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Microstructural influence on heat conduction

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Abstract—The influence of the microstructure of heterogeneous material on heat propagation was studied by the homogenization method of periodic media. This approach is based on the analysis of third-order heat balance equations. The physical interpretation of the corrective terms due to the existence of heterogeneities is also discussed in detail. It is shown that the higher terms introduce successive gradients of temperature and tensors, characteristic of the microstructure, which result in non-local effects. With respect to the heat plane wave, a dispersion phenomenon was shown. Finally, an application is described for periodically stratified composites.

1. INTRODUCTION

Many works have already been devoted to the description of heat conduction in heterogeneous materials. Different methods have been developed in order to determine the effective conduction coefficients of these heterogeneous materials such as: the experimental and phenomenological approach [1], numerical simulation [2–4], self-consistent theory [5], the volume averaging method [6, 7] and homogenization of periodic media [8–10].

However, these continuum descriptions are only valid when the considered heat conduction phenomenon implies a large number of heterogeneities [1, 11]. This hypothesis of 'good' scale separation means that the macroscopic size L, characteristic of heat conduction in a material, is very large in comparison with the size l of its heterogeneities ($\varepsilon = l/L \to 0$). In reality, this limit is never reached because of the microstructure, $l \neq 0$, and the macroscopic size, $L \neq \infty$. For these reasons, it is therefore interesting to investigate how the described theories could be modified when the hypothesis of scale separation is not perfectly respected.

This study deals with macroscopic conduction phenomena whose characteristic length L is 'relatively' large, with respect to the size l. Under this assumption one can expect that effects due to the microstructure will appear. In harmonic conditions, this corresponds to diffusion lengths of about 5–50 times greater than the heterogeneities. Under steady-state conditions, these phenomena would be observed in samples with few heterogeneities or because of a high gradient (for example near an angular boundary).

The homogenization method of describing periodic media, the principle of which is to take into account the existence of the two scales (L and l), is particularly well adapted to this type of analysis. This technique of asymptotic expansions allows for an improved definition by exploiting higher order equations, and considering their role in the macroscopic description. Such an approach, which, contrary to the common process, is not limited to the first significant terms, has already been proposed in the field of mechanics [12, 13] for statics and also in the field of dynamics [14]. It allows both the determination of the conditions in which the influence of the microstructure is negligible and also how the microstructure modifies the response of the material.

In the second part of this article, the author recalls the basic principles of the homogenization method. Equations up to third order governing the macroscopic heat conduction of a composite are also presented. In the third part, the results obtained are discussed and an analysis of microstructural effects is described. In the fourth section, we describe the application of the homogenization method to harmonic heat diffusion and we also point out the existence of a dispersion effect. Finally, in the fifth section, an application of the homogenization method to periodic stratified composites is described.

2. HOMOGENIZATION TO THIRD ORDER

2.1. *Principles of the homogenization method*

Described in this section are the main principles of the homogenization method [15, 16], which is an asymptotic method with double variables.

The existence of two distinct scales is represented by a system of double variables x and y. Variable x describes variations at the macroscopic scale, the characteristic length being L. Variable y describes the microstructure scale with characteristic length l. The small parameter ε is defined by the ratio of the two scales, such that:

$$\varepsilon = l/L \quad y = \varepsilon^{-1}x.$$

The use of the two variables x and y leads to a trans-

NOMENCLATURE

$\underline{a}$	$= 1/\langle 1/a \rangle$
C	specific heat capacity
$C\rho$	volume heat capacity
$\mathbf{k}$	conduction tensor
$\mathbf{K}^0$	macroscopic conduction tensor
$\mathbf{K}'$, $\mathbf{K}''$	macroscopic effective tensors
l	characteristic microscopic length
L	characteristic macroscopic length
L^{-j}	double variables conduction differential operators at different order ($i = 2, 1, 0$)
q	heat flux
q^j	heat flux of order j
$\mathbf{R}'$, $\mathbf{R}''$	macroscopic effective tensors
t	time
T	macroscopic temperature
T^j	macroscopic temperature of order j
x	macroscopic space variable
$\mathbf{X}$	tensor of first-order specific solutions
y	microscopic space variable
$\mathbf{Y}$	tensor of second-order specific solutions
$\mathbf{Z}$	tensor of third-order specific solutions.

Greek symbols

α	diffusivity
γ	ratio of volume heat capacity to their average: $\rho c/\langle \rho c \rangle$
ε	*small parameter ratio of micro and macro lengths*
θ	*temperature field*
θ^j	temperature field of order j
ρ	density
ω	pulsation
Ω	spatial period.

Other symbols

∇	gradient operator
.	contraction of tensor
$\langle\ \rangle$	average value on the period

formation of the common spatial derivatives into $\partial x + \varepsilon^{-1}\partial y$, and an expression of the variables in the form of asymptotic expansions in powers of ε. For example, with respect to the temperature, we have:

$$\theta(x,y) = \Sigma \varepsilon^j \theta^j(x,y) \quad \text{with}: \mathrm{O}(\theta^j/\theta^0) = 1.$$

Also, the periodicity of the microstructure induces the same periodicity of the functions θ^j related to the variable y. The homogenization process consists of introducing the expansions in the equations governing the physics at the local scale, then identifying terms of the same power in ε, and finally solving the problems obtained in series.

In principle, this method of asymptotic expansions is increasingly reliable the smaller ε is in comparison with 1, that is, when the separation of scales is clearly distinguished. In this case, the description obtained at the first significant order corresponds to the macroscopic behavior of the material, with an accuracy of ε.

For a given problem, the value of ε can be assessed by following the same reasoning as that in [17]. The homogenization process for heat conduction leads to an expansion of temperature of the form (see next section):

$$\theta(x,y) = T^0(x) + \varepsilon . \theta^1(x,y).$$

Therefore, the increment of $T^0(x)$ on the cell is such that (for example in direction x_1):

$$T^0(x_1 + l) - T^0(x_1) = O(\varepsilon . T^0(x)).$$

Since l, expressed with the macroscopic variable (x), is very small, in order to simplify it can be stated that:

$$\varepsilon = l|\nabla_x(T^0)|/|T^0| \quad \text{which gives} \quad L = |T^0|/|\nabla_x(T^0)|.$$

It is interesting to note that the expression of L is the same as the one which would have been obtained by a dimensional analysis at the macroscopic scale. With respect to the heat plane wave in a medium of diffusivity α we have:

$$T^0 = A \exp(-\mathrm{i}hx) \exp(\mathrm{i}\omega t)$$

so

$$\varepsilon = l.|h| = l\sqrt{(\omega/\alpha)}$$

$$\text{giving the classical value:} \quad L = \sqrt{\alpha/\omega}. \tag{1}$$

2.2. *Homogenization applied to heat conduction*

Homogenization has already been applied to the study of conduction in composites according to the period geometry, the contrasts of the conduction properties of the period components and the presence of thermal barriers [8–10, 18]. These descriptions are all given at the first significant order.

Let us consider a finely heterogeneous material for which the conductivity tensor $\mathbf{k}$ and the volume specific heat ρC vary locally with a period Ω (Fig. 1). For simplicity we assume that these parameters are of the same order of magnitude during the entire period. With a harmonic fluctuation of pulsation ω, conduction is denoted by the following equations:

$$\nabla.(-q) - \mathrm{i}\omega\rho C\theta = 0 \quad q = -\mathbf{k}.\nabla(\theta) \tag{2}$$

where θ is the temperature field and q the heat flux. The full-stop indicates a contraction (and double full-stop indicates double contraction, etc). ∇ is the nabla operator. If the variations of $\mathbf{k}$ are not continuous,

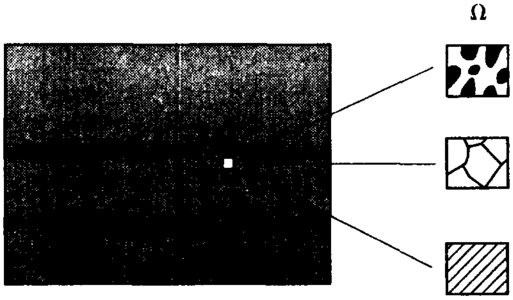

Fig. 1. Medium with periodic microstructure.

the equations have to then be interpreted in the form of the distributions, and θ and $q \,.\, n$ must be continuous through the discontinuity surfaces (n being normal).

As we are concerned with transient heat propagation at the macroscopic scale, equation (2) is therefore already scaled at the macroscopic level for which L is the reference length.

2.2.1. *The set of problems to be solved.* Using the system of double variables x and y, the heat flux takes the following form:

$$q = -\mathbf{k} \,.\, [\nabla_x(\theta) + \varepsilon^{-1}\nabla_y(\theta)]$$

where ∇_y and ∇_x are the gradients calculated according to the variables y and x respectively. The heat balance is then written as:

$$\varepsilon^{-1}\nabla_y \,.\, (-q) + \nabla_x \,.\, (-q) - \mathrm{i}\omega\rho C\theta = 0.$$

When using the temperature field only, the initial problem (2) can be transformed as follows:

$$\varepsilon^{-2}L^{-2}(\theta) + \varepsilon^{-1}L^{-1}(\theta) + L^{0}(\theta) = 0$$

where:

$$L^{-2}(\theta) = \nabla_y \,.\, [\mathbf{k} \,.\, \nabla_y(\theta)]$$

$$L^{-1}(\theta) = \nabla_y \,.\, [\mathbf{k} \,.\, \nabla_x(\theta)] + \nabla_x \,.\, [\mathbf{k} \,.\, \nabla_y(\theta)]$$

$$L^{0}(\theta) = \nabla_x \,.\, [\mathbf{k} \,.\, \nabla_x(\theta)] - \mathrm{i}\omega\rho C\theta.$$

When introducing asymptotic expansions into these differential equations, the following problems should be solved in sequence:

$$L^{-2}(\theta^0) = 0 \quad \text{i.e.}: \nabla_y \,.\, [-q^{-1}] = 0 \qquad (3a)$$

$$L^{-2}(\theta^1) = -L^{-1}(\theta^0) \quad \nabla_y \,.\, [-q^0] = \nabla_x \,.\, [q^{-1}] \qquad (3b)$$

$$L^{-2}(\theta^2) = -L^{-1}(\theta^1) - L^0(\theta^0)$$
$$\nabla_y \,.\, [-q^1] = \nabla_x \,.\, [q^0] + \mathrm{i}\omega\rho C\theta^0 \qquad (3c)$$

$$L^{-2}(\theta^3) = -L^{-1}(\theta^2) - L^0(\theta^1)$$
$$\nabla_y \,.\, [-q^2] = \nabla_x \,.\, [q^1] + \mathrm{i}\omega\rho C\theta^1 \qquad (3d)$$

$$L^{-2}(\theta^4) = -L^{-1}(\theta^3) - L^0(\theta^2)$$
$$\nabla_y \,.\, [-q^3] = \nabla_x \,.\, [q^2] + \mathrm{i}\omega\rho C\theta^2. \qquad (3e)$$

2.2.2. *Solutions.* Only the general ideas are discussed here. Detailed solutions of the problems for successive orders—close to those proposed in [14] for elastic wave propagation—are given in Appendix 1.

The problems, which are to be solved successively, all address the search for Ω-periodic temperature fields θ, such as:

$$\nabla_y \,.\, [-q^{j+1}] = \nabla_x \,.\, [q^j] + \mathrm{i}\omega\rho C\theta^j$$
$$\text{with} \quad q^j = -\mathbf{k} \,.\, [\nabla_y(\theta^{j+1}) + \nabla_x(\theta^j)] \qquad (4)$$

where temperatures θ^j, θ^{j+1} and fluxes q^j have already been determined by previous problems.

