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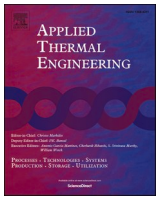

# Numerical modelling of radiant systems and phase change materials in building applications - a review

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ABSTRACT

As a result of increasing environmental and economic concerns, the demand for more efficient energetic systems has augmented, leading to a greater focus on investigating new solutions. The latest developments in the integration of radiant systems in buildings have shown promising results, being a feasible and more efficient technology. In this regard, an analysis of the current state of the radiant system's development is performed, focusing on several studies made in recent years. The aim of this article is to outline the current state of the numerical modelling of radiant systems, with a greater focus on the modelling of PCM in radiant systems, which hasn't been thoroughly done in the literature up until this moment. Its objective is to present researchers the necessary information about the function of PCM radiant systems, as well as to provide insight into the most used methods for numerical model development and their theoretical mathematical fundamentals, regarding its thermal behaviour. The accuracy and effectiveness of various numerical modelling methods are assessed and compared. Several experimental and numerical studies available in the literature are presented. A discussion between the various pros and cons of the most relevant studies is carried out, and possible solutions are suggested for future work.

## 1. Introduction

Over recent years, concerns have been raised about the effects of increasing energy consumption. As mentioned by the IEA, International Energy Agency, housing is one of the most energy-demanding activities, being responsible for more than 30 % of the world's energy consumption [1]. Academic and scientific researchers around the world have gathered their resources to develop new technologies and solutions in the hope of reducing this energy consumption [2,3]. The majority of the energy use of housing is used in climatization, as well as in the cooling and heating of indoor spaces. To reduce this energy consumption, a great diversity of methods was explored, including the coupling of HVAC (heat, ventilation and air conditioning) systems with renewable sources, and increasing the efficiency of equipment's by downsizing or the application of new and better materials. It is in this scope that phase change materials (PCM) have proven to have potential. Recently, companies and researchers have been making efforts to utilize these materials. Their integration in the various elements of building's façades and HVAC systems, such as radiant systems have been studied and demonstrated to have improved the building's thermal efficiency and proven to be a valid alternative [4–14].

In this review, the authors aim at reviewing and discussing articles presented in the literature, providing researchers the necessary resources to understand the theoretical basis of the numerical modelling of PCM radiant systems. The present review provides resources on the formulation of the methods used in the numerical modelling of PCM radiant systems. Furthermore, this article complements the presentation of the theoretical basis with its possible applications, through the analysis of numerical and experimental studies available in the literature. It is expected that this article will assist future researchers in accessing the best methods to model their study case.

The following subsections of the introduction provide context and insight to the composition of radiant systems, numerical modelling and already developed reviews on this subject, which provide further justification for the pertinence of the development of this work. The authors start with an in-depth state of the art on the different types of radiant systems, how they work, and the importance of the numerical modelling. In addition, other relevant review articles on the various topics are identified. This section is followed by a thorough description of the mathematical formulations required to model classic radiant systems, as

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well as methods to model more complex systems with PCM. Once the models are presented and discussed, their characteristics are compared. Multiple recent studies, making use of the previously presented numerical simulation methods, are then presented and discussed. Finally, a future direction of technology and a conclusion section provides a summary of the present review, as well as stating main findings and suggestions for further research.

### 1.1. Radiant systems description

Radiant systems in buildings are systems that aim to regulate the indoor conditions of the building and preserve thermal comfort. Radiant systems can be incorporated in most of the façade of a building, in walls, floors, or ceilings [8,15–23]. There are three types of radiant systems in the industry [24,25], hydronic systems, electrical systems, and thermoelectric systems, but the most used are the first two.

Hydronic radiant systems are composed of tubing system, fluid pumps, and fluid heaters/coolers [7,19]. In these systems, when used for heating purposes, heated circulating fluid (water in most cases) flows through the piping system and radiates heat to the room, which is at a lower temperature than the fluid. In case of cooling, the energy flows from the room (which is at a higher temperature than the circulating fluid) to the piping system, which will conduct the circulating fluid to a chiller to cool the fluid. Michal Krajčík *et al.* [26] studied a wide gamut of thorough information regarding water-based wall systems. Topics such as the classification of existing systems, benefits, and drawbacks of each, and design recommendations are discussed. Furthermore, the authors discuss the research opportunity by incorporating these systems with PCM and the chance of its implementation in building retrofit.

Electric radiant systems are used only for heating, but instead of using a heated circulating fluid, the temperature is increased through the Joule effect when electrical current is flowing through several resistors in the radiant system [27,28]. In thermoelectric systems an electrical current is formed between 2 materials, which generates a temperature differential, creating a “cool side” and a “hot side” [29,30]. Depending on which side is in contact with the exterior of the building and the interior of the room, these systems can be used for both cooling and heating. These three types of radiant systems can be further complemented with other systems, such as photovoltaic panels and heat pumps to create a high-energy efficient system [8,31,32].

Furthermore, PCM can be incorporated in radiant systems to provide increased energy efficiency. PCM are materials which have a high latent heat capacity that can be used to store large quantities of energy. Therefore, these materials have the capacity to collect what would be wasted or unnecessary energy used by the system, and release it whenever needed, reducing peak temperatures, temperature fluctuations and saving energy [33,34]. The benefits and intricacies of PCM integration in radiant systems can be comprehensively studied in Moreira *et al.* [35]. Further works, such as Michal Krajčík and Ondřej Šikula [36] carried out studies in this field, developing innovative indicators of thermal response and output of radiant systems that greatly benefit the scientific community by providing tools to comprehensively analyse data.

### 1.2. Numerical modelling

To develop radiant systems, experimental trials must be developed to gather the required data from the thermal system. Generally, the experimental setup regarding radiant systems requires large spaces and a lot of material. If the system has PCM embedded, whether through the usage of PCM macrocapsules in the system [10,11,37] or PCM microcapsules mixed in mortar/cement [12,31], the macrocapsules must be prototyped [38] and the cement/mortar mixtures must be specially developed and tested. Developing these experimental trials has a high cost, both in time and money [39].

Numerical models allow researchers to explore different variations of a base scenario, allowing the assessment of the consequences of variables changes in the system without much effort and no additional experimental investment [37,40,41]. Thus, numerical modelling is of extreme importance as it allows researchers to solve complex problems with ease. Predicting the behaviour of PCMduring the phase change period is still a challenge. This challenge results from the nonlinear nature of the moving interface separating the liquid and solid phases, as well as the varying thermodynamic properties of both phases [42–45]. To try to solve these complex problems, the sharp interface model or Stefan model assumed the solid phase and the liquid phase to be separated by an infinitely thin surface, called sharp interface. This model is the basis of the outgoing models to develop numerical models. When performing one-dimensional (1D) or two-dimensional (2D) models with a fixed melting temperature, the analytical solution can be derived. However, when more complex shapes are used and a PCM melting temperature range is considered, the sharp interface model becomes difficult to implement, requiring the help of computer-based calculations [45,46].

Although there is a necessity for developing accurate numerical models, it is usually linked to an increase in model complexity. This comes at an increased computational cost. Researchers need to find compromises to obtain usable results and to do it as quickly as possible [47,48]. This led to the development of numerous methods for solving the numerical models, such as the enthalpy method and the heat capacity method [49–54]. Moreover, it is important not only to have accurate but also valid ones. A numerical model is validated by comparing its results to those of an experimental trial and verifying if the numerical model accurately describes reality.

Regarding the software used to perform numerical modelling, there is plenty of commercially available software. According to Hassan and Abdelaziz [54], the most used software up until 2020 are the ANSYS® Fluent, TRNSYS®, EnergyPlus™ and COMSOL Multiphysics®. However, in scientific research, there are several alternatives used to develop numerical models and methods to simulate thermal systems.

### 1.3. Previous reviews and stat-of-art

Many reviews were developed in this field, which mention and explore the numerical modelling aspect of hydronic radiant systems and PCM. These reviews are necessary to outline the current state of the subject, summarise data, and provide relevant conclusions to guide authors on the most adequate modelling methods for their work, as well as to arouse new problems and areas which require more research.

Hassan *et al.* [54] developed an overall review on the simulation, control, and integration of hydronic radiant cooling systems. Regarding the numerical modelling of the systems, the authors present the most

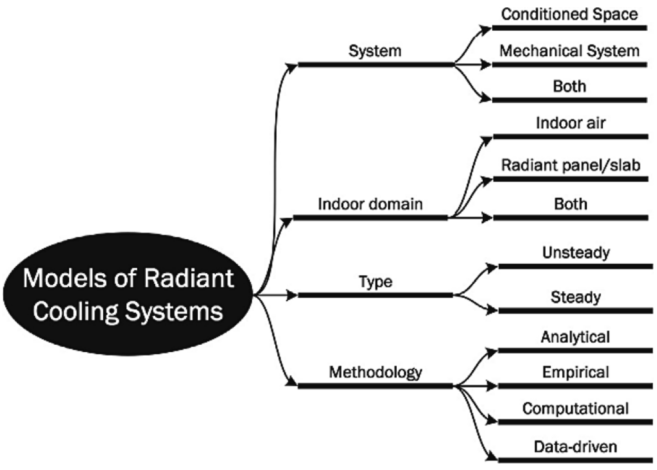


**Fig. 1.** Classification of radiant cooling system models [54].

common forms of classifying the developed models, which are presented in Fig. 1. The authors grouped the modelling techniques into 4 categories, *i)* computational models of indoor air, *ii)* computational models of radiant slabs or panels, *iii)* simplified analytical or numerical models of the conditioned space and radiative terminals, and *iv)* regression data-driven models. This review gave insight into the need for more transient-state computational models and the lack of discussion in the literature on exergy analysis.

In another article, *Kim et al.* [55] reviewed modelling approaches for passive ceiling cooling systems. The modelling techniques were grouped into 3 groups, *i)* passive ceiling cooler models, *ii)* indoor environment models, and *iii)* integrated models as shown in Fig. 2), where simplified models, detailed models, empirical models, and black box methods, such as transfer functions, were explored.

