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Data-Driven Integrated Decision Model for Analysing Energetic Behaviour of Innovative Construction Materials Capable of Hybrid Energy Storage

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Abstract: Aligning the European Union goals for climate neutrality by 2050 and the ambition for carbon equivalent emissions reduction to almost half by 2030 demands the exploration of alternative decarbonisation pathways. Energy consumption across all sectors is identified as a crucial contributor to this challenge, with a number of legislative and regulatory frameworks and commitments to be introduced every year. In response to these trends, the concept of exploiting a building's thermal mass through the integration of phase change materials (PCMs) enhances the ability of building elements to reserve and deliver large amounts of energy during phase transitions. However, the incorporation of PCMs into building elements requires the thorough understanding of their thermal behaviour. This study evaluates and predicts the thermophysical properties of mineral particles carrying PCMs and coated with a cementitious layer able to be utilised as fillers in construction applications. By employing deep learning and predictive modelling techniques, the numerical data-driven model developed in this paper enhances accuracy and efficiency in property estimation and prediction, facilitating material selection, system design, and optimisation. A model in a MATLAB simulation environment is presented, evaluating and predicting the thermophysical properties of semi-organic particles able to enhance building envelope thermal mass as a hybrid energy storage solution. These findings show the time needed for a building block to undergo cooling, demonstrating a clear upgrade in the thermal discharge of the walls. Substituting traditional EP with PCM-enhanced EP leads to a minimum reduction of 1 °C per hour in the discharge rate, thereby extending the comfort duration of indoor spaces without necessitating additional space heating. These models offer the potential for assessing diverse material compositions and usage scenarios, offering valuable insights to aid decisions in optimizing building energy efficiency.

Keywords: thermal mass; hybrid PCM; thermal performance; construction materials; data-driven modelling; thermal conduction; phase change; transient heat transfer



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1. Introduction

The European Commission has set climate neutral targets to reduce carbon emissions by 40% by 2030, while in parallel increase the penetration of Renewable Energy Sources (RES) up to 32% and enhancing energy performance by 32.5%. This can be quantified under the European climate law that expects the EU countries to overall minimise their carbon-related emissions by 55% by 2030. Investigating the benefits deriving from shifting electricity demand in buildings highlights the potential for exploiting the available thermal energy storage capacity resulting from the fabric mass of a building for applying pre-heating or pre-cooling strategies to the building. This concept introduces a passive energy storage system named “structural thermal energy storage” which employs the mass of the structural elements—i.e., walls, slabs and ceilings—to store thermal energy and retrieve it at a later time [1]. The efficiency of this strategy has been proven for ages, with a typical

case being the passive night cooling of heavyweight buildings as a traditional way to treat the heated thermal mass of stone or concrete in hot climates. Extending further to a smart grid context, the effective activation of structural thermal energy storage is also promising.

Furthermore, the Materials 2030 Manifesto stresses the European need for developing innovative, sustainable, solution-oriented construction materials which will enable accelerated, scalable, and cost-effective responses to the energy and climate challenges today and in the future. As an essential milestone in advancing the European Materials Initiative, the draft Materials 2030 Roadmap emphasises the incorporation of digitalization into materials development, presenting a significant opportunity to expedite the entire materials design and innovation process. This vision entails the adoption of cutting-edge research and development methodologies that seamlessly integrate computational and experimental materials sciences, capitalizing on techniques such as modelling, simulation, and high throughput characterization. A critical factor for its successful implementation revolves around ensuring reliable and unrestricted access to data. This forward-looking approach holds the potential to revolutionize the creation of novel materials, transcending the limitations of traditional discovery pathways, and granting precise control over material behaviours [2].

In response to these trends, thermal storage in buildings can be achieved at both high and low temperatures, aligning with the respective heating and cooling processes. The utilisation of PCMs for conserving thermal energy assumes a crucial significance in the context of building cooling and heating. The incorporation of these materials results in a reduction in energy consumption within the cooling and heating systems, achieved through load reduction or load shifting strategies. Furthermore, the integration of these materials contributes significantly to enhancing indoor thermal comfort by effectively mitigating indoor temperature fluctuations, thus creating a more stable and pleasant indoor environment. Rao et al. [3] conducted a comprehensive review focusing on the potential of PCM-mortar as a thermal energy storage medium in buildings. Moreover, they delved into an examination of the mechanical properties exhibited by these materials. Their findings revealed a strong correlation between the mechanical characteristics of PCM-mortar and their ability to efficiently store thermal energy, a relationship attributed to the microstructure of the materials. An intriguing prospect for building applications lies in the impregnation of phase change materials into porous construction materials commonly utilized in buildings, such as gypsum, concrete, and plasterboard. This integration serves to enhance the thermal mass of the building components, thereby positively impacting thermal performance and energy efficiency. However, the integration of PCMs into building materials requires a thorough understanding of their thermal behaviour [4]. The correlation between the compression, deformation, thickness, and thermal performance of porous composites should be specified because it has a direct influence on the energy efficiency of the building.

Certain porous materials, such as expanded perlite, exhibit the ability to adsorb phase change materials through their inherent capillary actions, even when in a liquid state. The structure of expanded perlite consists of approximately spherical particles that possess pores on their surface, known as intra-particle pores (refer to Figure 1). These pores are formed when the chemically bound water (2–6%) in volcanic glass transforms into steam due to rapid heating (700–1260 °C). As a result, the volcanic glass expands by about 20 times its original volume, giving rise to the term “expanded perlite” (EP). When utilized as an insulating material, the spherical EP particles arrange themselves in a random pattern [5].

In its conventional form, EP exhibits irregular shapes and possesses an extensive network of open pores that become evident on their fractured surfaces, consequently affecting their performance characteristics in end-use applications. Among the crucial quality attributes of EP, the loose bulk density, compression strength, and distributions of inner and surface pores hold significant importance [6]. The grades of EP can vary widely in terms of size distribution, offering diverse applications in the realm of construction technologies. Typically, particle sizes ranging from 2.5 to 0.6 mm are well-suited for use

in plasters, mortars, lightweight concrete, and loose-fill insulation, while finer grades, such as 1.4 to 0.3 mm, find application in the manufacturing of ceiling tiles and boards. Introducing EP into construction mixes, such as concrete, mortars, or plasters, leads to an array of improved physical properties. These improvements comprise a reduction in product density and an enhancement of its thermal insulation characteristics [7]. The porous nature of EP holds exudation during the phase change process, primarily due to the interplay of capillary and surface tension forces. Additionally, expanded graphite is considered as a viable option for improving heat transfer in PCMs, including exceptional stability, compatibility with organic PCMs, high thermal conductivity, and low weight.

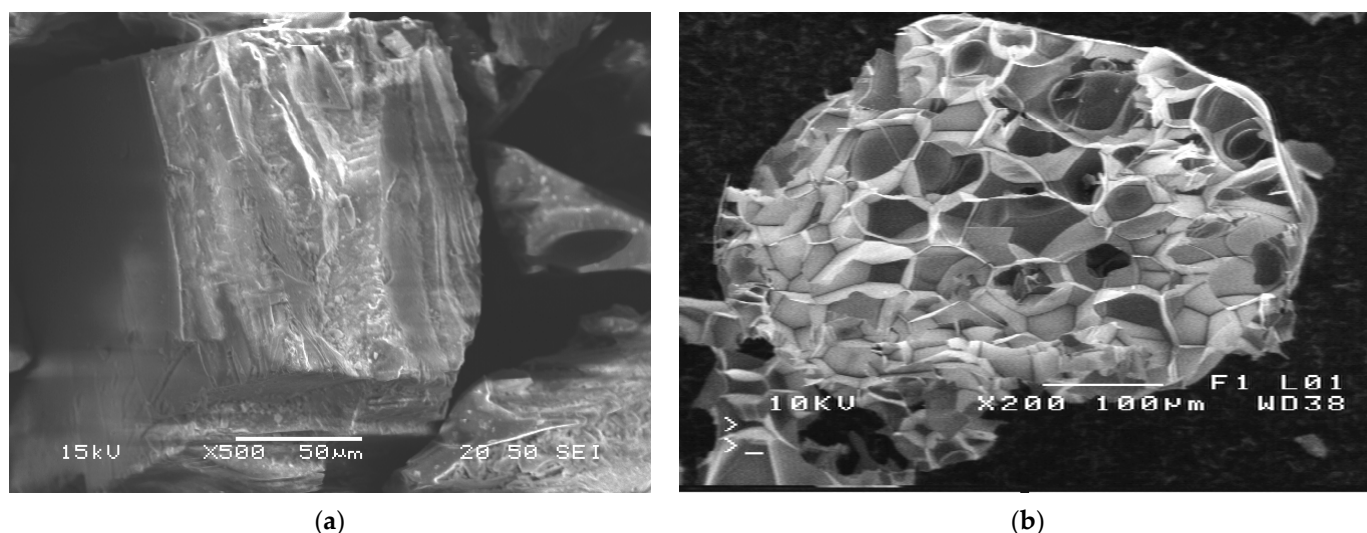


Figure 1. SEM images of (a) unprocessed perlite at 500 $\times$, 50 μ m; (b) expanded perlite at 200 $\times$, 100 μ m.

