# VARIATIONAL ESTIMATES OF THE EFFECTIVE THERMAL CONDUCTIVITIES OF TRANSVERSELY ISOTROPIC COMPOSITES

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A study is made of a type of composite material that is widely used in practical applications – a composite with fibers of constant cross section arranged parallel to one another in the matrix. The effective thermal conductivities of transversely isotropic composites is estimated on the basis of dual variational principles from thermostatics. Certain geometric models that are of practical interest are examined and refined estimates of their effective conductivities are obtained. Due to mathematical equivalence, the results obtained can also be used for effective electrical conductivity, the effective diffusion coefficient, effective permittivity, and effective permeability.

1. Formulation of the Problem. We will examine a two-dimensional problem of heat conduction in the plane of isotropy of a composite with a Cartesian coordinate system $\{x_1, x_2\}$. A representative element of the heterogeneous medium, confined to the volume V, consists of N continuous, transversely isotropic phases. Each phase occupies the multiply connected region $V_\alpha \subset V$ and in the plane of isotropy has a transverse thermal conductivity $\lambda_\alpha$, $\alpha = \overline{1, N}$. We will designate the area of $V_\alpha$ as $v_\alpha$. Without loss of generality, we can assume that the area of V = 1.

The equation of thermostatics for this problem has the form

$$Q_{i,i} = 0, \tag{1}$$

where $Q_i = -\lambda T_{,i}$, $\lambda = \lambda_\alpha$ in $V_\alpha$.

Conditions of continuity of the heat flux $Q_i n_i$ and temperature T are satisfied at the phase boundary. Here, $n_i$ represents components of the unit normal to the line of the boundary. The comma in front of the subscript i denotes differentiation with respect to $x_i$. Here and below, the English-letter indices take values of 1 and 2, while summation from 1 to 2 is carried out over repeating indices of this kind.

Let us determine the value of $Q_i$, averaged over the region V, from the following formula:

$$\langle Q_i \rangle = \int_V Q_i d^2x. \tag{2}$$

If the relations $\langle Q_i \rangle = -\lambda_c \langle T_{,i} \rangle$ are always established, then the quantity $\lambda_c$ is termed the effective transverse thermal conductivity of an isotropic composite.

We use $\kappa_\alpha (\alpha = \overline{1, N})$ to designate the coefficients of the phases in the direction perpendicular to the plane of isotropy. Then the effective longitudinal thermal conductivity of the composite $\chi_c$ is found from the familiar formula [1]

$$\varkappa_c = \sum_\alpha v_\alpha \varkappa_\alpha.$$

Here and below, the letters under the summation sign run through integers from 1 to N.

We are left with the problem of determining $\lambda_c$. Existing mathematical methods of finding effective thermal conductivity and the results that are obtained are well documented in

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[1-7]. In these studies, the variational approach [3, 4] was developed to obtain estimates of $\lambda_c$. The investigators constructed general estimates that depend on the coefficients characterizing the phase geometry of the composite. Obtained in particular from these coefficients were the Hashin–Shtrikman estimates for the general case. Explicit values of $\lambda_c$ were obtained for N-phase composites with fibers of circular cross section.

2. Derivation of Estimates. If we assign the heat flux

$$Q_i n_i|_{\partial V} = Q_i^0 n_i, \quad Q_i^0 = \text{const}, \tag{3}$$

at the boundary of the representative element, then the field T satisfying Eq. (1) and boundary condition (3) is the solution of the following variational problem:

$$\underline{I} = \inf_T I(T), \quad I = \int_V \left( \frac{\lambda}{2} T_{,i} + Q_i^0 T_{,i} \right) d^2x. \tag{4}$$

Convoluting (3) with $x_k$ and integrating over $\partial V$, we obtain $\langle Q_k \rangle = Q_k^0$. It follows from (2) and (4) that

$$\underline{I} = -\frac{Q_i^0 Q_i^0}{2\lambda_c}. \tag{5}$$

We introduce a certain positive number $\lambda_0$ and construct a new functional

$$I_q = \int_V \left[ \frac{\lambda_0}{2} T_{,i} T_{,i} + (q_i + Q_i^0) T_{,i} \right] d^2x - \Phi(q) + U(T), \tag{6}$$

where

$$\Phi(q) = \frac{1}{2} \sum_\alpha v_\alpha \frac{q_i^\alpha q_i^\alpha}{\lambda_\alpha - \lambda_0}, \quad q_i = q_i^\alpha = \text{const in } V_\alpha;$$

$$U(T) = \frac{1}{2} \sum_\alpha (\lambda_\alpha - \lambda_0) \int_{V_\alpha} (T_{,i} - \langle T_{,i} \rangle_\alpha)(T_{,i} - \langle T_{,i} \rangle_\alpha)\, d^2x.$$