Romaní *et al.* [56] reviewed thoroughly the simulation and control of thermally activated building systems (TABS), taking into consideration systems for both cooling and heating. The TABS simulation techniques are enlisted and described as numerical models (including finite element/difference/volume method analysis – FEM, FDM, and FVM), analytical models, semi-analytical models, resistor–capacitor (R-C) models, transfer-function models, and identification models. From this review, it was ensured that detailed numerical models such as the FEM, FDM, and FVM give the most accurate results and are often used for model verification. Despite this, many simplified models are used in integrated building simulation packages and control strategies, presenting good levels of accuracy whilst lowering the computational cost of the simulations. Furthermore, the usage of a transient state is required for accurate studies of the dynamic behaviour of TABS.

Garcia and Cabeza [57] present a review of numerical models for PCM packed bed systems. After giving a brief description of all the mentioned models, the authors elaborated on the methods, classified as single-phase models, Schumann's model, concentric dispersion model, continuous solid phase model, and empirical models. The authors provide comparisons between the usage of several of the beforementioned models. With the development of this review, the authors concluded that the single-phase models are computationally inexpensive but are only viable when the system has a heat transfer fluid and particles with high thermal capacity or when the particles are very small. Schumann's model is the simplest, as it removes thermal gradients from the equation by considering infinite thermal conductivity. Both the concentric dispersion and solid phase models require high computational effort. However, the solid phase model was one of the few available in the literature that could discretize the packed bed system.

In a review by Ghasemi *et al.* [58], PCM fundamentals, categories, fabrication, numerical models, and applications were discussed.

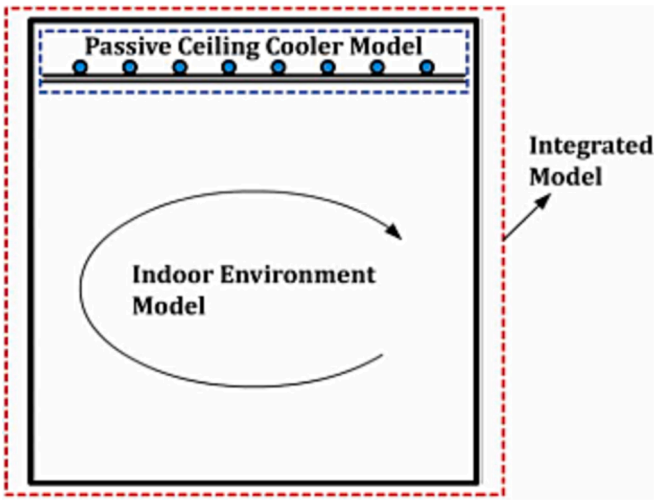


**Fig. 2.** Numerical model domains [55].

Regarding the numerical models, four were disclosed, *i)* the porous medium method, *ii)* the enthalpy method, *iii)* the enthalpy-porosity method, and *iv)* apparent and effective heat capacity. It was concluded that there are multiple numerical models for PCM and that they should be chosen depending on the specific purpose. Apparent heat capacity and enthalpy-porous are the most implemented methods in COMSOL and ANSYS that solve latent heat problems by using an equivalent heat capacity and simulate the solid/liquid interface. Also, despite a large number of studies on PCM, limited work was done on encapsulated PCM (EPCM) by considering both the shell and core interactions. Despite existing available reviews of PCM radiant systems, the information they explore related to numerical modelling methods is not very deeply discussed or is very specific to a determined application. Furthermore, there is no scientific work solely on the numerical modelling of PCM radiant systems, as this information is spread across multiple reviews by different authors in a more summarized manner. This review aims at providing an insightful review that aggregates both topics, providing an extensive work with great added value to researchers in understanding the whole subject of numerical modelling of PCM radiant systems. This review separates the numerical modelling strategies of generic radiant systems from the modelling of PCM, to give importance and comprehensively explore PCM modelling.

## 2. Mathematical formulations and numerical models

### 2.1. Conventional radiant systems

As previously mentioned in the introduction, radiant systems contribute to the improvement of the thermal comfort of buildings. With conventional radiant systems, the authors refer to radiant systems which are not complemented with PCM solutions. Multiple studies [46,47,50–56] have focused on developing these types of systems, recurring to numerical modelling as a way to predict the thermal behaviour of the system and comparing multiple scenarios to assess energetic gains. This chapter discloses the methods utilized for the numerical model development of radiant systems.

#### 2.1.1. Computational numerical models

Here, finite element and finite volume methods are used to examine the flow and thermal distribution inside a given space, through the usage of CFD (computational fluid dynamics) tools. Elements such as air inlets/outlets, radiative terminals, doors, windows, furniture, and human bodies are considered mass or thermal boundaries. Instead of solving the temperature in the radiant slabs or panels, those surfaces are represented by surface-specific mean temperatures, and conservation equations of mass, momentum and energy are solved in parallel with a radiation model of the space, typically discrete ordinate, or surface to surface models. The solar radiation can be solved using ray-tracing methods or defined as heat flux. These simulations are usually performed in a steady state due to computational cost.

Z. Cheng and S. Cheng [66] developed a numerical model of a radiant cooling floor of a large waiting hall room (Fig. 3). The radiation heat exchange between the radiant floor and the interior ambient temperature was described as:

$$\boldsymbol{Q}_{\mathrm{f}} = \boldsymbol{\sigma}_{\mathrm{b}} \sum \left( \boldsymbol{T}_{\mathrm{f}}^{4} - \boldsymbol{T}_{\mathrm{r}}^{4} \right), \tag{1}$$

where $\sigma_b$ is the black sphere radiation constant, $T_r$ is the absolute temperature of the radiant floor surface and $T_f$ is the absolute wall temperature. The indoor cooling load ($Q_r$) and the humidity cooling load ($D$) are described by equations (2) and (3) respectively:

$$\boldsymbol{Q}_{\mathrm{r}} = \boldsymbol{G}(\boldsymbol{h}_{\mathrm{n}} - \boldsymbol{h}_{\mathrm{s}}), \tag{2}$$

$$\boldsymbol{D} = \boldsymbol{G}(\boldsymbol{d}_{\mathrm{n}} - \boldsymbol{d}_{\mathrm{s}}), \tag{3}$$

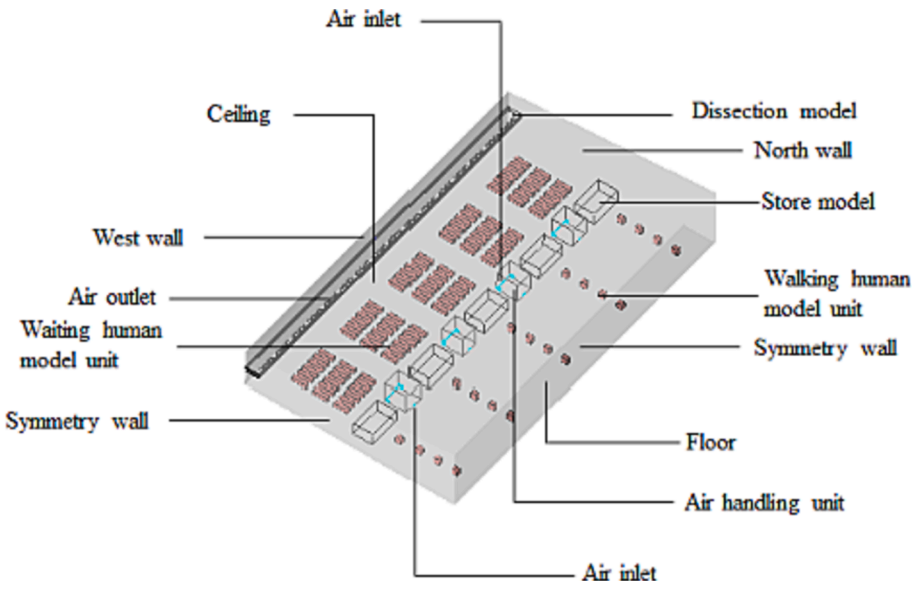


**Fig. 3.** Diagram of the waiting hall [66].

where $G$ is the mass flow of fresh air (kg/s), $h_s$ is the enthalpy of supply air (kJ/kg), $h_n$ is the enthalpy of indoor design state point (kJ/kg), $d_s$ the humidity ratio of supply air ($kg_{water}/kg_{air}$) and, $d_n$ the humidity ratio of indoor air ($kg_{water}/kg_{air}$).

This category includes numerical models such as finite difference (FDM), volume (FVM), or element (FEM), which are used to examine temperature distributions in radiant bodies, to determine condensation risk or cooling capacities. The volume of indoor air is represented as a boundary condition on the surface of the slab/panel. Usually, steady state is used to characterize the performance of the slab/panel for specific mean temperatures of water and surface. The neglect of the end losses of the panel, variations in water temperature, and fluid properties are often considered to simplify the body geometry. The reduction of the model to 2D is often considered.

Dong *et al.* [65] developed a CFD simulation study on heat transfer of chilled water flow in a capillary ceiling radiant cooling panel system (Fig. 4), using the finite volume method.

Six influence variables were studied, among them, the chilled water inlet parameters, the structural parameters of the gypsum plaster and the capillary mats. The models assumed that (*i*) heat transfer to the semi-circular tube extremities was inexistent; (*ii*) the side walls and top of the panel were considered to be adiabatic; (*iii*) the thickness of the capillary pipes and their respective thermal contact resistance were negligible; (*iv*) the fluid properties of the chilled water were considered to be constant. The author describes the governing equations as follows:

$$\frac{\partial}{\partial X_i}(\rho u_i) = 0, \tag{4}$$

where $X$ is the coordinate axis in the direction $i$, $u_i$ is the velocity in the direction $i$ and $\rho$ is the inlet water density,

$$\frac{\partial}{\partial X_i}(\rho u_i u_j) = \frac{\partial P}{\partial X_j} + \mu \frac{\partial}{\partial X_i}\left(\frac{\partial u_i}{\partial X_j} + \frac{\partial u_j}{\partial X_i}\right), \tag{5}$$

where $\mu$ is the kinetic viscosity of the inlet water and $P$ is the pressure,

$$\frac{\partial(\rho_s u_i T)}{\partial X_i} = \frac{\lambda_s}{c_p}\frac{\partial}{\partial X_i}\left(\frac{\partial T}{\partial X_i}\right), \tag{6}$$

where $\lambda$ is the thermal conductivity, $T$ is for temperature, and $c_p$ is the specific heat capacity of the plaster layer, with the subscript $s$ referring to the medium water or plaster layer. Under the condition of heat transfer of plaster layer, $u_i$ is set to 0. Lastly, the $q$ represents the total sensible heat flux of the radiant panel and is given by equation (7):

$$q = (q_c + q_r)_b, \tag{7}$$

with $q_c$ ($W/m^2$) being the convective term of the heat flux, and $q_r$ the radiant heat flux. Here, the subscript $b$ stands for the bottom of the capillary radiant panel. Heat will be exchanged both by thermal convection and radiation between the ceiling surface and the indoor environment.