Since 2018, the field of heat transfer analysis for PCMs has been a dynamic and evolving area of research [8–20]. Computational methods and numerical simulations were widely used to analyse and predict the behaviour of PCMs under complex thermal conditions and facilitate the design and optimization of PCM-based systems. The utilisation of empirical and numerical simulation and modelling offers several advantages, including efficacious, cost-effective analyses while reducing the costs required for conducting physical experiments, especially when studying complex systems or when dealing with expensive or hazardous materials. In addition, the realisation of different scenarios under a wide range of conditions without putting personnel or equipment at risk provides flexibility, safety, as well as in-depth insight and detailed understanding of PCM behaviour which may not be achievable through experiments alone [21]. In view of this, numerical simulation and modelling are valuable tools for understanding and optimizing the thermal behaviour of PCMs. Regardless, taking into account their limitations and the need for careful validation, numerical simulation and modelling should be used in a way to establish whether the generated data meet the physical requirements for thermal energy storage applications [22].

Assumptions and simplifications are an essential part in the study of PCMs. They are used to make complex problems more tractable, but they also introduce a level of approximation. For that reason, models may not capture the level of accuracy of real-world systems. In this frame, the selection between steady-state and transient analysis can impact the programming cost, accuracy, and complexity of the models. Steady-state analysis is computationally less demanding than transient analysis, making it faster and more suitable for parametric studies and initial assessments of PCM systems. However, it may lead to inaccurate results when the time-dependent behavior of the PCM is crucial to the study or application. For example, it cannot accurately represent the behavior during the charging and discharging of a PCM energy storage system. On the other hand, transient analysis

is highly accurate when the behaviour of the PCM system over time is essential. It can capture dynamic changes, including phase change, heat flux fluctuations, and temperature responses. Yet, transient simulations are computationally expensive and may require longer simulation times compared to steady-state simulations. In Ghani et al.'s study [23], a dynamic neural network has been developed to characterize the thermal properties of a latent heat storage system. The model achieved a remarkable accuracy during the slow melting of the PCM, whereas some disparity emerged during the rapid solidification process. When compared with experimental data, the errors for the charge and discharge phases were approximately 5.1 and 7.1%, respectively. Nevertheless, the limitation of this approach is the experimental data required for training the network. Compared to a steady neural network, transient operations are a computationally time-consuming process.

Heat transfer phenomena can be studied in either one dimension (1D) or more than one, (2D) or (3D). Modelling in 1D can be assumed when the system is relatively uniform along one dimension and accuracy can be maintained with this simplification. It is appropriate for initial assessments and when computational efficiency is crucial. Accordingly, when accuracy is crucial, particularly in scenarios with complex geometries or where non-uniform temperature distributions occur, the modelling is performed in 2D or 3D. While more computationally demanding, it provides a realistic representation of the physical processes and is essential for capturing accurate results in such cases. Gao et al. [14] performed an experimental and numerical analysis on the determination of the two-stage heat transfer characteristics of the constrained melting process of PCMs. In this study, a two-dimensional domain was analysed with the open source CFD software OpenFOAM, neglecting the heat transfer in the axial direction. The results were that the generated data agreed well with the experimental measurements, with the relative deviation within $-2\% \sim -7\%$. The development and validation required melting experiments by a combined use of photography and infrared technique. Günther et al. [24] introduced a 1D model for a simple but expedient simulation of subcooling and solidification processes in the PCM, based on the explicit finite volume method and the enthalpy method. An experimental validation was then performed to prove the adequate prediction of PCM quantitative behaviour. The geometry is assumed linear and one dimensional and the phenomena of convection or radiation are neglected. The results reflect the experimentally observed phenomena well, based on visual comparison, while further investigation is suggested.

In continuation of the reviewed studies performed at the material scale, this study aligned the Energy Efficiency Directive and the Materials 2030 Manifesto aims to evaluate and predict the thermophysical properties of mineral particles carrying PCMs and coated with a cementitious layer able to be utilised as fillers in construction applications at a macro scale. A model in a MATLAB simulation environment is presented, evaluating and predicting the thermophysical properties of semi-organic particles able to enhance building envelope thermal mass as a hybrid energy storage solution.

2. Phenomena under Study: Basics on Heat Transfer

The key feature of exploiting the energy potential of the hybrid PCM-enhanced construction material is to handle and moderate the heat transfer phenomena occurring between the building's elements (i.e., walls, roof, etc.) and the internal and external environment. Gaining insight into the main mechanisms that govern the heat transfer, the physical problem description, and the theoretical and numerical approach will be presented.

2.1. Thermodynamics and Heat Transfer Theory

Thermodynamics studies the amount of heat being transferred under steady equilibrium states and changes from one equilibrium state to another. The Heat Transfer theory analyses nonequilibrium thermal phenomena that are closer to the real ones. The fundamental condition for heat transfer between two mediums is to apply a temperature difference. The amount of temperature difference determines the rate of heat transfer, which depends on the temperature gradient per unit length or the rate of change of temperature

in that direction [25]. The heat transfer rate by definition represents the thermal energy transferred per unit of time. Thermal energy can be divided into sensible and latent heat. The sensible energy or sensible heat of a system corresponds to the kinetic energy of the molecules. Respectively, latent energy or latent heat is associated with the intermolecular forces between the molecules of a system, which once changed, can enforce a phase change process because of the added or removed energy.

2.2. Heat Transfer Mechanisms

Heat transfer occurs in three different ways, including conduction, convection, and radiation. Conduction describes the transfer of energy from a more energetic particle to the adjacent less energetic one as a result of interactions between the particles, and can take place in solids, liquids, or gases. Similarly, convection is associated with the macroscopic mass motion and involves the combined effects of conduction and fluid motion. The radiation is the energy emitted by matter and is facilitated by the propagation of electromagnetic waves, rendering it the sole heat transfer mechanism in a vacuum environment. [25,26].

For the purpose of this study, the heat transfer mechanisms that are considered for evaluating the thermal behaviour of a wall under charging and discharging processes are the conduction. The governing equations and approach will be described below.

Conduction Mechanism

According to the “Fourier Law”, the heat conduction rate is related to the geometry of the medium, its thickness, and the material of the medium, as well as the temperature difference across the medium.

$$q = -k \cdot \nabla \cdot T \quad (1)$$

where q is the local heat flux [W/m^2], k is the material's conductivity [$\text{W}/\text{m}\cdot\text{K}$], and ∇T is the change in temperature [K]. The minus signifies that the heat is being conducted in the reverse direction of the thermal gradient. Conductivity can be affected by external but only thermodynamic factors, such as temperature and pressure.

In this frame, the differential form of Fourier's law when it is applied on a continuous system (integrating the Continuous Equation) is expressed as follows:

$$\rho \cdot c_p \cdot \partial T / \partial \tau = -k \cdot \nabla \cdot T + q \quad (2)$$

where ρ is the material's density, [kg/m^3], c_p is the specific heat capacity [$\text{J}/\text{kg}\cdot\text{K}$], T is the temperature [K], τ is the time [s], k is the thermal conductivity [$\text{W}/\text{m}\cdot\text{K}$], and q is the internal power source [W].

