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On the use of numerical inverse Laplace transform applied to heat conduction in multilayer materials

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--***ABSTRACT***--

This article presents an approach to the semi-analytical treatment of the heat conduction problem applied to a multilayer material. At its interface (especially if its thermal conductivities are of very different orders of magnitude), the ``barrier effects'' are felt more intensely in the solution, impacting it in terms of its derivability at the point of contact. The proposal to use the Laplace transform to, in this space, obtain the analytical solution to the problem and then use the inverse numerical transform to obtain results, aims to introduce greater reliability in the response data in the interface region between the materials, given how the transform acts on discontinuities.

Keywords: *heat conduction problem, inverse Laplace transform, numerical methods, diffusion phenomena, composite materials, Fourier's law, partial differential equations*

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I. Introduction

Diffusion phenomena are a recurrent theme in Physics and Engineering. It deals with the transport of mass or energy through a homogeneous or composite medium. Practical applications of the second case involve the construction of closed insulating systems (e.g., walls of cold chambers), in which the composition consists of the juxtaposition of materials with different thermophysical properties, aiming to minimize thermal exchanges between the interior and the external environment. In physical terms, the union of different materials is not perfect: microscopically, the roughness inherent to their surfaces produces spaces that cause the presence of gases whose influence is perceived during the energy transit through the forming layers of the medium, in the form of currents convectives (Incropera, 1985). The gases present in the interstices between the materials offer a natural resistance to the energy flow, which does not exist in an ideal case of conduction, in which the energy is totally transferred without losses (perfect contact).

In mathematical terms, perfect contact is considered as a simplifying hypothesis in the study of the thermal transient in a composite medium. Fourier's Law, which therefore applies here, guarantees that the energy flow is kept constant at the interface between two of the consecutive materials that make it up and leads to one of the boundary conditions of a variation of the heat conduction problem, main theoretical framework used in the formulation of the present case, in which a function of position and time is sought to indicate the temperature in any part of the medium (by "medium", we understand the forming wall of the cold chamber).

Every substance has thermal conductivity and diffusivity constants, a density and a specific heat. The difference in the order of magnitude of thermal conductivity between insulating and non-insulating materials can vary by more than (Çengel, 2012). This discrepancy, observable in the use of similar materials in the composition of a cold room (eg, when using concrete associated with polyurethane aggregates) produces a "barrier effect", which can be interpreted as the difficulty of the heat flow to pass through a material more conductor to less conductor at the interface point. This phenomenon must be taken into account when choosing the numerical method for solving the resulting mathematical model; Hojjati (2010), for example, using the Crank-Nicolson numerical method, obtained a dataset that reveals a function in which the temperature profiles at the interface of the composite material accentuate a "non-derivative" character at the interface point. However, being a solution of a homogeneous partial differential equation, it is reasonable to expect that this differentiability is a characteristic of the function throughout its domain.

In an attempt to obtain a "smooth" curve that represents the temperature at the interface of multilayer materials (indicative of a "better-behaved" function in the determination of e), this study will address the possibility of using the Laplace transform in the original model. , allowing the solution in "Laplace space" to generate a dataset estimated by the inverse transformation, treated numerically in order to avoid excessive work in determining an algebraic solution (with a high possibility that this is even impossible).

II. Methodology

Consider the scenario sketched in Figure 1 below, in which a one-dimensional body is made up of 2 parts with distinct thermophysical characteristics (denoted C_1 and C_2 , with lengths respectively a and b), located on the x −axis (horizontal direction) of an orthogonal Cartesian coordinate system, restricted to the domain $[a, b] \in \mathbb{R}$:

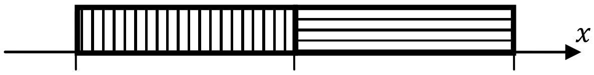

Figure 1: Arrangement of composite material on the x-axis of the orthogonal Cartesian coordinate system

With this arrangement, the classical modeling of the heat conduction problem states that:

$$\frac{\partial^2 u_1(x,t)}{\partial x^2} - \frac{1}{\kappa_1}\frac{\partial u_1(x,t)}{\partial t} = 0, a \leq x \leq 0, (t > 0) \quad [1]$$

$$\frac{\partial^2 u_2(x,t)}{\partial x^2} - \frac{1}{\kappa_2}\frac{\partial u_2(x,t)}{\partial t} = 0, 0 < x \leq b, (t > 0) \quad [2]$$