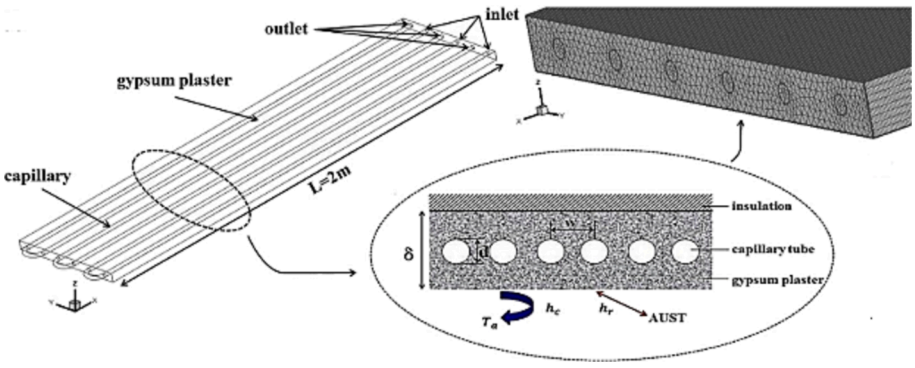


**Fig. 4.** Radiant cooling panel of the capillary ceiling [65].

#### 2.1.2. Analytical and semi-analytical models

Analytical models are models that are based on exact solutions of differential equations regarding heat transfer. The complexity of these equations limits the use cases of these models, which require assumptions to accurately describe the heat transfer process. Thus, analytical models are limited to 1D or simple 2D steady-state conditions. When developed, analytical models require low computational efforts, and thus are easily implemented in building environment simulation, being used in control purposes as well.

To overcome the limitations in geometries and conditions of the pure analytical models, some authors proposed correlations between different analytical solutions, developing more complex solutions such as TABS heat transfer. These models are referred to as semi-analytic models.

In a study, Tye-Gingras and Gosselin [64] aimed to determine the optimal modelling technique for heat transfer calculations of low thermal mass hydronic radiant cooling and heating panels that were composed of a serpentine lube layout. The authors concluded that the 2D FVM model could reproduce any tube pattern but was uselessly heavy. It had a very slow convergence because it relied on analytical solutions for its iterations. The authors stated that analytical models are fast and accurate but were not very versatile, as they required the heat transfer coefficient, the fin efficiency, and the tube spacing to be constant. In comparison, the semi-analytical model was fast to converge, accurate, and more versatile, as it allowed the calculation of the fluid temperature profile with nonconstant parameters, thus being potentially good when paired with CFD simulation programs for detailed convection and radiation calculations.

#### 2.1.3. Resistor-Capacitor models (R-C)

These models usually are zero-dimensional (0D) or (1D), meant to be used in transient simulation tools to assess the dynamics of the thermal systems through a generic/typical cooling or heating day or throughout an entire season. The most popular method is the resistor–capacitor model (R-C) (Fig. 5) suggested by Ren and Wright [63], which proceeds to calculate the heat flux ($q_{12}$– W/m$^2$) correlating the resistance of a material ($R_{12}$-Ω) with the temperature at both extremes of the material ($\theta_1, \theta_2$- °C), given by equation (8):

$$\boldsymbol{q}_{12} = \frac{\boldsymbol{\theta}_2 - \boldsymbol{\theta}_1}{\boldsymbol{R}_{12}}. \tag{8}$$

Bueno *et al.* [62] developed an R-C model for the analysis of interactions between urban climate and energy performance of buildings. The R-C model was assessed against advanced computational simulation tools that are well-evaluated and accepted. The authors stated that, because of its simplicity and reduced computational cost, the R-C model allowed for better comprehension of the physics involved in the problem, as well as making it possible to evaluate modeling hypotheses and the sensitivity of different parameters with greater ease. The authors concluded that the R-C model was able to be used both as a research and didactic tool [62].

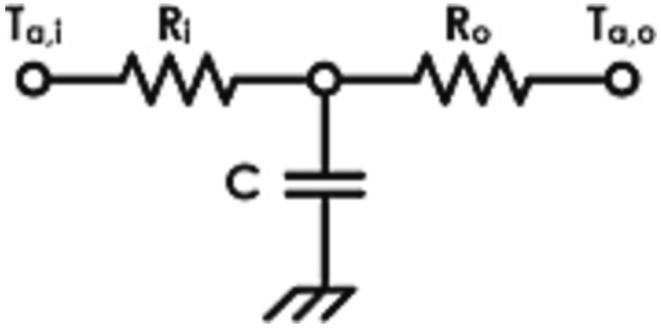


**Fig. 5.** Resistor-Capacitor model example [63].

In a study developed by Weber and Jóhanneson [61], the authors compared FEM, FDM, and the Boundary element method (BEM), to the R-C model approach, and stated that although they provided very accurate solutions, they were time consuming and often caused instability problems. Thus, it is of major interest to find simplified models that have limited complexity but still manage to be sufficiently accurate, as is the case with the R-C network [61].

Liu *et al.* [60] developed a study in which a star-type R-C network was modeled to simulate the dynamic thermal performance of a concrete cooling slab. Heat transfer through the slab is defined as heat transfer from chilled fluid to the core layer and heat transfer from the core layer to slab surfaces. In the star R-C-network the central node is treated as the core layer. The results demonstrated that the R-C model was in good agreement with a finite element method (FEM) in representing the dynamic and steady cooling performance.

#### 2.1.4. Regression data driven and identification models

These types of models are usually developed as part of predictive and adaptive control strategies. They can be used to predict the cooling loads of different zones of the building for determining a control strategy that manages to lower the power consumption whilst keeping the indoor environment within the comfort temperature range. With the advancements in database technologies, collecting data has become easier, allowing these methods to be more easily implemented. Compared to traditional first principle-based modelling methods, data-based models are more flexible and can be utilized in more complicated processes [59].

Identification models recur to statistical methods to obtain a model from a set of data. These models need to have previous measurements of the involved building, however, once developed these models are very easy to apply. Identification models are usually related to Model Predictive Control (MPC) [56].

### 2.2. Phase change materials

In recent years, the increase in popularity of thermal energy storage (TES) in buildings has attracted attention due to its numerous advantages, such as reducing temperature fluctuations and increasing the thermal efficiency of buildings [3,69]. TES is defined as the process of storing cold and heat for different applications [68,69]. The use of TES techniques in buildings is often the basis for thermally activated building systems (TABS), systems that are thoroughly reviewed in [56]. PCM have been shown to have a great potential to increase energy efficiency in buildings due to their potential to accumulate energy, resulting from their high latent heat when changing phase [70]. This phase change is what creates the complexity of its numerical models [71]. The most common methods for resolving these problems are the enthalpy method and the heat capacity method [19,72].

The governing equations for numerical models have three pillars of construction, often referred to as governing equations. Most methods for solving the melting problem have evolved from their initial formulation by Stefan [73]. The following equations are used to describe the melting problem:

$$\frac{\partial \boldsymbol{T}_s}{\partial \boldsymbol{t}} = \boldsymbol{a}_s \frac{\partial^2 \boldsymbol{T}_s}{\partial \boldsymbol{z}^2}, \tag{9}$$

$$\frac{\partial \boldsymbol{T}_l}{\partial \boldsymbol{t}} = \boldsymbol{a}_l \frac{\partial^2 \boldsymbol{T}_l}{\partial \boldsymbol{z}^2}, \tag{10}$$

$$\frac{\partial \boldsymbol{S}(\boldsymbol{t})}{\partial \boldsymbol{t}} = \frac{\boldsymbol{\lambda}_s \partial \boldsymbol{T}_s}{\boldsymbol{\rho}_s \boldsymbol{L} \partial \boldsymbol{z}} - \frac{\boldsymbol{\lambda}_l \partial \boldsymbol{T}_l}{\boldsymbol{\rho}_l \boldsymbol{L} \partial \boldsymbol{z}}, \tag{11}$$

where $\lambda$ is the thermal conductivity (W/m·K), $T$ is the temperature (K), $L$ is the latent heat diffusion (J), $a$ is the thermal diffusivity (m$^2$/s), $\rho$ the material's density, $t$ time,$z$ the spatial coordinate and $S$ the position of

the interface. Alternatively, Lin *et al.* [74] provide a variant governing equation for the enthalpy method:

$$\rho\frac{\partial H}{\partial t}=\lambda\frac{\partial^2 T}{\partial x^2} \tag{12}$$

where $\rho$ (kg/m$^3$), $H$ (kJ) and $\lambda$ are the density of the material, the enthalpy, and the thermal conductivity, respectively.