Because of the periodicity of q^{j+1}, a first condition called 'compatibility', can be obtained directly by integrating equation (4) over the period:

$$\int_\Omega \nabla_y \,.\, [-q^{j+1}]\,\mathrm{d}v = -\int \partial_\Omega[q^{j+1}] \,.\, n\,\mathrm{d}s = 0$$
$$= \int_\Omega (\nabla_x \,.\, [q^j] + \mathrm{i}\omega\rho C\theta^j)\,\mathrm{d}v$$

i.e.

$$\nabla_x \,.\, [-\langle q^j\rangle] - \mathrm{i}\omega\langle\rho C\theta^j\rangle = 0$$
$$\text{with} \quad \langle . \rangle = |\Omega|^{-1}\int_\Omega .\,\mathrm{d}v.$$

These are fundamental equations, since they involve only the macroscopic variable x, and express the heat balance of the fluxes with an order ε^j acting on the cell. With this compatibility condition being considered, the determination of the Ω-periodic field $\theta(x, y)$ is calculated by using the variational formulation of the problem. To avoid indetermination due to fields of constant temperature $T(x)$, it is necessary to seek the solution in the vectorial space U defined by:

$$U = \{u/u\ \Omega\text{-periodic}, \langle u\rangle = 0\}.$$

Taking the scalar product of (4) by any test field u and integrating over Ω, we get:

$$\int_\Omega \nabla_y \,.\, [-q^{j+1}] \,.\, u\,\mathrm{d}v$$
$$= \int_\Omega q^{j+1} \,.\, \nabla_y(u)\,\mathrm{d}v - \int \partial_\Omega[q^{j+1}] \,.\, n \,.\, u\,\mathrm{d}s$$
$$= -\int_\Omega (\nabla_x \,.\, [-q^j] - \mathrm{i}\omega\rho C\theta^j) \,.\, u\,\mathrm{d}v.$$

The boundary term being zero by periodicity, we obtain after introducing the compatibility equation:

$\forall u \in U$

$$\int_\Omega \mathbf{k}\,.\,\nabla_y(\theta^{j+2})\,.\,\nabla_y(u)\,\mathrm{d}v = \int_\Omega \mathbf{k}\,.\,\nabla_x(\theta^{j+1})\,.\,\nabla_y(u)\,\mathrm{d}v$$
$$-\int_\Omega \nabla_x\,.\,[\langle q^j\rangle - q^j]\,.\,u\,\mathrm{d}v$$
$$-\mathrm{i}\omega\int_\Omega (\langle\rho C\theta^j\rangle - \rho C\theta^j)\,.\,u\,\mathrm{d}v.$$

The conductivity tensor $\mathbf{k}$ satisfies an ellipticity condition, under which the Lax–Milgram lemma ensures the existence and uniqueness of a field θ^{j+2} of U. This solution depends linearly on the forcing terms obtained from the previously solved problems. The general solution is obtained by adding to θ any constant field $T(x)$.

2.2.3. *Results* (*see Appendix* 1).

Temperature. The temperature field can be expressed by:

$$\theta(x,y) = T^0(x)$$
$$+\varepsilon[T^1(x)+\mathbf{X}(y)\,.\,\nabla_x(T^0)]$$
$$+\varepsilon^2[T^2(x)+\mathbf{X}(y)\,.\,\nabla_x(T^1)+\mathbf{Y}(y)\,.\,.\,\nabla_x\nabla_x(T^0)]$$
$$+\varepsilon^3[T^3(x)+\mathbf{X}(y)\,.\,\nabla_x(T^2)+\mathbf{Y}(y)\,.\,.\,\nabla_x\nabla_x(T^1)$$
$$+\mathbf{Z}(y)\,.\,.\,.\,\nabla_x\nabla_x\nabla_x(T^0)].$$

Tensors $\mathbf{X}$, $\mathbf{Y}$, $\mathbf{Z}$ of ranks 1, 2 and 3 respectively, are obtained from specific solutions, θ. These ones having a zero average, the mean temperature $T(x)$ is given by:

$$\langle\theta(x,y)\rangle = T(x) = T^0(x)+\varepsilon T^1(x)$$
$$+\varepsilon^2T^2(x)+\varepsilon^3T^3(x)+\ldots.$$

The gradient of temperature is given by:

$$\nabla\theta_{(x,y)} = \nabla_x(T^0)+\nabla_y[\mathbf{X}\,.\,\nabla_x(T^0)]$$
$$+\varepsilon\{\nabla_x(T^1)+\nabla_y[\mathbf{X}\,.\,\nabla_x(T^1)]+\nabla_x[\mathbf{X}\,.\,\nabla_x(T^0)]$$
$$+\nabla_y[\mathbf{Y}\,.\,.\,\nabla_x\nabla_x(T^0)]\}+\varepsilon^2\{\nabla_x(T^2)+\nabla_y[\mathbf{X}\,.\,\nabla_x(T^2)]$$
$$+\nabla_x[\mathbf{X}\,.\,\nabla_x(T^1)]+\nabla_y[\mathbf{Y}\,.\,.\,\nabla_x\nabla_x(T^1)]$$
$$+\nabla_x[\mathbf{Y}\,.\,.\,\nabla_x\nabla_x(T^0)]+\nabla_y[\mathbf{Z}\,.\,.\,.\,\nabla_x\nabla_x\nabla_x(T^0)]\}+\ldots.$$

Tensors $\mathbf{X}$, $\mathbf{Y}$, $\mathbf{Z}$ are periodic with a zero mean value. By averaging, we obtain the mean gradient which is also the gradient of the mean temperature:

$$\langle\nabla\theta_{(x,y)}\rangle = \nabla_x(T^0)+\nabla_x(\varepsilon T^1)$$
$$+\nabla_x(\varepsilon^2T^2)+\nabla_x(\varepsilon^3T^3)+\ldots = \nabla_x(T).$$

Fluxes. The local flux is calculated directly from $\mathbf{k}(y)$ and $\nabla\theta(x,y)$:

$$q(x,y) = -\mathbf{k}(y)\,.\,\nabla\theta(x,y).$$

The averaged values of these fluxes define the tensors $\mathbf{K}^0$, $\varepsilon\mathbf{K}^1$, $\varepsilon^2\mathbf{K}^2$, $\varepsilon\langle\rho C\mathbf{X}\rangle$, $\varepsilon^2\langle\rho C\mathbf{Y}\rangle$, which together characterize the macroscopic behavior.

$$\langle q(x,y)\rangle = -\{\mathbf{K}^0\,.\,\nabla_x(T^0)$$
$$+\mathbf{K}^0\,.\,\nabla_x(\varepsilon T^1)+\varepsilon[\mathbf{K}^1\,.\,.\,\nabla_x\nabla_x(T^0)$$
$$+\mathrm{i}\omega\langle\rho C\mathbf{X}\rangle\,.\,\nabla_x(T^0)]$$
$$+\mathbf{K}^0\,.\,\nabla_x(\varepsilon^2T^2)+\varepsilon[\mathbf{K}^1\,.\,.\,\nabla_x\nabla_x(\varepsilon T^1)$$
$$+\mathrm{i}\omega\langle\rho C\mathbf{X}\rangle\,.\,\nabla_x(\varepsilon T^1)]$$
$$+\varepsilon^2[\mathbf{K}^2\,.\,.\,.\,\nabla_x\nabla_x\nabla_x(T^0)+\mathrm{i}\omega\langle\rho C\mathbf{Y}\rangle.\nabla_x\nabla_x(T^0)]\}$$

where, using formal writing:

$$\mathbf{K}^0 = |\Omega|^{-1}\int_\Omega(\mathbf{k}+\mathbf{k}\,.\,\nabla_y(\mathbf{X}))\,\mathrm{d}v: \quad \text{2nd rank tensor}$$
$$\mathbf{K}^1 = |\Omega|^{-1}\int_\Omega(\mathbf{kX}+\mathbf{k}\,.\,\nabla_y(\mathbf{Y}))\,\mathrm{d}v: \quad \text{3th rank tensor}$$
$$\mathbf{K}^2 = |\Omega|^{-1}\int_\Omega(\mathbf{kY}+\mathbf{k}\,.\,\nabla_y(\mathbf{Z}))\,\mathrm{d}v: \quad \text{4th rank tensor}$$
$$\langle\rho C\mathbf{X}\rangle = |\Omega|^{-1}\int_\Omega(\rho C\mathbf{X})\,\mathrm{d}v: \quad \text{1st rank tensor}$$
$$\langle\rho C\mathbf{Y}\rangle = |\Omega|^{-1}\int_\Omega(\rho C\mathbf{Y})\,\mathrm{d}v: \quad \text{2nd rank tensor.} \tag{5}$$

The expressions (5) of the different tensors, show that their orders of magnitude are given by:

$$\mathbf{K}^1 = \mathrm{O}(\mathbf{k}l_\mathrm{m}) \quad \mathbf{K}^2 = \mathrm{O}(\mathbf{k}l_\mathrm{m}^2)$$
$$\langle\rho C\mathbf{X}\rangle = \mathrm{O}(\rho Cl_\mathrm{m}) \quad \langle\rho C\mathbf{Y}\rangle = \mathrm{O}(\rho Cl_\mathrm{m}^2)$$

where l_m is the dimension of the period expressed according to the *system of dilated variables y*. Consequently:

$$\varepsilon\mathbf{K}^1 = \mathrm{O}(\mathbf{k}l) \quad \varepsilon^2\mathbf{K}^2 = \mathrm{O}(\mathbf{k}l^2)$$
$$\varepsilon\langle\rho C\mathbf{X}\rangle = \mathrm{O}(\rho Cl) \quad \varepsilon^2\langle\rho C\mathbf{Y}\rangle = \mathrm{O}(\rho Cl^2)$$

where l is the dimension of the cell expressed in the *system of reference variables x*. Therefore, in macroscopic equations, we are lead to use the effective tensors $\mathbf{K}' = \varepsilon\mathbf{K}^1$, $\mathbf{K}'' = \varepsilon^2\mathbf{K}^2$, $\mathbf{R}' = \varepsilon\langle\rho C\mathbf{X}\rangle$, and $\mathbf{R}'' = \varepsilon^2\langle\rho C\mathbf{Y}\rangle$, which are *independent of* ε (and can be directly calculated from known geometry and thermal characteristics of period components).

It should be noted that the closer the period comes to being homogeneous, the smaller are the values of $\mathbf{K}'$, $\mathbf{K}''$, $\mathbf{R}'$, $\mathbf{R}''$. Finally, it is important to note that tensors $\mathbf{K}'$ and $\mathbf{R}'$ are of odd rank and therefore anisotropic. Therefore, if the material is macroscopically isotropic (up to 2nd order) $\mathbf{K}' = 0$ and $\mathbf{R}' = 0$.

