled with different degrees of accuracy, ranging from the solution of the full radiative heat transfer equation (Ishimaru, 1978) with the 3-flux approximation (Weinläder, Beck, & Fricke, 2005) by use of a scaling concept (McKellar & Box, 1981), to modelling strategies that reduce the computational effort in the simulation by always treating the PCM layer as a non-diffuse medium (Goia, Perino, & Haase, 2012; Gowreesunker Stankovic, Tassou, & Kyriacou, 2013; Li et al. 2016, Liu et at. 2016) – but incorporating the complexity of the optical behaviour in the solar coefficient used in the models. In any case, these optical properties must be temperature dependent.

Modelling based on raytracing techniques through the bulk material (and in the adjacent room) are mandatory when detailed daylighting analyses (both in terms of natural light distribution and of visual comfort) are to be carried out. In these cases (Giovannini, Goia, Lo Verso, & Serra, 2017), the full set of optical properties for the solar range (i.e. the absorption coefficient and the scattering coefficient, which together give the extinction coefficient and the phase function, giving the probability that radiation with a certain propagation direction is scattered into a certain solid angle around the direction) is necessary. Alternatively, the use of experimentally characterised (Andersen, Roecker, & Scartezzini, 2005) Bidirectional (Optical) Distribution Functions (in the visible range) can represent a suitable alternative that reduces the simulation complexity by avoiding the modelling of the light ray paths within the bulk of the material.

Further assumptions on the optical properties of the PCM layer, supported by spectrophotometric analysis (Goia et al., 2015), may lead to the consideration of a PCM layer with a thickness greater than a few millimetres as a perfectly diffusive material, when in solid state, and as a fully homogeneous and non-scattering material, when in liquid state. In such an approach, the modelling of the PCM layer can be carried out by considering it as a Lambertian surface (in solid and musky state) and a conventional non-scattering material when in liquid state (Giovannini et al., 2017).

Finally, control strategies can be crucial for the correct operation of PCM systems. For passive systems, no control strategy is directly applied, since the phase change process is controlled by the boundary conditions – and, therefore, possible control strategies must rely on the control of, for example, ventilation rate, or indoor air temperature. On the other hand, for active and hybrid systems, different control strategies can be applied, and their influence in the PCM behaviour is very important (de Gracia et al., 2013; de Gracia, Navarro, Castell, & Cabeza, 2015a; de Gracia, Fernández, Castell, Mateu, & Cabeza, 2015b).

The need to adopt suitable control strategies is particular evident when PCMs are integrated in transparent/translucent building envelope systems, since in these configurations the systems can easily receive more (solar) energy than the latent heat available. The control over the incoming radiation – either through shading systems (Manz, Egolf, Suter, & Goetzberger, 1997), prismatic glass panes (Grynning, Goia, Rognvik, & Time, 2013), or other dynamic layers such as, for example, thermotropic layers (Bianco, Cascone, Goia, Perino, & Serra, 2017a; Bianco, Cascone, Goia, Perino, & Serra, 2017b) – as well as of the discharge of the collected latent heat – for example, through a transparent ventilated cavity in which the PCM layer is installed (Elarga, Goia, Zarrella, Dal Monte, & Benini, 2016) is of great importance.

3 IMPLEMENTATION OF PCMS MODELLING IN BUILDING ENERGY SIMULATION TOOLS

There are many numerical models available, capable of simulating the inclusion of PCM in building envelopes. Those most widely used are in TRNSYS (cf. section 3.1) and EnergyPlus (cf. section 3.2), because they have, for a long time, been integrating direct methods for simulating PCM layers (at least in opaque components).

However, there are also other software tools that have had for a long time (ESP-r, cf. section 3.3), or have just recently added (IDA-ICE, cf. section 3.5), dedicated sub-routines that allow the simulation of PCM layers (again, in opaque components only) to be carried out in a rather straightforward way.

The use of different simulation approaches, not based on dedicated sub-routines, has also been applied in other tools (e.g. IES-VE, cf. section 3.4) to replicate the performance of a PCM layer even if this is not directly modelled as such because of the limitations of the simulation environment.

