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An overview on Finite Different Method (FDM) in multilayer thermal diffusion problem

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Abstract. Numerous mathematical models have been developed for thermal diffusion through single-layer materials, while further developments are needed for multi-layer materials. Diffusion processes through a multilayer material are of interest in industrial, applied thermodynamics, physics, electrical and civil engineering applications. The proposed scheme is easily applicable in various fields, demonstrating that Finite Different Methods (FDMs) are flexible, simple to implement and help to represent multilayer materials even without associating them with other numerical methods. The numerical method studied is a FDM in a civil engineering application. Through the study of a multilayer wall, its criticalities are highlighted, and a possible implementation is proposed.

1. Introduction

Diffusion is an occurrence that draws interest from a wide range of fields such as heat, mass, and electric charge transport [1-4]. It is possible to use the Finite Different Method (FDM) alone or with mixed methods [1], analytical [5], or semi-analytical solutions [6]. Diffusion processes through a multilayered material are of interest for a wide range of applications, including industrial annealing steel coils [7-9], semiconductors [10,11], geological profiles [12,13], or medical applications [14,15]. A dynamic thermal model of a building wall must include a method for obtaining solutions to the diffusion equation for heat flow in solid multilayers. When a finite difference method is used, it is necessary to represent the continuous materials by a network of nodes and associated thermal capacities. The walls of buildings usually contain materials of widely differing properties in close conjunction. In 1985, Waters and Wright [16] studied the criteria for the distribution of nodes in multilayer walls in finite difference thermal modeling and suggested a simple criterion for the distribution. They suggested a given number of nodes throughout a model and discussed the distribution of nodes with respect to the internal boundaries of a multilayer wall. They studied the discontinuity created by an internal boundary using Taylor expansions, and this approximation in the time derivative was applied at a point on the boundary. This method is used to calculate the spatial changes in temperature. The results of the work are interesting in terms of the distribution of nodes and provide evidence of the difference in temperature obtained from the analytical model in boundary layers and the temperature obtained from a finite difference model. In

1999, Antonopoulos and Koronaki [17] proposed a procedure for analyzing the effective thermal capacitance, time constant, and thermal delay of buildings into components corresponding to discrete sections of an envelope to develop different parts of an architectonic composition and even the layers of exterior multilayer walls. The developed procedure was based on a finite-difference solution. The focus of their work [17] was to estimate the thermal parameters of building components corresponding to different parts of exterior walls and develop a procedure for the effective thermal parameters of an entire house. In 2000, Iliev [18] notably used an averaging of diffusivities across an interface, and during a lecture [19] to the Scientific School of Applied Environmental Thermodynamics in 2008, Orioli A. proposed an efficient distribution of nodes and provided evidence of the difference from the temperature obtained from an analytical model in layers and the temperature obtained from a finite difference model. In [19], Orioli proposed using the finite difference method – in an explicit form - in a multilayer wall. In particular, about heat conduction, Orioli proposed a solution in the case of internal physical boundary layers, suggesting that the dynamic parameters of the wall are weighted linearly with the distance between the left and right nodes; this is applicable when the layers have similar thermal properties but not when the thermal parameters are different, as often occurs in a wall, like better explained with more details in the following sections. Among the many disseminated books and papers regarding the numerical solutions of equations, Carlslaw in 1950 [20], Lapidus in 1999 [21], Canale in 2015 [22], and Tabares-Velasco and Griffith in 2012 [23] proposed a finite element method, as a numerical solution, for many science and engineering problems; however, the application of conduction phenomena in multilayer walls does not include the calculation of the temperature in the plane between two inner wall layers. At present, it is easy to believe that commercial software implements the best technical and scientific solutions. The most popular commercial building energy simulation software programs in research applications, such as CoDyBa [24], ESP-r [25–27], and TRNSYS [28–30], propose similar approaches to calculate the thermal resistivity (mK/W) and heat capacity (J/K) of walls. In recent years, new numerical models have been developed because of the study of early PCM (phase change material) models added to the layer walls [31,32], and the initially modified empirical models were obtained using an equivalent heat transfer coefficient [30] to fully implement finite difference models [29,33] and control volume models [27]. These models are used as prediction models [33]. TRNSYS and EnergyPlus are software programs that implement a routine FDM but do not easily validate the model, particularly with a multilayer wall. Kuznik et al [34] presented good results with these methods. In particular, Tabares-Velasco et al [35] tested EnergyPlus version 8 with a PCM application in a multilayer wall and noted improvements over version 6, which showed at most a half degree of difference between the experimental and simulation results. In addition, the difference between the simulated and measured heat flux was approximately 1 W/m^2 from approximately 4 W/m^2.To evaluate the thermal conductivity at the interface between nodes (layers), EnergyPlus uses a linear interpolation between nodal points [36] and the Conductance Finite Difference (CondFD) algorithm outputs the heat flux at each node and the heat capacitance of each half-node. During the CondFD solution iterations, the heat capacitance of each half node is stored similarly to the method discussed in [18]. In this work, an application of the FDM is proposed to model the diffusion of one-dimensional heat in a multilayer wall and is verified through an experimental test of a civil engineering application.