Macroscopic heat balance. With respect to the first three significant orders, the macroscopic heat balances are the following:

$$\nabla_x\,.\,[-\langle q^0\rangle]-\mathrm{i}\omega\langle\rho C\rangle T^0 = 0;$$
$$\text{where}: \langle q^0\rangle = -\mathbf{K}^0\,.\,\nabla_x(T^0) \tag{6a}$$
$$\nabla_x\,.\,[-\langle q^1\rangle]-\mathrm{i}\omega\langle\rho C\rangle T^1 = 0$$
$$\langle q^1\rangle = -\mathbf{K}^0\,.\,\nabla_x(T^1)-\mathbf{K}^1\,.\,.\,\nabla_x\nabla_x(T^0)$$
$$+\mathrm{i}\omega\langle\rho C\mathbf{X}\rangle\,.\,\nabla_x(T^0) \tag{6b}$$

$$\nabla_x . [-\langle q^2 \rangle] - \mathrm{i}\omega\langle \rho C\rangle T^2 = 0$$

$$\langle q^2 \rangle = -\mathbf{K}^0 . \nabla_x(T^2) - \mathbf{K}^1 .. \nabla_x\nabla_x(T^1) + \mathrm{i}\omega\langle \rho C\mathbf{X}\rangle . \nabla_x(T^1) - \mathbf{K}^2 ... \nabla_x\nabla_x\nabla_x(T^0) + \mathrm{i}\omega\langle \rho C\mathbf{Y}\rangle \nabla_x . \nabla_x(T^0). \quad (6c)$$

2.2.4. *Physical significance of macroscopic variables.* The variables used in the macroscopic description are in fact the volume averages of variables defined at the microscopic scale. Their physical significance should therefore be specified.

Temperature. The macroscopic temperature of any order $T^j(x)$ is given by the volume averages of local fields $\theta^j(x, y)$. These temperatures $T^j(x)$ can therefore be defined as the mean temperature of the cell.

There is no difficulty in interpreting macroscopic gradients of order j, since they correspond to macroscopic temperature gradients of the same order, j.

Heat fluxes. The homogenization introduces *volume averages* of heat fluxes of an order j. It is important to determine whether the quantities defined correspond to the usual physical definition of fluxes which are normally obtained by the average heat transfer across the elementary surface.

In order to verify this statement, we transform volume integrals into surface integrals using the identity:

$$\nabla_y . [qy_j] = y_j \nabla_y . [q] + q_j$$

and, by integrating over any volume V, and using the divergence theorem we have:

$$\int_{\partial V} y_j(q . n)\, \mathrm{d}s = -\int_V (\nabla_y . [q]) y_j\, \mathrm{d}v + \int_V q_j\, \mathrm{d}v. \quad (7)$$

Flux of zero order. Flux q^0 is of zero divergence (according to y), and therefore when applying (7) to the cell Ω, one obtains:

$$\langle q_j^0 \rangle = |\Omega|^{-1} \int_{\partial\Omega} y_j(q^0 . n)\, \mathrm{d}s.$$

Considering the periodicity of q^0, only the integrals on the boundaries S_j and S_j' (where the normal $n = \pm e_j$) are not equal to zero, the others equate to zero in pairs

$$\langle q_j^0 \rangle = |\Omega|^{-1} \int_{S_j} q_j^0 . y_j\, \mathrm{d}s - |\Omega|^{-1} \int_{S_j'} q_j^0 . y_j\, \mathrm{d}s$$

l_j being the period length in e_j direction, we have, $|\Omega| = l_j . S_j$ (Fig. 2). Using the periodicity of q^0, the final equation becomes:

$$\langle q_j^0 \rangle = l_j . |\Omega|^{-1} \int_{S_j} q_j^0\, \mathrm{d}s = |S_j|^{-1} \int_{S_j} q_j^0\, \mathrm{d}s.$$

Thus, the volume average $\langle q_j^0 \rangle$ is actually the surface average of elementary fluxes crossing the surface having e_j as normal.

This result can be generalized to fluxes crossing any oriented surface $|S| . m = \mathbf{A} \wedge \mathbf{B}$, where vectors $\mathbf{A}$ and $\mathbf{B}$ are linear combinations—with integer coefficients—of the vectors defining the elementary cell. Let us prove that the vector $\mathbf{f}$ obtained by surface averaging of elementary fluxes crossing S:

$$\mathbf{f} = |S|^{-1} \int_S q^0 . m\, \mathrm{d}S \quad \text{is equal to} \quad \langle q^0 \rangle . m.$$

To do this consider the cell Ω' (Fig. 2), defined by ($\mathbf{A}$, $\mathbf{B}$, ml'), the distance l' between the two faces of normal $\pm m$ being such that: $l' = |\Omega'|/S = l_j(e_j . m)$ (no summation over j). When applying (7) to Ω' and taking the scalar product by m, one obtains:

$$\int_{\Omega'} q^0 . m\, \mathrm{d}v = \int_{\partial\Omega'} (q^0 . n)(y . m)\, \mathrm{d}s.$$

From the definition of Ω', q^0 is also Ω' periodic, and we have:

$$|\Omega'|^{-1} \int_{\Omega'} q^0\, \mathrm{d}s = |\Omega|^{-1} \int_{\Omega} q^0\, \mathrm{d}s = \langle q^0 \rangle$$

hence:

$$\langle q^0 \rangle . m = |\Omega'|^{-1} \int_{\partial\Omega'} (q^0 . n)(y . m)\, \mathrm{d}s.$$

As previously stated, due to the periodicity, only the terms associated with the surfaces having $\pm m$ as normal remain in the boundary integral. Since the distance between these faces is l' we get:

$$\langle q^0 \rangle . m = (l'/l' . |S|) \int_S q^0 . m\, \mathrm{d}s = \mathbf{f}.$$

Thus $\langle q^0 \rangle = -\mathbf{K}^0 . \nabla_x(T^0)$ actually defines a macroscopic flux vector. In the same manner all the terms $-\mathbf{K}^0 . \nabla_x(T^i)$ are also flux vectors.

Fluxes at higher orders. Different from q^0, the fluxes with an order p ($p > 0$) satisfy an equation of the form:

$$\nabla_y . [-q^p] = s^p$$

where s^p is a periodic term not equal to zero but having a zero mean value in y. Following the same reasoning as above, gives:

$$\langle q^p \rangle . m = |S|^{-1} \int_S q^p . m\, \mathrm{d}s + |\Omega'|^{-1} \int_{\Omega'} s^p(y . m)\, \mathrm{d}v. \quad (8)$$

From equation (8) it is possible to make two remarks concerning the surface average $\mathbf{f}^p$ of q^p on face S:

$$\mathbf{f}^p = |S|^{-1} \int_S q^p . m\, \mathrm{d}s$$

is not a macroscopic quantity. In fact, with:

$$\mathbf{f}^p = \langle q^p \rangle . m + |\Omega'|^{-1} \int_{\Omega'} s^p(y . m)\, \mathrm{d}v$$

and as $s^p . (y . m)$ is *not a periodic* term, the value of f^p will depend on the choice of the period used in the

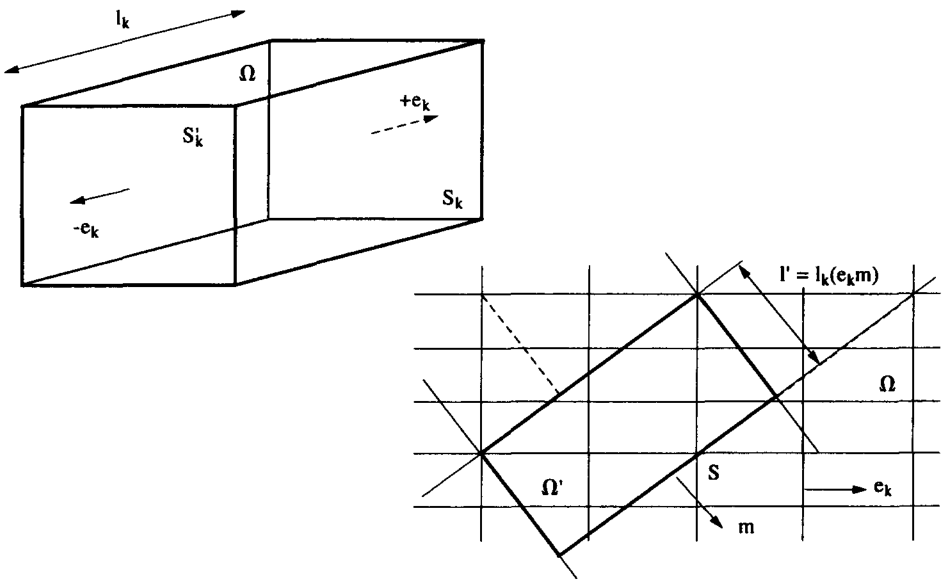

Fig. 2. The periods Ω and Ω′.

calculation. This means that the surface average of q^p will vary at the microscopic scale.

Moreover this expression proves that the operator connecting m to $f^p(m)$ is not linear, and consequently, the *surface average of fluxes q^p does not define a tensor.* On the contrary, it is volume averages that define a tensor, but these averages cannot be interpreted in terms of a flux. In the next section the meaning of the macroscopic equations which involve $\langle q^p \rangle$ tensors will be explained.

3. ANALYSIS OF THE DESCRIPTION INVOLVING HIGHER ORDER TERMS

This section studies the role of higher order expressions. Taking into account the difficulties in the interpretation of averaged fluxes $\langle q^p \rangle$ $(p > 0)$, their influence will be analysed by use of macroscopic heat balance equations.

3.1. *Interpretation of balance equations*

3.1.1. *Macroscopic conduction equation.*The balance equation (6a) with zero order, corresponds exactly to the Fourier equation of heat conduction. Field T^0 is the value which one would expect to appear in a continuum medium with a conductivity tensor $\mathbf{K}^0$ and a volume specific heat of $\langle \rho C \rangle$. However, this description is valid only with an accuracy of ε.

3.1.2. *Heat sources due to microstructure.* Let us now examine equations (6b) and (6) with respective orders of 1 and 2. As vector $-\langle q^p \rangle$ $(p > 0)$ is not a flux, these equations cannot be directly interpreted. Since the terms $-\mathbf{K}^0 . \nabla_x(T^p)$ in $-\langle q^p \rangle$ are fluxes, it is then possible to rewrite equations (6) to allow for a physical interpretation, so:

$$\nabla_x . [\mathbf{K}^0 . \nabla_x(T^0)] - i\omega\langle \rho C \rangle T^0 = 0 \qquad (9a)$$

$$\nabla_x . [\mathbf{K}^0 . \nabla_x(\varepsilon T^1)] - i\omega\langle \rho C \rangle \varepsilon T^1 = -\nabla_x . [\mathbf{K}' .. \nabla_x \nabla_x(T^0)] + i\omega \mathbf{R}' . \nabla_x(T^0) \qquad (9b)$$

$$\nabla_x . [\mathbf{K}^0 . \nabla_x(\varepsilon^2 T^2)] - i\omega\langle \rho C \rangle \varepsilon^2 T^3 = -\nabla_x . [\mathbf{K}' .. \nabla_x \nabla_x(\varepsilon T^1)] + i\omega \mathbf{R}' . \nabla_x(\varepsilon T^1) - \nabla_x . [\mathbf{K}'' ... \nabla_x \nabla_x \nabla_x(T^0)] + i\omega \mathbf{R}'' .. \nabla_x . \nabla_x(T^0)]. \qquad (9c)$$

Equations (9b) and (9c) are Fourier equations applied to the fields εT^1 and $\varepsilon^2 T^2$ respectively, in which heat source terms resulting from temperature fields at lower orders appear. Therefore, unlike what we would expect to happen in a perfectly homogeneous material, the presence of a microstructure results in a distribution of source which then generates a series of temperature fields of an increasingly lower amplitude: fields of order inferior to the value of i generate sources of an order j which themselves generate a field of order j, and so on.

These heat sources arise from the fact that the equations which express the heat balance of the cell with order ε^j do not take into account contributions of order ε^{j+1}. The latter then become forcing terms in the balance equation with an order of ε^{j+1}. Consequently, in order to counterbalance these sources, a temperature field T^{j+1} arises which then satisfies the conduction equations of the *homogeneous equivalent medium*.