A crucial aspect is always the attention that must be paid to the physical phenomena considered, and the experimental validation (especially when the simulation strategy includes the use of non-validated, already implemented sub-routines). These kinds of models usually require the Temperature–Enthalpy curve, the thermal conductivity, and the specific heat of the PCM as input data. These models are application oriented and integrated in Building Energy Simulation (BES) software, and are primarily developed for the application of PCMs in opaque building elements.

3.1 OVERVIEW OF MODELS

Most of the models that simulate the PCM behaviour in building envelopes analysed or presented in this paper are implemented in TRNSYS (59%), followed by ESP-r (18%), EnergyPlus (9%), IDA-ICE (9%), and IES-VE (5%) (Fig. 1).

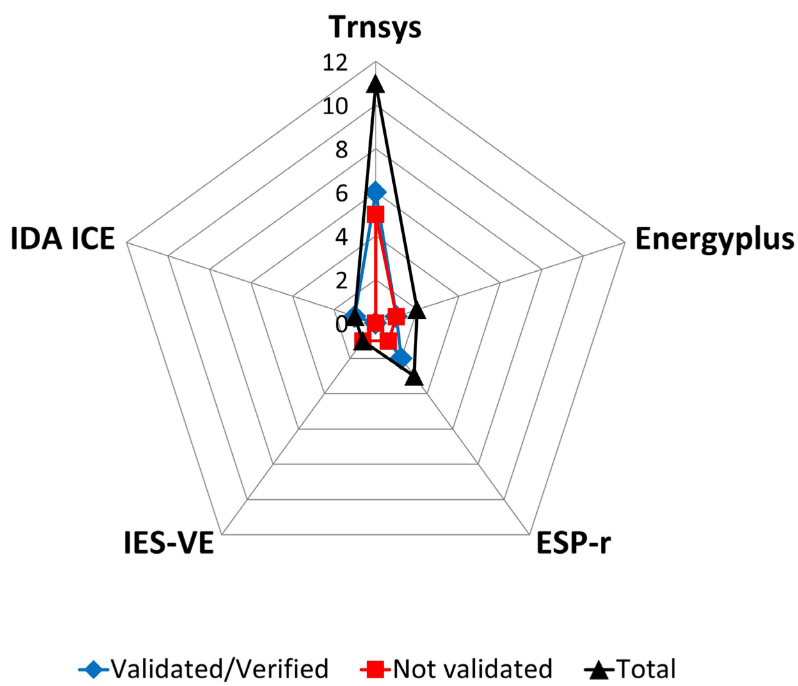

FIG. 1 PCM models implemented in BES software

Most of the analysed models are based on the enthalpy method or the effective heat capacity method (Fig. 2). Regarding the capability to simulate additional physical phenomena, most of the models do not include any additional capability. Six of them are capable of simulating hysteresis; two are capable of simulating subcooling; and none is capable of simulating natural convection inside the PCM (Fig. 2).

