Estimation of Thermal Parameters of a Sandwich Panel using Numerical Solutions for the Inverse Heat Conduction Problem

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Abstract. In thermal parameter identification problems of sandwich wall panels using the theoretical-experimental method, the property commonly estimated is the homogenized thermal diffusivity, which is insufficient for transient thermal simulations. In this work, a numerical formulation for solving the inverse heat transfer problem, based on the implicit finite difference method and the Monte Carlo method, is developed to estimate the thermal properties of each layer of the sandwich panel. Experimental temperature data are used in the numerical formulation to determine the thermal properties (conductivity and specific heat) of the layer materials and to predict the thermal behavior of the panel. The results obtained show that the formulation estimates the thermal properties of the materials with adequate accuracy.

Keywords: Thermal properties, Finite difference, Inverse problem, Parameter estimation, Sandwich panel.

1 Introduction

The increase in population and demand for housing, combined with the need to reduce the consumption of non-renewable natural resources and energy, has driven the search for low-cost, safe, and sustainable construction solutions. Besides cost and sustainability, it is crucial that new materials and construction systems can ensure the thermal performance of buildings. The evaluation of conventional materials for social housing production has shown that many buildings fail to provide the required thermal comfort, making their use nonviable according to the performance standard NBR 15575:2013 ABNT [1], as user comfort is reduced to a very low level, according to Soares et al. [2].

In civil engineering, new research must develop materials and products that can be used both for improving the thermal comfort of old buildings ("retrofit") and for ensuring the thermal and acoustic performance of new buildings, considering the bioclimatic zone defined in NBR 15220-3 ABNT [3]. In Brazil, most construction systems used as enclosure elements (walls) are limited to solid concrete walls, solid brick walls, or hollow brick walls (blocks), whereas in various other countries, sandwich panels have been an alternative to traditional masonry walls to improve the thermal and acoustic performance of buildings. In these cases, during the evaluation of the thermal performance of new sandwich panel systems, experimental tests have been conducted to estimate the global diffusivity for the transient analysis, and the transmittance or thermal resistance for the steady-state analysis, according to Owczarek [4] and R. Hegarty [5].

Studies on the use of sandwich panels with a steel-reinforced face and EPS core have shown that this type of element has sufficient mechanical resistance for use as ceiling slabs and enclosure walls, according to Bertini [6], Medeiros [7], and Mashal et al. [8]. However, the verification of the thermal performance of panels is still little studied experimentally, and there is a need to develop systematic methods for estimating thermal parameters from laboratory tests Silva [9]. Such parameters are generally defined directly or indirectly through standardized laboratory tests, using experimental setups where the system variables are controlled within a predefined range, and the required parameters are obtained from the measured behavior. According to Neto and Neto [10], in some parameter estimation problems, also called parameter identification problems, the theoretical-experimental approach is used. In this case, the inverse problem of the transient mathematical model is solved when the temperature values of the system are measured at several points on the sandwich panel during the respective experimental test.

In this work, such an approach was used to estimate the thermal parameters (thermal conductivity k and specific heat c) of each material in the sandwich panel, as well as the natural convection coefficient h. The inverse problem was formulated as an optimization problem, where the objective function was minimized for n monitored points in the domain and m time instants. To reduce computational cost, the Monte Carlo method was used for parameter selection based on a probability density function, which was then used in the simulation of the direct problem of transient heat flow, based on the implicit finite difference method, and error evaluation.

The following sections are organized as follows: Section 2 presents the mathematical model of the transient heat flow problem. Section 3 develops the numerical modeling of the problem based on the implicit finite difference method. Sections 4, 5, and 6 present the systematic approach for estimating the thermal parameters of the sandwich panel, the obtained results, and the conclusions, respectively.