The source terms are connected to the successive gradients of the temperature, and therefore introduce a weak non-local effect in the conduction phenomena. It is clear that the closer the temperature comes to being homogeneous, the weaker will be the sources. Conversely, when temperature gradients are significant, the corrective terms become significant, and so amplify the non-local effect and modify the solution T^0 of the equivalent homogeneous medium.

The sharper the heterogeneities at the microscopic scale, then the larger the values of $\mathbf{K}'$ and $\mathbf{K}''$ will be, and also the greater will be the significance of non-local terms (for a given level of the macroscopic gradient). Finally, if the material presents an isotropic macroscopic behavior the first significant source term will appear with an order of ε^2 (since $\mathbf{K}' = 0$ and $\mathbf{R}' = 0$).

3.2. *Solutions to boundary condition problems*

For a material of known microstructure, tensors $\mathbf{K}^0, \mathbf{K}', \mathbf{K}'', \mathbf{R}', \mathbf{R}''$ can all be calculated. In spite of this, the determination of macroscopic solutions, up to the third order, for any given boundary condition problem, necessitates the knowledge of the limit conditions to be applied to the fields $T^j(x)$.

3.2.1. *Macroscopic solution.* Let us now consider, at the macroscopic scale, a body B, the boundary of which is ∂B, which is submitted to the following conditions on its border:

—on the portion ∂B_F of ∂B, an imposed flux $F(x)$;
—on the complementary portion $\partial B_T = \partial B - \partial B_F$, an imposed temperature $\Theta(x)$.

At zero order, the field $T^0(x)$ is determined by the conduction equation (9a) and the following boundary conditions:

$$-\mathbf{K}^0 . \nabla x(T^0(x)) . N = F(x) \quad \text{on } \partial B_F \text{ (having } N \text{ as normal)}$$

$$T^0(x) = \Theta(x) \quad \text{on } \partial B_T. \qquad (10a)$$

The calculation of the field $T^1(x)$ is done by solving another conduction problem governed by the equation (9b) where the microstructural sources are deduced from the value of $T^0(x)$. The boundary conditions applied to $T^1(x)$ must be such that the *global* field $T^0(x)+\varepsilon T^1(x)$ meets the macroscopic conditions imposed on ∂B, i.e.

$$-\mathbf{K}^0 . (\nabla_x(T^0(x)+\varepsilon T^1(x))) . N = F(x) \quad \text{on } \partial B_F$$

$$T^0(x)+\varepsilon T^1(x) = \Theta(x) \quad \text{on } \partial B_T.$$

Taking into account (10a), $T^1(x)$ follows a Neumann condition on ∂B_F, and a Dirichlet condition on ∂B_T such that:

$$\begin{aligned} -\mathbf{K}^0 . \nabla_x(\varepsilon T^1(x)) . N &= 0 \quad \text{on } \partial B_F \\ \varepsilon T^1(x) &= 0 \quad \text{on } \partial B_T. \end{aligned} \qquad (10b)$$

By the same principle, the macroscopic field $\varepsilon^2 T^2(x)$ is fully determined by equation (9c), which calculates the microstructural sources from $T^0(x)$ and $\varepsilon T^1(x)$ obtained beforehand, and also the boundary conditions of zero flux and temperature on ∂B_F and ∂B_T respectively (i.e. conditions (10b) where $\varepsilon^2 T^2(x)$ replace $\varepsilon T^1(x)$).

By this type of reasoning with respect to the macroscopic scale, we obtain the macroscopic temperature which appears in the interior of the body B (up to the third order). However, this solution does not take into account the edge effects existing on a thin layer around ∂B.

4. PROPAGATION OF A HEAT PLANE WAVE

In this section we consider the incidence of the terms of superior order on the propagation of a macroscopic plane wave. We consider an homogenized medium (anisotropic) in which an harmonic plane wave propagates in any direction e_p.

In order to simplify the calculations (without limiting the scope of reasoning) we switch to a one-dimensional problem. In order to achieve this, we assume that the equations (and the tensors) are expressed in an orthonormal frame E_p whose first axis ox_1 direction coincides with e_p.

In the following, we simplify by suppressing the suffix x for the macroscopic operators and by writing x for the variable x_1. In the frame E_p, we look for plane waves of the following form:

$$T^0 = A \exp(-ihx)\exp(i\omega t).$$

Fourier equation (9a) leads to the classic dispersion equation:

$$A[(-ih)^2\mathbf{K}_1^{01} - i\omega\langle\rho C\rangle)] = 0$$

which then gives:

$$h^2 = -i\omega\langle\rho C\rangle/\mathbf{K}_1^{01} = -i\omega/\alpha$$

$$h = \pm\sqrt{(\omega/\alpha)} . (1-i)/\sqrt{2}$$

where α is the macroscopic thermal diffusivity in direction e_p.

We then assume that at zero order, a wave of unit amplitude propagates. That is to say:

$$T^0 = \exp(-i\sqrt{(\omega/2\alpha)} . x) \times \exp(-\sqrt{(\omega/2\alpha)} . x)\exp(i\omega t). \qquad (11)$$

This definition of the wave is correct only to $\varepsilon = l . \sqrt{(\omega/\alpha)}$. In the case of very long wavelengths, this precision is acceptable. However, for wavelengths of only 5–50 times greater than the size of the heterogeneities, more precision must be sought by considering terms of higher order.

For a given order we can calculate the heat sources resulting from temperature fields of inferior orders. This allows us to focus on the field induced by its sources. Then we obtain the macroscopically observable temperature field by adding the fields at different orders.

As these problems are linear, all the fields oscillate at the same frequency, and therefore the term exp (iωt) can be suppressed.

4.1. *Correction of first order*

Equation (9b), expressing the macroscopic heat balance with first order, shows that T^1 is the sum of any field solution of the homogeneous problem (but without interest in this case) and of the field generated by the following heat source:

$$-\nabla_x . [\mathbf{K}^1 .. \nabla_x \nabla_x (T^0)] + i\omega \langle \rho C \mathbf{X} \rangle . \nabla_x (T^0)$$

the explicit expression of which is (using index notation):

$$-\mathbf{K}_i^{1\,lm} T^0_{,lmi} + i\omega \langle \rho C \mathbf{X}^j \rangle T^0_{,j}.$$

In introducing expression (11) of T^0, we get:

$$-ih[(-i\omega/\alpha)\mathbf{K}_1^{1\,11} + i\omega\langle \rho C \mathbf{X}^1 \rangle] \exp(-ihx)$$
$$= -ih . (-i\omega/\alpha)(\mathbf{K}_1^{1\,11} - \mathbf{K}_1^{0\,1} \langle \rho C \mathbf{X}^1 \rangle / \langle \rho C \rangle) \exp(-ihx).$$

This volume source is *equal to zero*, since it can be demonstrated (as shown in Appendix 2) that:

$$\mathbf{K}_j^{1\,lm} - \mathbf{K}_m^{0\,l} \langle \rho C \mathbf{X}^j \rangle / \langle \rho C \rangle = \langle k_m^{0\,j} \mathbf{X}^l - k_m^{0\,l} X^j \rangle.$$

This result gives a field T^1 equal to zero. Thus, there is no correction with this order.

4.2. *Second order: dispersion effects*

Equation (9c) shows that the correction obtained from using the second-order terms comes only from the source resulting from field T^0 (since $T^1 = 0$). To calculate these sources:

$$\nabla_x . [-\mathbf{K}^2 .. \nabla_x \nabla_x \nabla_x (T^0)] + i\omega \langle \rho C \mathbf{Y} \rangle . \nabla_x \nabla_x (T^0)$$

and, with index notation:

$$-\mathbf{K}_i^{2\,lmn} T^0_{,lmni} + i\omega \langle \rho C \mathbf{Y}^{lm} \rangle T^0_{,lm}.$$

So finally, when introducing expression (11) for T^0 we have:

$$(i\omega/\alpha)[-(i\omega/\alpha)\mathbf{K}_1^{2\,111} + i\omega\langle \rho C \mathbf{Y}^{11} \rangle] \exp(-ihx).$$

Field T^2 is specifically obtained from this source, which is not necessarily zero (whereas it is with respect to first order).

Notice that this source respects the geometry of the plane wave: its amplitude is identical at every point of planes parallel to the wave front and oscillates spatially according to the wavelength. Therefore this forcing term excites the dynamic conduction operator according to its eigen mode. This is expressed by a perturbation which is amplified as the wave progresses. Now T^2 is expressed in the following form:

$$T^2 = -a(-ihx)(i\omega/\alpha)\exp(-ihx).$$

The application of the Fourier operator to this expression gives:

$$\nabla_x . [\mathbf{K}^0 . \nabla_x T^2] - i\omega\rho C T^2$$
$$= -a(i\omega/\alpha)\exp(-ihx)\{[(-ih)^2 \mathbf{K}_1^{0\,1} - i\omega\langle \rho C \rangle](-ihx) + 2(-ih)^2 \mathbf{K}_1^{0\,1}\}$$
$$= 2a(h)^2 (i\omega/\alpha)\mathbf{K}_1^{0\,1} \exp(-ihx).$$

By identification with the source term calculated above, we can deduce the value of the real coefficient a:

$$a = (\mathbf{K}_1^{2\,111}/\mathbf{K}_1^{0\,1} - \langle \rho C \mathbf{Y}^{11} \rangle / \langle \rho C \rangle)/2$$

giving:

$$a'' = \varepsilon^2 a = (\mathbf{K}_1''^{\,111}/\mathbf{K}_1^{0\,1} - R^{11}/\langle \rho C \rangle)/2$$

so that $a'' = O(l^2)$.

Thus, up to second order, the field of macroscopic wave is given by:

$$T(x) = T^0(x) + \varepsilon^2 T^2(x)$$
$$= [1 - a''(-ihx)(i\omega/\alpha)]\exp(-ihx).$$

We can observe a correction of second order—with a phase shift of $\pi/4$—which increases linearly with x and perturbs the wave propagation. In order to analyse more closely the influence of this term, we transform the expression

$$[1 - a''(-ihx)(i\omega/\alpha)] \quad \text{into:} \quad \exp[(ihx)a''(i\omega/\alpha)].$$

This approximation is correct up to ε^3, provided that the value of x lies within the boundaries defined as follows:

$$O(hx) \leqslant \varepsilon^{-1/2} \quad \text{i.e.}: 0 < x < \delta$$
$$\text{with}: \delta = 1/|h|\sqrt{|h|l} = (\alpha/\omega)^{3/4}/\sqrt{l}.$$

Thus up to ε^3:

$$T(x) = \exp(-ihx[1 - a''(i\omega/\alpha)])$$
$$= \exp[-i(1 - a''(\omega/\alpha))\sqrt{(\omega/2\alpha)} . x]$$
$$\times \exp[-(1 + a''(\omega/\alpha))\sqrt{(\omega/2\alpha)} . x].$$

We conclude that the global temperature propagates with characteristics in celerity and attenuation slightly different from that which has been calculated at zero order. This is caused by a 'resonant' effect generated by the microstructural sources, and from interferences between the corrective waves and the zero-order wave. Macroscopically, heat propagates as if the diffusivity has a complex value α_c:

$$\alpha_c = \alpha . [1 - 2 . a''(i\omega/\alpha)] \quad (\text{up to } \varepsilon^3).$$

The relative correction of the diffusivity coefficient is of an order ε^2 that is to say $O(\omega l^2/\alpha)$ and this dispersion effect varies linearly with frequency. It is important to note that in spite of this dispersion, diffusivities α and α_c stay within the same range of magnitude (since $\varepsilon \ll 1$).