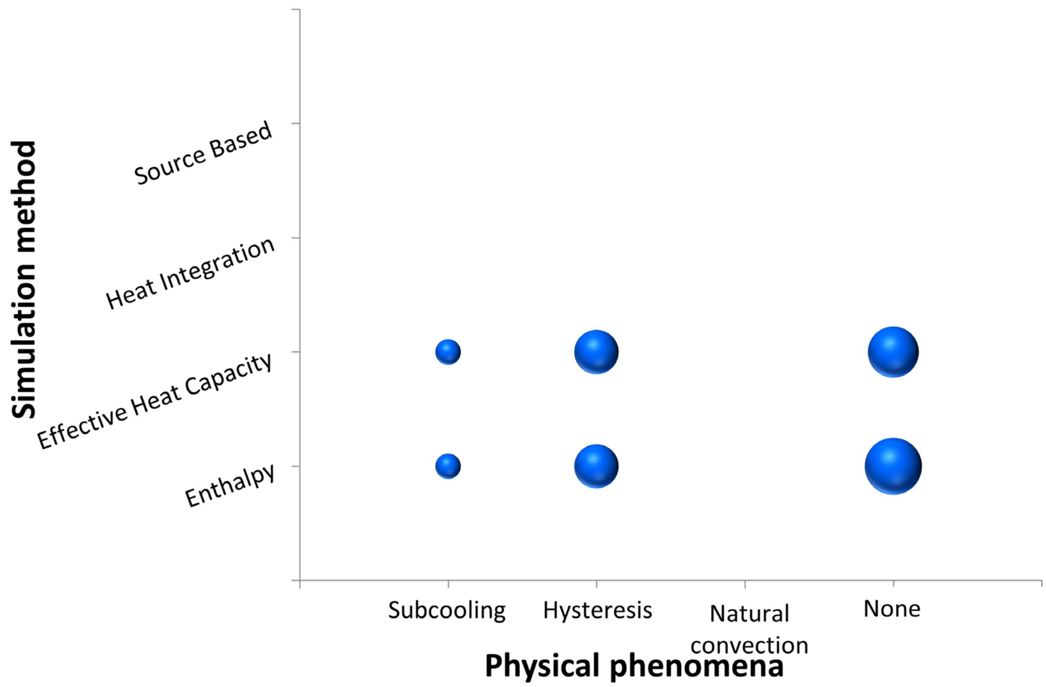

FIG. 2 Simulation method used and physical phenomena considered in PCM models

3.2 TRNSYS

Several PCM modelling efforts have been proposed for TRNSYS in the period 1991-2010 (Ghoneim, Klein, & Duffie, 1991; Stritih & Novak, 1996; Lamberg, Jokisalo, & Sirén, 2000; Jokisalo, Lamberg, & Sirén, 2000; Koschenz & Lehmann 2004; Ibañez, Lázaro, Zalba, & Cabeza, 2005; Ahmad, Bontemps, Sallée, & Quenard, 2006; Schranzhofer, Puschnig, Heinz, & Streicher, 2006; Kuznik, Virgone, & Johannes, 2010; Dentel & Stephan, 2010). Most of these were 1-D models based on finite difference and enthalpy methods. They were compiled in the form of several Types in TRNSYS (Type58, Type 204, Type 232, Type 101, Type 241, and Type 260, Type 399). All were proposed for PCM walls or ceilings and only a few included validations with experimental data. Only two included subcooling (Type 204) or hysteresis effects (Type 399).

In 2014, (Lu, Liu, Huang, & Kong, 2014) developed a new type to simulate PCM in walls. The model is one-dimensional and uses the Finite Volume Method. The apparent specific heat capacity method is used to simulate the PCM behaviour. Hysteresis can also be taken into account; however, convection within the PCM cannot be simulated, nor phase change in microcapsules. Although an experimental validation was performed, significant differences between the numerical and the experimental results were observed.

In 2015, Al-Saadi and Zhai (2015a) used different approaches to model PCM in walls: enthalpy method, heat capacity method, and heat source method, using as solvers the Gauss-Seidel and the TDMA methods and also considering some correction steps. The model is one-dimensional and a fully implicit scheme is used with a spatial discretisation based on the finite volume method. After experimental validation, they concluded that only two schemes out of the eight developed could be considered as potential candidates for integrating into whole building simulation tool: the linearised enthalpy method with the iterative correction scheme and the hybrid correction scheme.

Later, Al-Saadi and Zhai (2015b) validated the model with experimental data at building level, achieving good accuracy.

In 2017, Delcroix, Kummert, and Daoud (2017) presented a new model implemented in TRNSYS as Type 3258, which was dedicated to modelling phase change materials in building envelopes. The model considered 1-D conduction heat transfer and used an explicit finite-difference method coupled with an enthalpy method to consider the variable PCM thermal capacity. The model included temperature-dependent thermal conductivity and PCM-specific effects like hysteresis and subcooling. The model was verified by comparing results with those of other numerical models, following the approach presented in Haghighat et al. (2013) and Johannes et al. (2011). Results of the verification were successful.