2. Theory

With an evolution of temperature over time and space in a wall, it is possible to apply the finite difference method (FDM) at the heat equation written as a continuous version of energy balance equation (1) and in the case of a single layer with a homogeneous and uniform material:

$$\rho c_p \frac{\partial T}{\partial t} = \lambda \frac{\partial^2 T}{\partial x^2} \tag{1}$$

Where:

- $\rho c_p \frac{\partial T}{\partial t}$ is the heat stored
- $\lambda \frac{\partial^2 T}{\partial x^2}$ is the variation of the temperature gradient in the x direction (temperature Laplacian operator with a vector in the x direction).

In terms of finite difference elements, it is possible to have a discrete version in equation (2):

$$\rho c_p \frac{T_i^{n+1} - T_i^n}{\Delta t} = \lambda \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{\Delta x^2} \quad (2)$$

where "n" refers to the evolution over time Δt and "i" refers to the evolution over space Δx.
In explicit finite difference schemes, the temperature at time n+1 depends explicitly on the temperature at time n. The explicit finite difference discretization of equation (3) is:

$$T_i^{n+1} = T_i^n + \frac{\lambda}{\rho c_p} \Delta t \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{\Delta x^2} \quad (3)$$

the internal diffusivity coefficient k [m2/s] is equal to:

$$k = \frac{\lambda}{\rho C_p} \quad (4)$$

Where:

- ρ is the density [kg/m^3]
- Cp is the specific heat = heat capacity [J/kgK]

It is thus possible to calculate the interface temperature of each individual layer.
Implementing equation (3) in time and space x, it is possible to discern a trend of temperature, for example, in a homogeneous and isotropic wall or in general condition in a solid introduced in the first part of this paragraph.

3. Stationary model

When considering a multilayer wall, some authors [8-11] use EnergyPlus with a linear interpolation between nodal points equidistant from the interface plane between the two layers of different and a constant Δx distance for the whole thickness of the wall. Some authors [8 -11] modify equation (8) by introducing average values for the following elements:

$$k_M = \frac{\lambda_M}{\rho_M C_{pM}} = \frac{1}{2}\left(\frac{\lambda_1}{\rho_1 C_{p1}} + \frac{\lambda_2}{\rho_2 C_{p2}}\right) \quad (5)$$

where k_M is the average value of the internal diffusivity coefficient (m^2/s) by two layers, 1 and 2 in Figure 1, or:

$$\rho_M C_{pM} = \frac{1}{2}\left(\rho_1 C_{p1} + \rho_2 C_{p2}\right) \quad (6)$$

$$\lambda_M = \frac{1}{2}(\lambda_1 + \lambda_2) \quad (7)$$

If the Δx distance in the whole thickness of the wall is not constant, equation (7) becomes equation (9):

$$\rho_M C_{pM} = \left(\frac{\rho_1 C_{p1}\Delta x_1 + \rho_2 C_{p2}\Delta x_2}{\Delta x_1 + \Delta x_2}\right) \quad (8)$$

$$\lambda_M = \left(\frac{\lambda_1 \Delta x_1 + \lambda_2 \Delta x_2}{\Delta x_1 + \Delta x_2}\right) \quad (9)$$

$$T_{M-SM} = \left(\frac{T_{cold}\frac{\lambda_2}{\Delta x_2} + T_{Hot}\frac{\lambda_1}{\Delta x_1}}{\frac{\lambda_1}{\Delta x_1} + \frac{\lambda_2}{\Delta x_2}}\right) \quad (10)$$

