A MIXTURE THEORY FOR THERMAL DIFFUSION IN UNIDIRECTIONAL COMPOSITES WITH CYLINDRICAL FIBERS OF ARBITRARY CROSS SECTION[†]

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Abstract—A binary mixture theory is developed for heat conduction in a unidirectional, fibrous composite containing a two dimensional periodic array of cylindrical fibers of *arbitrary* cross section. The case considered concerns a class of problems for which conduction occurs primarily in the direction of the fiber axis. Model construction is based upon an asymptotic scheme wherein the ratio of transverse-to-longitudinal diffusion times is assumed to be small; this premise, and the problem class studied, are appropriate for many composites designed primarily for thermal protection. The resulting theory, which retains information on the temperature distribution in the microstructure, contains a mixture interaction coefficient; the latter is determined from the solution of a time-independent boundary value problem in a unit cell. A variational principle-based finite element method is proposed for the solution of this boundary value problem. Consequently, the theory is closed in the sense that no unknown coefficients exist, i.e. the theory is completely determined by the material properties and geometrics of the constituents.

Numerical analyses are carried out for several microstructural geometries of practical interest. The results indicate that, for achievable volume fractions, the concentric circular cylindrical approximation often used in practice provides an adequate measure of global and averaged local temperature fields for composites containing circular fibers in a hexagonal array, and square fibers arranged in a square array. It is found, however, that such an approximation may not be accurate for composites containing rectangular fibers in a similar unit cell. Here a parametric study reveals that the interaction coefficient is a strong function of the unit-cell aspect ratio.

INTRODUCTION

The influence of environmental factors on advanced composite materials has received considerable attention in the past several years (e.g. see [1-3]). Among these factors, temperature and moisture are primary environmental conditions that affect the behavior of a structural composite during its service life. It is evident that the first step in the analysis of such phenomena is the prediction of thermal and/or moisture fields in the composite.

In this paper the problem of thermal diffusion in unidirectional fibrous composites is addressed. In particular, a binary mixture theory is developed for a class of problems, typical of many materials utilized in primary thermal protection systems, in which heat conduction takes place primarily in the fiber axis-direction. This effort generalizes the theoretical development described in [4] to include general two dimensional cells with cylindrical fibers of arbitrary cross section. In [4] a unidirectional fibrous composite with hexagonal periodic microstructure was modeled by approximating a typical cell by concentric circular cylinders.

As in earlier works on diffusion in laminated composites [5, 6], the mixture theory construction technique is based upon an asymptotic method introduced by Hegemier [7] and successfully applied to the solution of wave propagation and diffusion problems [4, 8, 9]. A unique feature of this method is the retention of the heterogeneous character of the composite and the description of temperature fields in each constituent. Moreover, the approach is advantageous in that all constant and interaction terms associated with the theory are explicitly determined from the knowledge of the geometry and material properties of each constituent. In contrast, most general mixture theories, as for example discussed in [10], require a series of experiments for the evaluation of the above quantities.

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It should be noted that a self-contained heat conduction theory for composite materials has been recently developed[11] using a variational formulation. A crucial step of the method is an *a priori* assumption concerning the microstructure temperature field and the relation between micro- and macro-temperature fields.

In this paper, however, the microstructure temperature field is, via the asymptotic procedure adopted, obtained as a solution to a well-posed time independent, microstructure boundary value problem in a unit cell. This solution is obtained for arbitrary geometries by use of a finite element technique based on a variational principle proposed herein. From this solution one can determine the mixture interaction coefficient which relates heat transfer between the fiber and the matrix to the difference of the averaged temperatures in the constituents. With a rationally determined law of heat conduction for "partial" heat flux quantities, and the interaction coefficient, the mixture theory furnishes differential equations for an initial boundary value problem in which the axial coordinate and time are the only independent variables.

Because of the above reduction of the number of spatial coordinates from three to one, the mixture equations offer an attractive economical alternative to a direct numerical attack on the original problem.

It should be emphasized that, for the problem considered in this paper, there are layers adjacent to the boundary wherein the diffusion process is three dimensional. The mixture theory proposed here yields an *outer* solution, strictly valid in a region outside such boundary layers, the thickness of which is expected to be on the order of the composite microdimension. However, as evidenced by numerical results presented in an earlier paper[4], the accuracy of the mixture theory solution, both within and outside the boundary layers, is of higher order than that associated with the elementary effective diffusivity theory which treats the composite as a homogeneous material.

Following presentation of the basic theory, the proposed procedure is used to examine the accuracy of the axisymmetric approximation employed in [4] for the case of the circular fiber int a hexagonal cell. Subsequent to this, the case of a square fiber† in a square cell is studied and the values of the obtained interaction coefficients are compared with results based on the axisymmetric approximation and equivolume fractions. Finally, the results of a parametric study are presented to exhibit the influence of aspect ratio in the case of a rectangular fiber in a similar rectangular cell.

FORMULATION

Basic relations

Consider a periodic, two-dimensional array of unidirectional cylindrical fibers of arbitrary cross section embedded in a matrix, as illustrated in Fig. 1(a). Let a "cell" be associated with each fiber as depicted in Fig. 1(b). Each such cell consists of regions $\bar{A}^{(1)}$ and $\bar{A}^{(2)}$ occupied by the fiber and matrix, respectively. The interface between the two constituents shall be denoted by $\bar{\mathcal{I}}$, and the outer boundary of the cell by $\bar{\mathcal{C}}$.



Fig. 1(a). Geometry of fiber-reinforced composite and coordinate system.

†Rectangular fibers (actually-fiber bundles) result from the manufacturing processes associated with such materials as carbon-carbon composites.



Fig. 1(b). Cell geometry $\overline{A} = \overline{A}^{(1)} U \overline{A}^{(2)}$.

With respect to rectangular Cartesian coordinates \bar{x}_1 , \bar{x}_2 , \bar{x}_3 as shown in Fig. 1(a), let the composite occupy the domain $0 \le \bar{x}_3 \le L$, $-\infty < \bar{x}_2 < \infty$, $-\infty < \bar{x}_1 < \infty$. Let the two constituents in each cell be homogeneous and isotropic, and assume that the interface is perfectly bonded in the sense that any interface thermal resistance can be neglected. Finally, let the initial conditions, and the boundary conditions on $\bar{x}_3 = 0$, L, be such that the temperatures field is similar in each cell.