The symbol $\langle \cdot \rangle$ denotes the average over $V_\alpha$:

$$\langle T_{,i} \rangle_\alpha = \frac{1}{v_\alpha} \int_{V_\alpha} T_{,i} d^2x.$$

If the following equalities exist:

$$q_i^\alpha = (\lambda_\alpha - \lambda_0) \langle T_{,i} \rangle_\alpha, \tag{7}$$

then it can be shown that $I_q = I$. We will examine the problem

$$\underline{I}_q = \inf_T I_q(T). \tag{8}$$

It is clear that $I \le I_q$ if (7) occurs at the point of the extremum of the function $I_q(T)$. The substitution of variables

$$T = -\frac{1}{\lambda_0} (Q_i^0 + \langle q_i \rangle) x_i + T', \quad q_i = \langle q_i \rangle + q_i' \tag{9}$$

transforms problem (8) to the form

$$\underline{I}_q = \inf_{T'} [J_V(T') + U(T')] - \Phi(q) - \frac{1}{2\lambda_0} (Q_i^0 + \langle q_i \rangle)(Q_i^0 + \langle q_i \rangle), \tag{10}$$

$$J_V(T') = \int_V \left( \frac{\lambda_0}{2} T'_{,i} T'_{,i} + q_i' T'_{,i} \right) d^2x.$$

We will examine the region of integration of the functional $J_V(T')$ for all spaces $R_2$ and we obtain the new functional

$$J_\infty(T') = \int_{\mathscr{R}_2} \left( \frac{\lambda_0}{2} T'_{,i} T'_{,i} + q_i' T'_{,i} \right) d^2x$$

with the restrictions

$$q_i' = 0 \text{ in } R_2 \setminus V, \quad T'_{,i} = O\left(\frac{1}{|\bar{x}|}\right) \text{ for } |\bar{x}| \to \infty, \tag{11}$$

where $\bar{x}$ is the position vector of the points; $|\bar{x}| = \sqrt{x_1^2 + x_2^2}$. It is evident that $J_V(T') \leq J_\infty(T')$. We seek the minimum of the functional

$$\underline{J}_\infty = \inf_{T' \in (11)} J_\infty(T').$$

Here, inf means that the lower bound of the functional $J_\infty$ must be sought among the functions T' that satisfy restriction (11). The Euler equation for T' is as follows:

$$(\lambda_0 T'_{,i} + q'_i)_{,i} = 0. \tag{12}$$

The solution of (12) with restrictions (11) has the form

$$T'(\bar{x}) = -\frac{1}{\lambda_0} \sum_\alpha q'^{\alpha}_m \varphi^{\alpha}_{,m}, \tag{13}$$

where $\phi_\alpha(\bar{x})$ is the attraction potential of masses filling $V_\alpha$ with a unit density:

$$\varphi^\alpha(\bar{x}) = \int_{V_\alpha} G d^2 y, \quad G = \frac{1}{2\pi} \ln |\bar{x} - \bar{y}|.$$

Here and below, we choose V to be a circle whose center coincides with the origin of coordinate system $\{x_i\}$. Since the phases are distributed uniformly and are isotropic in the representative element of the heterogeneous medium, then [2]

$$\langle \varphi^\alpha_{,mi} \rangle_\beta = \frac{1}{2} \delta_{im} \delta_{\alpha\beta}, \tag{14}$$

where $\delta_{im}$ is the Kronecker symbol. With allowance for the last equality and (13), we can calculate $\underline{J}_\infty$:

$$\underline{J}_\infty = \frac{1}{2} \int_V q_i T'_{,i} d^2 x = -\frac{1}{4\lambda_0} (\langle q_i q_i \rangle - \langle q_i \rangle \langle q_i \rangle).$$

Since $J_V(T') \leq J_\infty(T')$, substitution of $J_\infty(T')$ in place of $J_V(T')$ in (10) gives

$$\begin{aligned}
\underline{I}_q &\leqslant \inf_{T'} [J_\infty(T') + U(T')] - \Phi(q) - \frac{1}{2\lambda_0} (Q_i^0 + \langle q_i \rangle)(Q_i^0 + \langle q_i \rangle) \leqslant \\
&\leqslant \underline{J}_\infty + U_J(q) - \Phi(q) - \frac{1}{2\lambda_0} (Q_i^0 + \langle q_i \rangle)(Q_i^0 + \langle q_i \rangle) = \\
&= \Big[ -\frac{1}{4\lambda_0} (\langle q_i q_i \rangle - \langle q_i \rangle \langle q_i \rangle) - \Phi(q) - \\
&\quad - \frac{1}{2\lambda_0} (Q_i^0 + \langle q_i \rangle)(Q_i^0 + \langle q_i \rangle) \Big] + Q_J(q).
\end{aligned} \tag{15}$$

Here, $U_J(q)$ is the value of the functional U(T') at the extremum point of the functional $J_\infty(T')$.

