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A method of recursive images to solve transient heat diffusion in multilayer materials

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ABSTRACT

An innovative method of recursive images is presented to obtain solutions to the transient diffusion equation in a N-layered material based on the superposition of Green functions for a semi-infinite material. Through a sequential sum of image reflected functions a temperature solution is initially built for a structure of one layer over a substrate. These functions are chosen in order to satisfy in sequence the boundary conditions, first at the front interface then at the back interface then again at the front interface and so on until the magnitude of the added functions becomes negligible. Based on this so-called 1-layer algorithm, a 2-layer algorithm is obtained. This is accomplished through a sequential application of the 1-layer algorithm first to layer 1 then to layer 2 then again to layer 1 and so on. After that it is suggested how the sequential application of the $N-1$ algorithm leads to the N-layer algorithm. This present scheme is valid for boundary conditions of the first and second kind but it will not applicable neither to the case where there is a contact resistance between layers or to the case of convective heat transfer at the end interfaces.

1. Introduction

Diffusion through multiple layers is an occurrence which has applications in a wide range of areas of heat and mass transport [1,2]. The partial differential equation [3,4] governing this phenomenon and in particular that of the heat diffusion in an N layer material, is given for each layer i in its simplest form by,

$$D_i \frac{\partial^2 T_i}{\partial x^2} = \frac{\partial T_i}{\partial t} \quad i = 1, 2, \ldots N \tag{1}$$

where t (s) is time and T (K) and D (m^2/s) are the temperature and the thermal diffusivity of a layer material respectively. The boundary condition at each interface involves the continuity of both the temperature and of the heat flow i.e.

$$T_i = T_{i+1} \tag{2}$$

$$\kappa_i \frac{\partial T_i}{\partial x} = \kappa_{i+1} \frac{\partial T_{i+1}}{\partial x} \tag{3}$$

where κ (W/m-K) is the thermal conductivity for a material. The boundary condition at the front face of the first layer will depend on the specific problem under study.

The diffusion equation is known for its difficulty in rendering closed form analytical solutions. Nevertheless, diffusion in multilayer materials has been solved analytically using the method of separation of variables,[5–8] the Laplace and Fourier transforms [9–11] and also numerically through the method of fundamental solutions [12] or using proprietary or commercial software packages employing finite elements, finite differences [1] or boundary element algorithms. For a thorough account of the state of the art in this subject one can take a look at the papers of de Monte [5,6].

The method of separation of variables in particular, is a widely used method even though it becomes quite involved once the number of layers increases [13]. In this paper, we propose a conceptually simple method based on the principle of superposition whose rules are easy to apply to a multilayer material, once the heat diffusion solution for a semi-infinite material is known together with the thermal properties of the various layers.

2. Theory: Green functions for an interface between different media

The Green function for a heat source $T_{si}(x_1, t)$ whose origin is located at $x_1 = 0$ of medium-1, whose interface with a back medium is at $x_1 = d_1$ (see Fig. 1) is as follows [3] (see pp. 363–364). The total temperature function for medium-1 $T_1(x_1, t)$, consists of a sum of the temperature function $T_{si}(x_1, t)$ with the temperature

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x	thickness coordinate	r_b, r_f	"reflection" strengths
d	thickness of a layer (m)	κ	thermal conductivity (W/m-K)
t	time	D	thermal diffusivity (m^2/s)
$T(x,t)$	temperature solution (K)	ρ	density (kg/m^3)
$T_{si}(x,t)$	semi-infinite temperature solution (K)	c	specific heat (J/kg)
t_b, t_f	"transmission" strengths		

function $r_bT_{si}(2d_1 - x_1, t)$, whose origin is thus symmetrically located a distance d_1 to the right of the back interface and whose strength is r_b. The total solution in medium-1 is thus (see Fig. 1),

$$T_1(x_1,t) = T_{si}(x_1,t) + r_bT_{si}(2d_1 - x_1,t) \tag{4}$$

where the "reflection strength" r_b is given by,

$$r_b = \frac{\kappa_1\sqrt{D_b} - \kappa_b\sqrt{D_1}}{\kappa_1\sqrt{D_b} + \kappa_b\sqrt{D_1}} \tag{5}$$

One should realize that both terms in Eq. (4) satisfy the diffusion equation (i.e. Eq. (1)) as can be verified for a generic function of the form $CT_{si}(b + ax_1, t)$ where a, b and C are constants. Upon substituting this function in Eq. (1) one gets,

$$C\frac{\partial T_{si}(b + ax_1, t)}{\partial t} = Ca^2 \quad D_1\frac{\partial^2 T_{si}(b + ax_1, t)}{\partial (b + ax_1)^2} \tag{6}$$

This statement is true if $T_{si}(x,t)$ is a solution of the diffusion equation which is obviously true, and $a = \pm 1$ which is also true for both terms of Eq. (4).

For the back medium, the "transmitted" temperature function is given, after some manipulation of Eq. (9), Section 14.6 in Carslaw and Jaeger [3] by

$$T_b(x_b,t) = t_bT_{si}\left(d_1 + x_b\sqrt{\frac{D_1}{D_b}}, t\right) \tag{7}$$

where the "transmission strength" t_b is given by,

$$t_b = \frac{2\kappa_1\sqrt{D_b}}{\kappa_1\sqrt{D_b} + \kappa_b\sqrt{D_1}} \tag{8}$$

One realizes that Eq. (7) also verifies the diffusion equation for the back medium as can be concluded from the discussion of Eq. (6). Furthermore, one can verify by direct substitution that the above solutions for $T_1(x_1,t)$ and $T_b(x_b,t)$ (i.e. Eqs. (4) and (5) and (7) and (8)) verify the conditions for continuity of both the temperature and heat flow at the back face, (i.e. Eqs. (2) and (3)),

$$T_1(x_1,t)|_{x_1=d_1} = T_b(x_b,t)|_{x_{b=0}} \text{ and}$$
$$\kappa_1\frac{\partial T_1(x_1,t)}{\partial x_1}\bigg|_{x_1=d_1} = \kappa_b\frac{\partial T_b(x_b,t)}{\partial x_b}\bigg|_{x_b=0} \tag{9}$$