The subscripts refer to the solid and liquid phases of the material, s and l respectively. At the interface, both the temperature of the liquid phase and the solid phase are equal to the melting temperature of the material:

$$T_s = T_l = T_{melt}\text{at}z = S(t). \tag{13}$$

Saleel and Ahamed [75] studied the melting and heat transfer characteristics of paraffins using the enthalpy-porosity mode. In modelling the study. Both conduction and convection in the PCM were acknowledged. The PCM was assumed to be incompressible and a Newtonian fluid inside its enclosure. Furthermore, variations in the paraffin's density, thermal conductivity and viscosity were considered to vary linearly with temperature. As one of the paraffins was a mixture of paraffin and SiC nanoparticles, it was assumed that both substances were in thermal equilibrium and had the same flow velocity. This resulted in the following governing equations:

Continuity

$$\frac{\partial\rho}{\partial t}+\nabla(\rho V)=0 \tag{14}$$

Momentum

$$\frac{\partial(\rho V)}{\partial t}+\nabla(\rho V)=-\nabla p+\mu\nabla^2 V+\rho g+S \tag{15}$$

Energy

$$\frac{\partial(\rho E_s)}{\partial t}+\nabla(\rho E_s)=K_t\nabla^2 T \tag{16}$$

Xion *et al.* [76] presents the various components of the absorbed and released heat of a PCM. The sensible energy of a material, $Q_s$, is stored in the system through differences in temperature ($\Delta T$), and depends on the mass (m) and the material's specific heat capacity ($C_p$) (J/kg.K):

$$Q_s = mC_p.\Delta T. \tag{17}$$

Latent energy $Q_l$ (J) is the absorbed or released energy necessary for a material to change from phase A to phase B, which takes place at the phase change temperature of each material ($T_{pc}$) and it is dependent on the enthalpy $H_l$ (kJ/kg) of each material's phase

$$Q_l = m\Delta H_l. \tag{18}$$

For two given temperatures, $T_1 < T_{pc}$ and $T_2 > T_{pc}$, the total stored energy ($Q$) of a PCM when increasing its temperature from $T_1$ to $T_2$, including a phase change, is given can be given by:

$$Q=\int_{T_1}^{T_{pc}} mC_{p,S}\Delta T+m\Delta H_l+\int_{T_{pc}}^{T_2} mC_{p,L}\Delta T, \tag{19}$$

with $C_{p,s}$ (J/kg.K) being the specific heat of the material in the solid phase and $C_{p,L}$ (J/kg.K)being the specific heat of the material in the liquid state. As latent heat can be 5 to 14 times higher than its sensible heat counterpart [77], phase change materials have proven to be of special interest in the incorporation in buildings [18,78]. The method used by this author is known as the enthalpy method. There are more methods for calculating the latent energy gathered or released by a PCM, such as the apparent and effective heat capacity method, the porous medium method, and the enthalpy-porosity approach. These models are used to describe the thermal behaviour of the mushy zone of the PCM, where during the phase change, liquid surrounds solid volumes of the material.

### 2.2.1. Enthalpy method

The enthalpy method is one of the methods to numerically model problems known as the "Stefan problem", where there are phase changes, made up by the solid phase, liquid phase and their interface [71,79,80]. Multiple authors have recurred to this method to develop their numerical models.

Muriel *et al.* [79] developed a numerical study in ANSYS utilizing this method to model two computational fluid dynamics models of an air-thermal energy storage unit. Although the study obtained an almost horizontal curve phase change curve, appropriate for pure PCM, most commercial PCM are compounds, hence the non-linearity during the phase change. Du *et al.* [81] used the enthalpy method to simulate the influence of PCM that detained different thermo-physical parameters in the indoor thermal temperature of solar greenhouses in China. *Zhang et al.* [50] recurred the enthalpy method and the effective heat capacity method, which is discussed previously, and compared the results from the simulations regarding three impact-factors. The enthalpy method proved to be more accurate with narrower temperature ranges.

If the enthalpy is the dependent variable, the problem construction equations from Stefan ((9),(10) and (11)) can be replaced by:

$$\frac{\partial H}{\partial t}=\frac{k\partial^2 T}{\rho\partial z^2}+\frac{\varnothing}{\rho}, \tag{20}$$

where $H$ is the enthalpy (J) and $\varnothing$ (J.m$^3$/kg.s)the body heating term. The previous equation is valid throughout all domains (liquid, solid, and interface) and can be solved by any method (implicit or explicit). The temperature term of the equation is then replaced by the Heaviside function, dependent on the enthalpy, of the form

$$T = F(H), \tag{21}$$

where:

$$F(H)=\begin{cases}\dfrac{H}{C_p}, H<L\\ T_{melt}, 0\le H\le L\\ \dfrac{(H-L)}{C_p}, H>L\end{cases}. \tag{22}$$

Being $C_p$ the specific heat. Rewriting the previous equation, it is obtained

$$\frac{\partial H}{\partial t}=\frac{k\partial^2 F(H)}{\rho\partial z^2}+\frac{\varnothing}{\rho}. \tag{23}$$

If the problem is solved recurring the other governing equation proposed by Zhang *et al.* [50] (Equation **(12)**), the enthalpy is calculated by the following equation:

$$H=\begin{cases}c_{p,s}T, T<T_m-\varepsilon\\ c_{p,s}(T-\varepsilon)+\dfrac{L}{2\varepsilon}[T-(T_m-\varepsilon)], T_m-\varepsilon\le T\le T_m+\varepsilon\\ c_{p,s}(T-\varepsilon)+L+c_{p,l}[T-(T_m+\varepsilon)], T_m<T_m+\varepsilon\end{cases} \tag{24}$$

where $c_{p,s}$ and $c_{p,l}$ represent the specific heat of the PCM in solid and liquid states, $\varepsilon$ is the phase change radius, representing half the length of the phase change temperature range and $T_m$ is the mean temperature of the phase change transition temperature and $L$ is the latent heat during the phase change. Having this, the lower temperature limit of the phase change is given by $T_m-\varepsilon$ and the upper limit of the phase change gamut is $T_m+\varepsilon$-. When the temperature $T<T_m-\varepsilon$, the PCM is in the solid phase and the specific heat is equal to $c_{p,s}$. Opposingly, when T > $+-\varepsilon$, then the specific heat is equal to $c_{p,l}$. When the temperature was inside the phase change range, $T_m-\varepsilon<T<T_m+\varepsilon$, the value of the equivalent specific heat was $c_{p,equ}=\frac{L}{2\varepsilon}$.

Typically, the numerical techniques used to solve equations are explicit or implicit. The method of lines, combined with the enthalpy

method is a more effective mathematical technique which presents itself as being more stable and easier to implement and solve boundary problems [71].

#### 2.2.2. Heat capacity method/Neumann solution

Another typical method for solving phase change problems is the heat capacity method. Lu *et al.* [19] developed a numerical model of a casing PCM radiant floor heating system where he recurred to this method to formulate and solve the simulation.

The initial formulation of the phase change process correlates the transient term, convection term, diffusion term, and source term, respectively, as shown in the follow equation:

$$\boldsymbol{\rho C_p}\frac{\partial \boldsymbol{T}}{\partial \boldsymbol{t}}+\boldsymbol{\rho C_p V}.\nabla \mathbf{T}=\mathbf{div}(\lambda \nabla \mathbf{T})+\boldsymbol{S_T}, \tag{25}$$

where $\rho$ is the density, $C_p$ is the heat capacity, $T$ is temperature, V the velocity, λ the thermal conductivity. If the material is completely solid or completely liquid, there are no density variations. However, during the phase change process the material's properties changes. The Rayleigh number ($R_a$) is calculated to determine whether conduction or convection plays the major role in the thermodynamic process. If its value is lower than 1708, the buoyant force is lower than the resistance imposed by the viscous force heat conduction exclusively occurs [82]. The liquid fraction, $\alpha$, is given by:

$$\boldsymbol{\alpha}=\begin{cases} 0, T<\boldsymbol{T_s} \\ \dfrac{\boldsymbol{T}-\boldsymbol{T_s}}{\boldsymbol{T_l}-\boldsymbol{T_s}}, \boldsymbol{T_s}<T<\boldsymbol{T_l} \\ 1, \boldsymbol{T_l}<T \end{cases}. \tag{26}$$

where $T$ is the temperature of the PCM, with $l$ and $s$ representing the state of the material, it being liquid or solid, respectively. This value changes between 0 and 1 – when the material is fully liquid is one and zero when the PCM is completely solid. With this, the effective density ($\rho_{eff}$) and effective thermal conductivity ($\lambda_{eff}$) changes linearly in accordance with the liquid fraction, and can be calculated by the equations **(27) and (28)**, as presented in Lu *et al.* [19]:

$$\boldsymbol{\rho_{eff}}=\boldsymbol{\alpha \rho_l}+(1-\boldsymbol{\alpha})\boldsymbol{\rho_l}, \tag{27}$$

and

$$\lambda_{\mathbf{eff}}=\boldsymbol{\alpha}\lambda_{\mathbf{l}}+(1-\boldsymbol{\alpha})\lambda_{\mathbf{l}}. \tag{28}$$

From this point, the effective specific heat capacity is calculated by equation **(29)**, where $T_1$ and $T_2$ are the initial and final temperatures of the phase change process, respectively, $L$ the latent heat and $\Delta T$ is half the phase change temperature range (equation **(30)**):

$$C_{\mathrm{eff,p}}=\begin{cases} C_{\mathrm{p,S}}, T<T_1 \\ \dfrac{(C_{\mathrm{p,S}}+C_{\mathrm{p,l}})}{2}+\dfrac{L}{2\Delta T}, T_1\le T\le T_2 \\ C_{\mathrm{p,l}}, T>T_2 \end{cases}, \tag{29}$$

$$\Delta T=\frac{1}{2}(T_2-T_1). \tag{30}$$

Using the previous equations, a simplified equation can be developed:

$$\boldsymbol{\rho_{eff}C_{eff,p}}\frac{\partial \boldsymbol{T}}{\partial \boldsymbol{t}}+\boldsymbol{\rho C_{eff,p}V}.\nabla \mathbf{T}=\mathbf{div}\left(\lambda_{\mathbf{eff}}\nabla \mathbf{T}\right)+\boldsymbol{S_T}, \tag{31}$$

or even further simplified, in case of ignored convective heat, as in Lu et al [19], given by:

$$\boldsymbol{\rho_{eff}C_{eff,p}}\frac{\partial \boldsymbol{T}}{\partial \boldsymbol{t}}=\mathbf{div}\left(\lambda_{\mathbf{eff}}\nabla \mathbf{T}\right)+\boldsymbol{S_T}. \tag{32}$$

The heat capacity method presents itself as being a relatively easy method to implement and managed to provide accurate results [19].