These results, valid for any kind of microstructure, agree with those obtained in [19, 20] where transient heat transfer is studied analytically in stratified composites.

4.3. *Superior orders*

The calculation of superior terms becomes very complex even in the case of a plane wave. However, as these terms can only generate (at superior orders) phenomena of the same nature as those that have already treated elsewhere, it is therefore not necessary to develop them here.

4.4. *Description beyond the distance δ*

From the preceding study, it is clear that the analysis of the effects of scattering at superior orders is only correct for a distance of propagation δ which is large but also limited in comparison with the wavelength.

Such a restriction of the domain of analysis comes from the amplification phenomenon which generates wave fields that increase with the distance of propagation. As a result, beyond distance δ terms of order j change with respect to range and interact with terms of order $j-1$. Since the fundamental hypothesis of discrimination of different orders is not longer respected, the results of the homogenization are therefore incorrect.

To avoid this difficulty we reason as follow: in the vicinity of the distance δ, in a plane parallel to the wave front, the medium is now not only influenced by the temperature at zero order. In order to satisfy these new boundary conditions a new wave of first order, and propagating in the same direction as the wave of zero order is added. For each of these waves, the analysis conducted earlier is still applicable and the global wave field can be described theoretically.

4.5. *Application to transient heat conduction*

Until now the results have been established for harmonic heat variations. Because of the linearity of the phenomena, the description for transient variations can be directly deduced by inverse Fourier transform, provided that the scale separation condition is fulfilled:

$$\varepsilon = l\sqrt{(\omega/\alpha)} \ll 1.$$

That means that the pulsation spectrum of the temporal signal must lie within the range:

$$0 < \omega \ll \omega_c = \alpha/l^2.$$

Under this assumption it was shown that the microstructural effects modify the usual diffusivity, by adding an imaginary part which linearly depends on the pulsation. Therefore one can expect that the modification of the response will essentially concern the highest frequency part of the signal (i.e. the fastest variations). The main consequences of this corrective coefficient will be an increase of the attenuation and a delay in the time arrival of the heat wave. Moreover, as this correction is dispersive, it will induce a progressive modification of the signal during its propagation.

Finally, let us notice that the pulsation $\omega_c = \alpha/l^2$ corresponds to a characteristic time $\tau_c = 2\pi l^2/\alpha$ for the heterogeneous medium. Oscillations with a period shorter than τ_c do not generate a macroscopic wave front associated with a macroscopic flux, since heat is scattered in any direction by the diffraction on the heterogeneities. Therefore, according to thermal macroscopic waves, the medium behaves as a 'low-pass' filter.

5. EXAMPLE: STRATIFIED COMPOSITES

The preceding results have been applied to periodic stratified composites, which have already been studied in a number of papers, for example [8–10, 19, 20]. This kind of microstructure presents an advantage of simplicity, which allows for an analytical expression of the tensors $\mathbf{K}^0$ and $\mathbf{K}''$. But, its 1D structure induces some specific properties.

We assume that the period (Fig. 3) is constituted of two isotropic layers a and b, with respective thicknesses of $(l\text{-}c)\,.\,l$ and $c\,.\,l$. As we use microscopic variables to solve elementary problems, in this system of variables, the period size is $l_m = \varepsilon^{-1}l$. Let k_a and k_b equal the conductivity constants of the layers a and b respectively. $\mathbf{k}$ is a function having the value k_a in the layer a and k_b in the layer b.

Owing to the 1D geometry, the fields depend locally on variable y_1 (noted simply as y). Thus, the differential operators L^{-2}, L^{-1}, L^0 take the following expressions:

$$L^{-2}(\theta) = \partial[\mathbf{k}\,\partial(\theta)/\partial y]/\partial y$$

$$L^{-1}(\theta) = \partial[\mathbf{k}\,\partial(\theta)/\partial x_1]/\partial y + \partial[\mathbf{k}\,\partial(\theta)/\partial y]/\partial x_1$$

$$L^0(\theta) = \partial[\mathbf{k}\,\partial(\theta)/\partial x_1]/\partial x_1 + \partial[\mathbf{k}\,\partial(\theta)/\partial x_2]/\partial x_2 + \partial[\mathbf{k}\,\partial(\theta)/\partial x_3]/\partial x_3 - \mathrm{i}\omega\rho C\theta.$$

5.1. *The conductivity tensor $\mathbf{K}^0$ and $\langle \rho C\mathbf{X}\rangle$*

Denoting as $T^0_{,j}$ the components $\partial(T^0)/\partial x_j$ of the macroscopic temperature gradient, problem (3b) is rewritten in the simple form:

$$\partial[k\,\partial(\theta)/\partial y + kT^0_{,1}]/\partial y = 0$$

with $\mathbf{X}$; $-\mathbf{k}(\partial(\mathbf{X}^1)/\partial y + T^0_{,1})$ continuous and l_m-periodic, and $\langle \mathbf{X}\rangle = 0$. We now define three solutions $\mathbf{X}^j$ associated with $\mathbf{T}^0_{,j}$. It is clear that $\mathbf{X}^2 = \mathbf{X}^3 = 0$ and the expression of $\mathbf{X}^1$ is as follows:

$$\mathbf{X}^1(y) = f(y)\,.\,\underline{\mathbf{k}}D(1/k)$$

where, by convention, for each function ϕ taking a constant value ϕ_a in layer a and ϕ_b in layer b, we introduce the notations:

$$\underline{\phi} = [(1-c)/\phi_a + c/\phi_b]^{-1}$$

$$D(\phi) = c(1-c)l_m(\phi_a - \phi_b)$$

and $f(y)$ being the function:

$$f(y) = \begin{cases} [y/l_m - (1-c)/2]/(1-c) & \text{in layer } a \\ -[y/l_m + c/2]/c & \text{in layer } b. \end{cases}$$

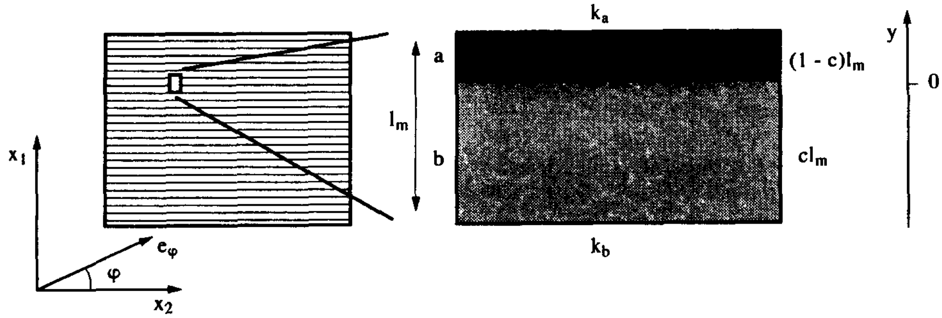

Fig. 3. Period of the stratified composite.

Consequently, the heat fluxes $-k^{0j}$ associated with $T^0_{,j}$ are:

$$\mathbf{k}^{01} = (\underline{\mathbf{k}}, 0, 0) \quad \mathbf{k}^{02} = (0, \mathbf{k}, 0) \quad \mathbf{k}^{03} = (0, 0, \mathbf{k}).$$

We obtain the macroscopic conductivity tensor by averaging. The components different from zero have the classical values:

$$\mathbf{K}^{01}_1 = \underline{\mathbf{k}} \quad \mathbf{K}^{02}_2 = \mathbf{K}^{03}_3 = \langle \mathbf{k} \rangle. \tag{12}$$

From the expression of $\mathbf{X}$, we also have: $\langle \rho C \mathbf{X} \rangle = 0$. It is easy to verify that the conductivity tensor given by expression (12) is valid for any 1D distribution of conductivity coefficients. Moreover the results can easily be generalized to anisotropic layers for which the components of the macroscopic conduction tensor are given in the formula:

$$\mathbf{K}^{0j}_i = \langle \mathbf{k}^j_i \rangle - \langle \mathbf{k}^1_i \mathbf{k}^1_j / \mathbf{k}^1_1 \rangle + \langle \mathbf{k}^1_i / \mathbf{k}^1_1 \rangle \langle \mathbf{k}^1_j / \mathbf{k}^1_1 \rangle / \langle 1/\mathbf{k}^1_1 \rangle.$$

5.2. *Tensor* $\mathbf{K}'$

The tensor $\mathbf{K}^1$ is determined from elementary solutions $\mathbf{Y}$ of the problem (3c). These solutions depend on the double gradient of temperature $\nabla_x \nabla_x (T^0)$ whose components are denoted $T^0_{,lm}$. We now treat (see Appendix 1):

$$\partial[\mathbf{k}\,\partial(\theta)/\partial y + \mathbf{k}\mathbf{X}^1 T^0_{,11}]/\partial y = (\gamma - 1)\underline{\mathbf{k}} T^0_{,11} + (\gamma \langle \mathbf{k} \rangle - \mathbf{k})(T^0_{,22} + T^0_{,33}).$$

Solving these problems, whilst taking into account the continuity and periodicity of flux and temperature, we deduce the expressions of $\mathbf{Y}^{lm}$ which do not equal zero:

$$\mathbf{Y}^{11} = [\langle \mathbf{F} \rangle - \mathbf{F}(y)] D(1/\mathbf{k})\underline{\mathbf{k}} - [\langle \mathbf{F}/k \rangle - \mathbf{F}(y)/\mathbf{k}]\underline{\mathbf{k}} D(\gamma)$$

$$\mathbf{Y}^{22} = \mathbf{Y}^{33} = [\langle \mathbf{F}/\mathbf{k} \rangle - \mathbf{F}(y)/\mathbf{k}][(D(\mathbf{k}) - \langle \mathbf{k} \rangle D(\gamma)]$$

where:

$$\mathbf{F}(y) = \int f(u)\,\mathrm{d}u = \begin{cases} y[y/l_m - (1-c)]/2(1-c) & \text{in layer } a \\ -y[y/l_m + c]/2c & \text{in layer } b. \end{cases}$$

We deduce the expression of the components of heat fluxes $\mathbf{k}^1$ resulting from the double gradient of temperature. The ones which do not equal zero are those associated with:

$$T^0_{,11}: \quad \mathbf{k}^{111}_1 = D(\gamma)\underline{\mathbf{k}} f(y)$$

$$T^0_{,22}, T^0_{,33}: \quad \mathbf{k}^{122}_1 = \mathbf{k}^{133}_1 = f(y)[D(\gamma)\langle \mathbf{k} \rangle - D(\mathbf{k})]$$

$$T^0_{,12}, T^0_{,13}: \quad \mathbf{k}^{112}_2 = \mathbf{k}^{113}_3 = f(y)\mathbf{k} D(1/\mathbf{k})\underline{\mathbf{k}}.$$

It appears that even though these fluxes of order ε are different from zero, they still have a zero average on the cell. Thus, this 1D microscopic geometry presents the particularity of defining an anisotropic material, for which:

$$\mathbf{K}^1 = 0 \quad \text{thus}\, \mathbf{K}' = 0.$$

This is due to the fact that the gradients of first order are constant in each constituent. In the more general case where the microstructure has a 2D or 3D geometry, this point no longer holds and $\mathbf{K}' \neq 0$.