We remark that if the back medium is highly thermally conductive, more specifically if $\kappa_b/\sqrt{D_b} >> \kappa_1/\sqrt{D_1}$, then $r_b \approx -1$. In that case the temperature at the back face will be,

$$T_1(x_1,t) = T_{si}(x_1,t) - T_{si}(2d_1 - x_1,t) \ \Rightarrow\ T_1(d_1,t) = 0 \tag{10}$$

and therefore it will not change from its initial value which is an indication of a thermal reservoir at the back face. If, on the contrary, the medium-2 is an highly insulating material (i.e. $\kappa_b/\sqrt{D_b} << \kappa_1/\sqrt{D_1}$) then $r_b \approx 1$ and very little heat will flow across the back interface, i.e.

$$T_1(x_1,t) = T_{si}(x_1,t) + T_{si}(2d_1 - x_1,t) \ \Rightarrow\ \frac{\partial T_1(x_1,t)}{\partial x_1}\bigg|_{x_1=d_1} = 0 \tag{11}$$

Using the results of this section one can solve for the temperature in a multilayer material through a sequential sum of "reflected" temperature solutions which satisfy the boundary conditions at the reflecting interface, as will be described in the next section.

3. Temperature solution for a layer in-between two semi-infinite media

Going back to Fig. 1 one realizes that Eq. (4) for $T_1(x_1,t)$ even though obeying the BC (Boundary Conditions) at the back interface now fails to fulfill the BC at the front face. We thus ought to change Eq. (4) so that the series solution for $T_1(x_1,t)$ obeys the front face BC too. Of the two terms of Eq. (4) the initial function $T_{si}(x_1,t)$ satisfies the BC at the front face but the second term does not. We are thus facing an analogous problem as that of the previous section although for a different interface and temperature function. The second term of Eq. (4) appears as a result from the first image reflection at the back interface (i.e. $T_{rb,1} = r_bT_{si}(2d_1 - x_1,t)$) and has its source located at $x_1 = +2d_1$ as was mentioned in Section 2. Thus its image at the front face should have its source symmetrically located relative to the front interface and thus its source should be positioned at $x_1 = -2d_1$. Furthermore the strength of its image should be affected by coefficient r_f which takes into account the thermal properties of medium-1 and those of the front medium. We thus obtain the third term which will make the series satisfy the BC at the front face (see Fig. 2),

$$T_{rf,1} = r_fr_bT_{si}(2d_1 + x_1,t) \tag{12}$$

Analogously to Eq. (7), the first "transmitted" temperature function into the front medium will be given by,

$$T_{tf,1}(x_f,t) = t_fr_bT_{si}\left(2d_1 + x_f\sqrt{\frac{D_1}{D_f}}, t\right) \tag{13}$$

One can appreciate that this adjustment process should not stop because now the BC at the back face will again fail to be fulfilled. Thus a fourth term should be added to the series in order to fulfill again the BC at the back face of the slab. If one proceeds with this method of recursive images, the series solution we are seeking will be given by,

$$T_1(x_1,t) = T_{si}(x_1,t) + \sum_{i=1}^{\infty}T_{rb,i}(x_1,t) + \sum_{i=1}^{\infty}T_{rf,i}(x_1,t) \quad 0 \leqslant x_1 \leqslant d_1 \tag{14}$$

where $T_{rb,i}(x_1,t)$ represents the successive temperature solutions "ith reflected" at the back face of the slab (see Fig. 2), i.e.

$$T_{rb,i} = r_f^{i-1}r_b^iT_{si}(2id_1 - x_1,t) \tag{15}$$

while $T_{rf,i}(x_1,t)$ represents those "ith reflected" at the front face (see Fig. 2),

$$T_{rf,i} = r_f^ir_b^iT_{si}(2id_1 + x_1,t) \tag{16}$$

These terms, summed at each image reflection, are chosen in such a way that the boundary conditions are satisfied in turn according to the rules set out by Eqs. (4)–(8). In addition, the

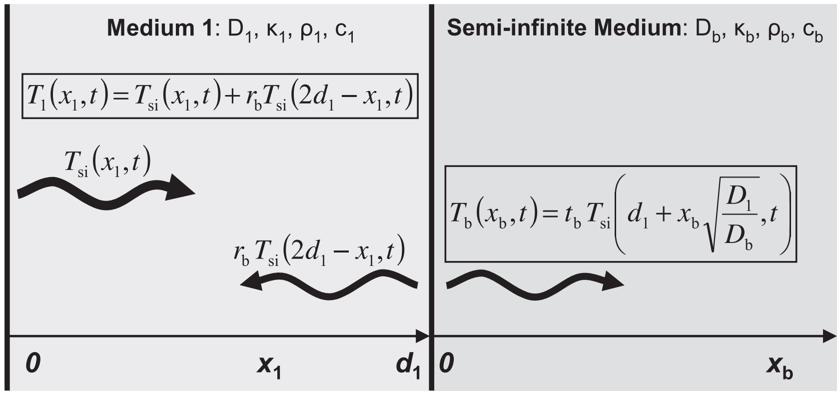

Fig. 1. The temperature in two different media assuming a temperature source located in $x_1 = 0$ of medium 1. The interface between the media is located in $x_1 = d$ ($x_b = 0$). Parameters r_b and t_b can be thought of as the "reflection" and "transmission" coefficients respectively of the temperature solution "incident" on the interface between the media.