#### 2.2.3. Porous medium method

For this method, a continuous medium for PCM particles is assumed, as well as the usage of a heat transfer fluid and a coupled heat transfer formula for PCM. According to [58], several assumptions must be made, as follows:

- Thermophysical properties of PCMs and heat transfer fluid are independent of temperature variations, except for heat capacity
- There is no heat generation and radiation within the domain
- No chemical reactions occur between the materials
- Plug flow for fluid flow through the voids
- Radial dispersion is negligible
- 1D energy conversion model with negligible temperature variations within PCM

Therefore, the derived energy equations are given by

$$\boldsymbol{\varepsilon(\rho C)_{ht}}\left[\frac{\partial \boldsymbol{T}}{\partial \boldsymbol{t}}+\boldsymbol{V}\frac{\partial \boldsymbol{T}}{\partial \boldsymbol{x}}\right]=\frac{\partial}{\partial \boldsymbol{x}}\left[\boldsymbol{k_{ht}}\frac{\partial \boldsymbol{T}}{\partial \boldsymbol{x}}\right]+\boldsymbol{UA}\left(\boldsymbol{T_p}-\boldsymbol{T_{ht}}\right), \tag{33}$$

$$(1-\boldsymbol{\varepsilon})\boldsymbol{(\rho C)_p}\frac{\partial \boldsymbol{T}}{\partial \boldsymbol{t}}=\frac{\partial}{\partial \boldsymbol{x}}\left[\boldsymbol{k_p}\frac{\partial \boldsymbol{T}}{\partial \boldsymbol{x}}\right]+\boldsymbol{UA}\left(\boldsymbol{T_{ht}}-\boldsymbol{T_p}\right), \tag{34}$$

where A, $\varepsilon$, U, and V are superficial particle area per bed, porosity, overall heat transfer coefficient, and mean velocity, respectively. Their correspondent physical units were not available in the original literature. Different correlations for PCM heat capacity, related to the temperature variations, must be introduced to incorporate the latent heat effect along the phase change. The governing equations for this method can be solved by FDM with fidelity. The major downside of this method is that it neglects the temperature variation within PCM. This causes considerable deviation from experimental results as PCM usually have low thermal conductivities, resulting in a temperature gradient.

#### 2.2.4. Enthalpy-Porosity method

The enthalpy-porosity approach is a common way to develop a numerical model of a PCM [75,86–88]. It is a single domain model in which the melting front is not explicitly calculated. Alternately, a scalar liquid fraction is associated with each computational node in the domain, while the semi-solid porous regions called "mushy zone" are created at the solid/liquid interface as a function of the liquid fraction value. The method greatly depends on two modelling parameters, them being the mushy zone constant and the phase change temperature interval ($\Delta T_{l-s}=T_{liquid}-T_{solid}$). While the first parameter influence has been studied quite extensively for different PCM types, its connection with the phase transition temperature gamut is currently less noticeable. Recurring to this method, the total energy of a material ($h$) is the sum of its latent enthalpy ($h_l$) with the sensible enthalpy ($h_s$):

$$\boldsymbol{h}=\boldsymbol{h_s}+\boldsymbol{h_l}. \tag{35}$$

Having this, the latent heat, $\Delta H_l$, varies from 0, when the PCM is in the solid state to $L$ (which depends on the properties of the material) when the PCM is in the liquid state. In the interval between solid and liquid state, the latent heat depends on the liquid fraction of the PCM, $\alpha$, which is calculated by equation (26) Therefore:

$$\boldsymbol{\Delta H_l}=\boldsymbol{\alpha L}, \tag{36}$$

and the sensible enthalpy of the material, given by

$$\boldsymbol{h}=\boldsymbol{h_{ref}}+\int_{T_r}^{T}\boldsymbol{c_p}\mathbf{d}\boldsymbol{T}, \tag{37}$$

where $h_{ref}$ is the enthalpy of reference and $c_p$ the specific heat at a

constant pressure. From this, the energy equation can be written as equation (38):

$$\frac{\partial(\rho V)}{\partial t}+\nabla(\rho V) = -\nabla \mathbf{p}+\mu\nabla^2 V+\rho g+S, \tag{38}$$

where $k$ is the thermal conductivity, $\rho$ the density and the enthalpy $H = h+\Delta H$ and $\vec{V}$ the fluid's velocity. The source term $S$ accommodates the porosity of the PCM. As the material changes from solid to liquid, it becomes porous, originating the called mushy zone. To describe the porosity of the material, a porosity function is used, which was defined by Brent et al [85]. This porosity function, $\beta$, is dependent on the liquid fraction and is given by:

$$\beta(\alpha) = \frac{M_z(1-\alpha)^2}{\alpha^2+\omega}, \tag{39}$$

where $M_z$ is the mushy zine constant (10,000) and $\omega$ is a constant of value (0.001) to prevent the denominator from being zero. The porosity function must be equal to zero when the material is in liquid phase to allow free motion of the particles. Opposingly, there must be a substantial value when in the solid phase to impose the velocity to be close to zero. The previously mentioned source term $S$ is dependent on the porosity function $\beta(\alpha)$ as is defined as:

$$S = \beta(\alpha)\left(\vec{V}-\vec{V}_p\right), \tag{40}$$

being $\vec{V}_p$ the solid velocity due to the constant pulling of the solidified material out of domain.

## 3. Computational models' layouts and systems

There is an increasing number of researchers that have been developing studies in PCM radiant systems, where multiple numerical tools are created and developed. This section presents practical use cases of numerical modelling in PCM radiant floor affairs, disclosing insightful information, such as the utilized methods, grid properties, attained accuracies, and other properties of the developed models.

Xu *et al.* [12] presented an innovative three phase zone heat transfer model. The phase change zones were referred to as the liquid zone, mushy zone, and solid phase region. The authors recurred to the momentum and energy equation for describing the liquid zone (Equation (15)). As for the mushy zone, the enthalpy method was used to characterize the nonlinear phase change in porosity. Lastly, the continuity equation and momentum equation were based on the modified Brinkmann-Forchheimer-Darcy flow model [86]. As for the modelling tool, COMSOL® was chosen to perform FVM simulation. In the calibration of the numerical model, grids with multiple node counts were tested and compared. 3050, 6388, and 12,778 nodes were used and insignificant differences of only 0.05 K were attained, so the opted node number was the one that required less computing power (3050). Several timesteps of 5, 10 and 20 were used, being the 10 s interval the one with the best results. Furthermore, an analysis and evaluation of the error between the experimental and numerical results were performed and an error of less than 5 % was achieved. The numerical simulation results are shown in Fig. 6.

In Plytaria *et al.* [31], the authors opted to use the TRNSYS® software to model the experimental layout (Fig. 8). The TRNSYS® Type 1270, which is a material type that describes the behaviour of a PCM wall from the TRNSYS® library, was selected to represent the PCM. To achieve the most adequate timestep, a sensitivity analysis was performed. This analysis resulted in the usage of a timestep of 5 min. The final temperature was calculated resourcing to the equation (41). Experimental data from a previous study [87] was used to validate the numerical model.

$$T_{final} = T_{initial}+\frac{\left(\dot{q}_1+\dot{q}_2\right)}{m_{PCM}.C_p}. \tag{41}$$

In another study by Gallardo and Berardi [11], a method for calculating the necessary cooling requirements from a radiant ceiling (Fig. 9) is developed, based on [88] with the aim of dimensioning radiant cooling systems. Surface cooling load is a concept that represents the heat that is to be removed from the convective and radiant components, the surface being the area of the ceiling where the radiant system is integrated (equation (42)).

$$q''_{surf} = q''_{conv}+q''_{lw_{surf}}+q''_{lw_{int}}+q''_{sw_{sol}}+q''_{sw_{int}}, \tag{42}$$

where $q''_{surf}$ is the heat transferred through convection between the radiant surface and the room air (W/m$^2$); $q''_{lw_{surf}}$ is the net heat transferred to the radiant surface by longwave radiation flux from other surfaces in the room (W/m2); $q''_{lw_{int}}$ is the heat transferred onto the