By assuming that there is no internal power source to the system and the thermal conductivity is constant, the Equation (3) gives:

$$\rho \cdot c_p \cdot \partial T / \partial \tau = -k \cdot (\partial^2 T / \partial x^2 + \partial^2 T / \partial y^2 + \partial^2 T / \partial z^2) \quad (3)$$

where x , y , and z are coordinates in the three dimensions.

2.3. Phase Change Heat Transfer

As discussed before, adding thermal energy by heat transfer mechanisms to a system increases the temperature of a substance. In addition to heat transfer being classified into thermal conduction, thermal convection, and thermal radiation, thermal energy can be transferred by phase change. During a phase change, a substance undergoes a change from one phase to another without changing its temperature. Instead, the excess thermal energy (also known as latent heat) acts to loosen bonds between molecules or atoms and causes a phase change [27].

The key feature in a phase change problem is the presence of a moving boundary (or region) in which heat and mass balance conditions have to be met [26]. In the scope of

this study falls the solid–liquid phase change problem, also known as the Stefan problem, which aims to determine the evolution of the moving boundary between two phases of a phase change material (i.e., ice to melting water) over time.

The one-dimensional single-phase Stefan problem [13] is based on having a PCM block (with width of W) that is primarily in a solid state and an imposed constant heat flux q'' is imposed at its left boundary, leaving a region $[0, s(t)]$ occupied by water. The temperature T_{ini} in the solid region is equal to its melting point T_m . Hereby, the PCM is divided into two subregions, the solid region on the right and the liquid region on the left. The term $s(t)$ indicates the melted depth moving towards the right over time (see also Figure 2).

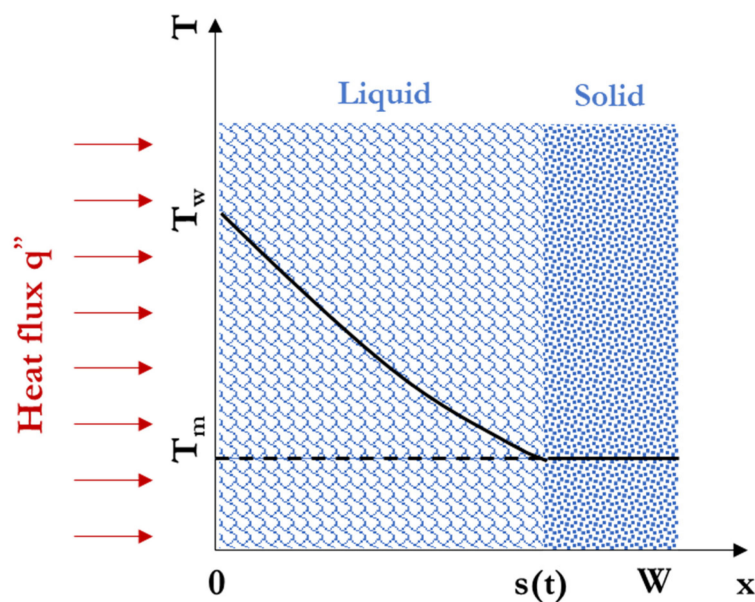


Figure 2. Schematics of the 1D single-phase melting problem under constant heat flux condition.

The main assumptions made include the neglect of the natural convection inside the liquid region, as only heat conduction is considered. Additionally, it is considered that the thermophysical properties of the PCM are dependent only on the phase of the PCM and not the temperature.

The Stefan Problem, after considering the restrictions above, facilitates a straightforward solution, considering one-dimensional semi-infinite PCM layer model. This model can be solved by applying some thermal restrictions:

1. At $\tau = 0$ s, the composite is in liquid form heated at the melting temperature: ($T_0 = T_{melt}$);
2. At $x = 0$ m, the temperature is set to T_0 and remains constant.

The governing equations for the liquid and solid state are described below.

Heat transfer when only thermal conduction is considered on the x axis derives from Equation (4):

$$\rho \cdot c_p \cdot \partial T / \partial \tau = -k \cdot (\partial^2 T / \partial x^2), \quad (4)$$

The liquid–solid interface is governed by the enthalpy equation as:

$$\rho \cdot \Delta H_{pc} \cdot ds(\tau) / d\tau = -k \cdot (\partial T / \partial x) \quad (5)$$

where ΔH_{pc} is the latent heat of fusion of the PCM [J/kg] and $s(\tau)$ is the position of interface [m]. In this regard, Stefan introduced several analytical solutions [27–30]. The solutions to this problem were mainly one-dimensional, while the assigned boundary as well as the initial conditions used were simple and mostly constant, hence excluding the mushy zone of the considered solutions. On this ground, numerical techniques can be found in the literature aiming to determine the moving boundary of phases as well as estimate the velocity of the mushy region.

Solving the Stefan problem is also approached through different techniques, including finite difference, finite element, and finite volume. Such techniques provide reliable and widely acceptable results for several engineering problems. It is evident that the methods and models for PCMs rely on discretization techniques using mathematical equations to describe the physical phenomenon. Among the abovementioned models, the enthalpy method is the most frequently used method, as reported by Madad, Mouhib [10].

3. Methods

3.1. Model Development Concept

The understanding and evaluation of the thermal properties of composites using high sorptive industrial minerals carrying PCMs is necessary for the analysis of the energetic behaviour of innovative construction materials capable of hybrid energy storage. In this line, the concept of the models developed is to combine numerical formulations and experimental measurements in order to successfully simulate the thermal behaviour of the hybrid materials throughout a thermal cycle, as well as predict their behaviour based on selected external parameters. Through the development of data-driven models and application of deep learning techniques, the generated thermophysical properties of mineral particles carrying PCMs and coated with a cementitious layer can be corrected, and the model's accuracy can be enhanced. The delivery of this system facilitates the material selection, system design, and optimisation for thermal energy storage able to enhance building envelope thermal mass as a hybrid energy storage solution. The structure of the algorithm comprises the following modules: 1. data collection; 2. data-driven objects; and 3. heat transfer Performance module.

3.2. Data Collection Module

Numerous studies can be found in the literature, with the main scope being to experimentally investigate the thermophysical properties of hybrid PCM composites. The structure of the studies includes the preparation of the composite by mixing the melted PCM with an inorganic carrier and then the testing and measuring of their behaviour with laboratory equipment. The exploitation of these results and measurements is investigated to develop a detailed, in-depth catalogue comprising different materials (i.e., PCMs), analytical methods, and quantified properties. A popular way of sharing results is to design diagrams and figures depicting the evolution of thermal and physical parameters corresponding to an independent variable (i.e., temperature, pressure), which can be controlled and managed externally. Therefore, designing a tool for extracting data points from image files enables the fast and efficient acquisition of data from diverse system options, materials, and tests.

The Image-to-Data conversion tool is developed in a MATLAB environment and is capable of reading the image formats of BMP, JPG, TIF, GIF, and PNG files (anything that is readable by `IMREAD`). The application is based on four steps and its structure derives from GRABIT tool [31]. The tool consists of the functions summarised in Table 1.

3.3. Data-Driven Objects

The data collection module is required to store, manage, and exchange the acquired information for further processing. In this frame, object-oriented programming (OOP) can facilitate these actions by enabling the grouping of the model's data parameters (properties) with its functions (methods) into a single definition, or class [32]. Object properties hold different types of data, including numbers, text, or other objects. The functions and methods execute numerical and logical calculations on the objects themselves. In this sense, functions enable modifications on the object properties or act as an object. The objects can then be used as building blocks in applications in order to simulate and analyse complex systems. The benefits of using object-oriented programming in MATLAB also include avoiding code duplication by creating reusable objects with well-defined interfaces that hide the complexity of the underlying code.

Table 1. Image-to-Data conversion tool functions description.

Function	Description
selectData	The callback is executed for selecting the data points from the image. When the variable is clicked, it enables the verification of the selected points by plotting the data in a Preview area. It also ensures that the variable in the base workspace is the same copy as the variable stored in the tool's workspace.
loadImage	This function loads an image file and draws the image to the display window. It also initializes image data.
adjustImage	The function performs calibration of the image by prompting the user to select points for where the X and Y axes are located and set values for X limits min and max and Y limits min and max. It is also makes sure the axis fills the whole axes extent.
extractPoints	This function is used to extract data points by prompting the user to select by clicking points on the image.
interpValues	This function is used for interpreting the calibration values of the selected points based on the axes' ranges.