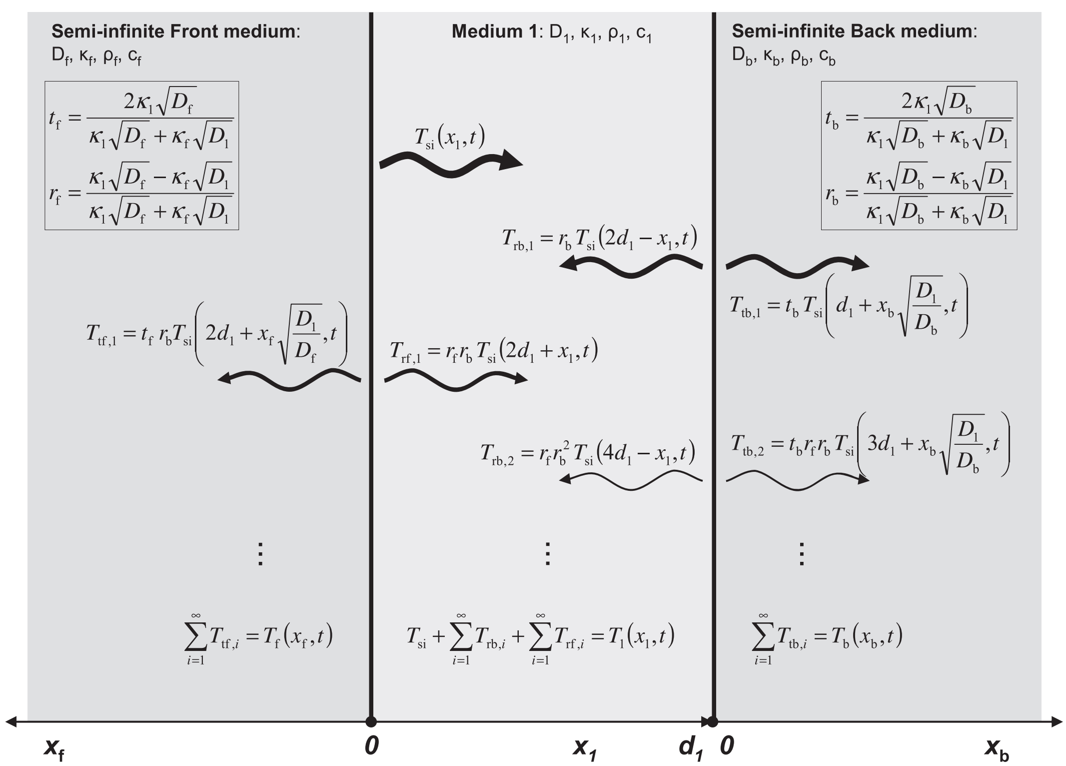

Fig. 2. A computation scheme for calculating the temperature for a sandwich structure consisting of a front semi-infinite medium, a layer medium and a backside semi-infinite medium. All media have different thermal properties. We assume a heat source at $x_1 = 0$ whose temperature function is $T_{si}(x, t)$ applicable inside the layer medium, considered semi-infinite. This temperature function is assumed to be consistent with the boundary condition at the front face.

temperature solutions for the semi-infinite media at the back and the front faces will be given respectively by,

$$T_b(x_b, t) = \sum_{i=1}^{\infty} T_{tb,i}(x_b, t) \quad x_b \geqslant 0 \tag{17}$$

$$T_f(x_f, t) = \sum_{i=1}^{\infty} T_{tf,i}(x_f, t) \quad x_f \geqslant 0 \tag{18}$$

where each term in the right member of the above equations represents the "transmitted" temperature solution into the semi-infinite media, due either to an image reflection at the back or at the front faces as described by Eqs. (7) and (8) (see Fig. 2), i.e.

$$T_{tb,i}(x_b, t) = t_b r_f^{i-1} r_b^{i-1} T_{si}\left((2i-1)d_1 + x_b\sqrt{\frac{D_1}{D_b}}, t\right) \tag{19}$$

$$T_{tf,i}(x_f, t) = t_f r_f^{i-1} r_b^{i} T_{si}\left(2id_1 + x_f\sqrt{\frac{D_1}{D_f}}, t\right) \tag{20}$$

Since the diffusion equation (Eq. (1)) is a linear equation, the temperature solution for the slab $T_1(x_1, t)$ (Eq. (14)) as well as the temperature solutions for the back $T_b(x_b, t)$ (Eq. (17)) and for the front semi-infinite media $T_f(x_f, t)$ (Eq. (18)) will all verify the diffusion equation in their respective media because they are all linear combinations of functions which verify Eq. (1) as pointed out above in the discussion of Eq. (6).

We can also verify that the proposed temperature solutions verify the BC both at the back and front faces. For the continuity of the temperature at the back face we obtain the following equation,

$$T_1(x_1,t)|_{x_1=d_1} = T_b(x_b,t)|_{x_b=0} \tag{21}$$

while for the continuity of the heat flow we get,

$$\kappa_1 \frac{\partial T_1(x_1,t)}{\partial x_1}\bigg|_{x_1=d_1} = \kappa_b \frac{\partial T_b(x_b,t)}{\partial x_b}\bigg|_{x_b=0} \tag{22}$$

Upon expanding Eq. (21) through the use of Eqs. (14) and (17) and grouping all the terms in the left member we realize that Eq. (21) is true, i.e.

$$\underbrace{T_{si}(d_1,t) + T_{rb,1}(d_1,t) - T_{tb,1}(0,t)}_{=0} + \underbrace{T_{rf,1}(d_1,t) + T_{rb,2}(d_1,t) - T_{tb,2}(0,t)}_{=0} + \cdots = 0 \tag{23}$$

In fact the first three terms are the result of the first image reflection at the back face and thus they verify the continuity of temperature at the back face then the next three are the result of the second reflection at the back face and thus they also verify the continuity of temperature at that interface and so on. If we expand Eq. (22) for the continuity of the heat flow and group all the term in the left member we obtain a similar equation as Eq. (23) which, in groups of three terms, verify the BC of continuity of heat flow at the back face. We conclude therefore that the temperature series solution for the slab $T_1(x_1,t)$ and for the semi-infinite medium at the back face $T_b(x_b,t)$ verify the BC at the back face.