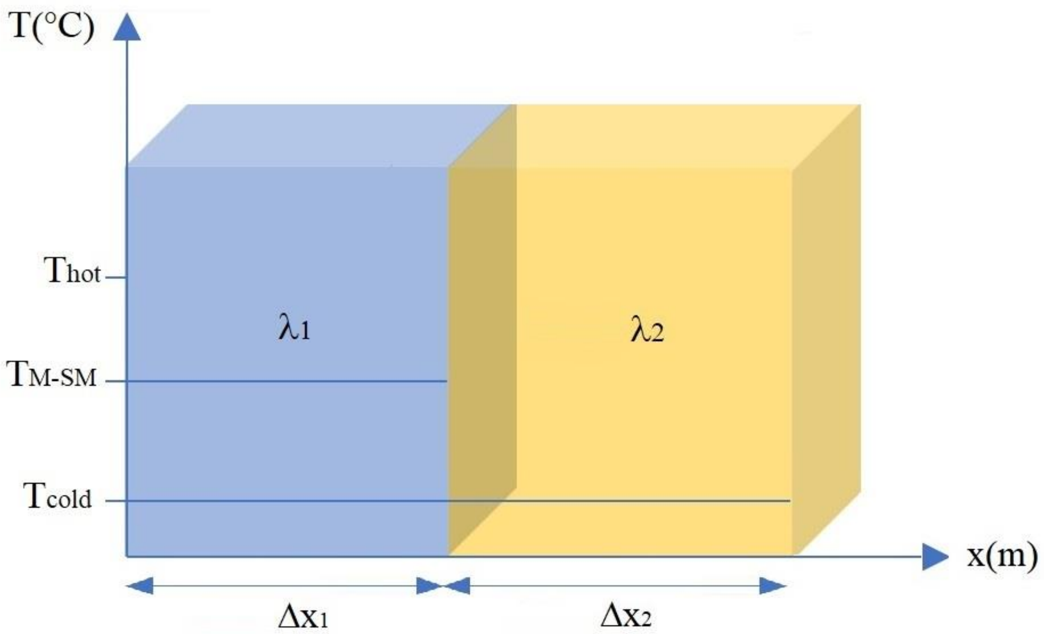

Figure 1. Scheme and equation to apply the stationary model.

4. FDM and stationary methods comparison

By compiling a MATLAB script, the FDM was applied to equation (3). Given an initial thermal state, the variation in time t and in space x of the temperatures inside a wall consisting of two layers with very different thermal properties between them was calculated. The two layers, having a different thermal conductivity, are defined according to a classification of building materials: one is an insulating layer, polyurethane, and the other is a good heat conductor, brick.

Table 1 shows the characteristic parameters of the finite difference model, the initial thermal state, and the thermophysical properties of the two materials and the temperature value for the node in the middle of the two layers for the wall after the results have thermally stabilized.

The specific heat flux (W/m^2) can be calculated by applying the Fourier law, the values of the specific heat fluxes on the two faces of the interface plane should be equal. Table 1 shows that the specific thermal fluxes calculated with the method of [19] does not have the same values.

Table 1. Data and results of stationary and dynamic thermal model.

$\Delta\tau^a$ (s) = 60	Δx^a (m) = 0.01	$T_{Hot}{}^a$ (°C) = 30	$T_{cold}{}^a$ (°C) = 20	Tw^a (°C) = 10
$x_1{}^b$ (m) = 0.1	$\lambda_1{}^b$ (W/mK) = 0.04	$Cp_1{}^b$ (J/kgK) = 1400	$\rho_1{}^b$ (kg/m^3) = 100	
$x_2{}^c$ (m) = 0.1	$\lambda_2{}^c$ (W/mK) = 0.55	$Cp_2{}^c$ (J/kgK) = 1000	$\rho_2{}^c$ (kg/m^3) = 1600	
$T_{Hot}{}^d$ (°C)	$T_{M\text{-}WA}{}^d$ (°C) (Fourier)	$T_{M\text{-}SM}$ (°C) ref.[19] ^{d}	$T_{Cold}{}^d$ (°C)	
(30.0)	(24.5)	(20.7)	(20.0)	

	layer 1 (W/m^2)	layer 2 (W/m^2)
q_x ^{e}	0.037	0.037
q_x ^{f}	0.02	0.25

[a] Data of finite differences model parameters
[b] Data layer 1 (polyurethane)
[c] Data layer 2 (brick)
[d] Data at regime Temperatures
[e] Results by Fourier Law
[f] Results by weighted average ref.[19]

Were:

- **$\Delta\tau$** is the discrete time (s)
- **q** is the specific heat flux (W/m^2)
- **Δx** is the discrete distance (m)
- **$T_{M\text{-}WA}$** is the Weighted Average Temperature (K)
- **$T_{M\text{-}SM}$** is the Stationary Method Temperature (K)

At the established temperatures in Table 1, it is evident the difference in the temperature values between the standard FDM application in the middle node between the two layers and the stationary model.

5. Discussion of the results and conclusions

The authors propose the calculation of the dynamic temperature for a multilayer wall according to a unidimensional heat flux model through a numerical method. The authors were interested in determining the values of the temperature in the transient time until the temperature stabilizes over time (steady state) in the interface between the physical layers. The proposed numerical method uses the FDM without a mixed method, i.e., FDM with a semi-analytical model.

The temperature simulated by the FDM in the literature (in particular in [5]) in the interface between physical layers of a wall provides results at a steady state, with a difference of 5% compared to the measured value in the laboratory in the same multilayer wall.

The referenced model in [19] is compared with the stationary model (Fourier) the difference at about 25°C of the middle temperature from both surfaces temperature are of about 4°C.

This difference could be critical when studying a point of humidity condensation between the layers or if linked to the internal comfort temperature which, as we know, is limited to a few degrees.

To the future, the authors intend to find a mathematical/numerical physical model of the heat equation that best models the temperature variation over time and space in the specific case of layers with specific heat values and thermal conductivity and density very different that will be a little computational capacity.

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