For the purpose of this study, an object is developed, setting the physical and thermal properties to be dependent on the temperature (corresponding to atmospheric pressure of 1 atm) of the RT27 by Rubitherm PCM. The RT27 object constitutes of constant properties, such as the average Phase Change Temperatures (onset, peak, end) [°C] measured in differential scanning calorimetry (DSC), adiabatic scanning calorimetry (ASC) [33–35], and the thermal expansion coefficient [K^{-1}] [9]. In addition to that, it provides curves of the enthalpy [kJ/kg], the heat capacity [KJ/kgK], the dynamic viscosity [Pa.s], the thermal conductivity [W/m.k], the thermal diffusivity [m^2/s], and the density [kg/m^3] in relation to the temperature for both the solid, liquid, and solid–liquid phases. The data derives from different measurements and studies [9,18,34–37] and the temperature ranges from 5 °C to 45 °C. The interpolation used for these curves is the interp1 using the LINEAR method and the EXTRAP method for predicting data outside the temperature boundaries. Interp1 returns interpolated values of a 1D function at specific query points using linear interpolation. Once using the Linear interpolation, the interpolated value at a query point is estimated on linear interpolation of the values at neighbouring grid points in each respective dimension. In addition, the extrapolation strategy is applied to evaluate points outside the domain using the same method it uses for interpolation based on the Akima algorithm for one-dimensional interpolation, described in [38]. The object is used for the thermophysical calculations and predictions described in Section 3.4.

3.4. Heat Transfer Performance Module

Thermal properties such as the melting point, the fusion latent heat, and the specific heat capacity are determined by the DSC. However, the costs of this method, especially when there is large number of samples, is relatively expensive and therefore developing simpler methods as well as simulation models is considered of high importance for studying the phase change properties [13]. The principal thermal properties to be studied are the latent heat of fusion (J/g) and the melting and freezing temperatures (°C), when considering the purpose of the hybrid PCM-loaded materials. However, these properties are mainly determined by the type of PCM used. In the context of PCM-mortars, their ability to store and release heat is defined by the properties of the thermal conductivity (W/m.K) and the latent heat (J/g), which provide an efficient thermal energy storage capacity and heat transfer of hybrid materials.

In this frame, the numerical approach enables solving transient problems based on the quantitative determination of the constrained melting process of encapsulated PCM integrated on a wall layer. The numerical models are established based on the enthalpy method [14,26,39]. It is worth mentioning that the enthalpy method is believed to be an

attractive method in comparison with the other methods due to several reasons, such as (i) computational efficiency, (ii) modelling accuracy, and (iii) flexibility in selecting solution schemes covering both corrective iterative schemes (i.e., a fast and energy conservative approach), or non-iterative schemes (i.e., a quick but conservative approach at low time steps) [12,13,40]. For the purpose of this work, the thermal and physical parameters are investigated to analyse and predict the heat transfer properties of the hybrid PCM-enhanced material based on the enthalpy method by assuming organic PCM constrained inside an open pore of inorganic porous carrier. The Heat Transfer Performance Model generates the temperature of the material in relation to time and space inside the wall.

4. Heat Transfer Performance Model

The Heat Transfer Performance Module relies on the respective model, which aims to simulate the thermal behaviour and performance of real hybrid PCM replacing expanded perlite loose fill in a wall. The model implements a physically expedient concept of air natural cooling of a building applying a suitable numerical scheme.

4.1. Physical Problem Description

The developed algorithm is to be utilised for analysing the heat transfer phenomena on a PCM-enhanced multi-layer building block. To understand and highlight the potential of the PCM-enhanced material, two building blocks are analysed [8]. The conventional building block contains four layers of 2 cm Plaster, 16 cm brick, 10 cm expanded perlite loose fill, and 2 cm of Extruded Polystyrene Foam insulation (see Figure 3a). The PCM-enhanced building block considers the same structure and sizes, while the loose fill is replaced by the hybrid PCM material (see Figure 3b). Thermal properties of the wall layers are provided in Table 2, while the thermal and physical properties of the PCM are provided from the Data Collection Module for RT27 Rubitherm. The model considers air natural cooling of a preheated building block up to 30 °C. The expected result includes the quantification of time required to cool down the block and therefore raise the demand for space heating.

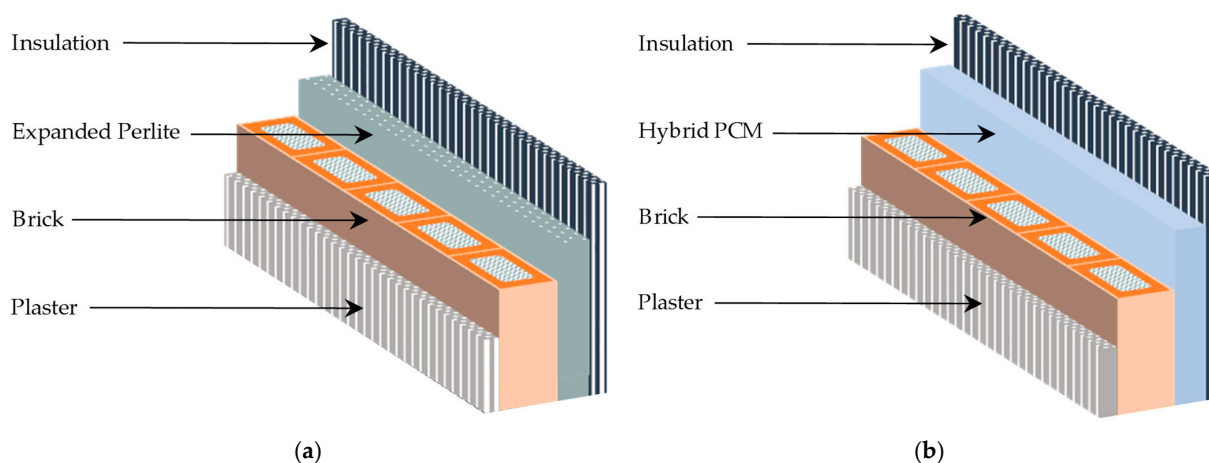


Figure 3. Building wall layers (a) with loose fill; (b) with hybrid-PCM.

Table 2. Physical and thermal properties of building construction materials used in this study [41–43].

Properties	Plaster	Brick	Expanded Perlite	Insulation
Layer Thickness [m]	0.02	0.16	0.10	0.02
Density [kg/m ³]	1300	1700	49 (32–66)	1050
Specific heat capacity [J/kg·K]	1000	800	1090	1100
Thermal conductivity [W/m·K]	0.50	0.73	0.04 (0.039–0.046)	0.12

4.2. Basic Simulation Setup, Geometry and Grid

The convective heat transfer within the building blocks in the unit of time can be approached as a 1D problem, solved with a finite difference method [24–26,44]. This method enables solving the governing partial differential Equations (6) and (7) into numerical solutions in a heat transfer system. The domain geometry is one dimensional and linear. This provides an approximate temperature value at each grid point in the domain of length L and divided in equal ds elements, identified by an index i , as depicted in Figure 4.

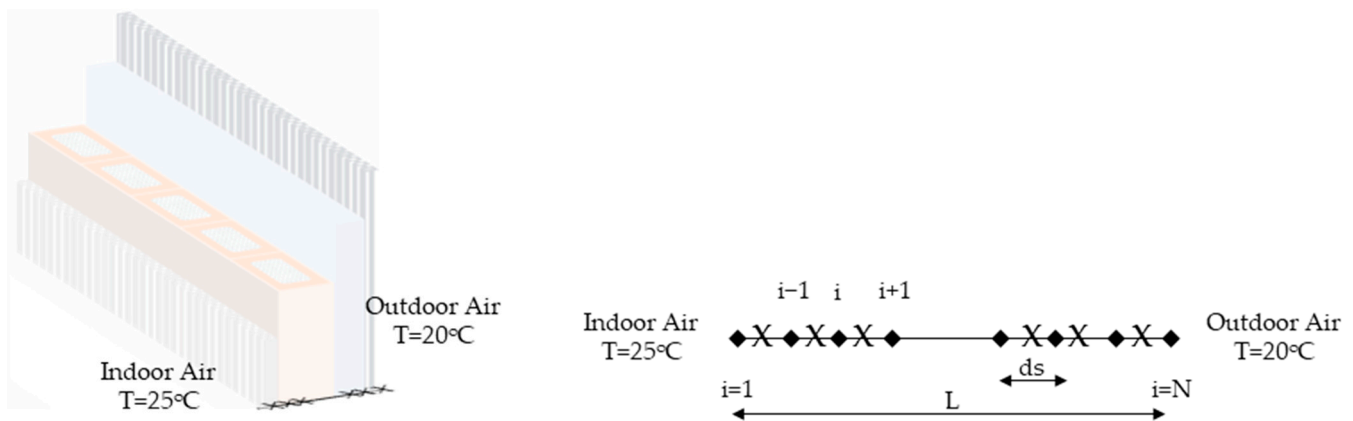


Figure 4. 1-d Numerical building block domain showing boundary conditions.