There is no evidence in the literature of the direct modelling of transparent systems incorporating PCMs through TRNSYS. However, a Matlab-based model of a PCM layer within a double skin façade has been coupled with TRNSYS to replicate the behaviour of this advanced façade solution (Elarga et al., 2016; Elarga, Dal Monte, Andersen, & Benini, 2017), though through the so called 'ping-pong' coupling that Hensen (1999) implemented by means of Type 155. Furthermore, given the possibility to compile a deliberate Type, it seems reasonable to expect that a dedicated Type could be developed in the future, based on the different numerical models available in literature for PCM glazing systems, as explained in the simulation requirements section.

3.3 ENERGYPLUS

A new approach to simulate PCM in walls in EnergyPlus was studied by Barbour and Hittle (2006). Conduction Transfer Functions (CTF) were used to implement a numerical model for annual simulations, requiring less calculation capacity. The model was one dimension and was based on an ASHRAE Toolkit. The model was validated with real data from previous experiments, but when implemented in EnergyPlus, the simulations showed unacceptable errors when using PCM.

In 2007, a new improved version of EnergyPlus was presented, incorporating the capability to simulate PCM in building envelopes (Pedersen, 2007) in 1-D. To solve the limitations of CTF to simulate PCM, a new implicit finite difference thermal model of building surfaces was incorporated into EnergyPlus, making it possible to use temperature dependent thermal properties. The model simulates the performance of PCMs using the enthalpy method. Later on, in 2012, (Tabares-Velasco et al. 2012) presented a validation of the EnergyPlus model to simulate PCM in walls. The procedure used was the one proposed by ASHRAE Standard 140, consisting of analytical verification, comparative testing, and empirical validation. Two bugs were identified and fixed, providing EnergyPlus with a validated PCM model.

In version 8.8 of EnergyPlus, released in 2017, a dedicated module was first integrated in the simulation code to model hysteresis phenomena. However, such a sub-routine was only applicable to building envelope systems fully realised with PCMs (i.e. not to multilayer walls), making it, in practice, of little or no use. This limitation has been overcome with the latest release of EnergyPlus (v. 8.9) in March 2018 (EnergyPlus, 2018). Alternative approaches to model hysteresis with EnergyPlus includes the use of the Energy Management System module in EnergyPlus (Goia, Chaudhary, & Fantucci, 2018) to impose a different enthalpy-temperature curve depending on the direction of the phase change (i.e. whether melting or solidifying).

As far as the simulation of PCM layers in transparent components is concerned, the literature review reveals no example of models or approaches developed in the EnergyPlus environment. The so-called Conditioned Cavity Method (Kendrick & Walliman, 2007), which is explained in more detail in Section 3.4, might be used in combination with EMS functions and glass panes characterised by (controllable) dynamic optical properties, as a suitable strategy to carry out this modelling. However, the complexity of such an approach would probably be very high and some intrinsic limitations in EnergyPlus might limit the verifications of the results too.

Preliminary attempts to overcome the current limitations of EnergyPlus were made by one of the authors, by connecting an Matlab/Simulink based model with EnergyPlus for co-simulation through the use of the external interface's Building Controls Virtual Test Bed (BCVTB) as well as the Functional Mock-up Units (EnergyPlus, 2015). However, in both cases the two coupled models solve the two sets of partial differential equations using a fixed synchronisation time step, which means that there is no iteration between the two simulation environments. This 'ping-pong' coupling may limit the reliability of the results for a system where inertial effects are crucial.

Given the open-source nature of EnergyPlus, the implementation of custom model in the source code of the simulation environment is a feasible option. This might be a more suitable solution for expanding EnergyPlus's capabilities in simulating a transparent PCM-based layer than the co-simulation approach – though such an activity would require a significant programming effort resulting in the compilation of an entirely new code for the software.