In [1] and [2], $u_i(x,t)$ and κ_i are the temperature function and the thermal diffusivity in the material i $(i = 1,2)$. Assuming that there is no contact resistance between the surfaces at x=0 , the boundary conditions are, for $t > 0$:

$$K_1 \frac{\partial u_1(0,t)}{\partial x} = K_2 \frac{\partial u_2(0,t)}{\partial x} \quad [3]$$

$$u_1(0,t) = u_2(0,t) \quad [4]$$

$$u_1(a,t) = U_1 \quad [5]$$

$$u_2(b,t) = U_2 \quad [6]$$

In [3], K_1 and K_2 are the thermal conductivities of materials. The initial condition is:

$$u_1(x,0) = u_2(x,0) = U_0 \quad [7]$$

The application of the Laplace transform in equations [1] and [2] (also for $t > 0$) leads to:

$$\frac{d^2\overline{u}_1}{dx^2} - q_1^2\overline{u}_1 = 0, a \leq x \leq 0 \quad [8]$$

$$\frac{d^2\overline{u}_2}{dx^2} - q_2^2\overline{u}_2 = 0, 0 < x \leq b \quad [9]$$

where $\overline{u}_1 = \overline{u}_1(x)$, $\overline{u}_2 = \overline{u}_2(x)$, $q_i \equiv \sqrt{\frac{s}{\kappa_i}}$, $(i = 1,2)$, and s is the Laplace parameter. As a result, the boundary conditions will become:

$$K_1 \frac{d\overline{u}_1}{dx} = K_2 \frac{d\overline{u}_2}{dx}, x = 0 \quad [10]$$

$$\overline{u}_1(0) = \overline{u}_2(0) \quad [11]$$

$$\overline{u}_1(a) = U_1/s \quad [12]$$

$$\overline{u}_2(b) = U_2/s \quad [13]$$

Solving the problem in Laplace space by traditional mechanisms provides:

$$\overline{u}_1(x) = A\left[e^{q_1 x} - e^{q_1(2a-x)}\right] + \frac{U_1}{s}e^{q_1(a-x)} \quad [14]$$

$$\overline{u}_2(x) = C\left[e^{q_2 x} - e^{q_2(2b-x)}\right] + \frac{U_2}{s}e^{q_1(b-x)} \quad [15]$$

with:

$$A = \frac{1 - e^{2q_2 b}}{1 - e^{2q_1 a}} + \frac{U_2 e^{q_2 b} - U_1 e^{q_1 a}}{s(1 - e^{2q_1 a})} \quad [16]$$

and

$$C = \frac{\delta\varepsilon q_1 K_1 + \alpha\zeta}{\alpha\beta p q_2 K_2 - \gamma\delta q_1 K_1} \quad [17]$$

for which they are:

$$\alpha = 1 - e^{2q_1 a}$$
$$\beta = 1 + e^{2q_2 b}$$
$$\gamma = 1 - e^{2q_2 b}$$
$$\delta = 1 + e^{2q_1 a} \quad [18]$$
$$\varepsilon = U_2 e^{q_2 b} - U_1 e^{q_1 a}$$
$$\zeta = U_2 q_2 K_2 e^{q_2 b} - U_1 q_1 K_1 e^{q_1 a}$$

The problem with this approach is the obvious infeasibility of inverting the solution to return to the function space that contains the analytic solutions we want to obtain. The alternative was, therefore, to proceed with the numerical inversion of the set of equations [14] to [18], for which an implementation of the algorithm of Stehfest (1970) and Gaver (1966) was used, according to which:

$$u_i(x,t) \cong \frac{ln2}{t} \sum_{j=1}^{M} w_j \overline{u_i}(s_j), i = 1,2 \quad [19]$$

$$s_j = j \frac{ln2}{t}, j = 1,2,3, \ldots, M \quad [20]$$

$$w_j = \quad [21]$$

In equations [20] and [21], it is a natural pair.

III. Results

The numerical experiments carried out were based on a multilayer material with the thermophysical characteristics listed in Tab. 1. A numerical code was written, in *Fortran 77*, to deal with this problem. This particular language was chosen because of the authors' extensive experience with it and the fact that there are free and reliable compilers on the *Unix* operating system.

Table 1: data on the materials used.

Materials	**thermal conductivity (W/m*K)**	**thermal diffusivity (m^2/s)**
Plaster	0.510	0.470
Polyurethane (PUR)	0.029	0.430
Concrete	1.400	0.870
Galvanized steel	48.9	14.1

Previous approaches to the problem in question were solved by the finite element method (explicit) and by the implicit method (Cranck-Nicholson) using diffusivity constants of different orders of magnitude (as is the case for the materials listed in Tab. 1, in which it appears that galvanized steel and other materials present a difference of the order of 10^2 this variable) led to the discontinuity of the solution $u(x,t)$ at the interface point (Hojjati, 2010). In physical terms this is unacceptable as thermal equilibrium occurs gradually when two distinct surfaces are brought into contact.