2 Mathematical model of transient heat flow problem

From the first law of thermodynamics — the principle of energy conservation — the transient heat flux equation for an isotropic solid material medium can be derived as the problem of: Finding the temperature $\theta(x, y, z, t)$ and the heat flux density $\mathbf{q}(x, y, z, t)$ in a body $\Omega \subset \Re^3$ with boundary Γ, for each instant of time $t \in (0, T)$, given by the following equations:

$$\rho\, c\, \frac{\partial \theta}{\partial t} = -\mathrm{div}(\mathbf{q}) + \omega, \quad \text{in} \quad \Omega \times (0, T) \quad \text{(Energy Conservation Equation)} \tag{1}$$

$$\mathbf{q} = -k\, \nabla \theta \quad \text{in} \quad \Omega \times (0, T) \quad \text{(Fourier equation)} \tag{2}$$

where ρ is the density, c is the specific heat at constant pressure, and k is the thermal conductivity. All material properties can depend on position (nonhomogeneous material) and temperature θ. The term ω is a source or sink of heat energy in the material medium, with units of power per volume. In the SI system, density is given in $\frac{kg}{m^3}$, specific heat in $\frac{J}{kg\,K}$, and thermal conductivity in $\frac{J/s}{m\,K}$. It is worth noting that heat flux occurs through different physical phenomena, which are characterized by conduction, convection, and radiation. Optionally, considering that radiation is not involved or can be introduced indirectly, temperature can be expressed in degrees Celsius,$^\circ C$.

To complement Equations (1) and (2), the following boundary conditions and initial condition can be applied:

$$\theta = \bar{f} \quad \text{on} \quad \Gamma_1 \times (0, T), \quad \text{(Dirichlet b.c.)} \tag{3}$$

$$q = \mathbf{q} \cdot \mathbf{n} = \bar{g} \quad \text{on} \quad \Gamma_2 \times (0, T), \quad \text{(Neumann b.c.)} \tag{4}$$

$$q = \mathbf{q} \cdot \mathbf{n} = h\,(\theta - \theta_f) \quad \text{on} \quad \Gamma_3 \times (0, T), \quad \text{(Robin b.c.)} \tag{5}$$

$$\theta = \bar{\theta}_0 \quad \text{on} \quad \Omega \times \{0\}. \quad \text{(initial condition t=0)} \tag{6}$$

where $\bar{f}(x, y, z, t)$ is the prescribed temperature on the part of the boundary Γ_1; q is the heat flux density normal to the boundary surface; $\bar{g}(x, y, z, t)$ is the prescribed normal flux on the boundary Γ_2; $\theta_f(x, y, z, t)$ is the temperature in the fluid adjacent to the boundary Γ_3; h is the convection coefficient between the fluid medium and the solid surface at the boundary Γ_3, which depends on the nature of the fluid, the velocity of the fluid medium, and the temperature; $\mathbf{n}$ is the unit vector normal to the boundary Γ of the material medium Ω; and $\bar{\theta}_0$ is the temperature field function along the sandwich panel at time $t = 0$. The boundary surface is such that $\Gamma = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3$ and $\Gamma_1 \cap \Gamma_2 \cap \Gamma_3 = \varnothing$.

In the case of heat flow through a wall, it is common, under certain conditions, to consider the case as one-dimensional in the x direction of the thickness, with state variables independent of the y and z coordinates in the plane of the wall. Here, we will model an experiment conducted in a thermal chamber where the panel is positioned to divide the chamber into two environments, with one environment maintained at a specific temperature profile, aiming to simulate what happens to an external building wall when exposed to a sunny day's temperature. In this context, neglecting the source term ω and assuming the medium is homogeneous, the one-dimensional transient heat equation is given by:

$$\frac{\partial \theta}{\partial t} = \lambda \frac{\partial^2 \theta}{\partial x^2}, \tag{7}$$

and $\lambda = \dfrac{k}{\rho\, c}$ is called thermal diffusivity.