From the knowledge of $\mathbf{Y}$, we can easily derive the expression of the component different from zero of the tensor $\langle \rho C \mathbf{Y} \rangle$ or R''

$$\mathbf{R}''^{11} = (l^2/12)[D(\rho C)][\underline{\mathbf{k}} D(1/k) - D(\rho C)/\langle \rho C \rangle]$$

$$\mathbf{R}''^{22} = \mathbf{R}''^{33} = (l^2/12)[D(\rho C)]\langle 1/\mathbf{k} \rangle [D(\mathbf{k}) - \langle \mathbf{k} \rangle D(\rho C)/\langle \rho C \rangle].$$

5.3. *Tensor* $\mathbf{K}''$

Tensor $\mathbf{K}''$ is determined from the elementary solutions of problem (3d) depending on the third gradient of temperature. As $\mathbf{K}^1 = 0$ and $\langle \rho C \mathbf{X} \rangle = 0$, we have to solve the elementary problem (see Appendix 1):

$$\partial[\mathbf{k}\,\partial(\theta)/\partial y + \mathbf{k}(\mathbf{Y}^{11} T_{,111} + \mathbf{Y}^{22} T_{,221} + \mathbf{Y}^{33} T_{,331})]/\partial y$$
$$= -(\mathbf{k}^{111}_1 T_{,111} + \mathbf{k}^{122}_1 T_{,221} + \mathbf{k}^{133}_1 T_{,331} + \mathbf{k}^{112}_2 T_{,122} + \mathbf{k}^{113}_3 T_{,133}) + \gamma \mathbf{X}(\underline{\mathbf{k}} T_{,111} + \langle \mathbf{k} \rangle T_{,221} + \langle \mathbf{k} \rangle T_{,331}).$$

In order to obtain $\mathbf{K}^2$, it is only necessary to determine the expression $\partial(\mathbf{Z})/\partial y$, and the fluxes $\mathbf{k}^2$ associated with the third gradient of T^0; the final result being an average of these. After calculation we obtain the components (not equal to zero) of the tensor $\mathbf{K}''$ which are listed below and expressed in the system of macroscopic variables:

$$\mathbf{K}_1''^{111} = (l^2/12)\underline{\mathbf{k}}[D(1/\mathbf{k})\underline{\mathbf{k}}][\langle\rho C\rangle\underline{\mathbf{k}}D(1/\mathbf{k}) - D(\rho C)]/\langle\rho C\rangle$$

$$\mathbf{K}_1''^{122} = \mathbf{K}_1''^{133} = (l^2/12)\underline{\mathbf{k}}[D(1/\mathbf{k})\underline{\mathbf{k}}][\langle\mathbf{k}\rangle D(1/\mathbf{k})]$$

$$\mathbf{K}_1''^{221} = \mathbf{K}_1''^{331} = (l^2/12)\underline{\mathbf{k}}[D(1/\mathbf{k})][\langle\mathbf{k}\rangle(\langle\rho C\rangle\underline{\mathbf{k}}D(1/\mathbf{k}) - D(\rho C))/\langle\rho C\rangle + D(\mathbf{k})]$$

$$\mathbf{K}_2''^{112} = K_2''^{113} = (l^2/12)[D(\mathbf{k})][\underline{\mathbf{k}}D(1/\mathbf{k}) - D(\rho C)/\langle\rho C\rangle]$$

$$\mathbf{K}_2''^{222} = \mathbf{K}_2''^{332} = \mathbf{K}_3''^{223} = \mathbf{K}_3''^{333} = (l^2/12)[D(\mathbf{k})\langle 1/\mathbf{k}\rangle][D(\mathbf{k}) - D(\rho C)\langle\mathbf{k}\rangle/\langle\rho C\rangle].$$

5.4. *Application to heat propagation*

For example, consider a specific stratified composite with $\mathbf{k}_a = \mathbf{k}$, $\mathbf{k}_b = 15\mathbf{k}$, and $c = 0.5$. For simplicity assume that the two layers have the same specific volume heat. For this medium the values of the tensor's components are:

$$\mathbf{K}_1^{01} = \underline{\mathbf{k}} = \mathbf{k}\,.\,15/8 \quad \mathbf{K}_2^{02} = \mathbf{K}_3^{03} = \langle\mathbf{k}\rangle = 8\,.\,\mathbf{k}$$

$$\mathbf{R}_i''^{j} = 0$$

$$\mathbf{K}_1''^{111} = (l^2/12)\underline{\mathbf{k}}[D(1/\mathbf{k})\underline{\mathbf{k}}]^2 = (\mathbf{k}l^2/12)\,.\,49\,.\,15/32\,.\,64$$

$$\mathbf{K}_1''^{122} = \mathbf{K}_1''^{133} = (l^2/12)\underline{\mathbf{k}}[D(1/\mathbf{k})\underline{\mathbf{k}}][\langle\mathbf{k}\rangle D(1/\mathbf{k})] = (\mathbf{k}l^2/12)49/32$$

$$\mathbf{K}_1''^{221} = \mathbf{K}_1''^{331} = (l^2/12)\underline{\mathbf{k}}[D(1/\mathbf{k})][\langle\mathbf{k}\rangle\underline{\mathbf{k}}D(1/\mathbf{k}) + D(\mathbf{k})] = (\mathbf{k}l^2/12)49/16$$

$$\mathbf{K}_2''^{112} = \mathbf{K}_2''^{113} = (l^2/12)[D(\mathbf{k})][kD(1/\mathbf{k})] = (\mathbf{k}l^2/12)49/32$$

$$\mathbf{K}_2''^{222} = \mathbf{K}_2''^{332} = \mathbf{K}_3''^{223} = \mathbf{K}_3''^{333} = (l^2/12)[D(\mathbf{k})\langle 1/\mathbf{k}\rangle]D(\mathbf{k}) = (\mathbf{k}l^2/12)49.2/15.$$

Let us now study a plane heat wave propagating in a direction e_φ having as components $(\sin(\varphi), \cos(\varphi), 0)$ in the frame (Ox_1, x_2, x_3). In this direction, the thermal diffusivity α_φ is given by:

$$\alpha_\varphi = [\underline{\mathbf{k}}\sin^2(\varphi) + \langle\mathbf{k}\rangle\cos^2(\varphi)]/\langle\rho C\rangle$$

and the corrective coefficient a''_φ is such that:

$$a''_\varphi\,.\,[\underline{\mathbf{k}}\sin^2(\varphi) + \langle\mathbf{k}\rangle\cos^2(\varphi)] = -[\mathbf{K}_1''^{111}\sin^4(\varphi) + (\mathbf{K}_1''^{122} + \mathbf{K}_1''^{221} + \mathbf{K}_2''^{112})\cos^2(\varphi)\sin^2(\varphi) + \mathbf{K}_2''^{222}\cos^4(\varphi)].$$

Following the results of Section 4.2, the temperature field is given by:

$$T(x) = T(0)\exp[-\mathrm{i}(x\,.\,e_\varphi)(\sqrt{-\mathrm{i}\omega/\alpha_\varphi})(1 - \mathrm{i}a''_\varphi\omega/\alpha_\varphi)].$$

By introducing the dimensionless space variable x^* and pulsation ω^*, defined by:

$$x^* = (x\,.\,e_\varphi)(\sqrt{\omega/2\alpha_0})/\pi \quad \omega^* = \omega l^2/\alpha_0$$

we get:

$$T(x)/T(0) = \exp[-(1+\mathrm{i})(\sqrt{\alpha_0/\alpha_\varphi})(1 - \mathrm{i}\omega^* a''_\varphi\alpha_0/l^2\alpha_\varphi)\pi x^*]. \quad (14)$$

Expression (14) has been used to compute the perturbation on heat conduction at the limit dimensionless pulsation $\omega^* = 1$, in three directions ($\varphi = 0$, $\pi/4$, $\pi/2$) for which:

$$a''_0/l^2 = -49/720$$

$$\sqrt{\alpha_0/\alpha_{\pi/4}} = 1.273 \quad a''_{\pi/4}\alpha_0/l^2\alpha_{\pi/4} = -0.089$$

$$\sqrt{\alpha_0/\alpha_{\pi/2}} = 2.066 \quad a''_{\pi/2}\alpha_0/l^2\alpha_{\pi/2} = -49/720.$$

The results are shown in Fig. 4 where the temperature distribution for both descriptions—with and without microstructural effects—are presented for a given time ($t = 0 + 2\pi n/\omega$ if $T_{x=0} = T(0)\sin(\omega t)$).

In terms of transfer function of the medium, the amplitude and phase Φ_x of the temperature are easily deduced from (14):

$$\log(T(x)/T(0)) = -(\pi/\ln(10))(\sqrt{\alpha_0/\alpha_\varphi})(1 + \omega^* a''_\varphi\alpha_0/l^2\alpha_\varphi)x^*$$

$$\Phi_x = -\pi(\sqrt{\alpha_0/\alpha_\varphi})(1 - \omega^* a''_\varphi\alpha_0/l^2\alpha_\varphi)x^*.$$

Conversely to the usual description, these parameters depend on the pulsation. Since a''_φ is negative, the increases of attenuation and the phase retardation due to the microstructure clearly appear. In Fig. 5 the logarithm of temperature amplitude at different values of x^*, for a heat wave propagating in three directions ($\varphi = 0, \pi/4, \pi/2$), is presented according to the dimensionless pulsation. This Bode diagram shows that the microstructural effects essentially concern dimensionless pulsations higher than 0.05, and are more significant for large values of x^*.

6. CONCLUSION

The homogenization method is used to study the heat propagation in media with a periodic microstructure when the wavelength is relatively large in comparison with the dimension of the heterogeneities.

It is shown that when we consider only the zero order, the macroscopic description is identical to the one we would expect to obtain for a homogeneous material. Taking into account the terms of a superior order, we diverge from the classic conduction description, as non-local terms are introduced. The latter have to be interpreted in terms of microstructural heat sources.

For an harmonic plane wave, analysis of the effects of the corrective terms brings into evidence a dispersion effect (varying according to $\omega l^2/\alpha$). This phenomenon results from interferences between the initial wave of zero order and the waves generated by microstructural sources.

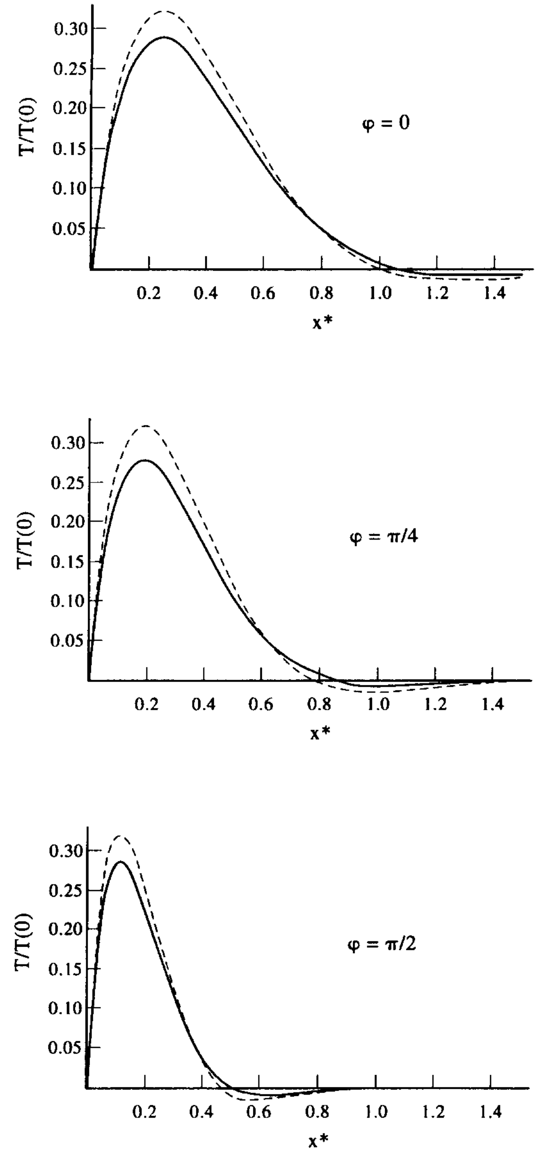

Fig. 4. Temperature at time $t = 0\ (+2\pi n/\omega)$ in a semi-infinite stratified composite subjected to harmonic oscillation ($\omega = \alpha_0/l^2$) of amplitude $T(0)\sin(\omega t)$ at the origin. The black line and the dotted line correspond to the descriptions with and without higher terms respectively. Three orientations of the composite were investigated—$\varphi = 0$: propagation in the direction of the layers; $\varphi = \pi/4$; $\varphi = \pi/2$: propagation in the direction normal to the layers.