The temperature of each node for each discrete timestep is calculated based on the values of the previous timestep. Nodes 1 to N represent the ds interface position within the building block, where the indoor air node is labelled 0 and the outdoor air node is $N + 1$. Boundary conditions are shown in Figure 4 for the surrounding air temperature, as well as the starting conditions for the preheated block, which are set to 30 °C for all cells. The output of the simulation is the temperature of the building layers as a function of time. The set of initial and boundary conditions, as well as the properties of the different materials are set for time $\tau = 0$ s.

4.3. Transient Heat Transfer

The main heat transfer mechanisms that are investigated are the thermal conduction (Section 4.3.1) and the heat transfer through phase change (Section 4.3.2).

4.3.1. Conduction in Plane Walls

The heat transfer in a certain direction is driven by the respective gradient of temperature. The Fourier Law for the rate of heat being transferred through the wall by performing integration and rearranging the Equation (1) for assuming steady-state can be expressed as:

$$Q_{\text{cond,wall}} = -k \cdot A \cdot (T_i - T_{i+1}) / L \quad (6)$$

By introducing the thermal resistance concept as a constant parameter characterising each material, the conduction resistance will be related to the thermal conductivity, the length, and the contact area of each layer.

In the scenario of transient conduction, employing a time discretization based on the Forward Euler's Method, coupled with spatial discretization, and assuming spatial and temporal constancy of thermal conductivity, the Equation (6) can be solved as:

$$T_i^{\tau+1} = T_i^{\tau} + (d\tau \cdot k) / (\rho \cdot c_p \cdot ds^2) \cdot (T_{i-1}^{\tau} - 2 \cdot T_i^{\tau} + T_{i+1}^{\tau}) \quad (7)$$

$$\text{Alpha} = d\tau \cdot k / (\rho \cdot c_p \cdot ds^2)$$

For the algorithm, the alpha value is considered proportional to the thermal resistance and will be used for calculating the temperature of each node I for every timestep.

4.3.2. Heat Transfer through Phase Change

In the case of the phase change, the temperature field is not correlated to the melting and solidifying behaviour as expressed in Equation (7). This is due to the sub-cooling effects and hysteresis phenomena occurring during the phase change. For this purpose, the enthalpy method is utilised, coupled with the modelling of statistical nucleation and subcooling effects in order to include the real behaviour of the PCM [24,26]. A phase change phenomenon is defined by the phase change temperatures, phase change enthalpy, and heat capacities in the solid and liquid states and the thermal conductivity [17]. In this frame, the enthalpy method relies on a fixed space grid, but a variable time step is used to ensure that the phase front is always on a node point. The spacial discretization, by assuming that the thermal conductivity is constant in time and space domain and integrating the thermal resistance values, solves the Stefan problem as expressed below:

$$H_i^{\tau+1} = H_i^{\tau} + ((1/R_{i-1} \cdot (T_{i-1}^{\tau} - T_i^{\tau})) + ((1/R_{i+1} \cdot (T_{i+1}^{\tau} - T_i^{\tau}))) \cdot d\tau / (A \cdot ds) \quad (8)$$

$$T_i^{\tau+1} = F(H_i^{\tau+1}, p) \quad (9)$$

Equations (8) and (9) are solved in a loop for all interfaces ds and all timesteps $d\tau$. The function $F(H, p)$ is a data-driven function that returns the corrected temperature based on the new enthalpy and the phase p of the PCM. The data used for the $F(H, p)$ function derive from the Data Collection Module acquired using calorimetric methods.

This approach enables to correct the new temperature using lab measurements and increase the precision of the model as shown in Figure 5. The complete algorithm flowchart is shown below (Figure 6).

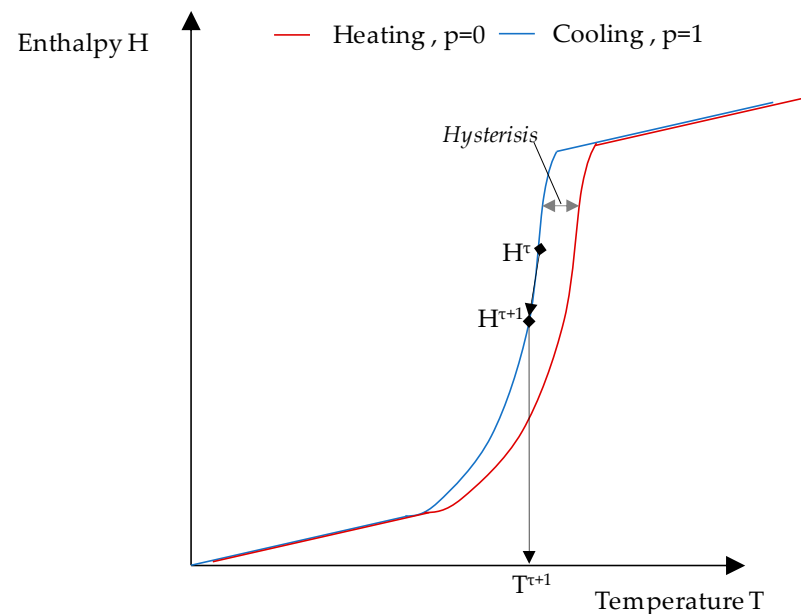


Figure 5. Enthalpy method illustration for data-driven correction function.