For the BC at the front face we proceed in a similar manner. Accordingly, for the continuity of the temperature solution we have,

$$T_{si}(0,t) + \underbrace{T_{rb,1}(0,t) + T_{rf,1}(0,t) - T_{tf,1}(0,t)}_{=0} + \underbrace{T_{rb,2}(0,t) + T_{rf,2}(0,t) - T_{tf,2}(0,t)}_{=0} + \cdots = T_{si}(0,t) \tag{24}$$

while for the continuity of the heat flow we get,[1]

$$\kappa_1 \frac{\partial T_{si}(0,t)}{\partial x_1} + \underbrace{\kappa_1 \frac{\partial T_{rb,1}(0,t)}{\partial x_1} + \kappa_1 \frac{\partial T_{rf,1}(0,t)}{\partial x_1} + \kappa_f \frac{\partial T_{tf,1}(0,t)}{\partial x_f}}_{=0} + \cdots = \kappa_1 \frac{\partial T_{si}(0,t)}{\partial x_1} \tag{25}$$

Therefore, in the case of the front face, the above continuity conditions show that this method of recursive images assures that the proposed solutions do not affect the BC for the front face imposed by the initial semi-infinite solution.

Finally it should be pointed out that, from a computational perspective, the number of terms needed to be included in the series of Eqs. (14), (17) and (18) depends on the time. Obviously for very short times the number of terms needed are few because those terms originating from multiple reflections will have a negligible value. As time progresses however, if the series is truncated too "early" then the BC either at the front face or at the back face will not be fully satisfied. Thus the number of terms needed in the series must increase due to the propagation of heat further and further away from the source located at $x_1 = 0$. As the semi-infinite diffusion equation is expressed in terms of the similarity variable [14] (i.e. $x/\sqrt{4Dt}$), it seems natural that for the last term of the series of Eq. (14) this variable should attain several units.

[1] Note that the positive signal for the "transmitted" heat flow into the front medium is due to the direction of the x_f axis (see Fig. 2).

Summing up, this method starts with an temperature solution $T_{si}(x_1,t)$ for Eq. (1), valid for a semi-infinite medium of constant properties, subject to boundary conditions coinciding with those at the front face of the slab. Then in essence, what this method does is a kind of folding of that solution (like "origami paper") according to certain rules which are set by the boundary conditions at each of the layer interfaces. At this point we should note again that a thermally insulated wall or a thermal reservoir are extreme cases of the general case of an interface between two different media.

4. Analytical solution for a layer in-between a thermal reservoir and a semi-infinite substrate

Using the results of the previous section, we look for the temperature solution for a layer over a semi-infinite substrate of zero initial temperature and whose front face comes into contact with a thermal reservoir ($T = T_o$) at time $t = 0$. For a semi-infinite medium the solution satisfying the BC at the front face, found in any textbook, is,

$$T_{si}(x_1,t) = T_o \,\mathrm{erfc}\left(\frac{x_1}{\sqrt{4Dt}}\right) \tag{26}$$

where erfc is the complementary error function. This temperature solution is thus the first term of the temperature series solution inside the layer $T_1(x_1,t)$ (see Eq. (14)). We assume that r_b and t_b are respectively the "reflection" and "transmission" strengths at the back interface given by Eqs. (5) and (8) while $r_f = -1$ is the "reflection" strength at the front face. This value for r_f implies that the front medium is a thermal reservoir and thus the temperature at the front face is kept constant and equal to T_o as discussed previously in Eqs. (24) and (25) relating to the BC at the front face.

Therefore the temperature series solution for the layer using Eqs. (14)–(16) is,

$$T_1(x_1,t) = T_{si}(x_1,t) + \sum_{i=1}^{\infty} (-1)^{i-1} r_b^i T_{si}(2id_1 - x_1, t) + \sum_{i=1}^{\infty} (-1)^i r_b^i T_{si}(2id_1 + x_1, t) \quad 0 \leqslant x_1 \leqslant d_1 \tag{27}$$

while the temperature for the substrate using Eqs. (17) and (19) will be given by,

$$T_b(x_b,t) = \sum_{i=1}^{\infty} t_b (-1)^{i-1} r_b^{i-1} T_{si}\left((2i-1)d_1 + x_b\sqrt{\frac{D_1}{D_b}}, t\right) \quad x_b \geqslant 0 \tag{28}$$

In Fig. 3 we show the results of the simulation of this heat conduction problem where a layer is placed over a substrate of lower thermal conductivity so that the "reflection strength" at the back face r_b is greater than zero and equal to 0.1716 while the value for t_b is 1.1716. In the same figure are also plotted curves calculated using PDETOOL from MATLAB [15] which uses Finite Elements to solve partial differential equations. An observation of the plot shows the excellent agreement between results of both methods although the number of terms used for the proposed method was just five reflections for each interface.

The temperature solution for this particular heat diffusion problem has been given before by Carslaw and Jaeger [3] (pp. 321–322 Eqs. (16) and (17)) which deduced it using Laplace transforms. Nevertheless we have chosen to solve this simple problem using the proposed method because it exemplifies the way in which the method of recursive images work. In addition it will be useful to compare the result for one layer of Fig. 3 with subsequent results for a number of layers over a substrate.

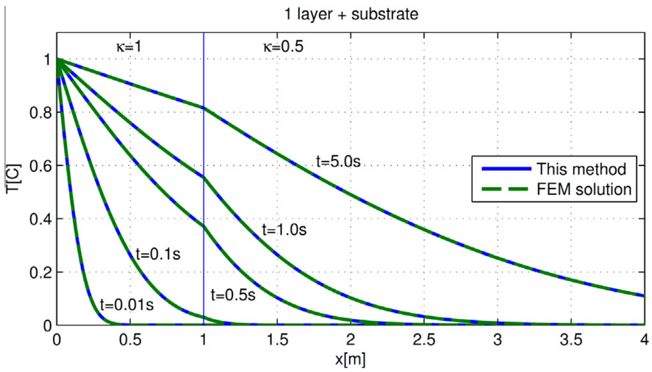

Fig. 3. Results of the simulation of a thermal reservoir in contact with a layer over a substrate (Eqs. (27) and (28)). All the parameters for the slab were taken as unity namely: thermal diffusivity κ_1 = 1 W/m-K, mass density ρ_1 = 1 kg/m^3, specific heat c = 1 J/kg-K and thickness d_1 = 1 m. Parameters for the substrate were the same as the layer except its thermal conductivity which is half that of the layer.

Finally we emphasize that this method of recursive images allows in a straightforward manner, the analytical solution for any 1-layer diffusion problem as long as a semi-infinite solution satisfying the front face boundary condition is known as will be illustrated below.