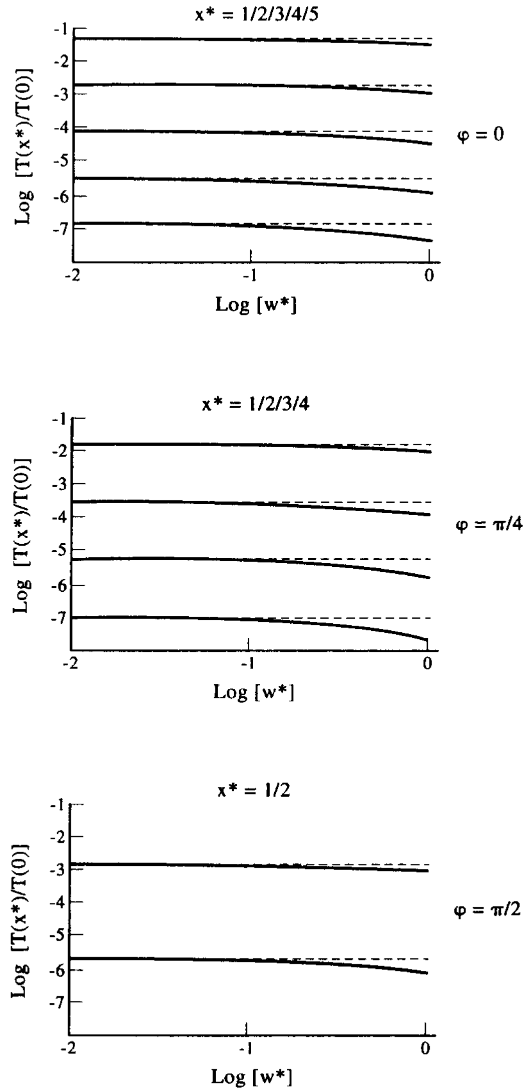

Fig. 5. Bode diagram of the thermal transfer function of a semi-infinite stratified composite (orientations $\varphi = 0$, $\pi/4$, $\pi/2$) for different values of x^* (logarithm of the temperature according to the logarithm of the dimensionless pulsation). The black line and the dotted line correspond to the descriptions with and without higher terms, respectively.

The method is a theoretical means to quantify these effects using the knowledge of the thermal properties of the period. The calculation of the different tensors that come into the macroscopic description is presented, taking periodic stratified materials as an example.

Finally these results have been established whilst assuming that the medium was microperiodic. If the hypothesis of periodicity is not verified the method is no longer directly applicable. However, in many problems, the *structure* of the equations of a homogenizable medium is identical, whether the microstructure of the medium is periodic or stochastic [11]. However, this point remains an open issue and for descriptions including higher orders.

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APPENDIX: HOMOGENIZATION OF HEAT CONDUCTION IN PERIODIC MICROSTRUCTURES

This Appendix states the theoretical developments which lead to the macroscopic heat balance equations up to second order.

Appendix 1. *Resolution of the problems encountered at different orders*

In order to simplify we will write $\mathbf{k}$ and $\rho\,.\,C$ instead of $\mathbf{k}(y)$ and $\rho(y)C(y)$, respectively.

Order ε^{-2}. The first problem solved is the following (3a):

$$L^{-2}(\theta^0) = \nabla_y\,.\,[\mathbf{k}\,.\,\nabla_y\,.\,(\theta^0)] = 0$$

whose evident solutions are constant fields on the period: $\theta^0 = T^0(x)$

Order ε^{-1}. At this order we imply the system (3b):

$$L^{-2}(\theta^1) = -L^{-1}(T^0)$$

which can be written:

$$\nabla_y\,.\,[\mathbf{k}\,.\,\nabla_y(\theta^1)]+\nabla_y\,.\,[\mathbf{k}\,.\,\nabla_x(T^0)] = 0.$$

As a consequence of the linearity of the problem, the general solution is given by:

$$\theta^1(x,y) = T^1(x)+\mathbf{X}(y)\,.\,\nabla_x(T^0).$$

The one rank tensor $\mathbf{X}$ is constructed from the particular solutions $\mathbf{X}^i$ such as:

$$\mathbf{k}^0(y) = \mathbf{k}+\mathbf{k}\,.\,\nabla_y[\mathbf{X}] \quad \nabla_y\,.\,[\mathbf{k}^0(y)] = 0 \quad \langle\mathbf{X}\rangle = 0.$$

The variational formulation is the following:

$$\int_\Omega \mathbf{k}^0(y)\,.\,\nabla_y(w)\,\mathrm{d}v = \int_\Omega [\nabla_y(w)\,.\,\mathbf{k}\,.\,\nabla_y(\mathbf{X})+\mathbf{k}\,.\,\nabla_y(w)]\,\mathrm{d}v = 0.$$

Using index notations, we have more explicitly:

$$\theta^1 = T^1+\mathbf{X}^j\nabla_{xj}(T^0).$$

The functions $\mathbf{X}^j$ being the solutions to the systems:

$$\mathbf{k}_i^{0j} = \mathbf{k}_i^j+\mathbf{k}_i^p\,.\,\nabla_{yp}[\mathbf{X}^j] \quad (\mathbf{k}_i^{0j})_{,i} = 0 \quad \langle\mathbf{X}^j\rangle = 0.$$

Order ε^0. From this order the macroscopic balance equations are no longer obvious. These equations are obtained by integrating in the cell the considered system (3c):

$$L^{-2}(\theta^2) = -L^{-1}(\theta^1)-L^0(T^0)$$

which is more conveniently written as:

$$-\nabla_y\,.\,q^1-\nabla_x\,.\,q^0-\mathrm{i}\omega\rho C T^0(x) = 0.$$

Taking into account the stress periodicity, we have:

$$\nabla_x\,.\,[-\langle q^0\rangle]-\mathrm{i}\omega\langle\rho C\rangle T^0 = 0$$
$$\langle q^0\rangle = -\langle\mathbf{k}\,.\,[\nabla_y(\theta^1)+\nabla_x(T^0)]\rangle.$$

Then, by putting the expression θ^1 in q^0, we deduce the macroscopic momentum equation at zero order (9a):

$$\nabla_x\,.\,[\mathbf{K}^0\,.\,\nabla_x(T^0)]-\mathrm{i}\omega\langle\rho C\rangle T^0 = 0 \quad K^0 = \langle\mathbf{k}^0\rangle.$$

The equation allowing the determination of θ^2 is:

$$\nabla_y\,.\,[\mathbf{k}\,.\,(\nabla_y(\theta^2)+\nabla_x(\theta^1)] = -\nabla_x\,.\,[\mathbf{k}\,.\,(\nabla_y(\theta^1)+\nabla_x(T^0))] + \mathrm{i}\omega\rho C T^0(x).$$

In this equation we substitute θ^1 by its expression and $\mathrm{i}\omega\rho C T^0(x)$ from the macroscopic equation (9a) obtained above. We then have:

$$\nabla_y\,.\,[\mathbf{k}\,.\,(\nabla_y(\theta^2))+\nabla_x(\mathbf{X}\,.\,\nabla_x(T^0))]+\nabla_y\,.\,[\mathbf{k}\,.\,(\nabla_x(T^1))] = -\nabla_x\,.\,[\mathbf{k}^0\,.\,\nabla_x(T^0)-\gamma\mathbf{K}^0\,.\,\nabla_x(T^0)].$$

In order to simplify this expression, we have introduced $\gamma(y)$, the ratio of the volume specific heat to the average value, such that:

$$\gamma(y) = \rho(y)C(y)/\langle\rho C\rangle.$$

We observe that the solution θ^2 depends on two forcing terms:

—the first one is associated with $\nabla_x(T^1)$,
—the second one is associated with $\nabla_x\nabla_x(T^0)$ i.e. the double gradient of the temperature T^0 at zero order.

As a consequence of the linearity of the system, the field solution is a linear combination of particular solutions associated with each of these forcing terms. It is important to notice that the problems linked to the temperature at first order are identical to those already treated at zero order. Consequently we have:

$$\theta^2(x,y) = T^2(x)+\mathbf{X}(y)\,.\,\nabla_x(T^1)+\mathbf{Y}(y)\,.\,.\,\nabla_x\nabla_x(T^0).$$

The second-rank tensor $\mathbf{Y}$ is constructed from the particular solutions $\mathbf{Y}^{lm}$ and verifies:

$$\mathbf{k}^1(y) = \mathbf{kX}+\mathbf{k}\,.\,\nabla_y[\mathbf{Y}] \quad \nabla_y\,.\,[\mathbf{k}^1(y)] = -[\mathbf{k}^0(y)-\gamma(y)\mathbf{K}^0] \quad \langle\mathbf{Y}\rangle = 0,$$

which corresponds to the variational formulation:

$$\int_\Omega \mathbf{k}^1(y)\,.\,\nabla_y(w)\,\mathrm{d}v = \int_\Omega [\nabla_y(w)\,.\,\mathbf{k}\,.\,\nabla_y(\mathbf{Y}) + \mathbf{k}\,.\,\mathbf{X}\,.\,\nabla_y(w)]\,\mathrm{d}v = \int_\Omega [\mathbf{k}^0(y)-\gamma(y)\mathbf{K}^0]\,.\,w\,\mathrm{d}v.$$

Or using the index notation:

$$\theta^2 = U^2+\mathbf{X}^j\nabla_{xj}(T^1)+Y^{lm}\nabla_x\nabla_x(T^0)_{lm}.$$

The vectors $\mathbf{Y}^{lm}$ being the solutions to the systems:

$$\mathbf{k}_i^{1\,lm} = \mathbf{k}_i^m\mathbf{X}^l+\mathbf{k}_i^p\nabla_{yp}[\mathbf{Y}^{lm}](\mathbf{k}_i^{1\,lm})_{,i} = \gamma\mathbf{K}_m^{0\,l}-k_m^{0\,l} \quad \langle\mathbf{Y}^{lm}\rangle = 0.$$

Order ε^1. As above, we first establish the balance equation at this order, and we obtain:

$$\nabla_x.[-\nabla q^1\rangle] = \mathrm{i}\omega\langle\rho C\theta^1\rangle \quad \langle q^1\rangle = -\langle\mathbf{k}\,.\,[\nabla_y(\theta^2)+\nabla_x(\theta^1)]\rangle.$$