The transformation of the partial differential equation (PDE) into an ordinary differential equation (ODE) with constant coefficients in the Laplace space guarantees the maintenance of the original solution's continuity, as can be seen in the results below:

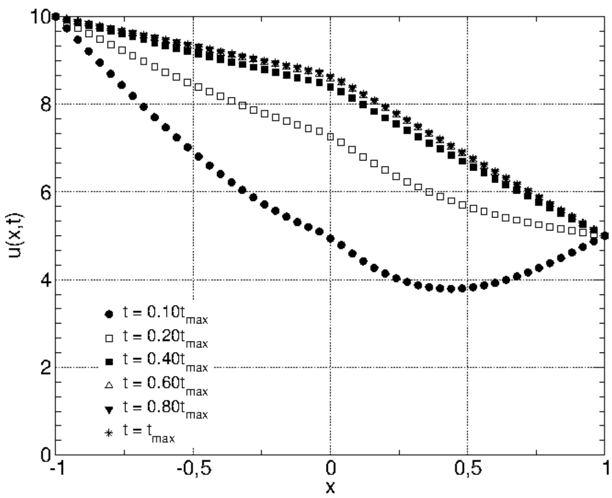

Figure 2: Composite material formed by plaster and concrete ($t_{max} = 6$s).

The first experiment simulates the situation of perfect contact between a material composed of plaster (left) and concrete (right). Tab.1 shows similar thermal diffusivities and a difference of the order of 10^1 between the respective conductivities. In such a scenario, it is reasonable to expect that temperature stabilization at the interface will occur smoothly, given the characteristics of the materials involved. Respectively, boundary and initial conditions were:

$$u_1(a,t) = 10^0C \quad [22]$$
$$u_2(b,t) = 5^0C \quad [23]$$
$$u_1(x,0) = u_2(x,0) = 0 \quad [24]$$

The second experiment simulates heat transmission in a composite material in a perfect contact situation. PUR and galvanized steel were used, whose thermal conductivities show a difference in their order of magnitude of approximately 10^3. Temperature profiles are shown in figs. 3 and 4. The boundary conditions used were the same as above.

The Fig 3 shows the temperature profiles for 6 different time points, with PUR on the left and galvanized steel on the right. Note that, as PUR has a greater resistance to thermal flow (better insulator), the curves evolve more slowly towards the thermodynamic equilibrium situation. On the other hand, the curves for galvanized steel evolve rapidly, as this material has a low thermal resistance (an excellent conductor of heat). But, most importantly, the functions do not have non-derivative points or discontinuities. This can be seen best in Fig. 4, where the region of perfect contact ($x = 0$) is shown in an enlarged form.

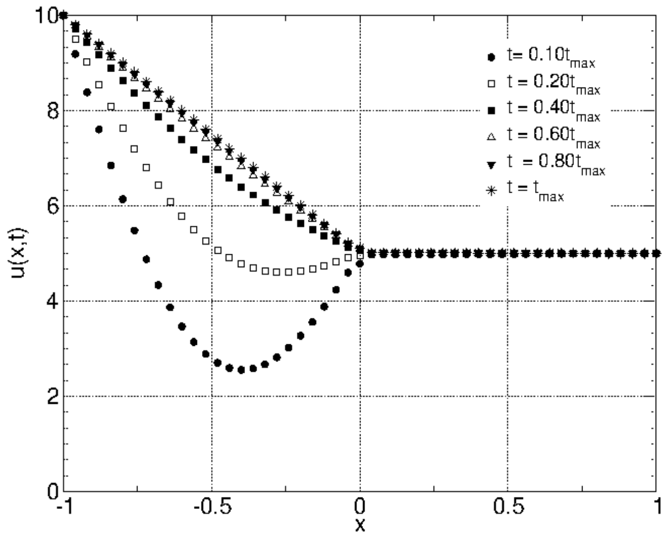

Figure 3: Composite material formed by materials with different thermal diffusivity (galvanized steel and PUR).