5. Numerical solution for two or more layers on a substrate

5.1. A brief description of the 1-layer algorithm

Although the ideas incorporated in Eqs. (14)–(20) are analytical in nature it is too complex to find analytical expressions, like Eqs. (27) and (28), for cases with more than one layer. Therefore a numerical procedure was employed whose details will be the object of a specific paper but which works along the steps described below. The basis of this numerical approach is that a temperature function, instead of an analytical expression, can alternatively be defined in tabular form by a two row matrix, one row for x and one row for the temperature values, whose length and spacing take into account the specifics of the problem to be solved.

Here we explain how the so-called 1-layer algorithm allows for the computation of the temperature solutions represented by Eqs. (14), (17) and (18). The problem consists of a layer-1 in-between a front and a back semi-infinite media (see Fig. 4), so that the "reflection" coefficients are r_b and r_f for the back and the front interfaces respectively while the "transmission" coefficients for those same interfaces are correspondingly t_b and t_f.

(a) The process starts for time t with the definition of a two-row matrix: one row containing the x values while the other row vector contains the corresponding values for the semi-infinite temperature solution (i.e. T_{si} row-vector) whose extension in length should be several times the similarity variable i.e. $x_{max} \geqslant 10\sqrt{4D_1t}$, sufficient for the temperature to decay to zero at the end of the row-vector. Therefore the minimum length of the initial T_{si} row-vector does not strictly depend on the thickness of the layer, but on the extent to which the temperature would have diffused if medium-1 was a semi-infinite medium. The resolution of the x row-vector is determined also by the similarity variable i.e. $\Delta x \leqslant 0.01\sqrt{4D_1t}$ but should also be high enough so that the number of points inside the layer allow for a fine interpolation of the semi-infinite solution. This is not too critical because diffusion solutions are in general well behaved functions except possibly for very short times in which case the layer will behave as a semi-infinite medium and this whole method of images will be meaningless [16,17].

(b) The first term of $T_1(x_1,t)$ of Eq. (14) is then a segment sliced out from the T_{si} row-vector from $x \geqslant 0$ to $x \leqslant d_1$, and which is set aside in a cumulative T_1 row-vector to evaluate the temperature in the layer. We remark that the interface points $x_1 = 0$ and $x_1 = d_1$, where there is a continuity of temperature and of heat flow, make also part of the temperature solutions for the front and back media respectively. An x_1 row-vector is also synthesized from a duplicate of the x values between $x \geqslant 0$ to $x \leqslant d_1$ which together with the cumulative T_1 row-vector constitute a table which in the final will represent the temperature in layer-1 $T_1(x_1,t)$.

(c) A duplicate is made from the remaining of the T_{si} row-vector (i.e. whose $x_{min} \geqslant d_1$) which after its multiplication by t_b is the first term of semi-infinite $T_b(x_b,t)$ (i.e. $T_{tb,1}(x_b,t)$, see Eqs. (17), (19) and Fig. 2). An x_b row-vector is also synthesized from a duplicate of the remaining x row-vector after multiplying it by $\sqrt{D_1/D_b}$ (see Eq. (7)). This two row matrix, the x_b and the cumulative T_b row vectors, will in the final constitute a table corresponding to the temperature solution of the back medium $T_b(x_b,t)$ (Eq. (17)).

(d) The remaining T_{si} row-vector (i.e. whose $x_{min} \geqslant d_1$) is then multiplied by r_b. The first reflection at the back interface $T_{rb,1}(x_1,t)$ (see Eqs. (14), (15) and Fig. 2), is subsequently a segment sliced out from the T_{si} row-vector between $x \geqslant d_1$ and $x \leqslant 2d_1$, which is after that flipped (mirror-reflected) and added to the cumulative T_1 row-vector.

(e) A duplicate is made from the remaining of the T_{si} row-vector (i.e. whose $x_{min} \geqslant 2d_1$) which after its multiplication by t_f is the first term of semi-infinite $T_f(x_f,t)$ (i.e. $T_{tf,1}(x_f,t)$, see Eqs. (18), (20) and Fig. 2). An x_f row-vector is also synthesized from a duplicate of the remaining x row-vector after

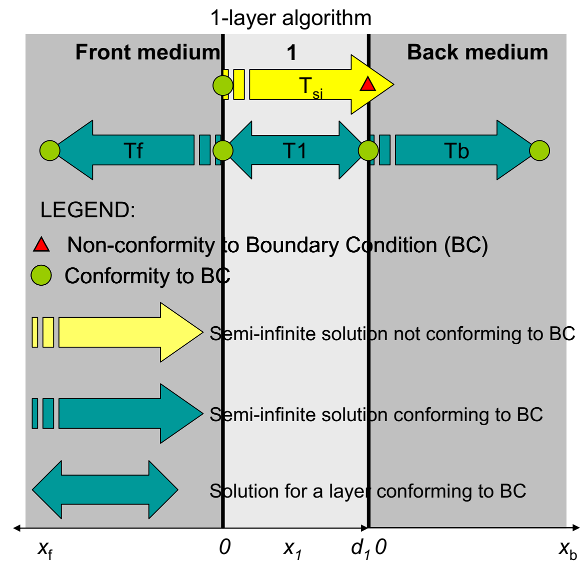

Fig. 4. Computation scheme to determine the temperature in a multilayer structure consisting of 1-layer over a substrate. The light yellow arrows represent a temperature function valid for a semi-infinite layer while the dark blue arrows represent temperature solutions conforming to its boundary conditions. The final temperature for each layer is determined from the sum of all of its temperature functions associated to dark arrows. The green round dots mean conformity of the temperature function to the boundary condition at the interface while red triangles represent non-conformity. (For interpretation of the references to colour in this figure caption, the reader is referred to the web version of this article.)

multiplying it by $\sqrt{D_1/D_f}$ (see Eq. (13)). This two row matrix will in the final, constitute a table representing the temperature solution for the front medium $T_f(x_f,t)$ (see Eq. (18)).