In order to have an equation where only average temperatures appear, we introduce expressions of the fields that have already been determined. Thus:

$$\begin{aligned} q^1 &= -\mathbf{k}\,.\,[\nabla_y(\mathbf{Y}\,.\,.\,\nabla_x\nabla_x(T^0)+\mathbf{X}\,.\,\nabla_x(T^1)) \\ &\quad +\nabla_x(\mathbf{X}\,.\,\nabla_x(T^0)+T^1)] \\ &= -\mathbf{k}^1\,.\,.\,\nabla_x\nabla_x(T^0)+\mathbf{k}^0\,.\,\nabla_x(T^1). \end{aligned}$$

Consequently, the momentum balance at the first order is (9b):

$$\nabla_x\,.\,[\mathbf{K}^0\,.\,\nabla_x(T^1)]-\mathrm{i}\omega\langle\rho C\rangle T^1 = -\nabla_x\,.\,[\mathbf{K}^1\,.\,.\,\nabla_x\nabla_x(T^0)] + \mathrm{i}\omega\langle\rho C\mathbf{X}\rangle\,.\,\nabla_x(T^0)\mathbf{K}^1 = \langle\mathbf{k}^1\rangle.$$

The determination of the field θ^3, is achieved by solving:

$$\nabla_y\,.\,[\mathbf{k}\,.\,(\nabla_y(\theta^3)+\nabla_x(\theta^2))] = -\nabla_x\,.\,[\mathbf{k}\,.\,(\nabla_y(\theta^2)+\nabla_x(\theta^1))] + \mathrm{i}\omega\rho C\theta^1.$$

That is, when expressing the different fields:

$$\begin{aligned} &\nabla_y\,.\,\mathbf{k}\,.\,[\nabla_y(\theta^3)+\nabla_x(\mathbf{Y}\,.\,.\,\nabla_x\nabla_x(T^0))] \\ &\quad +\nabla_y\,.\,\mathbf{k}\,.\,\nabla_x(\mathbf{X}\,.\,\nabla_x(T^1))+\nabla_y\,.\,\mathbf{k}\,.\,\nabla_x(T^2) \\ &= -\nabla_x\,.\,[\mathbf{k}\,.\,(\nabla_y(\mathbf{Y}\,.\,.\,\nabla_x\nabla_x(T^0))+\nabla_x(\mathbf{X}\,.\,\nabla_x(T^0)))] \\ &\quad -\nabla_x\,.\,[\mathbf{k}\,.\,(\nabla_y(\mathbf{X}\,.\,\nabla_x(T^1)) \\ &\quad +\nabla_x(T^1))]+\mathrm{i}\omega\rho C(\mathbf{X}\,.\,\nabla_x(T^0)+T^1). \end{aligned}$$

When one replaces T^1 by using the heat balance at the first order (9b), we have:

$$\mathrm{i}\omega\rho CT^1 = \gamma\,.\,[\nabla_x\,.\,[\mathbf{K}^0\,.\,\nabla_x(T^1)]+\nabla_x\,.\,\mathbf{K}^1\,.\,.\,\nabla_x\nabla_x(T^0)] - [\mathrm{i}\omega\langle\rho C\mathbf{X}\rangle\,.\,\nabla_x(T^0)]$$

and so, introducing the tensor $\mathbf{k}^0$ and $\mathbf{k}^1$.

$$\begin{aligned} &\nabla_y\,.\,\mathbf{k}\,.\,[\nabla_y(\theta^3)+\nabla_x(\mathbf{Y}\,.\,.\,\nabla_x\nabla_x(T^0))]+\nabla_y\,.\,\mathbf{k}\,.\,\nabla_x(\mathbf{X}\,.\,\nabla_x(T^1)) \\ &\quad +\nabla_y\,.\,\mathbf{k}\,.\,\nabla_x(T^2) \\ &= -\nabla_x\,.\,[\mathbf{k}^1-\gamma\mathbf{K}^1]\,.\,.\,\nabla_x\nabla_x(T^0)-\nabla_x\,.\,[\mathbf{k}^0-\gamma\mathbf{K}^0]\,.\,.\,\nabla_x(T^1) \\ &\quad -\gamma\,.\,[\langle\rho C\mathbf{X}\rangle/\langle\rho C\rangle-\rho CX]\,.\,\nabla_x\nabla_x\,.\,[\mathbf{K}^0\,.\,\nabla_x(T^0)]. \end{aligned}$$

We notice that the solution θ^3 depends of three forcing terms associated with:

—the gradient of the average temperature at second order;

—the double gradient of the average temperature at first order;

—the third gradient of the temperature at zero order.

The first two terms give the previously solved problems, and the latter introduces a different problem not yet solved. Because of the linearity, the solution to this problem is as follows:

$$\theta(x,y) = T^3(x)+\mathbf{X}(y)\,.\,\nabla_x(T^2)+\mathbf{Y}(y)\,.\,.\,\nabla_x\nabla_x(T^1) + \mathbf{Z}(y)\,.\,.\,.\,\nabla_x\nabla_x\nabla_x(T^0).$$

$\mathbf{Z}$ is the third-rank tensor constructed from the particular solutions $\mathbf{Z}^{npq}$. It verifies the equations:

$$\mathbf{k}^2 = \mathbf{kY}+\mathbf{k}\,.\,\nabla_y[\mathbf{Z}] \quad \langle\mathbf{Z}\rangle = 0$$

$$\nabla_y\,.\,[\mathbf{k}^2] = -[\mathbf{k}^1-\beta\mathbf{K}^1]-\gamma\,.\,[\langle\rho C\mathbf{X}\rangle/\langle\rho C\rangle-\rho C\mathbf{X}]\,.\,\mathbf{K}^0$$

or, with indicial notation:

$$\theta^3 = T^3+\mathbf{X}_{xj}^{\nabla}(T^2)+\mathbf{Y}^{lm}\nabla_x\nabla_x(T^1)_{lm}+\mathbf{Z}^{npq}\nabla_x\nabla_x\nabla_x(T^0)_{npq}$$

where the vectors $\mathbf{Z}^{npq}$ are the solutions to the systems:

$$\mathbf{k}_i^{2npq} = \mathbf{k}_i^n\mathbf{Y}^{pq}+k_{yr}^{r\nabla}[\mathbf{Z}^{npq}] \quad \langle\mathbf{Z}^{npq}\rangle = 0$$

$$(k_i^{2npq})_{,i} = \gamma\mathbf{K}_q^{1np}-k_q^{1np}-\gamma[\langle\rho C\mathbf{X}^q\rangle/\langle\rho C\rangle-\rho C\mathbf{X}^q]\mathbf{K}_p^{0n}.$$

Order ε^2. At this order we are only interested in the momentum balance, which is obtained as above:

$$\nabla_x\,.\,[-\langle q^2\rangle] = \mathrm{i}\omega\langle\rho C\theta^2\rangle \quad \langle q^2\rangle = -\langle\mathbf{k}\,.\,[\nabla_y(\theta^3)+\nabla_x(\theta^2)]\rangle.$$

After replacing θ^2 and θ^3 by their expression, we get (9c):

$$\begin{aligned} &\nabla_x\,.\,[\mathbf{K}^0\,.\,\nabla_x(T^2)]-\mathrm{i}\omega\langle\rho CT^2\rangle \\ &= -\nabla_x\,.\,[\mathbf{K}^1\,.\,.\,\nabla_x\nabla_x(T^1)]+\mathrm{i}\omega\langle\rho C\mathbf{X}\rangle\,.\,\nabla_x(T^1) \\ &\quad -\nabla_x\,.\,[\mathbf{K}^2\,.\,.\,.\,\nabla_x\nabla_x\nabla_x(T^0)]+\mathrm{i}\omega\langle\rho C\mathbf{Y}\rangle\,.\,.\,\nabla_x\nabla_x(T^0) \\ &\qquad \mathbf{K}^2 = \langle\mathbf{k}^2\rangle. \end{aligned}$$

Appendix 2. *Relation between the tensors* $\mathbf{k}^1$ and $\mathbf{k}^0$

From the variational formulations we can link $\mathbf{k}^1$ and $\mathbf{k}^0$. Let us transform the term including $\mathbf{Y}$, in the expression of the average value of:

$$\mathbf{k}^1(y) = \mathbf{kX}+\mathbf{k}\,.\,\nabla_y[\mathbf{Y}] \quad \mathbf{k}_i^{1\,lm} = \mathbf{k}_i^m\mathbf{X}^l+\mathbf{k}_i^p\nabla_{yp}[\mathbf{Y}^{lm}].$$

In order to achieve this, we use the variational formulations associated with the fields $\mathbf{X}^j$. They express that any continuous periodic field w verifies:

$$\int_\Omega \mathbf{k}_j^p\,.\,\nabla_{yp}(w)\,\mathrm{d}v = -\int_\Omega \nabla_y(w)\,.\,\mathbf{k}\,.\,\nabla_y(\mathbf{X}^j)\,\mathrm{d}v.$$

Letting $w = \mathbf{Y}^{lm}$ and taking into account the symmetry of $\mathbf{k}$, we obtain:

$$\int_\Omega [\mathbf{k}_j^{1\,lm}-\mathbf{k}_j^m\mathbf{X}^1]\,\mathrm{d}v = \int_\Omega [\mathbf{k}_j^{p\prime}\nabla_{yp}(\mathbf{Y}^{lm})]\,\mathrm{d}v = -\int_\Omega \nabla_y(\mathbf{Y}^{lm})\,.\,\mathbf{k}\,.\,\nabla_y(\mathbf{X}^j)\,\mathrm{d}v.$$

Now, using $\mathbf{X}^j$ as test field in the variational formulation associated with $\mathbf{Y}^{lm}$, we get:

$$-\int_\Omega \nabla_y(\mathbf{Y}^{lm})\,.\,\mathbf{k}\,.\,\nabla_y(\mathbf{X}^j)\,\mathrm{d}v = \int_\Omega [(\nabla_y\,.\,\mathbf{k}^{1lm})\mathbf{X}^j + \mathbf{k}_p^m\mathbf{X}^k\nabla_{yp}(\mathbf{X}^j)\,\mathrm{d}v.$$

So:

$$\int_{\Omega} \mathbf{k}_j^{1\,lm}\,\mathrm{d}v = \int_{\Omega} (\nabla_y\,.\,\mathbf{k}^{1\,lm})\mathbf{X}^j\,\mathrm{d}v + \int_{\Omega} [\mathbf{k}_p^m \mathbf{X}^l \nabla_{yp}(\mathbf{X}^j)] + \mathbf{k}_j^m \mathbf{X}^l\,\mathrm{d}v.$$

That is, when introducing $\mathbf{k}^0$:

$$\int_{\Omega} \mathbf{k}_j^{1\,lm}\,\mathrm{d}v = \int_{\Omega} (\nabla_y\,.\,\mathbf{k}^{1\,lm})\mathbf{X}^j\,\mathrm{d}v + \int_{\Omega} \mathbf{k}_m^{0\,j}\mathbf{X}^l\,\mathrm{d}v$$

and, by replacing the divergence by its expression, we establish the identity:

$$\mathbf{K}_j^{1\,lm} - \mathbf{K}_m^{0\,l}\langle \rho C \mathbf{X}^j\rangle / \langle \rho C\rangle = \langle \mathbf{k}_n^{0\,j}\mathbf{X}^l - \mathbf{k}_m^{0\,l}\mathbf{X}^j\rangle.$$

Note. In the case of a constant value of ρC this relation becomes:

$$\mathbf{K}_j^{1\,lm} = \langle \mathbf{k}_m^{0\,j}\mathbf{X}^l - k_m^{0\,l}\mathbf{X}^j\rangle$$

which proves the antisymmetry of tensor $\mathbf{K}^1$ with regards to the indexes (j, l).