In view of the last premise, it is sufficient to consider a typical cell with zero heat flux normal to the boundary $\overline{\mathscr{G}}$. Consequently, the basic equations for the temperature fields $\overline{T}^{(\alpha)}$ and heat flux vectors $\overline{Q}_i^{(\alpha)}$ are

(a) Conservation of energy:

$$\bar{Q}_{ii}^{(\alpha)} = -\bar{\mu}^{(\alpha)}\bar{T}^{(\alpha)} \quad \text{on} \quad \bar{A}^{(\alpha)}; \tag{1}$$

(b) Fourier heat conduction law:

$$\bar{O}_{i}^{(\alpha)} = -\bar{k}^{(\alpha)}\bar{T}_{j}^{(\alpha)} \quad \text{on} \quad \bar{A}^{(\alpha)}.$$
⁽²⁾

In the above the superscript $\alpha = 1, 2$ refers to the fiber and matrix, respectively. The quantities $\bar{\mu}$, \bar{k} denote heat capacity and thermal conductivity, respectively. Lower case Latin indices imply indicial notation and the usual summation convention, with range 1-3 unless otherwise noted. The notation $(\bar{})_{,i} \equiv \partial(\)/\partial \bar{x}_i$ and $(\bar{}) \equiv \partial(\)/\partial \bar{t}$ where \bar{t} denotes time.

In addition to (1) and (2), the complete problem specification requires

(c) Symmetry conditions:

$$\bar{Q}_i^{(2)}\bar{\nu}_i^{(2)} = 0 \quad \text{on} \quad \bar{\mathscr{C}} \tag{3}$$

where $\bar{\nu}_i^{(2)}$ is the unit outer normal to the boundary of $\bar{A}^{(2)}$ (note that $\bar{\nu}_3^{(2)} = 0$ since the fibers are cylindrical);

(d) Interface conditions:

$$\bar{T}^{(1)} = \bar{T}^{(2)}, \quad \bar{Q}_i^{(1)} \bar{\nu}_i^{(1)} = \bar{Q}_i^{(2)} \bar{\nu}_i^{(1)} \quad \text{on} \quad \bar{\mathscr{I}}$$
(4)

where $\bar{\nu}_i^{(1)}$ is the unit outer normal to the boundary of $\bar{A}^{(1)}$ (note that $\bar{\nu}_3^{(1)} = 0$);

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(e) Initial conditions at $\overline{t} = 0$ and appropriate boundary data at $\overline{x_3} = 0$, L.

Scaling procedure

Equations (1)-(4) and conditions (e) specify a well-posed problem involving three spatial variables \bar{x}_i and time, \bar{t} . The objective of the subsequent analysis is to derive simplified differential equations governing the macroscopic diffusion process which involve only one spatial dimension (\bar{x}_3) and yet reflect, at least approximately, the effect of conduction on the microscale. To this end, let Λ and Δ be associated with typical macroscopic and microscopic observational dimensions, respectively. The quantities Λ and Δ may be defined in terms of characteristic thermal diffusion times in the longitudinal and transverse directions according to

$$\bar{t}_{(\Lambda)} \equiv \bar{\mu}_{(m)} \Lambda^2 / \bar{k}_{(m)}, \qquad \bar{t}_{(\Lambda)} \equiv \bar{\mu}_{(m)} \Delta^2 / \bar{k}_{(m)}$$
(5a)

where $\bar{\mu}_{(m)}$, $\bar{k}_{(m)}$ denote mixture heat capacity and thermal conductivity; these variables will be defined later. In addition to (5a), it will be convenient to introduce a mixture heat flux $\bar{Q}_{(m)}$, based upon a reference temperature \bar{T} , according to

$$\bar{Q}_{(m)} = \bar{k}_{(m)}\bar{T}/\Lambda,\tag{5b}$$

and a parameter ϵ ,

$$\epsilon = \Delta/\Lambda = (\bar{t}_{(\Delta)}/\bar{t}_{(\Lambda)})^{1/2}$$
(5c)

which represents the ratio of micro-to-macro dimensions of the composite.

With the aid of the foregoing definitions, the following nondimensional variables are now defined:

$$(x_{3}, \epsilon x_{1}, \epsilon x_{2}) = (\bar{x}_{3}, \bar{x}_{1}, \bar{x}_{2})/\Lambda, \qquad t = \bar{t}/\bar{t}_{(\Lambda)},$$

$$(Q_{3}^{(\alpha)}, \epsilon Q_{1}^{(\alpha)}, \epsilon Q_{2}^{(\alpha)}) = (\bar{Q}_{3}^{(\alpha)}, \bar{Q}_{1}^{(\alpha)}, \bar{Q}_{2}^{(\alpha)})/\bar{Q}_{(m)} \qquad (5d)$$

$$T^{(\alpha)} = \bar{T}^{(\alpha)}/\bar{T}, \ \mu^{(\alpha)} = \bar{\mu}^{(\alpha)}/\bar{\mu}_{(m)}, \ k^{(\alpha)} = \bar{k}^{(\alpha)}/\bar{k}_{(m)}.$$

Under (5d), the basic equations can be rewritten as follows:

(a) Conservation of energy:

$$Q_{i,i}^{(\alpha)} = -\mu^{(\alpha)} \dot{T}^{(\alpha)} \quad \text{on} \quad A^{(\alpha)}; \tag{6}$$

(b) Fourier law of heat conduction:

$$(Q_{3}^{(\alpha)}, \epsilon^{2}Q_{1}^{(\alpha)}, \epsilon^{2}Q_{2}^{(\alpha)}) = -k^{(\alpha)}(T_{.3}^{(\alpha)}, T_{.1}^{(\alpha)}, T_{.2}^{(\alpha)}) \quad \text{on} \quad A^{(\alpha)};$$
(7)

(c) Symmetry conditions:

$$Q_i^{(2)} \nu_i^{(2)} = 0$$
 on \mathscr{C} ; (8)

(d) Interface conditions:

$$T^{(1)} = T^{(2)}, Q_i^{(1)} \nu_i^{(1)} = Q_i^{(2)} \nu_i^{(1)} \quad \text{on} \quad \mathscr{I};$$
(9)

(e) Initial conditions at t = 0 and boundary data on $x_3 = 0$, L/Λ .