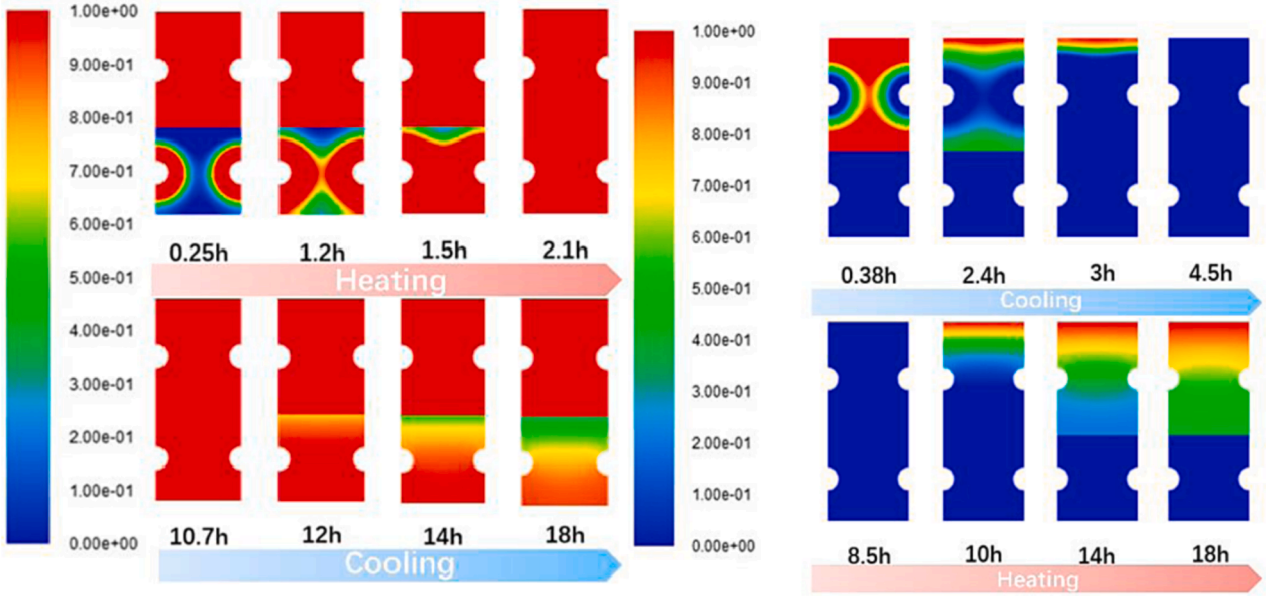


**Fig. 6.** Behaviour of the heat storage PCM layer in both heating and cooling stages [12].

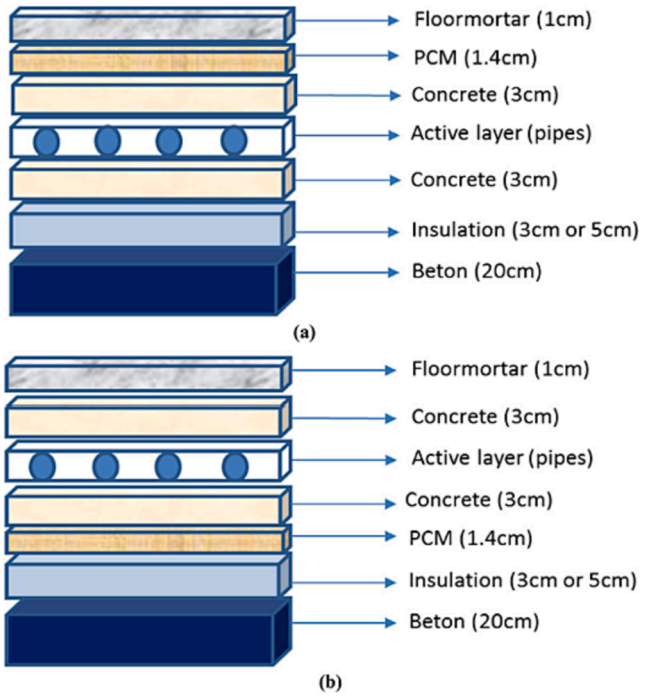


**Fig. 8.** Microencapsulated PCM experimental system layout a) PCM over the pipes and b) PCM under the pipes [31].

radiant surface by longwave infrared thermal radiation that emanated from internal gains such as lights, electric equipment, and people; $q''_{sw_{sol}}$ is the heat transferred by solar radiation onto the radiant surface; and $q''_{sw_{int}}$ is the heat transferred to the radiant surface by shortwave radiation that emanates from electric lighting equipment. The author refers that the conventional sizing of HVAC systems is usually based on peak instantaneous cooling loads during summer, quickly responding to control signals, thus not suitable to size PCM incorporated systems due to their response latency, derived from their high thermal capacitance. Having this, the author [88] proposes the usage of whole year simulations with the sums of hourly values from each 24 h day's total surface cooling loads, resembling methods such as in ISO 11855-4 [89].

The chosen simulation software was EnergyPlus™ v.9.4 to perform the dynamic simulations. The authors opted to use the fully implicit scheme because of its robustness and unconditional stability over time. Simultaneously with this algorithm, an enthalpy-temperature function was used, having in mind the phase change energy. Numerical model validation was done recurring to RMSE. Having the models validated, in order to optimize the system, a parametric design was developed. The models were calibrated with a deviation of ±0.78 °C for the piping location of the PCM panel and ±0.47 °C for the bottom of the same panel, being ±1.5 °C the maximum, according to the German Standard VDI 6020 [90]. Having the models calibrated, the author proceeded to simulate multiple case scenarios, changing the PCM type, the PCM thickness, the water temperature, and the tube length. The results showed that variables such as operation hours, water temperature, and especially the PCM thickness affect the effective storage capacity of the system. The information is presented by plotting graphs with the effective storage capacity of the PCM. The best scenario was with the lowest PCM thickness, pipe length, and operating hours. Then, the authors presented the percentage of occupancy time in an uncomfortable temperature (where the Predicted Mean Value (PMV) values are outside the range between $-0.5 <$ PMV less than 0.5).

González and Prieto [40] used ANSYS® Fluent to develop a numerical model of a PCM radiant system. For the solid domains, the equation (43) was used:

$$\frac{\partial}{\partial t}(\rho i) = \nabla \bullet (k \nabla T). \tag{43}$$

The authors opted for the enthalpy method to obtain the heat transfer rate in PCM, considering natural convection. The continuity and energy equations are solved. The liquid fraction was calculated, and the results are shown in Fig. 10. Due to the reduced porosity in the mushy zone, the momentum equation is considered. To solve the conservation equations, second-order implicit transient formulations were used. The SIMPLE algorithm with the PRESTO scheme was used for the pressure–velocity coupling. Tests were made to the grid refinement in both PCM and non-PCM scenarios. Multiple grid sizes were tested (with 3647, 8196 and 15,356 elements) which presented negligible deviations (from 0.057 to 0.058). The solution became independent from the grid when the timestep of 0.5 s and a mesh size of 8196 elements was used, thus the authors carried on with these values. For $A_{mush}$, the reference value of $10^5$ was used. For the permanent regime, the Turkish Standards Institute (TSI) model was used, as recommended by ASHRAE [91], despite its disregard for heterogeneities and nonlinear thermal diffusivity. The resistance of the PCM radiant floor was determined recurring to the parallel resistance calculation, using the mean conductivity value of the concrete layer and the macrocapsule.

Larwa *et al.* [37], developed and tested a 2D FEM model in COMSOL Multiphysics® considering both steady-state and transient-state. The model was validated in both scenarios in accordance with the experimental results. The mesh was refined close to the PCM containers, as shown in Fig. 11. A number of 21,949 elements were used and selected for the mesh, where 10,024 of them were dedicated to the PCM layer. To assess the independence of the results from the grid, a 45000-element grid simulation was performed, where the changes were negligible. The PCM was considered to be a porous media with both a solid and liquid phase. The definition of the specific heat capacity was made recurring to a normalized Dirac's pulse. The thermal properties of the PCM were calculated and evaluated using a multitude of conditions (flow rate, supply water temperature, etc.). The simulation managed to have an accuracy of 5 % at 23 °C.

Lu *et al.* carried out multiple studies [10,19,92] considering numerical simulations of a Type232 PCM performed in TRANSYS® to predict the behaviour of the system. A diagram of the developed simulation is shown in Fig. 12. To perform the dynamic heat transfer model, the analysis was split into 2 parts, one unsteady state when there is a mixture of both solid and liquid PCM and an unsteady state where only liquid or solid PCM exist. The mathematical description process includes the momentum conservation equation, the continuity equation, and the