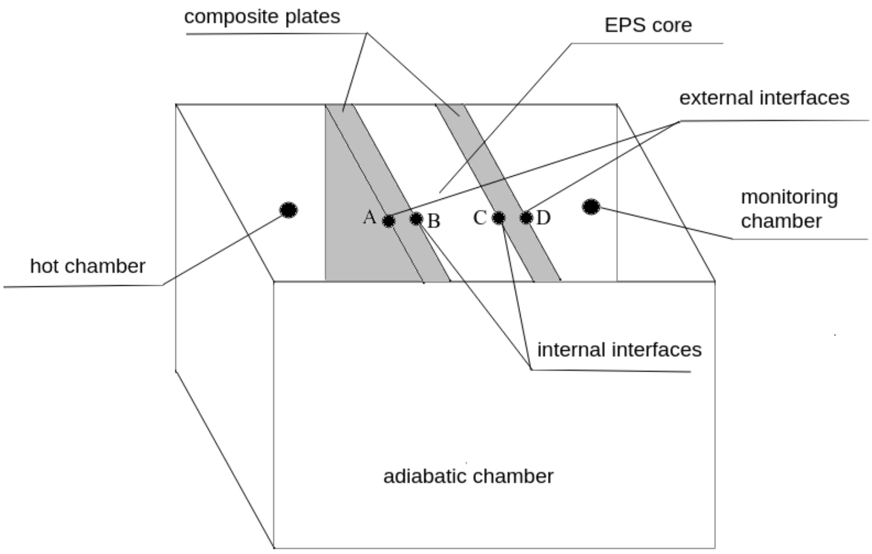

Figure 1. Assembly of the sandwich panel in the thermal chamber for evaluating thermal insulation capacity.

In this case, considering that the wall is formed by a sandwich panel, consisting of two cementitious composite plates and an XPS core, as shown in Figure 1, the system of equations for each homogeneous domain is such that

$$\frac{\partial \theta}{\partial t} = \lambda_i \frac{\partial^2 \theta}{\partial x^2}, \quad \text{in} \quad \Omega_i, \tag{8}$$

and $\lambda_i = \dfrac{k_i}{\rho_i\, c_i}$, i = 1,2 e 3, are the thermal diffusivity parameters of the materials of the layers represented by domains Ω_1, Ω_2 and Ω_3, respectively. Additionally, transmissibility conditions between the layers must be imposed, which state that the normal heat flux exiting one layer is equal to the normal heat flux entering the adjacent layer. That is,

$$q_1^B + q_2^B = 0, \qquad \text{on interface B}, \tag{9}$$
$$q_2^C + q_3^C = 0, \qquad \text{on interface C}, \tag{10}$$

with $q_i^j = \pm k_i \dfrac{\partial \theta}{\partial x}\Big|_j$ given as the flux in layer i ($i = 1, 2, 3$) across interface j ($j = B, C$). It is important to note that the normal flux is positive when it exits a material medium and negative when it enters. One should also consider the possible boundary conditions described by Equations (3), (4), and (5), and the initial condition given by Equation (6).

If we consider that thermal exchange at the two external faces of the panel occurs through convection with the surrounding fluid, the boundary conditions are given by:

$$k_1 \frac{\partial \theta}{\partial x} = h_A\,(\theta - \theta_{fA}) \qquad \text{on external interface A}, \tag{11}$$
$$k_3 \frac{\partial \theta}{\partial x} = -h_D\,(\theta - \theta_{fD}) \qquad \text{on external interface D}, \tag{12}$$

where θ_{fA} and θ_{fD} are the temperatures of the fluids adjacent to the external surfaces of interfaces A and D, respectively, and h_A and h_D are the respective convection coefficients.

3 Computational modeling of the one-dimensional transient heat equation in a piecewise nonhomogeneous domain

3.1 Implicit finite difference method at the internal nodes of the layers

Considering the panel by layers, the discretization of the one-dimensional domain into uniformly distributed points (or nodes) in each layer is such that the number of divisions per layer is N_i, $i = 1, 2, 3$, as shown in Figure 2, following the sequential numbering of the nodes. The points at the boundaries of the layers are: 1 and $N_1 + 1$ in layer 1, $N_1 + 1$ and $N_1 + N_2 + 1$ in layer 2, and $N_1 + N_2 + 1$ and $N_1 + N_2 + N_3 + 11$ in layer 3.

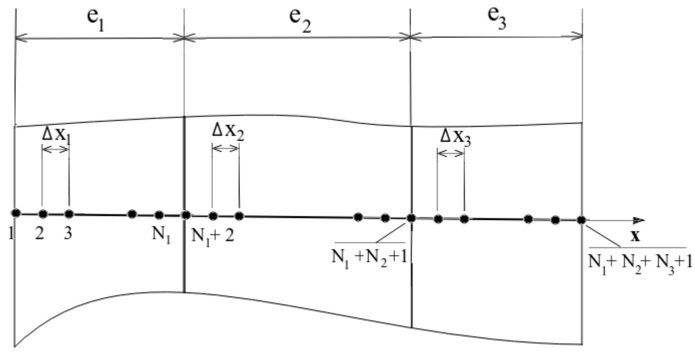

Figure 2. One-dimensional discretization of the panel by layers.