In the above $A^{(\alpha)}$, \mathcal{I} , \mathcal{C} denote $\overline{A}^{(\alpha)}$, $\overline{\mathcal{I}}$, $\overline{\mathcal{C}}$, respectively, in nondimensional coordinates; the vectors $\nu_i^{(\alpha)}$ are outer normals to the boundaries of $A^{(\alpha)}$; partial derivatives are now defined by $()_{,i} \equiv \partial()/\partial x_i, (\dot{}) \equiv \partial()/\partial t$.

Mixture equations

Mixture equations for the diffusion process are obtained by averaging (6) over the crosssectional area $A^{(\alpha)}$. For this purpose, let

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$$f^{(\alpha a)}(x_3, t) \equiv \frac{1}{A^{(\alpha)}} \iint_{A^{(\alpha)}} f^{(\alpha)}(x_1, x_2, x_3, t) \, \mathrm{d}x_1 \, \mathrm{d}x_2. \tag{10}$$

Integration of (6) according to (10) furnishes, with use of Gauss' Theorem,

$$(A^{(\alpha)}Q_3^{(\alpha\alpha)})_{,3} + \oint_{\partial A^{(\alpha)}} Q_i^{(\alpha)} \nu_i^{(\alpha)} \,\mathrm{d}s = -\mu^{(\alpha)} A^{(\alpha)} \dot{T}^{(\alpha)}, \tag{11}$$

where $\partial A^{(\alpha)}$ denotes the boundary of $A^{(\alpha)}$. With the aid of the boundary conditions (8) and (9), eqn (11) can be written in the standard binary mixture form as

$$Q_{3,3}^{(1p)} + \mu^{(1p)} \dot{T}^{(1a)} = -P$$

$$Q_{3,3}^{(2p)} + \mu^{(2p)} \dot{T}^{(2a)} = P.$$
(12)

In the above equation

$$Q_3^{(ap)} = n^{(a)} Q_3^{(aa)}, \qquad \mu^{(ap)} = n^{(a)} \mu^{(a)}$$
 (13a)

are "partial" heat fluxes and material constants, where

$$n^{(\alpha)} \equiv \bar{A}^{(\alpha)} / (\bar{A}^{(1)} + \bar{A}^{(2)}) = A^{(\alpha)} / (A^{(1)} + A^{(2)}) \equiv A^{(\alpha)} / A$$
(13b)

is the volume fraction of each constituent, and

$$P = A^{-1} \oint_{\mathcal{S}} Q_i^{(1)} \nu_i^{(1)} \, \mathrm{d}s = A^{-1} \oint_{\mathcal{S}} Q_i^{(2)} \nu_i^{(1)} \, \mathrm{d}s \tag{14}$$

is an "interaction" term reflecting heat transfer from the fiber to the matrix.

At this stage the mixture eqns (12) are exact. Approximations arise when one attempts to model the Fourier expressions for heat conduction, and the interaction term. The theory developed in [4] and pursued in this paper has the distinct advantage that both heat conduction and interaction relations are explicitly given as functions of the averaged temperature $T^{(ae)}$, $(\alpha = 1, 2)$ based upon a knowledge of constituent geometry and properties.

Asymptotic expansions

A fundamental premise is now introduced: the ratio of characteristic thermal diffusion times in the transverse and longitudinal (fiber axis) direction is small compared to unity, i.e.

$$\epsilon^{2} = \bar{t}_{(\Delta)}/\bar{t}_{(\Lambda)} = (\Delta/\Lambda)^{2} \ll 1.$$
(15a)

Equation (15a) is appropriate for many composites used for thermal protection.

The premise (15a) suggests the following regular asymptotic expansion for all dependent variables, denoted by $G^{(\alpha)}$:

$$G^{(\alpha)}(x_1, x_2, x_3, t; \epsilon) = \sum_{n=0}^{\infty} \epsilon^{2n} G^{(\alpha)}_{(2n)}(x_1, x_2, x_3, t).$$
(15b)

If (15b) is substituted into the governing eqns (6) and (7) and the coefficients of similar order of ϵ are equated, one obtains a system of equations for each n = 0, 1, 2, ... In what follows a mixture theory is developed based upon the lowest order system.

MIXTURE THEORY BASED ON LOWEST ORDER SYSTEM The lowest order system corresponding to (6) and (7) is

$$Q_{i(0),i}^{(\alpha)} = -\mu^{(\alpha)} \dot{T}_{i(0)}.$$
 (16)

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$$Q_{3(0)}^{(\alpha)} = -k^{(\alpha)} T_{(0),3}^{(\alpha)}, \tag{17a}$$

$$T_{(0),1}^{(\alpha)} = T_{(0),2}^{(\alpha)} = 0.$$
(17b)

Equations (17b) yield

$$T_{(0)}^{(\alpha)} = T_{(0)}^{(\alpha)}(x_3, t).$$
(18)

Thus, eqn (17a) may be averaged according to (10) which furnishes, to lowest order accuracy,

$$Q_3^{(ap)} = -k^{(ap)}T_3^{(aa)}(x_3, t).$$
⁽¹⁹⁾

To "close" the mixture formulation (12), the functional dependence of the interaction term P on the averaged temperatures $T^{(aa)}$ must be determined. For this purpose it is necessary to consider $Q_{j(0)}^{(a)}$, $T_{(2)}^{(a)}$, (j = 1, 2), and to satisfy the continuity of temperature, eqn (9), including $O(\epsilon^2)$ terms, as has been discussed in detail in [7].