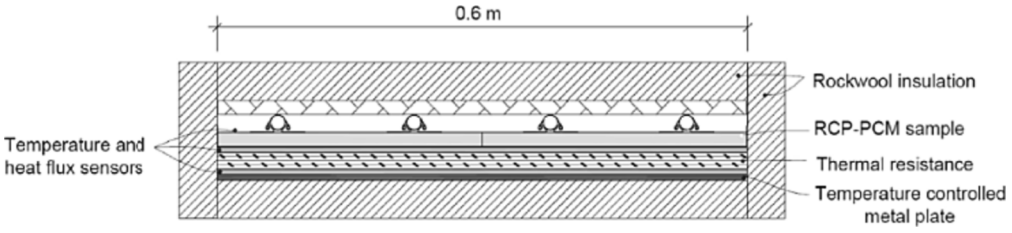


**Fig. 9.** Radiant ceiling modelled system [11].

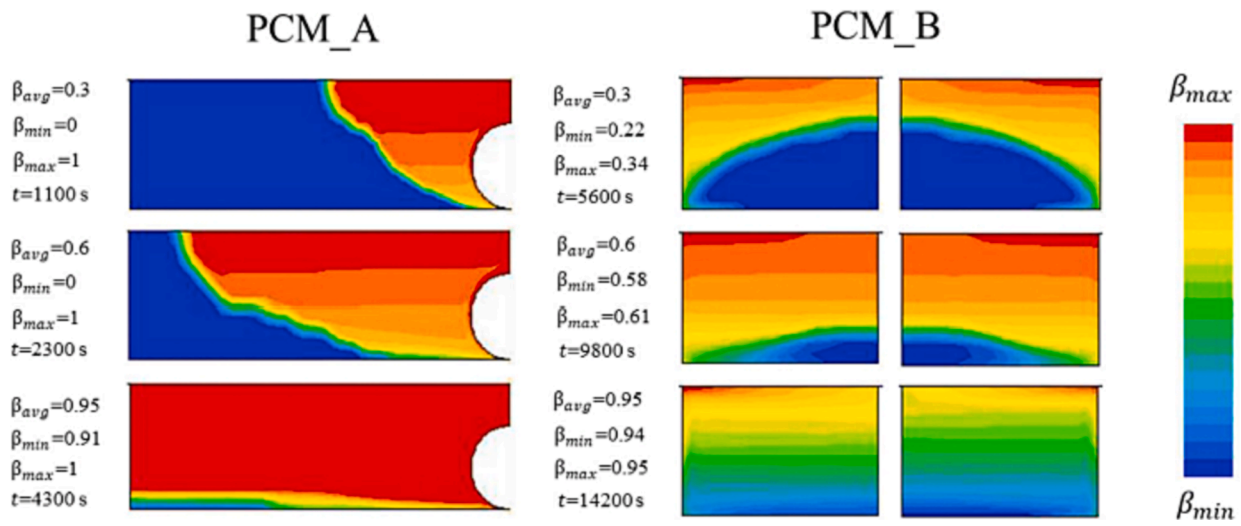


**Fig. 10.** Liquid fractions of the PCM in the macrocapsules A and B [40].

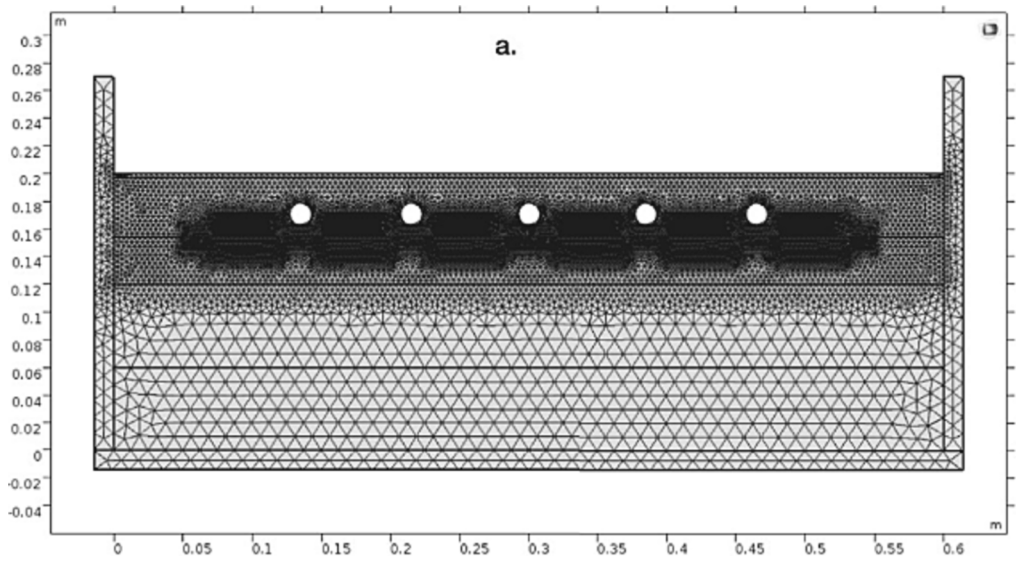


**Fig. 11.** System layout's mesh with varying density [37].

energy conservation equation. The first 2 are not considered as the PCM is enclosed in space. Energy conservation calculation is given by equation (25) using the heat capacity method.

In this model, the source term is a time-varying input term according to the circulating water. The heat transfer is determined to be mainly convection or conductive by calculating the Rayleigh number (Ra). If Ra is smaller than 1708, the buoyancy force is superior to the viscous force, thus the convection term may be ignored.

To assess the melting and solidification stages, the liquid fraction was used, which was then used in a linear interpolation alongside the PCM's fully liquid and solid density ($\rho_l$ and $\rho_s$), as well as the PCM's fully liquid and solid thermal conductivity ($\lambda_s$ and $\lambda_l$) in order to calculate the effective density ($\rho_{eff}$) and the effective thermal conductivity ($\lambda_{eff}$) of the PCM as demonstrated in equations (27) and (28).

To solve the partial differential equations, the interface tracking method and the fixed grid method are used. The first converts the irregular interface into a discretizable regular interface, allowing to know every node's temperature at any time, which increases the difficulty of solving the equations. The former was chosen as it does not require the determination of the solid–liquid interface, which makes it simpler. The fixed grid method can be solved by recurring to both the enthalpy method and the apparent heat capacity. The apparent heat capacity method was chosen as it solves the temperature directly, facilitating calculation and because due to experimental conditions, the enthalpy of the PCM could not be tested at different temperatures. To represent the nonlinear variation of the specific heat capacity ($C_{eff.p}$) with a simplified step, equations (29) and (30) were used.

when validating the data from the numerical model, a couple of strategies were used, the relative error (MRE) and the Bland-Altman consistency analysis. The results show an MRE of 4.82 %. The Bland-Altman consistency analysis of the reference building shows that $\bar{d}$ is (−0.005), Sd is 0.38, ($\bar{d} \pm 1.96$Sd) is (−0.79,0.70) and 97 % of the data are set in the consistency interval. Thus, the established model is both approximately accurate and reliable.

Mohammadzadeh and Kavgic [93] developed a simulation-based optimization of a PCM radiant floor system. Two scenarios were studied, the first being the optimization of the design variables PCM melting temperature and thickness. The second scenario was composed of the study of seven parameters, including PCM melting temperature and thickness, insulation thickness and thermal conductivity, floor thickness, thermal conductivity, and solar absorbance. For the numerical simulation, EnergyPlus was used and the results for the optimization

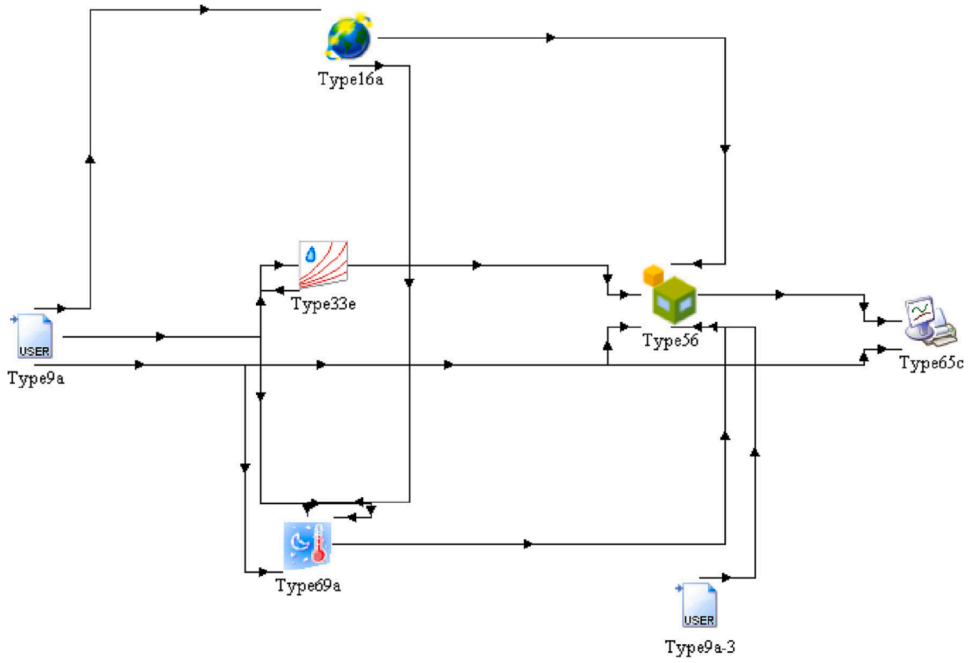


**Fig. 12.** TRNSYS diagram for the system layout [92].

were to be used in MATLAB. The integration of this software can be seen in Fig. 13. A sensitivity analysis was made to assess the impact of small changes in circulating fluid flow and temperature, recurring to FDM. It concluded that an increase of 1 % of the circulating fluid temperature had more impact on the system's energy demand than the same increase in fluid flow - up to a magnitude of two times.

## 4. Discussion and analysis

### 4.1. Numerical model's mathematical formulations

While being highly accurate, compared to analytical models, CFD simulation models of indoor environments require extensive computational costs, leading researchers to develop steady state models, which do not provide the whole panorama of the expected performance of the systems under real-world dynamics [54]. This contradicts the nature of radiant systems, which store and release energy. To overcome this contradiction, quasi-steady state models can be developed. This, coupled with the advancements in computing makes transient finite volume-based simulations more accessible and feasible, opening opportunities to develop work in the literature. Semi-analytical models have advantages over purely analytical models, as they are more versatile and use non-constant parameters [64]. As previously mentioned, in Weber and Jóhanneson [61] and Liu *et al.* [60], R-C models have proven to be very accurate and have very little computational cost when compared to FEM, FMD and BEM methods, making them desirable in order to save time and complexity in numerical simulations.

Despite the vast number of articles regarding the numerical simulation of thermal systems, there is a lack of articles where comparisons are made between multiple methods, making it difficult to extract conclusions on which method is the most suited for a certain scenario.

### 4.2. Phase change materials modelling

In Iten *et al.* [79], a direct comparison between the enthalpy method and the heat capacity method was developed regarding the same numerical model of the air-PCM system. The authors concluded that the heat capacity methods showed the most promising results, especially regarding the PCM temperature. The errors of the heat capacity method were 2.6 % and 1.4 % when charging and discharging, respectively, compared to the worse 5.7 % and 4.9 % from the enthalpy method, due to the lever rule, which regards the temperature and enthalpy's relationship as linear, negatively affecting the sensible heating and cooling. Regarding the air intake, both had similar errors of about 1.4 %, as they are not sensitive to the lever rule. The authors finish their conclusions by recommending the usage of the heat capacity model.

In another study, Zhang [72] developed a numerical model using the heat capacity method and compared it's results to a former study in which the enthalpy method was utilized. The author concluded that the deviations of the enthalpy method were more significant. In this study, using the heat capacity method, the maximum relative errors were less than 2.7 % and 5.2 %.

Zang *et al.* [50] claimed that the accuracy of the heat capacity method was always higher than that of the enthalpy method, caused by the way how the methods treat the latent heat. While the enthalpy method treats the sensible heat as a linear function, data from the DSC showed it to have a parabolic behaviour. Three impact factors on the effectiveness of the methods were studied, them being whether the phase change range was unified, the phase change range and whether the liquid fraction was considered, which are in decrescent order of impact. Finally, the authors concluded that due to the way sensible heat is treated in the methods, the enthalpy method had lower accuracies than that of the heat capacity method.

In a study developed by Reichl *et al.* [94], a comparison was made between two CFD models in ANSYS. These models were a solidification and melting (SM) model based on the enthalpy porosity method and the apparent heat capacity model (AHC). Both methods showed small deviations lower than 2 %. In this study, the authors concluded that phase prediction sing both models is very accurate when natural convection behaviour is included. The AHC method allows for good prediction of phase front movement and temperature distribution. However, the SM model had more difficulty in being applied to different cases due to the mushy zone constant being very closely related to the experimental data. This made the AHC model the one recommended by the authors.