3.4 ESP-R

In 2004, Heim and Clarke (2004) developed a modified ESP-r program to simulate PCM-impregnated gypsum plasterboard. Using control volumes, the effective heat capacity method and assuming equivalent homogeneous properties of PCM-gypsum composite, several temperatures were studied. Unfortunately, the numerical model was not validated with real data and further macro-scale experiments are necessary. On the other hand, Schossig, Henning, Gschwander, & Haussmann (2005) developed an ESP-r model to simulate micro-encapsulated PCM in gypsum wallboard and experimentally validated the model.

In terms of ESP-r's prediction capability when it comes to effects such as hysteresis and subcooling, it must be mentioned that a dedicated subroutine (SPMCMP56) was programmed by Gelissier (2008) and included the possibility to model hysteresis, using the modelling approach developed by Hoffmann (2006).

Later, an experimental validation of the ESP-r PCM model was carried out by Fallahi, Shukla, & Kosny (2012), using a base case wall assembly experimentally tested in the Oak Ridge National Lab. testing facility located in Charleston, South Carolina, and by Heim and Wieprzkowicz (2016), which instead followed the methodology from the International Energy Agency (IEA) Annex 23 by Johannes et al. (2011).

There is no evidence in the literature about the use of ESP-r to simulate transparent envelope applications of PCM system. As for EnergyPlus, possible paths to enable simulation of PCM transparent system with ESP-r include the development of a dedicated subroutine, as well as the adoption of strategies (e.g. the conditioned cavity method) to work around the limitation of the current state of the software tool.

3.5 IES-VE

IES-VE (which stands for Integrated Environmental Solutions) does not incorporate, for the time being, any direct modelling possibility for PCM-based components (either in opaque or in transparent building envelope components). However, a successful work-around, using the ApacheSim model, was developed in the past few years, and the official support of the code (IES-VE 2018) recommends it – though highlighting some limitations.

This work-around is based on the so-called 'Conditioned cavity method' (Kendrick & Walliman, 2007), and is based on the modelling of the PCM layer as a virtual cavity, which is maintained at a set-point temperature corresponding to the nominal melting temperature of the PCM by means of an ideal heating and cooling system. Such a cavity has an infinitesimal volume, whose surface have (almost) no thermal resistance and no heat capacity, while the cavity boundaries themselves have a thermal resistance equal to that of the PCM layer. The equivalent heat capacity method is embedded in this approach.

The complexity of this work-around lies in the fact that the control of the energy to be delivered or removed (through an airflow) in the virtual cavity requires an iterative process to determine the schedule to control the fictitious heating and cooling system. This means that, in practice, due to the need to establish a very detailed control schedule, simulations are often limited to short periods (in the range of one or few weeks).

Favoino (2015) employed the "Conditioned cavity method" in IES-VE by choosing to control the air temperature of the virtual cavity and assuming an infinite latent heat storage capacity for the PCM layer. If, on the one hand, such an approach enables longer simulations to be carried out, on the other hand it requires further verification to be carried out (i.e., the energy balance on the fictitious PCM layer needs to be carried out to ensure that the sum of the virtual cavity's heating and cooling loads, at least on a daily basis, needs to be equal or lower than the actual latent heat storage capacity of the PCM layer.

Other examples of implementation of this method in IES-VE are reported in Padovani Jensen, and Hes (2010) and Ahmed, Mateo-Garcia, McGough, Caratella, and Ure (2018). However, it must be stated that there is no evidence in the literature about the validation of the simulation results obtained though this work-around in IES-VE. It is also not possible to find an application of this approach for transparent PCM-based envelope components.

3.6 IDA ICE

Until recently, IDA-ICE had not supported an open, direct modelling of PCM layers. The new explicit module to model PCM has been now (early 2018) embedded in the latest version 4.8 of this tool. Documentation on this new approach is not yet publicly and fully available, and this prevents a comprehensive understanding of the features of the modelling strategy implemented in the code, which, anyway, seems to be based on the enthalpy method equation.