To begin this task, one finds, from (7) and (15b), that

$$(Q_{1(0)}^{(\alpha)}, Q_{2(0)}^{(\alpha)}) = -k^{(\alpha)}(T_{(2),1}^{(\alpha)}, T_{(2),2}^{(\alpha)}).$$
(20)

Next, with use of (17) and (20), eqn (16) can be written

$$(k^{(\alpha)}T^{(\alpha)}_{(2)})_{,jj} = \varphi^{(\alpha)}(x_3, t), \qquad (j = 1, 2).$$
(21)

The functions $\varphi^{(\alpha)}(x_3, t)$ can be related to the interaction term P, defined by (14), by integration of (21) over $A^{(\alpha)}$ with use of Gauss' Theorem and the symmetry conditions (8); the result is

$$n^{(1)}\varphi^{(1)} = -P, \qquad n^{(2)}\varphi^{(2)} = P.$$
 (22)

Thus, one obtains the following equations for the functions $T_{(2)}^{(\alpha)}$ in the x_1, x_2 plane:

$$n^{(1)}(k^{(1)}T^{(1)}_{(2),j})_j = -P$$
 on $A^{(1)}, \quad (j = 1, 2);$ (23a)

$$n^{(2)}(k^{(2)}T^{(2)}_{(2),j})_j = P$$
 on $A^{(2)}$, $(j = 1, 2)$. (23b)

The appropriate boundary conditions are, from (8) and (9),

$$T_{(2),j}^{(2)}\nu_j^{(2)} = 0$$
 on \mathscr{C} , $(j = 1, 2);$ (24)

$$T_{(0)}^{(1)}(x_3, t) + \epsilon^2 T_{(2)}^{(1)} = T_{(0)}^{(2)}(x_3, t) + \epsilon^2 T_{(2)}^{(2)} \quad \text{on} \quad \mathcal{I};$$
 (25a)

$$k^{(1)}T^{(1)}_{(2),j}\nu^{(1)}_j = k^{(2)}T^{(2)}_{(2),j}\nu^{(1)}_j$$
 on \mathscr{I} , $(j = 1, 2)$. (25b)

The solution to the above boundary value problem is unique within a function $H(x_3, t)$. Without loss in generality one can combine this function with $T_{(0)}^{(\alpha)}(x_1, t)$ as follows:

$$\tilde{T}_{(0)}^{(a)}(x_3,t) = T_{(0)}^{(a)}(x_3,t) + \epsilon^2 H(x_3,t).$$
(26)

Under (26), uniqueness for the field $T_{(2)}^{(\alpha)}$ can now be obtained by setting $T_{(2)}^{(1)} = 0$ at some point on $A^{(1)}$; for convenience the point $O \in A^{(1)}$ is selected; thus,

$$T_{(2)}^{(1)} = 0$$
 at point $O \in A^{(1)}$. (27)

It is noted that (25a) represents a jump condition for the dependent variables $T_{(2)}^{(\alpha)}$ in the foregoing boundary value problem, i.e.

$$T_{(2)}^{(2)} - T_{(2)}^{(1)} = \frac{1}{\epsilon^2} (T_{(0)}^{(1)} - T_{(0)}^{(2)}) \quad \text{on} \quad \mathscr{I}.$$
 (28)

A more convenient formulation of this problem without a jump condition can be obtained by introducing new field variables $T^{*(\alpha)}$ as follows:

$$PT^{*(1)} \equiv T^{(1)}_{(2)}; \qquad PT^{*(2)} \equiv T^{(2)}_{(2)} + \frac{1}{\epsilon^2} (\tilde{T}^{(2)}_{(0)} - \tilde{T}^{(1)}_{(0)}). \tag{29}$$

The boundary value problem in terms of the new dependent variables $T^{*(\alpha)}$ is

$$n^{(1)}k^{(1)}T^{*(1)}_{jj} = -1$$
 on $A^{(1)}$, $(j = 1, 2);$ (30a)

$$n^{(2)}k^{(2)}T^{*(2)}_{jj} = 1$$
 on $A^{(2)}$, $(j = 1, 2);$ (30b)

$$T^{*(2)}_{,j}\nu_{j}^{(2)} = 0$$
 on $\mathscr{C};$ (31)

$$T^{*(1)} = T^{*(2)}, \qquad k^{(1)}T^{*(1)}_{,j}\nu_j^{(1)} = k^{(2)}T^{*(2)}_{,j}\nu_i^{(1)} \qquad \text{on} \qquad \mathcal{I}(j=1,2);$$
(32)

$$T^{*(1)} = 0$$
 at point $O \in A^{(1)}$ (33)

The solution of the problem posed by (30)-(33) will be of the form

$$T^{*(\alpha)} = T^{*(\alpha)}(x_1, x_2). \tag{34}$$

Once these functions are known, the temperature field can be written to $O(\epsilon^2)$ accuracy using (26) and (29); thus

$$T^{(1)} = \tilde{T}^{(1)}_{(0)}(x_3, t) + \epsilon^2 P T^{*(1)}(x_1, x_2) + O(\epsilon^4),$$

$$T^{(2)} = \tilde{T}^{(2)}_{(0)}(x_3, t) + \epsilon^2 \left\{ P T^{*(2)}(x_1, x_2) - \frac{1}{\epsilon^2} (T^{(2)}_{(0)} - T^{(1)}_{(0)}) \right\} + O(\epsilon^4)$$

$$= \tilde{T}^{(1)}_{(0)}(x_3, t) + \epsilon^2 P T^{*(2)}(x_1, x_2) + O(\epsilon^4).$$
(35)

Upon averaging (35) according to (10) one now obtains

$$T^{(aa)}(x_3,t) = \tilde{T}^{(1)}_{(0)}(x_3,t) + \epsilon^2 P T^{*(aa)}.$$
(36)

With use of (36), the interaction term can be written as a function of the averaged temperature $T^{(aa)}(x_3, t)$:

$$P = \zeta [T^{(1a)}(x_3, t) - T^{(2a)}(x_3, t)]/\epsilon^2$$
(37a)

where

$$\zeta = (T^{*(1a)} - T^{*(2a)})^{-1}.$$
(37b)

The preceding development (eqns 12, 19 and 37) completes the mixture formulation of the diffusion process under the premise that $\epsilon^2 \ll 1$. The main result is the expression (37b) which can be used to determine the interaction coefficient ζ from the solution of the time independent problem defined by (30)-(33) over the unit cell. For future reference this problem will be termed the microstructure boundary value problem (MBVP).