(f) The remaining T_{si} row-vector (i.e. whose $x_{min} \geqslant 2d_1$) is then multiplied by r_f. The first reflection at the front interface (i.e. $T_{rf,1}(x_1,t)$, see Eqs. (14), (16) and Fig. 2), is then a portion taken out from the T_{si} row-vector between $x \geqslant 2d_1$ and $x \leqslant 3d_1$ and subsequently added to the T_1 cumulative row-vector.

(g) A duplicate is made from the remaining of the T_{si} row-vector (i.e. whose $x_{min} \geqslant 3d_1$) which after its multiplication by t_b is the second term of semi-infinite $T_b(x_b,t)$ (i.e. $T_{tb,2}(x_b,t)$, see Eqs. (17), (19) and Fig. 2). This row vector is added to the cumulative T_b row vector.

(h) The remaining T_{si} row-vector (i.e. whose $x_{min} \geqslant 3d_1$) is then multiplied by r_b. The second reflection at the back interface $T_{rb,2}(x_1,t)$ (see Eqs. (14), (15) and Fig. 2), is subsequently a segment taken out from the T_{si} row-vector between $x \geqslant 3d_1$ and $x \leqslant 4d_1$, which is flipped (mirror-reflected) and added to the cumulative T_1 row-vector.

(i) A duplicate is made from the remaining of the T_{si} row-vector (i.e. whose $x_{min} \geqslant 4d_1$) which after its multiplication by t_f is the second term of semi-infinite $T_f(x_f,t)$ (i.e. $T_{tf,2}(x_f,t)$, see Eqs. (18), (20)). This row vector is added to the T_f row vector.

(j) The remaining T_{si} row-vector (i.e. whose $x_{min} \geqslant 4d_1$) is then multiplied by r_f. The second reflection at the back interface $T_{rf,2}(x_f,t)$ (see Eqs. (14), (16)), is subsequently a segment sliced out from the T_{si} row-vector between $x \geqslant 3d_1$ and $x \leqslant 4d_1$, which is added to the cumulative T_1 row-vector.

This process then repeats from step (g) until exhaustion of the T_{si} row-vector which gets shorter upon the successive reflections. It should be mentioned here that the numerical implementation of this procedure was performed under MATLAB [15].

In Fig. 4 we have drawn schematically the 1-layer algorithm. The input of the algorithm is an arbitrary function T_{si} satisfying both the diffusion equation and the boundary conditions at the front interface of a semi-infinite media but which, therefore, does not conform to BC at the back interface of the layer-1. The 1-layer algorithm then works out, based on the thermal properties at play, what should be the temperature solutions in tabular form for all three media.

5.2. Theory and algorithm for a two layer problem

To extend this method to the case of two layers over a substrate, one should first observe that the temperature function for the semi-infinite back medium $T_b(x_b,t)$ (i.e. Eq. (17)) has the same merits as the initial semi-infinite solution $T_{si}(x_1,t)$ that was used to find the temperature solutions in 1-layer algorithm.

To solve a diffusion problem for a structure of two layers over a substrate, given the semi-infinite solution $T_{si}(x_1,t)$ for medium-1, we start by applying the 1-layer algorithm (see stage 1 of Fig. 5) to a structure made of a front-medium/medium-1/medium-2. Note that we are considering medium-2 to be semi-infinite. As a result we obtain, in tabular form, the temperature solutions for medium-1 (i.e. $T_1(x_1,t)$) and for the semi-infinite front medium (i.e. $T_f(x_f,t)$) both verifying their corresponding boundary conditions. We also get a temperature solution in tabular form for a semi-infinite medium-2 which does not conform to the BC at the interface between medium 2 and the back medium. We then reach stage 2 of this 2-layer algorithm (see stage 2 of Fig. 5) where we again apply the 1-layer algorithm for medium-1/medium-2/back medium, using as the initial semi-infinite solution, the solution

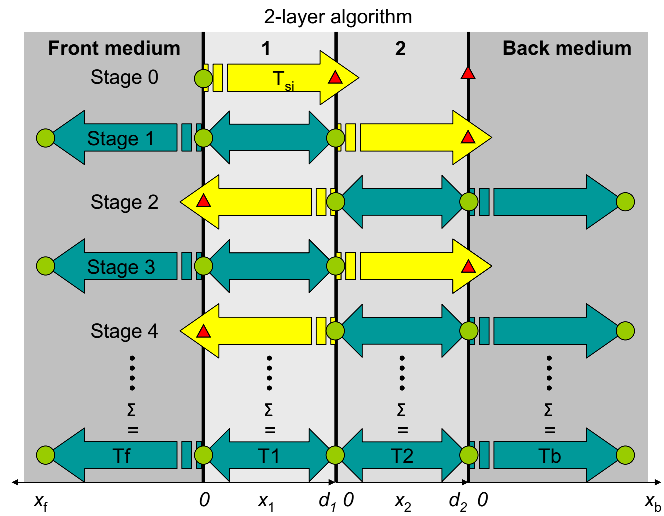

Fig. 5. The 2-layer algorithm based on the successive application of the 1-layer algorithm. For an explanation of the arrows see legend of Fig. 4. The final solutions for each region are the result of the summation of temperature functions represented by dark blue arrows.

obtained in stage 1 for medium-2. As a result of stage 2 the solution for medium-2 and for the semi-infinite back medium will now conform to the BC while the solution obtained assuming a semi-infinite medium-1 will not satisfy the BC at the interface between medium 1 and the front medium. Thus we reach stage 3 of this algorithm. This process should go on, back and forth, until the temperature solutions get sufficiently small to become negligible.

Finally, the temperature solution for each layer is given by the sum of all the temperature solutions satisfying both BC conditions obtained at each stage of the algorithm, while the same applies to the semi-infinite solutions for both the back and front media.

It should be emphasized that the 2-layer algorithm procedure, in its essence, is not different from the 1-layer algorithm. In both algorithms temperature solutions are added in sequence to satisfy the boundary conditions at each alternate interface, and thus build the complete solution.

An analytical implementation of the above 2-layer algorithm although theoretically possible is not as simple as in the case of the 1-layer algorithm. Therefore, we have opted in the present paper for the numerical approach where the initial analytical solution $T_{si}(x_1,t)$, is defined as an interpolating table. The temperature solution for each layer obtained at different stages of the algorithm is thus a table of temperature values calculated for a set of points along the thickness direction. This set of temperature values obtained at different stages of the computational algorithm are summed to obtain the final temperature in each of the regions of interest. The details of the implementation of this algorithm will be object of a companion paper to be submitted in a journal in the area of computational physics.