Using the centered finite difference approximation in space (Δx_j) and the implicit time approximation (Δt) (implicit finite difference method), Equations (8) at each internal point j of the layers Ω_i and at time t_{m+1} are given by:

$$\frac{\theta_j^{m+1} - \theta_j^m}{\Delta t} = \lambda_i \cdot \frac{\theta_{j-1}^{m+1} - 2\,\theta_j^{m+1} + \theta_{j+1}^{m+1}}{\Delta x_i^2} \quad \text{in} \quad \Omega_i, \tag{13}$$

or

$$-F_0^i \cdot \theta_{j-1}^{m+1} + \left(1 + F_0^i\right) \cdot \theta_j^{m+1} - F_0^i \cdot \theta_{j+1}^{m+1} = \theta_j^m \quad \text{in} \quad \Omega_i,\ i = 1, 2, 3. \tag{14}$$

with $F_0^i = \dfrac{\lambda_i \Delta t}{\Delta x_i^2}$ given as the Fourier number in the finite difference form, and θ_j^{m+1} is the temperature at the internal point j of the layers at time $t_{m+1} = t_m + \Delta t$. The parameters λ_i and Δx_i are the diffusivity and the uniform distance between the nodes of the grid of layer i. The time step Δt and space increments Δx_i were defined as the maximum values to ensure adequate accuracy with the least computational effort.

3.2 Heat flux compatibility at the internal interfaces of the layers

Additionally, the temperatures at nodes j of the internal interfaces B and C, at time t_m, are such that the heat flux leaving one layer is equal to the heat flux entering the adjacent layer. That is,

$$k_1 \cdot \frac{\theta_j^m - \theta_{j-1}^m}{\Delta x_1} = k_2 \cdot \frac{\theta_{j+1}^m - \theta_j^m}{\Delta x_2} \quad \text{on interface B,} \tag{15}$$

$$\Rightarrow \quad \theta_j^m = \frac{k_2 \cdot \Delta x_1 \cdot \theta_{j+1}^m + k_1 \cdot \Delta x_2 \cdot \theta_{j-1}^m}{k_1 \cdot \Delta x_2 + k_2 \cdot \Delta x_1}, \tag{16}$$

$$k_2 \cdot \frac{\theta_j^m - \theta_{j-1}^m}{\Delta x_2} = k_3 \cdot \frac{\theta_{j+1}^m - \theta_j^m}{\Delta x_3} \quad \text{on interface C,} \tag{17}$$

$$\Rightarrow \quad \theta_j^m = \frac{k_3 \cdot \Delta x_2 \cdot \theta_{j+1}^m + k_2 \cdot \Delta x_3 \cdot \theta_{j-1}^m}{k_2 \cdot \Delta x_3 + k_3 \cdot \Delta x_2}. \tag{18}$$

The possible boundary conditions for a wall with three layers in this case are: (i) temperature prescription, (ii) flux prescription, and (iii) mixed or convection prescription. It is worth noting that these conditions do not change if there are more or fewer layers, as long as the indices are used correctly. Also, no thermal interface resistance was considered here, which would create a discontinuity in the temperature field.

3.3 Dirichlet boundary conditions

When prescribing temperature boundary conditions at $x = 0$ and $x = L$, there is no need to establish any equation at the boundary, as the temperature values are already known. Therefore, it is sufficient to define for all times $t = t_m$ that:

$$\theta_1^m = \bar{\theta_0}(t_m) \quad (19)$$

$$\theta_{N_1+N_2+N_1+1}^m = \bar{\theta_L}(t_m) \quad (20)$$

with $\bar{\theta_0}(t)$ and $\bar{\theta_L}(t)$ being, respectively, the prescribed temperature fields at the boundaries $x = 0$ e $x = L$.

3.4 Neumann boundary conditions

To apply flux boundary conditions at the ends, we must use Fourier's equation at each boundary point, such that

$$\bar{q}_1^m = k_1 \cdot \frac{\theta_2^m - \theta_1^m}{\Delta x_1} \quad (21)$$

and

$$\bar{q}_{N_1+N_2+N_1+1}^m = -k_3 \cdot \frac{\theta_{N_1+N_2+N_1+1}^m - \theta_{N_1+N_2+N_1}^m}{\Delta x_3} \quad (22)$$

where $\bar{q}_1^m$ and $\bar{q}_{N_1+N_2+N_1+1}^m$ are, respectively, the prescribed flux fields at the boundaries $x = 0$ e $x = L$.