Inequality (15) is satisfied for any value of $q_i$. We will examine values of $q_i$ which are stationary points of the quadratic form in the square brackets in (15):

$$\begin{aligned}
q_i^\alpha &= \frac{-Q_i^0}{(1 + M/2)[1/2 + \lambda_0/(\lambda_\alpha - \lambda_0)]}, \\
M &= M(\lambda_0) = \sum_\alpha \frac{v_\alpha}{1/2 + \lambda_0/(\lambda_\alpha - \lambda_0)}.
\end{aligned} \tag{16}$$

It is easily proven that (7) follows from (16), (14), (13), and (9). Thus, after substitution of (16) into (15), we obtain

$$\underline{I} \leqslant \underline{I}_q \leqslant \left( -\frac{1}{\lambda_0} + \frac{1}{\lambda_0} \frac{M}{1 + M/2} \right) \frac{Q_i^0 Q_i^0}{2} + U_J,$$

where

$$U_J = \frac{1}{2} \sum_\alpha (\lambda_\alpha - \lambda_0) \frac{Q_m^0 Q_n^0}{(1 + M/2)^2 \lambda_0^2} \varphi^\alpha_{mn};$$

$$\varphi^{\alpha}_{mn}\sum_{\beta,\gamma}\left(\frac{1}{\frac{1}{2}+\frac{\lambda_0}{\lambda_\beta-\lambda_0}}-M\right)\left(\frac{1}{\frac{1}{2}+\frac{\lambda_0}{\lambda_\gamma-\lambda_0}}-M\right)\times$$
$$\times\int_{V_\alpha}\left(\varphi^{\beta}_{,mi}\varphi^{\gamma}_{,mi}-\frac{v_\alpha}{2}\delta_{\alpha\beta}\delta_{\alpha\gamma}\right)d^2x.$$

The quantity $\phi^{\alpha}_{mn}$ is a symmetric tensor of the second order with respect to the indices m and n. By virtue of the uniform and isotropic distribution of the phases in the representative element, this tensor is also isotropic, i.e.,

$$\varphi^{\alpha}_{mn}=C_\alpha\delta_{mn},\quad C_\alpha=\text{const.}$$

It is easily shown that $C_\alpha = (1/2)\phi(\alpha/mm)$ and $C_\alpha \geq 0$. Summing the results obtained here, we arrive at the inequality

$$\lambda_c\leqslant\lambda_0\left[1-\frac{M}{1+M/2}-\frac{1}{(1+M/2)^2}\sum_\alpha\frac{\lambda_\alpha-\lambda_0}{\lambda_0}C_\alpha\right]^{-1},\tag{17}$$

$$C_\alpha=\sum_{\beta,\gamma}\left(\frac{1}{\frac{1}{2}+\frac{\lambda_0}{\lambda_\beta-\lambda_0}}-M\right)\left(\frac{1}{\frac{1}{2}+\frac{\lambda_0}{\lambda_\gamma-\lambda_0}}-M\right)\times$$
$$\times\left(C^{\beta\gamma}_\alpha-\frac{v_\alpha}{4}\delta_{\alpha\beta}\delta_{\alpha\gamma}\right),\quad C^{\beta\gamma}_\alpha=\frac{1}{2}\int_{V_\alpha}\varphi^{\beta}_{,ij}\varphi^{\gamma}_{,ij}d^2x.\tag{18}$$

We take $\lambda_0 > \lambda_\alpha$, $V_\alpha = \overline{1, N}$. Discarding the last term in the square brackets in (17) as a positive number (which thus strengthens the inequality) and making $\lambda_0$ approach max $\{\lambda_\alpha\}$, we obtain the Hashin–Shtrikman upper bound.

A refined estimate can be obtained if we know the values of $C^{\beta\gamma}_\alpha$, which are dependent on the phase geometry of the composite. We then choose $\lambda_0$ such that the last term in the square brackets in (17) vanishes:

$$\sum_\alpha(\lambda_\alpha-\lambda_0)C_\alpha=0.\tag{19}$$

Equations (17) and (19) give

$$\lambda_c\leqslant\lambda_0\left[1-\frac{M}{1+M/2}\right]^{-1}=\lambda_0\frac{2+M(\lambda_0)}{2-M(\lambda_0)}.\tag{20}$$

The process of deriving the lower bound is similar. If we replace conditions (3) by assigned boundary values of temperature

$$T|_{\partial V}=T^0_ix_i,\quad T^0_i=\text{const},\tag{21}$$

then the flux $Q_i$ becomes the solution of the following variational problem:

$$\underline{I}'=\inf_{Q_i\in(1)}\int_V\left(\frac{1}{2\lambda}Q_iQ_i+Q_iT^0_i\right)d^2x=-\frac{\lambda_c}{2}T^0_iT^0_i.$$