5.3. Results for a two layer over a substrate

In Fig. 6a is shown the result of the simulation using the above theory and computing algorithm, for a structure of two layers over a substrate in contact with a thermal reservoir at the front layer. Again the simulation using the present method and that obtained using finite element modeling agree very well. The thermal conductivity values used in the simulation are, in SI units (W/m-K), 1 for the first layer, 0.5 for the second layer and 0.25 for the substrate. The thickness of the two layers are the same and equal to 1 m and therefore the x coordinate in the plot reflects the thickness

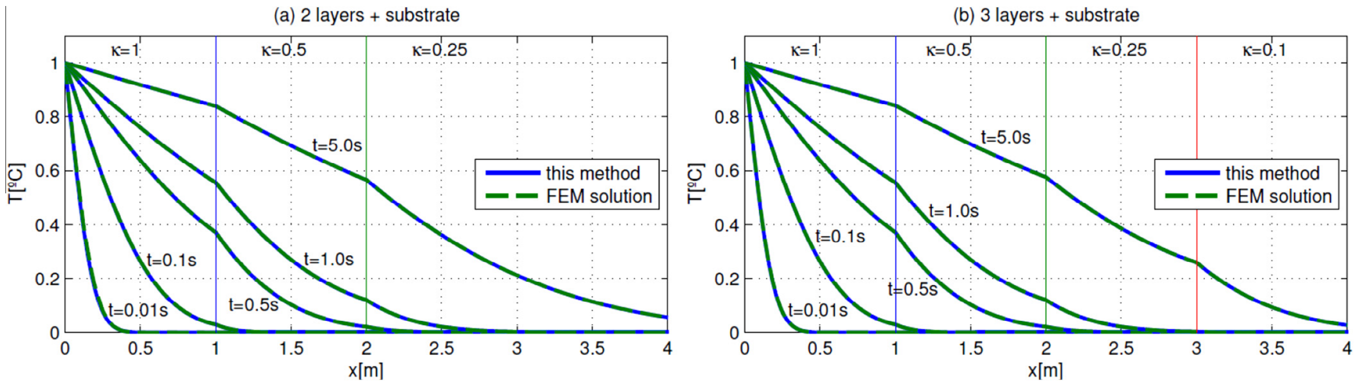

Fig. 6. Simulation of an heat reservoir in contact with (a) a two layer over a substrate; (b) a three layer over a substrate. In the simulation, all properties of the layers and the substrate are the same as in Fig. 3, except the thermal conductivity of the layers and the substrate which is indicated in the plot in SI units (i.e. W/m-K). The thickness of the layers is the same and equal to 1 m. The simulation times can be seen in the graphs.

wise dimension of the structure. The length of the initial tabular T_{si} solution for all times was 48.2 times the thickness of the first layer. This means that the similarity variable for $t = 5$ s would be 10.78 at the end of the T_{si} table so that the temperature would be nearly zero at the end of the table for all times in this simulation. The resolution used was such that there would be 1000 points for the first layer.

5.4. Three layers and more

To extend this method for a three layer over a substrate one has first to apply the previous 2-layer algorithm of Fig. 5. This is stage 1 in Fig. 7. Then, using the semi-infinite solution for layer 3 apply the 1-layer algorithm (stage 2 in Fig. 7). After that, in stage 3, apply the 2-layer algorithm again and so on. In Fig. 6b is shown the result of the simulation of three layers over a substrate with a thermal reservoir in contact with the front layer. Again the agreement between the method of recursive images and the FEM simulation is excellent. Both the length of the initial solution T_{si} and its resolution were the same as in the simulation of Fig. 6a.

It is now clear the way in which the Nth order algorithm can be constructed from the $(N-1)$th order algorithm. For example, for the case of a material with four layers over a substrate one would use the above 3-layer algorithm to reach stage 1 of the 4-layer algorithm. Then, the use of the 1-layer algorithm would take us to stage 2 of that algorithm, and so on.

6. A constant heat flux at the front face

Finally, we have simulated a different problem altogether in which a constant heat flux is entering through the front layer of a 3-layer over a substrate structure. For such a front face boundary condition, the semi-infinite solution is,

$$T(x,t) = \frac{\dot{q}}{\kappa}\left[\sqrt{\frac{4Dt}{\pi}}\exp\left(-\frac{x^2}{4Dt}\right) - x\,\mathrm{erfc}\left(\frac{x}{\sqrt{4Dt}}\right)\right] \tag{29}$$

where $\dot{q}$ (W/m^2) is the heat flux. The ideas as described in Figs. 1, 2, 4, 5 and 7 were used in this simulation. As is clear from Fig. 8, the results continue to be excellent as regards the agreement between the proposed method and FEM modeling. We point out that in this simulation, the substrate was assumed to be insulating and thus $r_b = 1$ while the specific heat of layer 2 was set to 2 J/kg. Furthermore the reflection strength at the front face is set to $r_f = 1$. This value for r_f means that all reflections taking place at the front face of the first layer do not involve an heat exchange. Therefore the only heat exchanged at the front face is that implied by the semi-infinite solution Eq. (29) (see also Eq. (25)).