This new integrated solution is based on a custom model, developed by the software house of IDA-ICE, but until version 4.7 was made available only for research purposes. In 2017 and 2018, Cornaro, Pierro, Puggioni, and Roncarati, (2017) and Cornaro, Pierro, Roncati, and Puggioni (2018) tested and compared the 'PCM wall' module, written in Neutral Model Format language (NMF, the programming language of IDA-ICE), with experimental data. This custom mode simulates the behaviour of a PCM layer based on the enthalpy method with a finite difference method, where one node represents the PCM layers and two nodes are placed a the two interfaces of the PCM, one at each surface of the layer. This model and implements two enthalpy-temperature curves, which may better replicate the behaviour of PCMs with strong hysteresis effects. On the contrary, no evidence is found to assess whether or not subcooling can be addressed. The validation of the model was done using paraffin wax as PCM, a type of PCM that shows little hysteresis and almost no subcooling.

A custom model for transparent PCM layers was developed and validated by (Plüss et al. 2014), and used to estimate the effect of PCM transparent glazed system by (Bionda, Kräuchi, Plüss, & Schröcker 2015). This model is the only model known to replicate PCM in transparent envelope components that is integrated (though through a custom version) in software for BES. The model, written in NMF, uses a 1-D formulation, and is aimed at accurately representing subcooling effects (as it was developed to reproduce the behaviour of a salt hydrate-based system), based on the equivalent capacity method. The optical part of the model is based on the work of Weinläder (2003) and Weinläder et al. (2005).

Since only recently, and primarily through custom releases, IDA-ICE is presently the only tool capable of addressing both opaque and transparent building envelope components that integrate PCMs. However, the potentials and limitations of the implemented simulation codes have not been extensively communicated and a comprehensive validation effort might be necessary to fully demonstrate the reliability of these codes.

4 VALIDATION OF PCM MODULES OR APPROACHES FOR BES TOOLS

Validation of numerical models is crucial to ensure accuracy, precision, and reliability of simulation results. Validation is usually referred to direct comparison between experimental data and simulation results by means of concepts as average errors or relative maximum errors. However, other processes can also be used, such as analytical validation and model verification. Analytical validation consists of comparing the simulation results of a simple case with its analytical solution, while model verification consists of comparing the simulation results with those of a validated model.

In a validation process, experimental errors must be considered, as well as errors in input data. When simulating PCM in building façades, errors in ambient conditions and in PCM thermo-physical properties are of great importance and must be carefully evaluated (Dolado, Lázaro, Marín, & Zalba, 2011). Moreover, special attention must be paid to the physical phenomena modelled, since some physical phenomena of the PCM may not be captured by the model, such as hysteresis or subcooling, and thereby affecting the accuracy of the results.

For validation processes, the variable to be analysed must be determined with care. When modelling PCM, this variable can be a PCM variable (energy stored/released, PCM temperature evolution, etc.) or a variable of the system (internal temperature of the building, energy demand of the building, etc.). When the validation process includes the system (latter case), errors from the PCM model can be hidden by the system.

Finally, when using PCM as a passive system (intrinsic control), one must remember that errors in the system model may result in incorrect temperature predictions of the PCM, thus predicting a complete different behaviour.

In the IEA Annex 23 (Johannes et al. 2011; Haghighat et al. 2013), a standardised procedure for validation of PCM-enhanced (opaque) walls was proposed. This procedure, based on nine different cases, allows a numerical benchmark of the simulation results to be established. On the contrary, and probably due to the limited amount of research activities in this field, as well as the limited market-ready solutions, no standardised procedures have been internationally agreed upon for the validation of PCM-enhanced transparent/translucent elements, where the role of the impinging solar radiation becomes very relevant (Grynning et al. 2013). Thus, a standardised procedure for PCM model validation in general is still required, based on detailed and reliable experimental data.