SOLUTION OF THE MICRO BOUNDARY VALUE PROBLEM

Variational principle

In general, it is difficult to obtain an analytical solution to the MBVP. As an alternative, a finite element procedure, valid for arbitrary two-dimensional cell geometry, is proposed. A prelude to this procedure is a variational principle, which is developed in this section.

At the outset it is noted that, if the effect of fiber geometry is to be adequately modeled, it is essential that both interface conditions (32) be satisfied. For this reason a modified Reissnertype variational principle is utilized. A significant feature of this principle is that it allows arbitrary variations of heat flux along the constituent interface and hence mitigates the kinetmatic constraint-difficulty associated with the usual extremum principles [12]. Consider the functional

$$\Pi = \sum_{\alpha=1}^{2} \iint_{\mathcal{A}^{(\alpha)}} \left[\frac{1}{2} k^{(\alpha)} T^{*(\alpha)}_{,j} T^{*(\alpha)}_{,j} + \frac{(-1)^{\alpha}}{n^{(\alpha)}} T^{*(\alpha)} \right] dA$$
$$+ \oint_{\mathcal{F}} Q^{*} [T^{*(1)} - T^{*(2)}] ds, \qquad (j = 1, 2)$$
(38)

which is defined in terms of $T^{*(\alpha)}$ on $A^{(\alpha)}$ and Q^* on \mathcal{I} . It is now shown that the microstructure boundary value problem for $T^{*(\alpha)}$ follows from the requirement that II be stationary with respect to arbitrary variations of $T^{*(\alpha)}$ and Q^* where Q^* is a Lagrange multiplier which physically represents heat flux normal to the boundary \mathcal{I} . Indeed, on setting the first variation of II equal to zero we obtain

$$\delta \Pi = \sum_{\alpha=1}^{2} \left\{ -\int_{A^{(\alpha)}} \int \left[k^{(\alpha)} T^{*(\alpha)}_{,ji} - \frac{(-1)^{\alpha}}{n^{(\alpha)}} \right] \delta T^{*(\alpha)} dA \right\}$$

+ $\oint_{\mathscr{C}} k^{(2)} T^{*(2)}_{,j} \nu_{j}^{(2)} \delta T^{*(2)} ds - \sum_{\alpha=1}^{2} (-1)^{\alpha} \oint_{\mathscr{C}} \left[Q^{*} + k^{(\alpha)} T^{*(\alpha)}_{,j} \nu_{j}^{(1)} \right] \delta T^{*(\alpha)} ds$
+ $\oint_{\mathscr{C}} \left[T^{*(1)} - T^{*(2)} \right] \delta Q^{*} ds, \quad j = 1, 2$
= 0. (39)

From (39) it is obvious that (30)-(32) are Euler equations for extemization of the functional Π .

The only "kinematic" constraint to be imposed on $T^{*(1)}$ for the uniqueness of the solutions is (33), as discussed in the last section. The other kinematic constraint, defined by (32a), has been eliminated by the introduction of Q^* as a Lagrange multiplier.

Finite element discretization

To use the variational principle of the last section for a finite element analysis, the closure of the domain $A^{(1)} + A^{(2)}$, which includes \mathcal{I} , is partitioned into unions of closed subdomains or elements overlapping only at the interelement boundaries. The field $T^{*(\alpha)}(\mathbf{r})$ is interpolated by nodal values $\varphi_I^{(\alpha)} = T^{*(\alpha)}(\mathbf{r}_I)$ in each finite element $A_{(\alpha)}^{(\alpha)}$, where (\mathbf{r}_I) is the position vector of the *I*th node of the element $A_{(\alpha)}^{(\alpha)}$. Thus

$$T^{*(\alpha)}(\mathbf{r}) = [N_1(\mathbf{r}), N_2(\mathbf{r}) \dots] \begin{cases} \varphi_1^{(e)} \\ \varphi_2^{(e)} \\ \vdots \\ \vdots \end{cases}^{(\alpha)} = N_{(e)} \varphi_{(e)}^{(\alpha)} \quad \text{on} \quad A_{(e)}^{(\alpha)} \tag{40}$$

where $N_l(\mathbf{r})$ are interpolation functions used for discretization of $T^{*(\alpha)}$ in the domain $A_{(\mathbf{r})}^{(\alpha)}$ such that

$$N_{I}(\mathbf{r}_{J}) = \delta_{IJ}, \quad \mathbf{r}_{J} \in A_{(e)}^{(\alpha)}.$$
(41)

Since the functional Π contains additional terms defined on the interface, one-dimensional interface elements must also be used. It is most convenient to choose these elements to be the boundaries of those 2-D elements $A_{(e)}^{(\alpha)}$ which are partly bounded by the interface \mathcal{I} . On such an interface element $\mathcal{I}_{(e)}$

$$T^{\star(\alpha)}(\mathbf{r}) = [\bar{N}_{1}(\mathbf{r}), \quad \bar{N}_{2}(\mathbf{r}) \dots] \begin{cases} \bar{\varphi}_{1} \\ \bar{\varphi}_{2} \\ \vdots \\ \vdots \\ \vdots \end{cases} = \bar{N}_{(e)} \bar{\varphi}_{(e)}$$
(42)

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$$Q^{*}(\mathbf{r}) = [\bar{N}_{1}(\mathbf{r}), \quad \bar{N}_{2}(\mathbf{r}) \dots] \begin{cases} \bar{\Psi}_{1} \\ \bar{\Psi}_{2} \\ \vdots \\ \vdots \\ \vdots \end{cases} = \bar{N}_{(e)} \bar{\Psi}_{(e)}$$
(43)

where $\bar{N}_{l}(\mathbf{r})$ are shape functions used for interpolation along the interface such that

$$\bar{N}_{I}(\mathbf{r}_{J}) = \delta_{IJ}, \quad \mathbf{r}_{J} \in \mathscr{I}_{(e)}.$$
(44)

Based on (40), the derivatives $T_{ij}^{*(\alpha)}$ (j = 1, 2) are discretized by

$$\begin{cases} T_{\perp 1}^{*(\alpha)} \\ T_{\perp 2}^{*(\alpha)} \end{cases} = \begin{bmatrix} N_{1,1} N_{2,1} \cdots \\ N_{1,2} N_{2,2} \cdots \end{bmatrix} \varphi_{(e)}^{(\alpha)} \equiv \mathbf{B}_{(e)} \varphi_{(e)}^{(\alpha)}.$$
 (45)

At this point it is appropriate to note the degree of continuity required of the interpolation functions so that conforming elements are obtained. As a minimum, the shape functions N_I must be of class C^1 on $A_{iei}^{(\alpha)}$, with continuity of functions imposed along the inter-element boundaries. The interpolants \bar{N}_I along the interface are required to be at least of class C^0 within each boundary element.