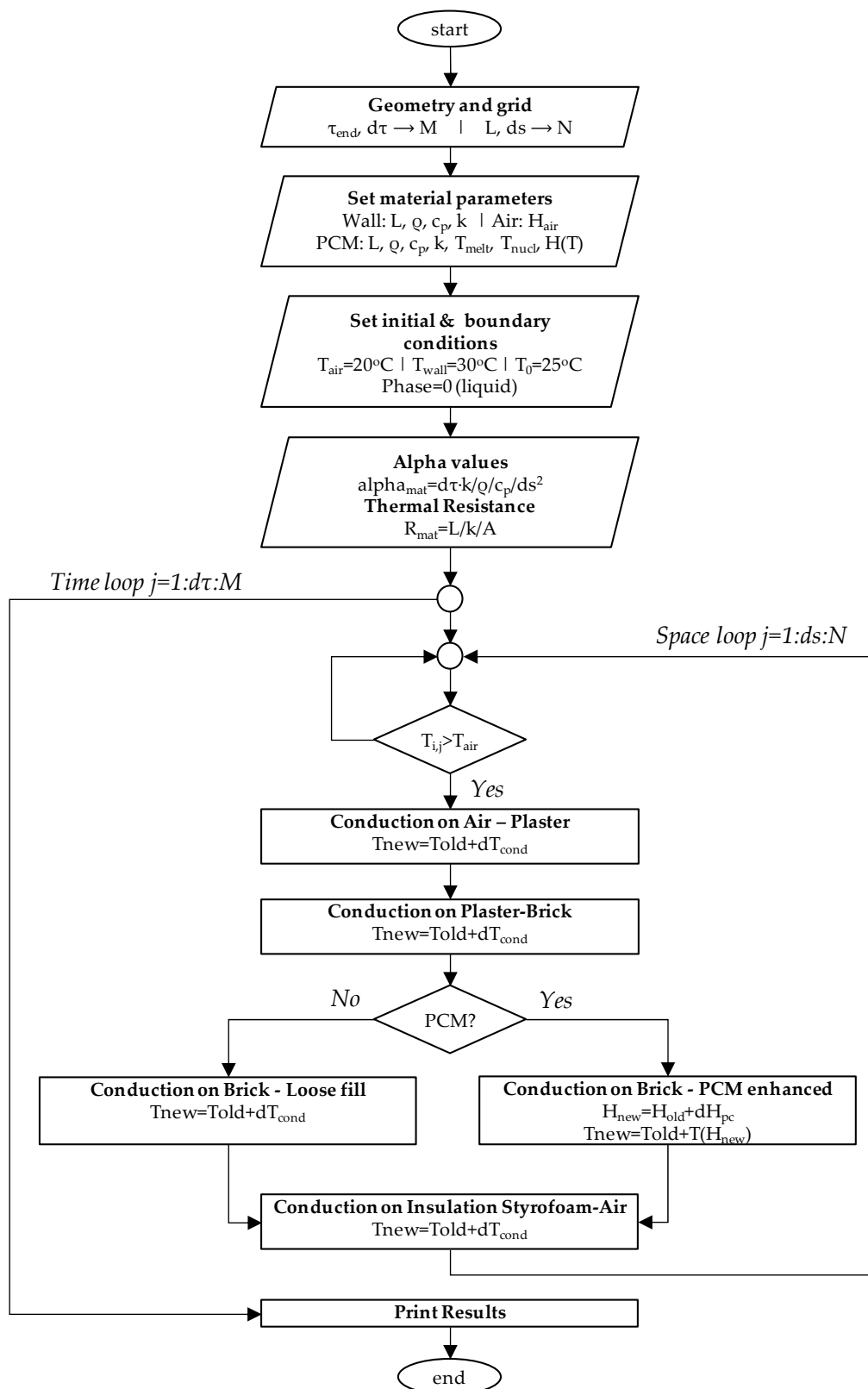


Figure 6. Heat transfer performance flowchart scheme.

5. Results

The data-driven models developed in this study facilitate the understanding of hybrid PCM integrated within a building block. The quantification of the temperature gradient

in the unit of time provides a solid base for the evaluation of the thermal properties of PCM composites as innovative construction materials capable of hybrid energy storage. To ensure the higher precision of the generated values and the minimum computational cost, both combine numerical formulations and experimental measurements are employed in order to successfully predict the thermal behaviour of the hybrid materials throughout a thermal cycle based on selected external parameters. The outcome of the tool and the results are presented below for the following modules: 1. data collection; 2. data-driven objects; and 3. heat transfer Performance module.

5.1. Data Collection

The data collection module processes figures and images in order to extract numeric data. The gathering of this material requires the execution of experiments and laboratory tests for analysing and capturing the property evolution in correlation with temperature and time. Alternatively, it allows the use of respective literature to collect images from previous works and build this database. For this study, an extensive review was performed to gather information for the selected PCM RT27 Rubitherm in relation to physical and thermal properties. The level of accuracy in the numerical simulations of PCMs can be significantly influenced by whether constant properties or temperature-dependent properties are used. For this reason, the model utilises temperature-dependent properties, which are captured from studies as mentioned in Section 3.2. Indicatively, the specific enthalpy of RT27 Rubitherm is measured in an ASC. Figure 7 depicts an original figure obtained from [34] and the extracted data from this figure. The number of nodes can be adjusted based on the complexity and the accuracy of the input image. This process is implemented for all the physical and thermal parameters required for the simulations.

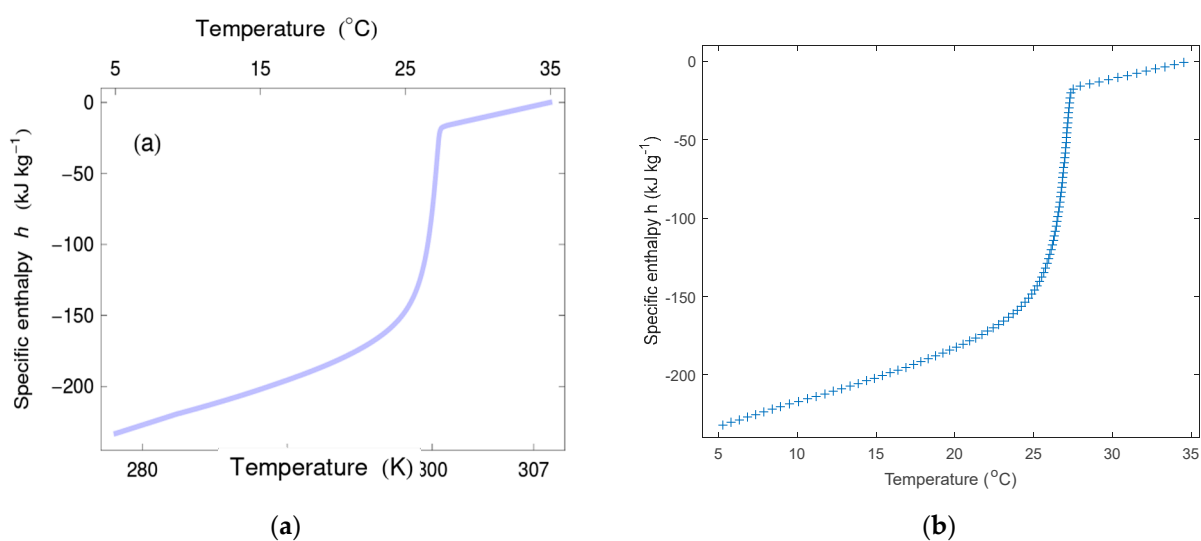


Figure 7. Image-to-Data tool (a) input; (b) output.

This approach enhances the quality, accuracy, and utility of scientific data, particularly when dealing with complex or large datasets where manual measurements would be impractical. It can also enable the integration of other datasets in statistical analysis computational models, facilitating a more comprehensive understanding of the phenomenon being studied. Once this process is fully automated, data collection can be more efficient and time saving compared to manual data entry.

5.2. Data-Driven Objects

The data-driven object performs the correlation of raw data derived from the data collection module. Its function relies on executing the least possible process on the data for minimising errors and inaccuracies related to data misinterpretations. For this reason, the

module cleans and filters the data to remove possible unwanted observations, including duplicate observations or irrelevant observations. Then, according to the method described previously, the module correlates the data points, creating a function of specific enthalpy in relation to temperature, $h(T)$, as shown in Figure 8.

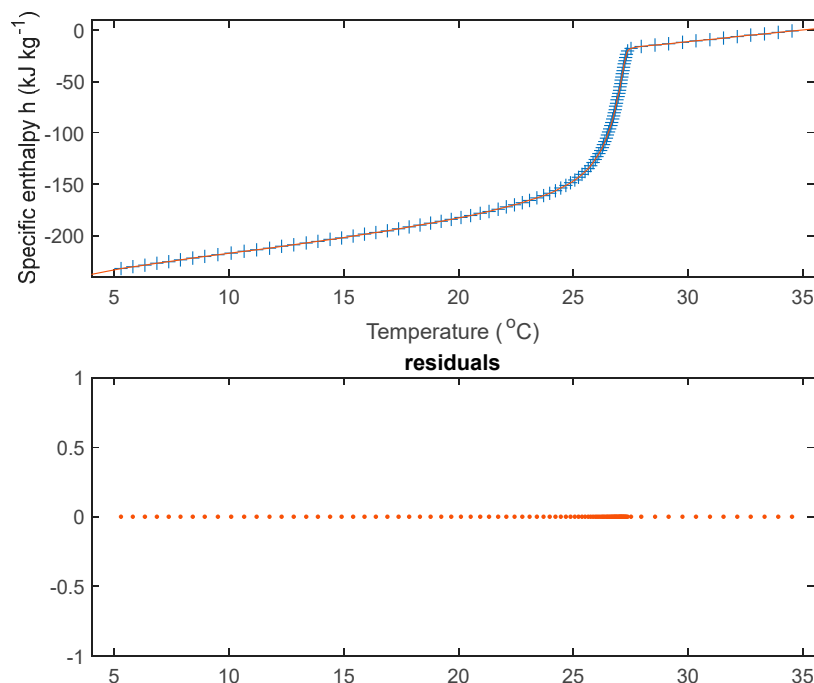


Figure 8. Data-driven object correlation of specific enthalpy for RT27.