BES programs usually attempt to experimentally validate their models (Kuznik & Virgone, 2009; Kuznik et al. 2010; Tabares-Velasco, 2012). However, these validations can be limited to certain situations and thus, attention must be paid to the validity range and conditions. From all of the presented models, 10 out of 18 (56%) were validated (Fig. 1). On the other hand, from the most recent models developed, three models in TRNSYS have been validated (Kuznik et al., 2010; Al-Saadi & Zhai, 2015a; Al-Saadi & Zhai 2015b; Delcroix et al., 2017). On the other hand, the model in EnergyPlus is also validated (Tabares-Velasco et al., 2012). A model in ESP-r (Fallahi et al., 2012; Heim & Wieprzkowicz, 2016) and a model in IDA-ICE (Cornaro et al., 2017; Cornaro et al., 2018) were also validated against experimental data.

The model developed by Kuznik et al. (2010) used experimental results from a test cell to compare both the internal ambient temperature and the internal surface temperatures for two external temperature evolutions (step and sinusoidal). For the internal air temperature, maximum differences between numerical and experimental results were 1.1°C and 0.8 °C for step and sinusoidal external temperature evolution, respectively. On the other hand, mean differences were 0.2°C and 0.3°C, respectively. For the internal surface temperature, the model presents good agreement for the step case (maximum difference of 1.1°C and mean difference of 0.2°C). For the sinusoidal case (maximum difference of 1.3°C and mean difference of 0.6°C), the model predicts the same behaviour for all walls, while experimental results demonstrate some differences that are not captured by the model. Although the model shows good agreement with the experimental results, there exist some differences, which can be caused by the aeraulic effects inside the test cells, which cannot be predicted by the model. This limitation could be overcome if the convective heat transfer coefficient is known.

Regarding the EnergyPlus model, the validation procedure performed by Tabares-Velasco et al. (2012) consisted of the analytical verification, comparative verification, and empirical validation of three PCM applications: PCM distributed in drywall, PCM distributed in fibrous insulation, and thin concentrated PCM layers. The analytical verification consisted of solving the Stefan problem. The three cases analysed showed similar results and were in good agreement with the analytical. However, results determined that the node spacing must be smaller (3 times smaller) than the default one in EnergyPlus. The verification process consisted of a comparative testing relative to the ideal PCM model in Heating 7.3, thus representing a more realistic case. Results were in good agreement when time steps where shorter than 4 minutes. Moreover, the PCM model also determined peak load reduction and shift accurately. Finally, experimental validation was performed based on data from the literature (Haavi Gustavsen, Cao, Uvsløkk, & Jelle 2011; Cao et al., 2010). Results were in good agreement in terms of temperature for the heating process, but significant differences were observed for cooling. This is due to the incapability of EnergyPlus to simulate PCM hysteresis, at least until the implementation of this feature in version 9, which was recently tested against dedicated experimental data (Goia et al. 2018). In this latter activity, it was shown that even if the capability to simulate the hysteresis has been embedded in the code, the reliability of the simulation to catch this phenomenon is still pretty low, especially in the case when the melting or solidification process is not completed.

Al-Saadi & Zhai (2015a) also used data from (Cao, 2010) to experimentally validate their models. They used the Root Mean Squared Error (RMSE) to analyse the accuracy of the models. Two different points in the PCM layer were analysed. All models except the non-iterative correction scheme showed an error close to or below 0.1°C, which was within the uncertainty range of the experimental equipment. They also performed a comparative analysis with EnergyPlus, analysing the interior and exterior surface temperatures. All models show good agreement with EnergyPlus, showing errors lower than 0.1°C for a duration of 3 minutes. Finally, the same authors (2015b) also validated the model with the experimental data from Kuznik et al. (2010), showing good agreement.

The model developed by Delcroix et al. (2017) was validated following the approach proposed by the International Energy Agency Annex 23 (Johannes et al., 2011; Haghighat et al., 2013). Results were in accordance with the ones from IEA Annex 23, both for the internal and external surface temperatures and for the heat fluxes.

Fallahi et al. (2012) validated the PCM model in ESP-r, against experimental field data obtained from the Oak Ridge National Lab. testing facility located in Charleston, South Carolina (Kośny, 2008; Kośny, Kossecka, & Yarbrough, 2009; Kośny, Kossecka, Brzezinski, Tleoubaev, & Yarbrough., 2011). To validate the model, the heat flux across the walls was compared with the measured one, showing a total heat gain difference of about 0.6%.