With (40)-(45), the discrete form of the functional Π in (38) can be written as (with $A_{(e)}^{(\alpha)} \subset \text{clos. } A^{(\alpha)}$).

$$\Pi \simeq \sum_{\alpha=1}^{\infty} \sum_{\mathcal{A}_{\{e\}}^{(\alpha)}} \left\{ \frac{1}{2} \varphi_{(e)}^{(\alpha)T} \mathbf{K}_{(e)}^{(\alpha)} \varphi_{(e)}^{(\alpha)} + \frac{(-1)^{\alpha}}{n^{(\alpha)}} \varphi_{(e)}^{(\alpha)T} \tau_{(e)}^{(\alpha)} \right\} + \sum_{\mathcal{I}_{\{e\}} \subseteq \mathcal{I}} \left[\bar{\Psi}_{(e)}^{T} \mathbf{H}_{(e)} \left(\bar{\varphi}_{(e)}^{(1)} - \bar{\varphi}_{(e)}^{(2)} \right) \right]$$
(46)

where

$$\mathbf{K}_{(e)}^{(\alpha)} = \iint_{A_{(e)}^{(\alpha)}} \mathbf{B}_{(e)}^{T} \mathbf{B}_{(e)} \, \mathbf{d}A \tag{47a}$$

$$\tau_{(e)}^{(\alpha)} = \iint_{A_{(e)}^{(\alpha)}} \mathbf{N}_{(e)}^T \, \mathrm{d}A \tag{47b}$$

$$\bar{\mathbf{H}}_{(e)} = \int_{\mathcal{S}_{(e)}} \bar{\mathbf{N}}_{(e)}^T \bar{\mathbf{N}}_{(e)} \, \mathrm{d}s \tag{47c}$$

are various quantities defined on the element level. By the usual finite element assembly process, corresponding global level quantities can be obtained, so that, finally,

$$\Pi \simeq \sum_{\alpha=1}^{2} \left\{ \frac{1}{2} \varphi^{(\alpha)T} \mathbf{K}^{(\alpha)} \varphi^{(\alpha)} + \frac{(-1)^{\alpha}}{n^{(\alpha)}} \varphi^{(\alpha)T} \tau^{(\alpha)} \right\} + \bar{\Psi}^{T} \bar{\mathbf{H}}^{T} (\bar{\varphi}^{(1)} - \bar{\varphi}^{(2)}).$$
(48)

It is convenient to number the global system such that interior nodal temperatures $\varphi^{*(\alpha)}$ appear as the leading components of the vector $\varphi^{(\alpha)}$, i.e.

$$\boldsymbol{\varphi}^{(\alpha)} = \begin{cases} \boldsymbol{\varphi}^{\ast(\alpha)} \\ \bar{\boldsymbol{\varphi}}^{(\alpha)} \end{cases}. \tag{49}$$

Equating to zero the first variation of Π in (48) with respect to Ψ and $\varphi^{(\alpha)}$ leads to

$$\mathbf{K}^{(\alpha)}\boldsymbol{\varphi}^{(\alpha)} + \frac{(-1)^{\alpha}}{n^{(\alpha)}} \tau^{(\alpha)} - (-1)^{\alpha} \begin{bmatrix} 0 & 0\\ 0 & \tilde{\mathbf{H}} \end{bmatrix} \begin{bmatrix} 0\\ \boldsymbol{\Psi} \end{bmatrix} = \mathbf{0}$$
(50)

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$$\bar{\mathbf{H}}^T(\bar{\boldsymbol{\varphi}}^{(1)} - \bar{\boldsymbol{\varphi}}^{(2)}) = 0.$$
(51)

In (50), $\mathbf{K}^{(1)}$ and $\boldsymbol{\tau}^{(1)}$ must be modified because of the kinematic condition (33). Let point O be chosen as the first node, then

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$$K_{1N}^{(1)} = \delta_{1N}, \quad \tau_1^{(1)} = 0, \quad 2 \le N \le M^{(1)}$$
(52)

where $M^{(\alpha)}$ denotes the total number of the nodal degrees of freedom in $A^{(\alpha)}$. To retain the symmetry of the "stiffness" matrix $K^{(\alpha)}$ it is preferable to modify the first column also; thus

$$K_{N1}^{(1)} = 0, \qquad 2 \le N \le M^{(1)}$$
 (53)

without any loss of generality.

Further details of the computational technique are best explained by partitioning $\mathbf{K}^{(\alpha)}$, $\tau^{(\alpha)}$ in accordance with (49), thus,

$$\mathbf{K}^{(\alpha)} = \begin{bmatrix} \mathbf{K}_{11}^{(\alpha)} & \mathbf{K}_{12}^{(\alpha)} \\ \mathbf{K}_{21}^{(\alpha)} & \mathbf{K}_{22}^{(\alpha)} \end{bmatrix}, \quad \boldsymbol{\tau}^{(\alpha)} = \begin{bmatrix} \boldsymbol{\tau}^{*(\alpha)} \\ \bar{\boldsymbol{\tau}}^{(\alpha)} \end{bmatrix}.$$
(54)