5.3. Heat Transfer Performance Module

Once the required parameters are well-defined, the heat transfer performance module is employed to evaluate and quantify the potential of delaying the wall's cooling in case natural air cooling is applied. The simulation is performed for the cases described in Section 4.1, including a conventional building block consisting of 2 cm plaster, 16 cm brick, 10 cm expanded perlite loose fill, and 2 cm of extruded polystyrene foam insulation and a PCM-enhanced building block that has the same structure and sizes; meanwhile, the loose fill is replaced by the hybrid PCM material (sizing and specifications in Table 2).

The module generates the temperature gradient for each grid point in the domain of length L . In Figure 9, a filled contour plot is presented that contains the isolines of temperature in °C ranging from 20 °C (outdoor air temp.) to 30 °C (preheated wall temp.) for each $d\tau$ (every 10 s) on the X axis and each ds interface position on the Y axis for 1 h.

To facilitate the understanding of the results, the position of the different layers is depicted in the figure. It is observed that the wall is thermally discharged, as the temperature losses occur on both directions with different rates. In this timescale, each node is 10 s. From Figure 9, it is shown that the plaster's temperature is completely cooled to the indoor temperature of 25 °C in about 30 min. This rapid cooling may have implications for indoor climate control and energy efficiency. Respectively, the insulation's temperature is completely decreased to nearly the outdoor temperature of 21 °C in about 60 min. This highlights the insulation's effectiveness in maintaining a temperature gradient and thermal comfort indoors. The data presented suggest that the EP loose fill follows a similar cooling trend as the insulation, reaching a temperature decrease of 26 °C in about 60 min. This observation is expected, as EP loose fill is a lightweight, thermally insulating, and fire-resistant insulation material used in the construction industry. Its ability to reduce heat transfer, resist moisture, and contribute to energy efficiency in buildings makes it a valuable choice for various insulation applications. After 1 h, the temperature of the brick is about 26 °C. This point provides insight into the thermal mass properties of the brick

and its ability to retain heat. Bricks with greater thermal mass can store more heat energy and will therefore take longer to discharge that heat.

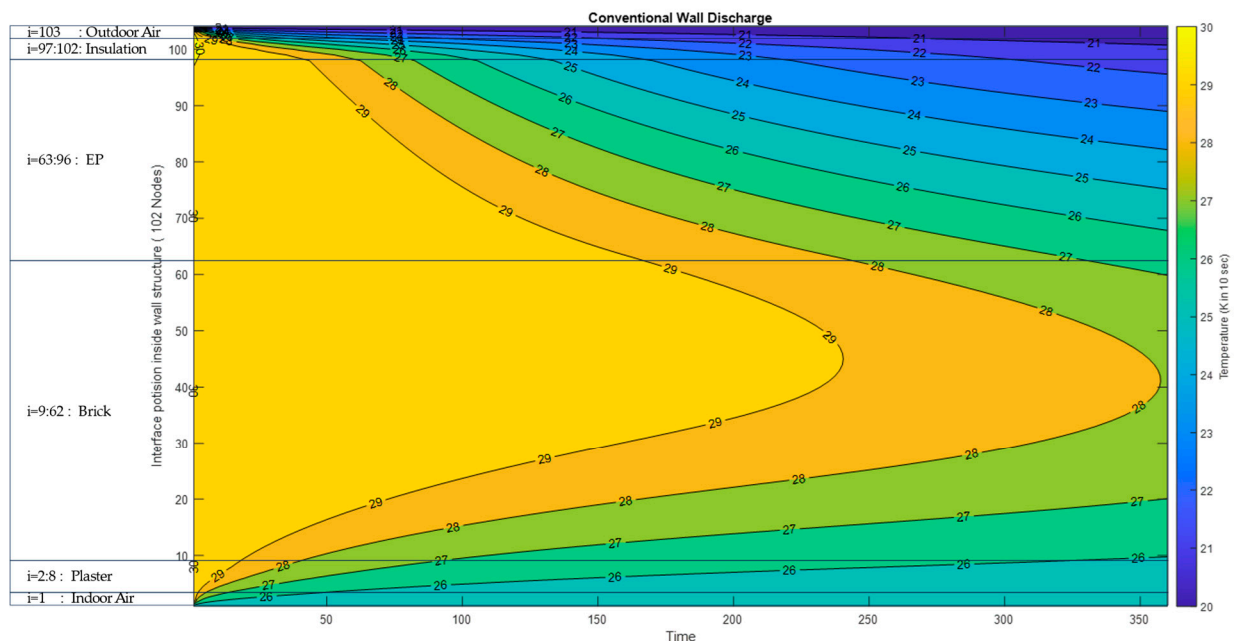


Figure 9. Temperature isolines for conventional wall cooling after 1 h.

Accordingly, Figure 10 represents the gradient of the wall's temperature for the PCM-enhanced wall for air cooling after an hour. Despite the fact that the thermal discharge is equivalent for the plaster and the insulation, the brick's thermal discharge presents a significant delay. After 60 min, its temperature is about 28 °C, as the integration of the PCM-enhanced composite clearly delays the temperature drop from the outdoor air. This expresses a better time lag performance for the whole building block provided by the increased latent heat of the PCM-enhanced composite layer. This layer effectively delays the transmission of temperature changes from the external environment to the interior, resulting in better thermal stability and enhanced energy efficiency.

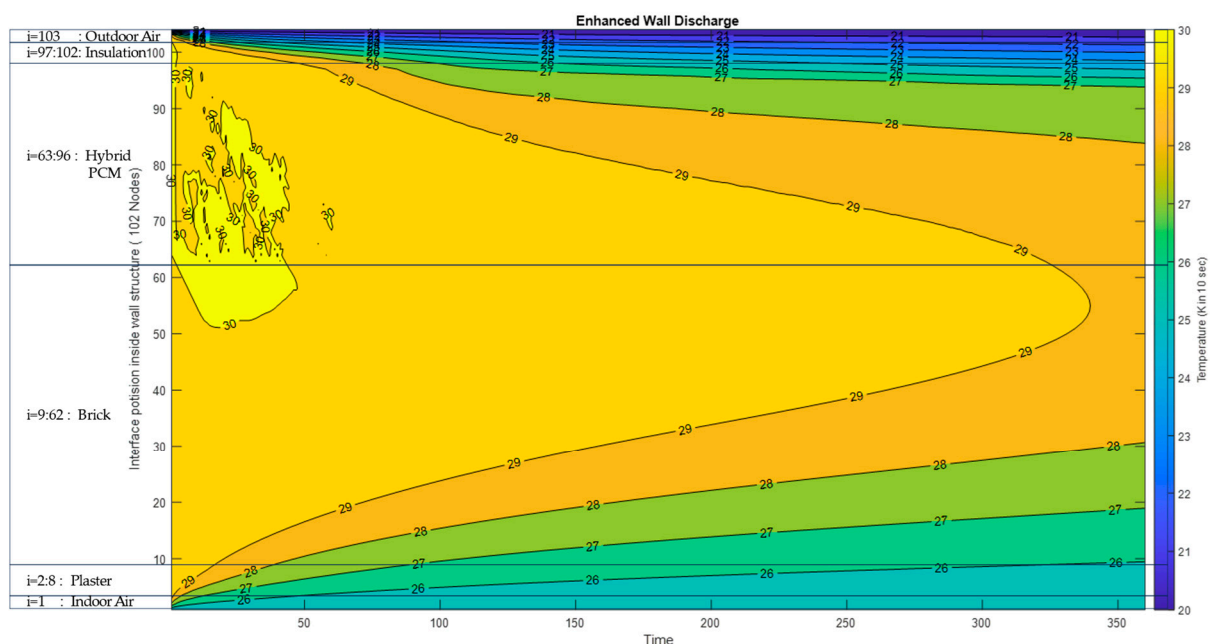


Figure 10. Temperature isolines for PCM-enhanced wall cooling after 1 h.

The temperature of the brick is considered to be of most importance for the building's energy performance and indoor temperature stability as it the layer with the higher thermal mass and the potential to store energy. In this line, emphasis is given to the temperature gradient per time for each interface position inside the brick for the conventional wall in Figure 11 and the PCM-enhanced wall in Figure 12.