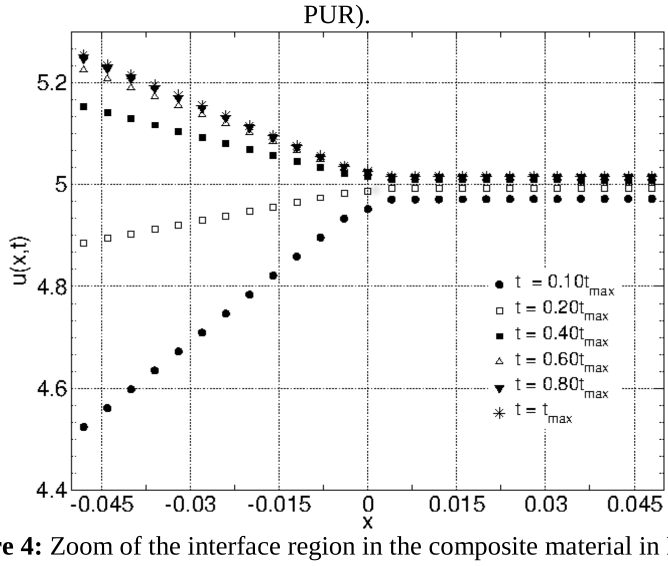

Figure 4: Zoom of the interface region in the composite material in Fig. 3.

IV. Discussions about the results

Locating the composite material with the interface at the origin of the orthogonal Cartesian coordinate system was the strategy found to prevent the beads from becoming too cumbersome both algebraically and computationally: the imposition of the perfect contact condition (equation [10]) in such a situation led , in the first approaches to this problem, the solutions in the forms [14] and [15] in which the arguments of the exponential functions that compose it turned out to be very extensive, mainly hindering the implementation in a high-level language. The positioning of the interface at the origin did not cause any loss of generality of the obtained results, facilitating later qualitative analysis and the creation of code whose visual results were presented in the previous section.

This strategy has also been shown to be effective in controlling the size of the composite material. Introducing negative values for the size of the material (before the origin – note that the interval is symmetric and the -1 from 1), an equilibrium in exponential terms was verified, avoiding divergent ($+\infty$ or $-\infty$) temperature values. Incidentally, this procedure is similar to that found in Iserles (2008), which parameterizes the heat conduction problem in a unit size bar, which allows subsequent extrapolation to a bar of any size, while this ensures the convergence of the numerical method used in its resolution, based on the Courant number.

Authors such as Carslaw (1959) cite the Laplace Transform as a more appropriate tool for treating the heat conduction problem in composite media. Mathematically, the transposition of an ODE defined in a space of continuous functions by parts to a "Laplace space" uniforms a finite amount of discontinuities arising from a non-homogeneous term. Physically, this is compatible with the parameterization of the temporal variable in the EDP of the problem under study, because as , the (possibly large) temperature variations along the material (including its interface) become irrelevant, something that is expected given the diffusive nature of heat conduction.

The equations derived from PDE plus original boundary conditions are (in the "Laplace space") ordinary and with constant coefficients. The "transformed" boundary conditions [10] to [13] guarantee not only the existence of the solutions $\overline{u}_1$ and $\overline{u}_2$ but also their continuity until the second derivative (it should be remembered that these equations are in the spatial variable), therefore guaranteeing the smoothness of the $u(x,t)$ obtained by the proposed numerical inversion process.

In the general case, the continuity (in parts) of the solution of a non-homogeneous ODE and its derivatives is directly linked to the continuity of the forcing term and its derivatives. It is proved that, if we impose on the solution that it and its first derivative are continuous, then a supposed forcing term must already present discontinuity in its definition; for$\overline{u}_1$, $\overline{u}_1'$ e $\overline{u}_1''$, and to be continuous, the forcing term must present discontinuity in its first derivative, and so on. Now, since this forcing term does not exist (or, more adequately, constant and null), its derivatives will always be continuous and, thus, it will be continuous, as well as any derivative of order *n*. If we consider that the same holds true for $\overline{u}_2$, it is expected that, for values close to, the solution at the interface presents a desired "derivability" behavior after being numerically estimated, which is effectively observed in the results obtained.

V. Conclusions

In this work, a study of the heat transfer in a composite material with significantly different conductive properties was carried out. The resulting "barrier effect", acting on the thermal flow, gave rise to a model whose solution showed problems of discontinuity at the interface, depending on the method used in its determination. The use of the Laplace transform in the original partial differential equation led to ordinary equations that, providing continuous solutions in "Laplace space", due to the way it was obtained (obtained by methods in the solution function of the PDEs that govern the problem is something not allowed To eliminate this problem, we use the Laplace transform and analytically calculate the new functions (in the Laplaca space).The inverse transform was done numerically due to the complexity of the solution functions.

Our results show that the use of Laplace transforms, and their numerical inverse, resulted in a smoothing of the solution function (temperature). In this way, we can accept them as, in fact, a solution for a PDE. Furthermore, our code is robust enough and can be used in future studies where materials that are not listed in Tab. 1 can be used. We should also emphasize the use of a high-level programming language, widely used in similar calculations, where there is total control of the mathematical procedures during the simulation. This is the opposite of what happens when we use paid programs, which do not make it completely clear and explicit how the calculations are being developed.

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