Wijesuriya *et al.* [95] compared and analysed the enthalpy method and the heat capacity method across several CFD simulation software (EnergyPlus, ESP-r and WUFI). The results presented a good accuracy, and to assess and evaluate the results they used the RMSE, CV(RMSE)

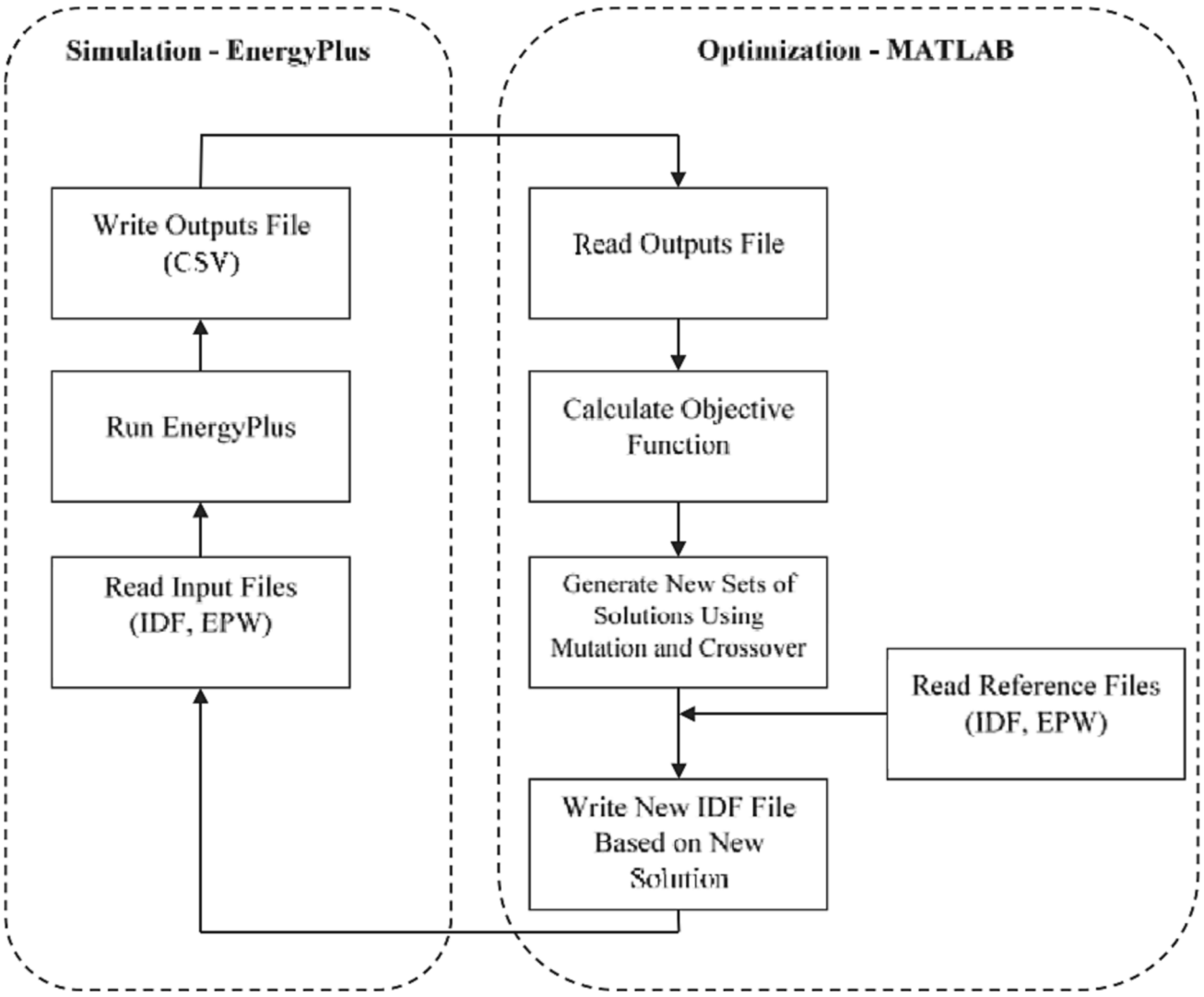


**Fig. 13.** Integration of EnergyPlus and Matlab for result optimization [93].

and NMBE statistical calculations. Furthermore, the authors compared two developed models, one in COMSOL and another in MATLAB, which demonstrated that there were no significant gains in performing a 2D analysis over a 1D. Furthermore, the authors admit that more work is needed regarding different types of macroencapsulated PCM applications when 2D and 3D (3 dimensional) both hysteresis and heat transfer effects have more intense effects.

Regarding the presented CFD modelling software and methods, the use of the heat capacity model provides the most accurate results and is the one that takes the least time to accomplish its results [96].

Phase change materials have a non-negligible change in density upon phase change, which can reach values of more than 10 % between solid and liquid phases. In real case scenarios, this behaviour can affect the mechanical stability of the system and its structural integrity. The presented models consider multiple ways for calculate the heat transfer, considering different variables, as the specific heat and enthalpy of the material in both physical states (solid, liquid) and during the transition phase. The lack of studies considering density changes and their impact on the PCM radiant system's structural integrity creates a possible area of research to be further explored by researchers in future works.

### *4.3. Computational model's layouts and systems*

Regarding the aforementioned literature, it can be stated that it is possible to successfully represent a PCM radiant system with any of the available methods and software with relatively low errors of 5 % or lower. Despite the heat capacity method being the most accurate among these, the enthalpy method is more adopted in the literature. All of the studies demonstrate varying degrees of timesteps and nodes in the simulations, depending on the developed system design. The authors experiment with multiple values and once the results stabilize, the authors utilize the lowest value possible, as to reduce the computational cost of the simulation. Regarding the node number of the simulation, it is a common practice to use a denser mesh in the interface between the PCM macrocapsules/ activated layer and the non-PCM materials, which is the zone with the most complex thermal behaviour due to the phase changes.

## 5. Future direction of technology

With the development of this article, it is noticeable the developments already made regarding numerical modelling and simulation in general. Other researchers have developed quality research work in this field, developing new algorithms to simplify and solve the system's behaviour and methods. Advancements in technical-scientific knowledge in the engineering field allow new developments considering more detailed and complete solving methods and algorithms. Together with the latest breakthroughs in computational science,

modern workstations, and commercial software, complex calculations can be performed in a fraction of the time. Besides the time savings, the model's accuracy improved, providing more reliable results and allowing researchers to further expand the boundaries of scientific knowledge. Further developments on computational science will enable us to compute already existing numerical models that were too complex for old technology to solve. Furthermore, new developments in the mathematical methods will describe more accurately the behaviour of a system whilst reducing its complexity, as to increase the reliability and efficiency of results. All these benefits will provide more accurate data in less time. The aggregate of these developments will result in information with more quality, accelerating the innovation of the science in this research areas.

However, there are some gaps of information in the literature, which create interesting opportunities for further developments. There is a lack of studies comparing multiple simulation approaches to the same problem, which limits the possibility of comparing and analysing data. Moreover, the dependence of current PCM numerical model techniques in enthalpy is very noticeable. There are plenty of other models that can be alternatively used, such as exergetic based models, which would result in novelty work. This, combined with the lack of exploration of the porous medium method would result in an innovative work. Furthermore, there aren't many 3D complex transient models developed, mainly due to the lack of computational power, leading researchers away from using these methods and focus the research on 2D simple models. One way to overcome this obstacle is to develop more efficient numerical models that would be less computationally costly or to embrace this hardship. Although, studies which take more time to complete can provide more insightful data, providing to the authors an opportunity to present and publish novel works. There is still more work to be develop regarding the capabilities of the simulation software and raw computational power, as well as the development of new less computationally costly numerical methods. Another area which lacks development is the presentation, comparison, discussion, and review of PCM modelling schemes. The use of numerical modelling is very diverse, changing from study to study, and according to the researcher's approach to the problem. More developments in this subject are welcome, as they could provide more insight into practical numerical modelling development, helping new researchers to give their first steps in this field with more thoughtful inputs and rationalized choices.

## 6. Conclusion

The development of this article aimed at compiling and critically reviewing relevant information in the literature to provide readers with a comprehensive outlook of the numerical modelling of thermal systems, focusing on numerical methods that describe phase change materials in radiant systems enhanced with PCM. This review begins with an introduction to the subject of general radiant systems, including their applications, types, and operation methods. This is followed by an introduction of the relevance of numerical modelling in the development of thermo-mechanical systems. Lastly, a multitude of existing reviews in the literature is reviewed, as to elaborate on the necessity and pertinence of the development of this new review. In section 2, numerical modelling methods are enumerated, described and compared. In subsection 2.2, the numerical modelling methods of PCM systems were more thoroughly focused, as this subject was lacking in the literature. In section 3, innovative recent studies with practical cases of numerical modelling applications are disclosed. Here, examples of the applications of the formerly exposed numerical modelling methods are presented. In section 4, the authors discuss and critically analyse the previously presented information. Model's accuracy, efficiency and use cases are compared. This is followed by a discussion of the future direction of technology in section 5. Lastly, in section 6, the authors summarize the article and state the most important conclusions.

Concerning generic numerical models of radiant systems:

- Simplified numerical models are easily integrated into building simulations, but have many limitations, such as considering solar incidence in the wall of a building. Opposingly, detailed models are very robust but unfeasible to adopt, as they are too computationally expensive, opening the opportunity for hybrid models.
- Transient state models should replace the currently developed steady state models as they represent more accurately the dynamic nature of the system's thermal behaviour.
- R-C models are computationally cheap and effective.
- Numerical simulations of general thermal systems are well available in the industry.
- There is a lack of studies comparing multiple simulation approaches. There is opportunity in the literature to develop work in this field, to further comprehend the benefits of each method.

Relatively to the numerical modelling of PCM systems:

- There are no articles that fully disclose a comparison between all methods of the numerical model of PCM, therefore there is no certainty about which model is best. This opens an interesting opportunity for further research, as in the development of an article which compares all methods with one set of experimental data.
- The choice of the method to use will always be dependent on the interests of the researcher, whether being the fastest to complete or the most accurate.
- There is very little information in the literature regarding the porous medium method.
- Most of the available literature refers to models that depend on the enthalpy of the system. The use of other alternatives, such as recurring to exergetic models is still lacking on the literature, creating a window of opportunity for researchers to develop innovative work on this subject.
- The literature agrees that the apparent heat capacity method is the one that gives the most accurate results.

## Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## Data availability

No data was used for the research described in the article.

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