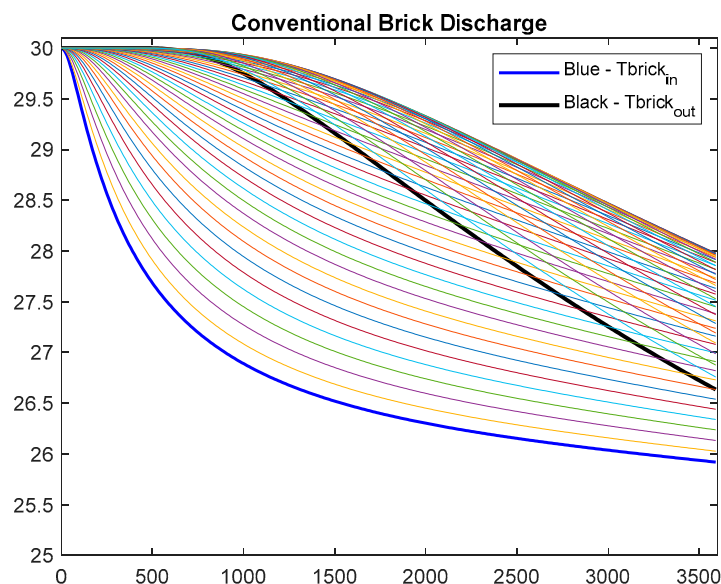


Figure 11. Gradient temperature of a brick's nodes in relation to time—conventional wall.

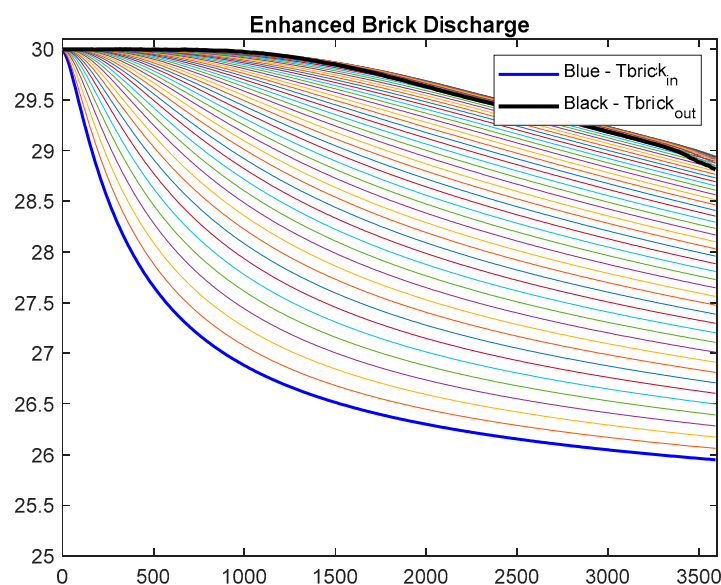


Figure 12. Gradient temperature of brick's nodes in relation to time—PCM-enhanced wall.

For the first case, the inner side of the brick drops from 30 °C to 25.9 °C after 60 min and the outer side of the wall drops from 30 °C to 26.6 °C, resulting in an average temperature drop rate of about 3.75 °C/h. This rate is higher than the accepted temperature fluctuations for maintaining thermal comfort inside a room. It is noted that for 80% occupant acceptability, the temperature fluctuations for maintaining a comfort zone width should be below $\pm 3.5^\circ$ for ASHRAE Standard 55 or $\pm 3^\circ$ for EN CEN 15251 standard d [45].

For the PCM-enhanced building block, the thermal discharge of the brick is delayed as the inner side of the brick drops from 30 °C to 25.9 °C after 60 min and the outer side of the wall drops from 30 °C to 28.8 °C. Compared to the conventional case, the temperature

in the outer side of the wall is 2 °C higher. This observation has also been demonstrated in Irsyad et al.'s study [46]. The average temperature drop rate is reduced to 2.65 °C/h, improving the thermal stability of the indoor environment and reducing the temperature variations. The temperature losses from the outdoor environment are minimised and the brick maintains its temperature for an extended duration. The PCM-enhanced rate indicates that dropping the brick's temperature to 25 °C requires about 180 min, which is also consistent with the study performed by Gupta et al. investigating the time lag of a brick filled with paraffin wax and coconut oil [47].

6. Discussion

This study aims to present a data-driven integrated decision model for analysing the thermal behaviour of hybrid PCM-enhanced composites for improving energy performance in buildings. The key feature of exploiting the energy potential is to handle the heat transfer phenomena occurring between the building's elements (i.e., walls, roof, etc.) and the internal and external environment.

The quantification of the thermal discharge rate of a wall when air natural cooling conditions are applied enables the investigation of innovative materials and composites in the direction of improving the thermal stability of indoors environment and meet the demand for space heating. Sudden temperature drops and large fluctuations are associated with disrupted thermal comfort. To overcome this issue, the buildings will present increased energy demands in order to correct and maintain the appropriate indoor temperature.

In this frame, the concept of increasing the thermal mass of buildings poses as a very promising solution for overcoming both energy and economic challenges deriving from these events. The integration of PCM-enhanced loose fill as a replacement for the insulating loose fill applied in many buildings is expected to improve the thermal behaviour and performance of the building elements. The PCM additional thermal capacity enables the storing of thermal energy which will then be released to the indoor environment by prolonging its temperature. This application is associated with a lot of advantages for building energy performance as it reduces the demand for energy consumption and the power peaks of equipment which would be reported otherwise.

The investigation of the PCM-enhanced composites under data-driven and numerical models allows the optimisation of the composites synthesis in order to achieve the physical and thermal properties tailored to each use case. The approach minimises the costs and time required for performing trial-and-error tests and reduces the resources required for the realisation of the final products. Nevertheless, the concept of PCM-hybrid composites has been investigated extensively over the last decade, as it is associated with a few challenges. Imposing the composites to thermal cycles can lead to PCM leakage of material within the building blocks and a reduction in its thermal performance, such as thermal conductivity. To overcome these challenges, several solutions are currently being investigated, including the impregnation and coating of PCM in order to secure the material and minimise the leakage. Furthermore, by including carbonated substances in the coating, the thermal properties of the PCM can be protected and even enhanced. To summarise, further research is required for optimising and commercialising the PCM-enhanced composites as materials for improving building energy performance. The development and exploitation of data-driven decision support models can facilitate this process and pave the path towards the EU-wide targets for the reduction in energy consumption by 2030.

7. Conclusions

The digitalisation of material development enables the acceleration of all aspects of materials design and the cost-effective and efficient development of innovative materials. The need for new research and development methodologies, merging computational and experimental materials sciences based on modelling, simulation, and high throughput characterisation is clear and urgent to align the building sector with the European Directives and sustainable goals. In particular, the exploitation of a building's thermal mass through

phase change materials due to their ability to store and release large amounts of energy during phase transitions has become quite popular in scientific and academic research. In this frame, by employing predictive modelling techniques and numerical data-driven models, the material selection, system design, and optimisation can act more effectively. This study evaluates and predicts the thermophysical properties of mineral particles carrying PCMs and coated with a cementitious layer able to be utilised as fillers in construction applications. The models aim to simulate the thermal behaviour of hybrid PCM replacing EP loose fill in a wall. The model implements a physically expedient concept of air natural cooling of a building, applying a suitable numerical scheme. The results show the quantification of time required to cool down the block and depict a clear improvement in the thermal discharge of the walls. The rate of discharge is reduced by at least 1 °C/h when replacing EP with PCM-enhanced EP, and the comfort level of the indoor environment can be prolonged without introducing space heating. The models can be exploited for analysing different material compositions and use cases, providing insightful information for decision support on optimising the energy performance of buildings. A key advantage of the models is that they leverage pre-existing datasets to establish predictive models. This can significantly reduce computational time and resources required for analysis. In addition to that, they allow for the integration of diverse data sources and features, enabling the incorporation of realistic variability and uncertainty. This flexibility is especially valuable when dealing with heterogeneous materials or conditions that may not be easily accounted for using traditional numerical methods. In view of this, as more data become available, this data-driven model can be updated and refined, continually improving its accuracy, especially for the analysis of phase change material behaviour, which is a main aim of this study.

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