3.5 Robin boundary conditions

Finally, the boundary conditions of Newton – thermal exchange through convection with the surrounding fluid medium – and the initial condition are such that:

$$-k_1 \cdot \frac{\theta_2^m - \theta_1^m}{\Delta x_1} = -h_A \cdot (\theta_1^m - \theta_{f_A}^m) \quad \text{(c. c. em A)}, \quad (23)$$

$$\Rightarrow \quad \theta_1^m = \frac{k_1 \cdot \theta_2^m + h_A \cdot \Delta x_1 \cdot \theta_{f_A}^m}{h_A \cdot \Delta x_1 + k_1}, \quad (24)$$

$$-k_3 \cdot \frac{\theta_{N_1+N_2+N_3+1}^m - \theta_{N_1+N_2+N_3}^m}{\Delta x_3} = -h_D \cdot (\theta_{f_D}^m - \theta_{N_1+N_2+N_3+1}^m) \quad \text{(c. c. em D)}, \quad (25)$$

$$\Rightarrow \quad \theta_{N_1+N_2+N_3+1}^m = \frac{k_3 \cdot \theta_{N_1+N_2+N_3}^m + h_D \cdot \Delta x_3 \cdot \theta_{f_D}^m}{h_D \cdot \Delta x_3 + k_3}, \quad (26)$$

$$\theta_j^0 = \bar{\theta}_0(x_j, t = 0) \quad j = 1, .., N_1 + N_2 + N_3 + 1. \quad (27)$$

Given the temperatures θ_{f_A} e θ_{f_D}, we can calculate the evolution of temperature at discrete points within the thickness of the panel at discrete times $t_{m+1} = t_m + \Delta t$, $m = 0, 1, 2, ..., N_t$, where the final time $T = N_t \cdot \Delta t$.

4 Estimation of thermal parameters

The development of new composite materials for use in civil construction requires their characterization, including the definition of physical, chemical, thermal, and mechanical properties. These properties are generally defined directly or indirectly through standardized laboratory tests, where an experimental setup controls the parameters and degrees of freedom of the system within a predefined range, and from the measured behavior, the desired properties are obtained. As presented by Neto Neto and Neto [10], in some cases, a theoretical-experimental approach is used, where the solution of an inverse problem of the mathematical model under study is obtained, with the variables (degrees of freedom) of the system known from measurements of the coupled experiment.

Specifically, for measuring thermal resistance and thermal conductivity, the Brazilian Standard NBR 15220-4 (ABNT, 2005) describes the method of the protected hot plate apparatus. This method involves measuring the average temperature gradient established in the sample, based on a well-known heat flux under steady-state conditions. In the case of buildings, since walls are made up of multiple layers of heterogeneous materials, it is common to conduct thermal testing with full-scale walls under conditions as close as possible to the actual construction of the wall, as outlined in Figure 1.

The **direct problem** of transient heat flow involves calculating the temperatures and heat fluxes at any point in the domain and at any time t within the analyzed interval of the problem $(0, T)$, given the boundary conditions and thermal parameters of the problem. However, when the goal is to estimate thermal parameters, one must solve a type of **inverse problem**, also known as a *parameter identification problem*, where temperature data and boundary conditions are known and some unknown parameters of the medium need to be calculated. Using a theoretical-experimental approach, the inverse problem is solved based on the mathematical model of transient heat flow, where temperature values of the system are measured at several points on the sandwich panel during the respective experimental test.

In this work, such an approach was used to estimate the thermal parameters (thermal conductivity and specific heat) of each material in the sandwich panel and the natural convection coefficient h. The inverse problem was formulated as an optimization problem, where the objective function minimized for n monitored points in the domain and at m time instants is given by equation (28).

$$E = \left(\sum_{i=1}^{n} \sum_{j=0}^{m} |\theta_{exp}(x_i, t_j) - \theta_{cal}(x_i, t_j)|^2 \right)^{1/2} . \tag{28}$$

where $\theta_{exp}(x_i, t_j)$ is the temperature measured experimentally at point x_i and time t_j, and $\theta_{cal}(x_i, t_j)$ is the temperature calculated from the computational simulation of the experiment at the same point and time x_i and t_j, respectively. The value of E is calculated for each parameter value p_k within the interval $I_{p_k} = [p_{k\ min}, p_{k\ max}]$, chosen based on literature results. From this interval, a pseudo-random value is selected using the Monte Carlo method, considering a normal probability distribution (for thermal conductivity and specific heat) and a uniform distribution (for the convection coefficient).