With (54), eqns (50) can be written in a more explicit form, which is

$$\mathbf{K}_{11}^{(\alpha)}\boldsymbol{\varphi}^{*(\alpha)} + \mathbf{K}_{12}^{(\alpha)}\bar{\boldsymbol{\varphi}}^{(\alpha)} + \frac{(-1)^{(\alpha)}}{n^{(\alpha)}}\boldsymbol{\tau}^{*(\alpha)} = 0,$$
(55a)

$$\mathbf{K}_{21}\boldsymbol{\varphi}^{*(\alpha)} + \mathbf{K}_{22}^{(\alpha)} \bar{\boldsymbol{\varphi}}^{(\alpha)} + \frac{(-1)^{\alpha}}{n^{(\alpha)}} \bar{\boldsymbol{\tau}}^{(\alpha)} - (-1)^{\alpha} \bar{\mathbf{H}} \boldsymbol{\Psi} = 0, \qquad \alpha = 1, 2.$$
(55b)

From (55) we obtain

$$\varphi^{*(\alpha)} = -\mathbf{K}_{11}^{(\alpha)-1} \mathbf{K}_{12}^{(\alpha)} \bar{\varphi}^{(\alpha)} - \frac{(-1)^{\alpha}}{n^{(\alpha)}} \mathbf{K}_{11}^{(\alpha)-1} \tau^{*(\alpha)}, \qquad \alpha = 1, 2.$$
(56)

On substitution of (56) into (55b), the following equations are obtained for the interface quantities

$$\mathbf{D}^{(\alpha)}\boldsymbol{\bar{\varphi}}^{(\alpha)} + (-1)^{\alpha} \left[\frac{\boldsymbol{\tau}_{1}^{(\alpha)}}{n^{(\alpha)}} - \boldsymbol{\bar{\mathbf{H}}} \boldsymbol{\Psi} \right] = 0, \qquad \alpha = 1, 2$$
(57)

where

$$\mathbf{D}^{(\alpha)} = \mathbf{K}_{22}^{(\alpha)} - \mathbf{K}_{21}^{(\alpha)} [\mathbf{K}_{11}^{(\alpha)}]^{-1} \mathbf{K}_{12}$$
(58a)

$$\tau_1^{(\alpha)} = \tau^{*(\alpha)} - \mathbf{K}_{21}^{(\alpha)} [\mathbf{K}_{11}^{(\alpha)}]^{-1} \bar{\tau}^{(\alpha)}.$$
(58b)

With proper choice of shape functions, the matrix $\bar{\mathbf{H}}$ is positive definite and, hence, it follows from (51) that

$$\bar{\boldsymbol{\varphi}}^{(1)} = \bar{\boldsymbol{\varphi}}^{(2)}.\tag{59}$$

Equation (59) can be used to eliminate Ψ from (57) to obtain

$$\left[\mathbf{D}^{(1)} + \mathbf{D}^{(2)}\right]\bar{\boldsymbol{\varphi}}^{(1)} + \left[\frac{\tau_1^{(2)}}{n^{(2)}} - \frac{\tau_1^{(1)}}{n^{(1)}}\right] = 0.$$
(60)

By virtue of the constraint (33), the matrix $[D^{(1)} + D^{(2)}]$ is nonsingular provided conforming elements are used for discretization. As a result we can solve (60) for $\bar{\varphi}^{(1)}$,

$$\bar{\boldsymbol{\varphi}}^{(1)} = \bar{\boldsymbol{\varphi}}^{(2)} = [\mathbf{D}^{(1)} + \mathbf{D}^{(2)}]^{-1} \left\{ \frac{\boldsymbol{\tau}_1^{(1)}}{n^{(1)}} - \frac{\boldsymbol{\tau}_1^{(2)}}{n^{(2)}} \right\}.$$
(61)

Substituting (61) into (56) we obtain $T^{*(\alpha)}$, ($\alpha = 1, 2$) and by the averaging process we get $T^{*(\alpha \alpha)}$ which are required for the calculation of the interaction coefficient ζ defined in (37).

So far we have considered the entire unit cell in the development of the theory and the finite element discretization procedure. However, for computational efficiency, any symmetry conditions, if they exist, must be fully exploited. Since no heat transfer occurs across the lines of symmetry, no major modification in either the theory or the discretization procedure is required even if a reduced cell obtained from symmetry considerations is used for computations.

MIXTURE QUANTITIES AND RECOVERY OF MICROSTRUCTURE

With the complete formulation of the mixture equations, the appropriate mixture heat capacity $\bar{\mu}_{(m)}$ and mixture thermal conductivity $\bar{k}_{(m)}$ introduced for scaling can be found in the following manner.

On substitution of (19) and (37) into (12) we get

$$k^{(1p)}T^{(1a)}_{,33} - \mu^{(1p)}\dot{T}^{(1a)} = \zeta [T^{(1a)} - T^{(2a)}]/\epsilon^2,$$
(62a)

$$k^{(2p)}T^{(2a)}_{,33} - \mu^{(2p)}\dot{T}^{(2a)} = -\zeta [T^{(1a)} - T^{(2a)}]/\epsilon^2.$$
(62b)

Elimination of either $T^{(1a)}$ and $T^{(2a)}$ from (62) yields

$$[(k^{(1p)} + k^{(2p)})T^{(aa)}_{,33} - (\mu^{(1p)} + \mu^{(2p)})\dot{T}^{(aa)} + O(\epsilon^2)] = 0.$$
(63)

Equation (63) suggests the following definitions for mixture thermal conductivity and heat capacity

$$\bar{k}_{(m)} = n^{(1)}\bar{k}^{(1)} + n^{(2)}\bar{k}^{(2)}, \tag{64a}$$

$$\bar{\mu}_{(m)} = n^{(1)} \bar{\mu}^{(1)} + n^{(2)} \bar{\mu}^{(2)}.$$
(64b)

It might be noted here that with the above definition of mixture properties the nondimensional constituent properties $k^{(\alpha)}$ and $\mu^{(\alpha)}$ are of order unity for a practical range of volume fractions.