Cornaro et al. (2017) compared the simulation results obtained with IDA-ICE with temperature data collected by means of solar test boxes. These are boxes with a linear scale factor of 1:5 and a surface scale factor of 1:25 with respect to a real room, with five opaque walls and one glazed wall, where the opaque walls are equipped with PCM layers. The results of the validation show that the RMSE, calculated for the indoor air temperature over a period of 3 days, was in the range 1.6 to 1.8 °C, corresponding to an error of ca. 5%.

5 LIMITATIONS AND DESIRABLE FURTHER IMPROVEMENTS

The use of PCM in building envelopes has focused in passive systems (intrinsic control systems), where the PCM is passively charged and discharged by either solar energy/external temperature or an internal heat source. The main goal of such systems is to reduce the energy demand of the building and/or improve the thermal comfort. However, these systems present difficulties in their design process and PCM selection, since they require very specific designs to achieve a suitable performance. For operating conditions (weather conditions, use and occupation of the building, etc.) different from the design ones, the behaviour of the PCM will change, and its phase change temperature may no longer be suitable, thus reducing or even eliminating its benefits.

Moreover, errors in the building model affect the PCM behaviour, and may result in inaccurate PCM system design (such as phase change temperature) that may reduce its benefits.

Additionally, the recharging of the PCM is sometimes limited in such applications, compromising the potential benefits of the system. Therefore, active systems (extrinsic control systems) are advisable in order to solve some of these problems.

Finally, other important issues in the simulation of the PCM remain to be solved. The accurate inclusion of hysteresis, subcooling, natural convection, and ageing in PCM simulation must be solved in future BES tools. Although some advances have been done in the newest versions of software tools, there is still room for improvement.

6 CONCLUSIONS AND FUTURE WORKS

This paper provides an overview of the successful implementation of the modelling and simulation of PCM-based building envelope systems in software tools for building energy simulation (BES). Five of the most common BES tools have been analysed and evidence from the scientific literature about their use for simulating PCM-enhanced envelope has been given.

In a time when the integration of detailed aspects typical of PCMs' behaviour (i.e. hysteresis and subcooling) is becoming more and more common in BES tools, it is necessary to highlight how validation of the models implemented in BES is probably an underestimated activity. Although there have been proposals on standardised procedures, these have not been extensively used, and the comparison of the simulation performance of BES has not been comprehensively carried out – at least as far as the latest developments are concerned. An overall comparison of the performance of BES tools in modelling and simulation of PCM-enhanced envelope would definitely be an important research task to fill a present-day knowledge gap. Coupling such a numerical benchmarking with reliable experimental activities would further increase the relevance of the effort. Apart from the standardised procedures proposed by the IEA Annex 23 for model verification (Johannes et al., 2011; Haghighat et al., 2013), two different sets of experimental data have been used in the literature for experimental validation of different models (Kuznik et al., 2010; Cao, 2010).

While almost all the BES tools analysed in this paper allow the simulation of opaque envelope systems incorporating PCMs to be carried out (and, with the help of a work-around, such a simulation is possible with all of them), it is almost impossible at present to simulate the transparent envelope, which includes PCMs exposed to solar radiation – only one custom model is available for one software tool. Modelling and simulation of transparent solutions incorporating PCMs is therefore way behind the simulation of opaque PCM envelope, and future development of tools by the BES community should also focus on enabling this simulation domain.

Acknowledgements
The authors would like to thank EU Cost Action TU1403 'Adaptive Facades Network' for providing excellent research networking. The authors Albert Castell and Marc Medrano would like to thank the Catalan Government for the project grant (2017 SGR 659) given to their research group. The author Francesco Goia would like to thank the Research Council of Norway and several partners through The Research Centre on Zero Emission Buildings (ZEB) (2009 – 2017, grant 193830) at the Norwegian University of Science and Technology.

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