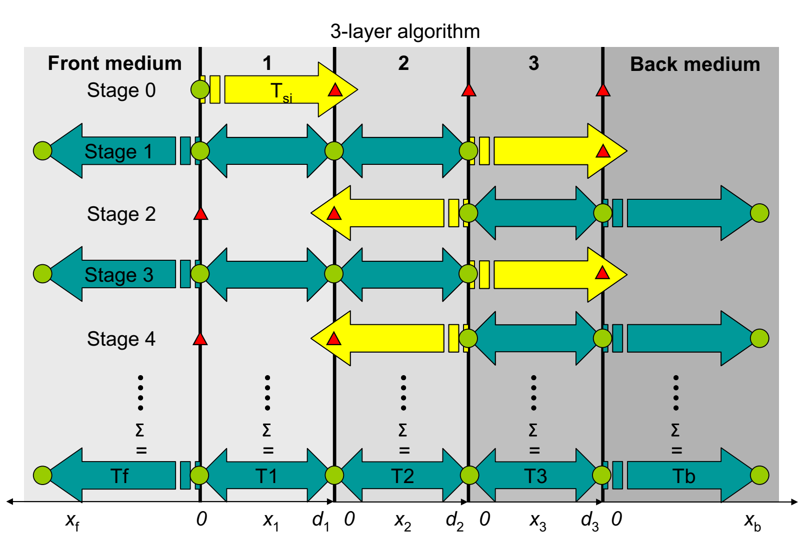

Fig. 7. The 3-layer algorithm based on the successive application of the 2-layer and the 1-layer algorithms. For an explanation of the arrows see caption of Fig. 4.

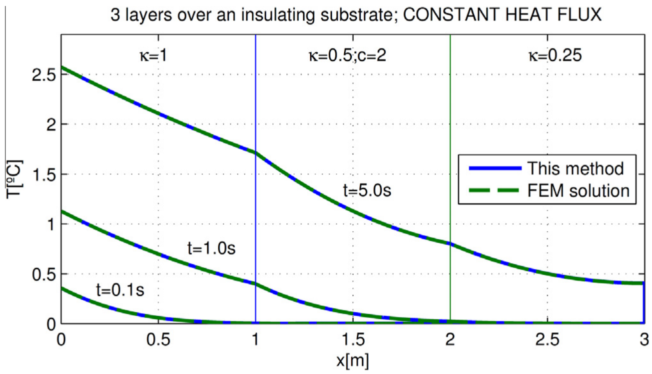

Fig. 8. Simulation of a constant heat flux into a three layer material placed over an insulating substrate. In the simulation, all parameter properties of the layers and substrate are the same as in Fig. 5 except their thermal conductivities whose values can be seen in the plot and the specific heat of layer 2 which was set to 2 J/kg. The simulation time can be seen in the graph. Properties in the plot are in SI units.

7. Discussion

The proposed method has its roots in the method of images as described by Carslaw and Jaeger [3] see Section 10.10. In effect, for heat conduction in one layer, whose boundary conditions are either thermally insulating or of fixed temperature, the proposed method and the method of images give identical results. Therefore, this method of recursive images first extends the boundary conditions to situations which are in-between these two limiting cases and secondly proposes a way to extend the method of images to the case where there is a structure made of multiple layers. It is interesting to note that the similar rationale as the present method has been used by Powles et al. in their work on partially permeable barriers [18].

As was demonstrated by the last example of the constant heat flux problem, the way in which this method of recursive images works, allows its use in a given heat diffusion problem whenever the temperature solution in a semi-infinite solid is known.

It should be mentioned that this method, as shown in Figs. 1 and 2, is inherently analytical. However its analytical implementation, beyond the algorithm for a one layer structure, although feasible is not easy. Therefore we have opted here for a numerical approach in order to prove the validity of this method of recursive images. Nevertheless, we acknowledge that an analytical device, valid for any number of layers should be a desirable result as it would allow in a straightforward manner to know, for example, the temperature at the interface between the first and second layer of a structure as a function of the thermal conductivity of the second layer. Even so we point out that the temperature solution for $t = 5$ s depends exclusively on the semi-infinite temperature solution at that particular time i.e. $T_{si}(t = 5\ \mathrm{s})$ and on the properties of the materials involved.

It is perhaps worth mentioning here, a resemblance between this method and that of the fundamental solutions [12]. Both of these methods use the fundamental solution for a given heat problem to solve the multilayer temperature problem however, the way in which the points that contribute to the solution are chosen as well as their weights is different. This point may be a key one to obtain an analytical expression for this method and will be addressed in the near future.

From Fig. 1 and Eq. (7) one realizes that for a multilayer structure the dimension of medium 2 is changed relative to that of the medium 1 in such a way that the solution valid for medium 1 is either stretched or compressed depending on the ratio $\sqrt{D_1/D_2}$. Using this result one can say that the total effective thickness of a N-layer material having the first layer as the reference is,

$$d_{\mathrm{eff}} = \sum_{i=1}^{N} d_i \sqrt{\frac{D_1}{D_i}} \tag{30}$$

This result is quite useful to evaluate the length with which the interpolating table should initiate. Regarding these thickness matters, care must be exercised when the effective thickness of a given layer is very thin compared to the other layers. In effect, the resolution of the interpolating table must be such that enough points are defined inside this layer. It is also worth noting that Eq. (13) and this whole method justifies, in a way, the "natural analytical approach" where in the separation of variables, the thermal diffusivity is retained on the side of the modified heat conduction equation where the time-dependent function is collected [5].

An important type of boundary condition such as convection is not contemplated in this study. This situation is not easy to simulate using this method of recursive images. This will be the object of a near future work as this would turn this method even more flexible.

Finally, this method of recursive images could be applicable with suitable modifications, to other geometries such as cylindrical and spherical as well as to problems of higher dimensionality taking profit of the superposition and linearity of the solutions. This is also a line of research worth pursuing.

8. Conclusions

In this paper, we propose a conceptually simple method to determine the diffusion of heat in a multi-layer material. It is based on the principle of superposition, whose rules are easy to apply, given the heat diffusion formula in a semi-infinite material together with the diffusion properties of the layers.

This method of recursive images was demonstrated to be valid for heat diffusion in a structure of three-layer on a substrate with its front face in contact with either a fixed temperature reservoir or with a constant heat flux passing through it. It was also shown the way in which this method of recursive images allows, in general, its extension to N-layered material.

Although the proposed method has proven its validity, improvements should be made in order to minimize its uncertainties. The length of the initial table solution and its resolution as a function of the thickness and thermal properties of the various layers are topics which need further consideration. This has been done in this paper but a detailed analysis will provide a procedure which may involve adimensionalization to minimize the errors in the calculations. It hoped that this task which also includes the detailed description of the actual numerical computation will be performed soon.

Conflict of interest

None declared.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.ijheatmasstransfer.2015.01.138.

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