The methodology for the use of the theory presented here is the following. For a given composite, the MBVP is solved by the finite element procedure to obtain the fields $T^{\phi(\alpha)}$ and the iteraction coefficient ζ defined by (37). This interaction coefficient can be used to calculate the average temperature fields $T^{(\alpha\alpha)}(x_3, t)$ from (62) with appropriate boundary and initial data. To recover the temperature microstructure one first calculates

$$\tilde{T}_{(0)}^{(1)}(x_3,t) = T^{(\alpha\alpha)}(x_3,t) - \zeta [T^{(1\alpha)} - T^{(2\alpha)}] T^{\#(\alpha\alpha)}, \quad \alpha = 1 \quad \text{or} \quad -2$$
(65)

from (36). Finally, the fields $T^{(\alpha)}(x_1, x_2, x_3, t)$, correct to $O(\epsilon^2)$, can be obtained from (35).

NUMERICAL RESULTS

The finite element procedure described in this paper has been used for the solution of the temperature microstructure problem (30)-(33) for the interaction coefficient for a variety of geometries and combination of material properties. Conforming triangular elements with six nodes and quadratic interpolation functions were used for discretization of the fields $T^{\phi(\alpha)}$ in the fiber and the matrix domains in the unit cell. For the heat flux quantities on the interface, compatible quadratic interpolation functions were used.

To estimate the size of the mesh required to obtain reliable results, the interaction coefficient ζ was calculated for a composite containing rectangular fibers in a similar unit cell, using a coarse and a fine mesh shown in Fig. 2(a, b). As can be seen in the figure, the corner of the fiber was rounded off to remove the singularity in the solution that would otherwise occur. Although the number of degrees of freedom of the two finite element models differs by more than one hundred, the computed values of interaction coefficient were within 0.06% of each other. Similar calculations for other values of volume fraction yielded a difference of no more than 0.15% between the interaction coefficients calculated using a fine and a coarse mesh,



Fig. 2(a). Coarse mesh for solution of MBVP for rectangular fiber in a similar unit cell, $(\Delta_1/\Delta_2 = 2, d_1/\Delta_1 = 0.4, k_1/k_2 = 10)$.



Fig. 2(b). Fine mesh for solution of MBVP for rectangular fiber in a similar unit cell, $(\Delta_1/\Delta_2 = 2, d_1/\Delta_1 = 0.4, k_1/k_2 = 10)$.

respectively. With this check on the convergence of the numerical solution, subsequent computations were conducted with meshes similar in size to the "fine" mesh of Fig. 2(b).

In an effort to check the validity of the concentric circular cylinders approximation used in [4] for circular fibers in a hexagonal array, the interaction coefficient was calculated as a function of fiber volume fraction and thermal conductivity ratio. From the results, shown in Fig. 3, the somewhat expected conclusion can be drawn that for a practical range of fiber volume fraction the theory presented in [4] can be used without any significant loss of accuracy.

For calculation of the interaction coefficient, the concentric circular cylinders approximation based on equal fiber volume fraction can also be used for composites containing square fibers arranged in a square array. This is borne out by the results shown in Fig. 4. The calculations for this figure were conducted by rounding off the corner of the fiber by a quarter circle whose radius was arbitrarily selected to be 10% of the fiber width.

The final set of calculations was conducted for composites containing rectangular fibers in a similar unit cell. The results for three values of the slenderness ratio of the unit cell are presented in Figs. 5(a-c). In these cases the corner was rounded by a quarter circle with radius equal to a quarter of the smaller of the sides of the rectangular fiber. As can be seen from these figures, the interaction coefficient is significantly overestimated when the concentric circular cylindrical approximation is used. This discrepancy illustrates the importance of the type of calculations reported here.

As has been noted previously, the fields $T^{*(\alpha)}(x_1, x_2)$ needed to calculate the interaction term can also be used for the calculation of the temperature distribution in a unit cell. From (35), (37a) and (65) we have

$$T^{(\alpha)}(x_1, x_2, x_3, t) = T^{(\alpha a)} + \zeta [T^{(1a)} - T^{(2a)}] [T^{*(\alpha)} - T^{*(\alpha a)}]$$
(66)



Fig. 3. Interaction coefficient for a hexagonal cell with a circular fiber.





Fig. 5(a). Interaction coefficient for a rectangular cell with a similar rectangular fiber, $\Delta_1/\Delta_2 = d_1/d_2 = 1.5$.



Fig. 5(b). $\Delta_1/\Delta_2 = d_1/d_2 = 2.0$.

Fig. 5(c). $\Delta_1/\Delta_2 = d_1/d_2 = 2.5$.



Fig. 6. Isothermal contours of $\zeta T^{*(\alpha)}$ in a square cell $(k_1/k_2 = 10)$.



Fig. 7. Isothermal contours of $\zeta T^{\pm(\alpha)}$, ($\alpha = 1, 2$) in a rectangular cell ($k_1/k_2 = 10, \Delta_1/\Delta_2 = 2$).

In the r.h.s. of the above equation, the only quantity dependent upon inplane coordinates x_1 and x_2 is $T^{*(\alpha)}$. It follows, therefore, that curves of equal $T^{*(\alpha)}$ are also isothermal lines within the framework of our theory. For this reason, and to illustrate the type of temperature microstructure that can be obtained from the mixture theory, contours of equal $T^{*(\alpha)}$, suitably normalized, are given in Figs. 6 and 7 for the case of rectangular fibers in a similar unit cell. Of course, the discontinuity in the slope of these contours arises because of the difference between the thermal conductivity of two materials.

CONCLUDING REMARKS

A binary mixture theory has been constructed for heat conduction in the direction of the fiber axis for unidirectional fibrous composites. The theory contains information on temperature microstructure. A mixture thermal property, the interaction coefficient, that relates the heat transfer between the fiber and the matrix to the difference between the average temperatures of the two constituents, is calculated from the solution of a static microstructure boundary value problem defined over the unit cell. A computational approach to the solution of the microstructure boundary value problem has been described and examples of its application have been given. The numerical results indicate that the concentric circular cylinder approximation is adequate for the prediction of the interaction coefficient and, consequently, the average temperatures for some geometries. However, if it is desired to obtain some information on the temperature distribution within the unit cell, it is necessary to solve the microstructure boundary value problem. Even though additional computational effort is needed, the ability of the theory to predict microstructure is unmatched by any other continuum model of heat conduction in composites.

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