5 Results and discussion

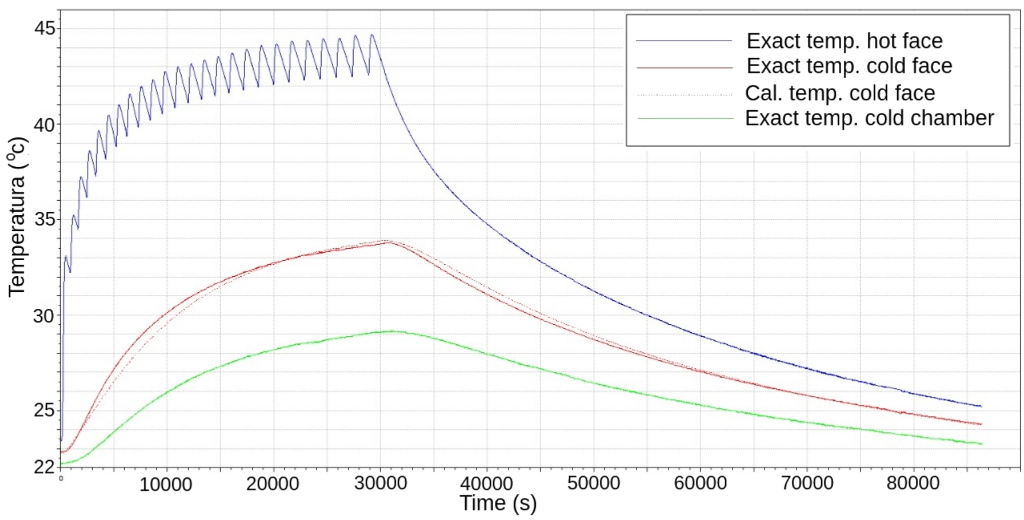

Figure 3. Comparison between the experimental and calculated results on the cold face, using the estimated parameters.

Using the implicit finite difference program developed for calculating thermal parameters through the inverse problem, the following measured data were used: thickness of the cement boards $e_1 = e_3 = 0,0079\,m$, thickness of the XPS core $e_2 = 0,0197\,m$, specific mass of the cement boards $\rho = 1690\,kg/m^3$, specific mass of the XPS core $\rho = 40\,kg/m^3$. The parameter ranges for sampling were defined based on the expected data range in the literature. The temperature data used in the objective function were the experimental and calculated temperatures of the cold face. Consequently, the boundary conditions used were the prescribed temperature on the hot face and the prescribed convection on the cold face, necessitating the estimation of the convection coefficient as well. To ensure the accuracy of the results without increasing computational cost, the time interval used was $\Delta = 10\,s$ and the number of grid points was 7 and 19 for the cement boards and XPS core, respectively. With this, the thermal conductivity and specific heat values of the materials were estimated, and the experimental thermal evolution curve at the interface of panel D (cold face) was compared with the numerical result, using the estimated parameters, as shown in Figure 3. The temperature fluctuation observed on the hot surface is due to the heating curve control system, which was based on an on-off relay used to maintain the medium's temperature within a range.

The estimated properties for the materials of the sandwich panel were a thermal conductivity of k = 1,05 W/(m K) and a specific heat of c = 1000 J/(kg K) for the cement board, as well as a thermal conductivity of k = 0,030 W/(m K) and a specific heat of c = 1450 J/ (kg K) for the XPS core. The estimated convection coefficient was h = 3,0 W/(m2 K), which is within the range of natural convection coefficients $(2,0 \leq h \leq 25,0)$ presented in the literature, according to Incropera et al. [11]. The result presented in Figure 3 indicates that the developed numerical model can predict the thermal behavior of the panel, allowing for the development of different face-core configurations depending on the thermal requirements of the construction environment.

6 Conclusions

In this study, a systematic approach was developed for the estimation of thermal parameters using a theoretical-experimental approach on a sandwich panel with cementitious composite faces reinforced with pineapple fabric and an XPS core.

From the results obtained, it is possible to conclude that by using the implicit finite difference method based on a numerical model, it is possible to determine, through an inverse problem and the Monte Carlo method, the thermal properties of the layers (face and core), which allow for an adequate simulation of the real problem.

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