Using the method being proposed here, we arrive at the inequality

$$\lambda_c\geqslant\lambda_0'\left[1+\frac{M}{1-M/2}-\frac{\lambda_0'}{(1-M/2)^2}\sum_\alpha\left(\frac{1}{\lambda_\alpha}-\frac{1}{\lambda_0'}\right)C_\alpha\right],\tag{22}$$

where $M = M(\lambda_0')$ is determined from (16). We choose $\lambda_0'$ as the solution of the following equation:

$$\sum_\alpha\left(\frac{1}{\lambda_\alpha}-\frac{1}{\lambda_\alpha'}\right)C_\alpha=0,\tag{23}$$

and we obtain a simple expression for the lower bound

$$\lambda_c\geqslant\lambda_0'\frac{2+M(\lambda_0')}{2-M(\lambda_0')}.\tag{24}$$

3. Geometric Models. In order to obtain estimates (20), (24), it is necessary to determine $\lambda_0$ and $\lambda_0'$ from Eqs. (19) and (23). This is equivalent to calculating $C_\alpha^{\beta\gamma}$ from (18). We will examine an N-phase composite consisting of a continuous matrix and inclusions in the form of cylinders of circular cross section. Each cylinder is made of one material and is surrounded by a hollow cylinder made of the matrix material. The ratio of the volumes of the cylinders is constant. For greater clarity, first we choose a two-phase composite.

Let the composite consist of the matrix phase $V_M$ and the inclusion phase $V_I$, having thermal conductivities $\lambda_M$ and $\lambda_I$, respectively. Each circle $S_I$ belonging to $V_I$ is enclosed within a larger circle $S_M$, the region $S_M \backslash S_I$ of the latter circle being filled with the matrix material. We will construct a cartesian coordinate system $\{x_i'\}$ whose origin coincides with the center of circle $S_I$. Then we have the relation $x_i' = A_{ij}x_j$ + const. It is known from potential theory that

$$\int_{S_I} Gd^2y = \begin{cases} \dfrac{x_i' x_i'}{4} + \text{const in } S_I, \\ \dfrac{a^2}{2} \ln \sqrt{x_i' x_i'} + \text{const in } V \backslash S_I, \ a \text{ — is the radius of } S_I \end{cases} \tag{25}$$

$$\int_V Gd^2y = \frac{x_i x_i}{4} + \text{const in } V.$$

Since the phases are distributed uniformly in V and since the dimensions of the circles $S_I$ and $S_M$ are small compared to V, we can assume that

$$\int_{V_I \backslash S_I} Gd^2y = v_I \int_{V \backslash S_I} Gd^2y, \quad x_i \in S_I,$$
$$\int_{V_M \backslash S_M} Gd^2y = v_M \int_{V \backslash S_M} Gd^2y, \quad x_i \in S_M. \tag{26}$$

It can be deduced from potential theory that Eqs. (26) are exact for the polydisperse model [2]. In the more general case, they can be used as a first approximation. We can use (25-26) to calculate the potentials $\phi^I(\bar{x})$, $\phi^M(\bar{x})$ everywhere in V. For example, for $x_i \in S_I \subset V_I$

$$\varphi^I(\bar{x}) = \int_{V_I} Gd^2y = \int_{S_I} Gd^2y + \int_{V_I \backslash S_I} Gd^2y = \int_{S_I} Gd^2y + v_I \int_{V \backslash S_I} Gd^2y =$$

$$= \frac{x_i' x_i'}{4} + v_I\left(\frac{x_i x_i}{4} - \frac{x_i' x_i'}{4}\right) + \text{const},$$

$$\varphi^I_{,ij} = \frac{A_{ki}A_{kj}}{2} + v_I\left(\frac{\delta_{ij}}{2} - \frac{A_{ki}A_{kj}}{2}\right) = \frac{\delta_{ij}}{2} \quad (\text{Since } A_{ki}A_{kj} = \delta_{ij}),$$

$$C_I^{II} = \frac{1}{2}\int_{V_I} \varphi^I_{,ij}\varphi^I_{,ij} d^2x = \frac{1}{2}\sum_{S_I \subset V_I} \int_{S_I} \varphi^I_{,ij}\varphi^I_{,ij} d^2x = \frac{v_I}{4}. \tag{27}$$

Similarly, we obtain

$$C_I^{IM} = C_I^{MM} = 0, \quad C_M^{II} = -C_M^{IM}\frac{v_I v_M}{2}, \quad C_M^{MM} = \frac{v_M}{4} + \frac{v_I v_M}{2}. \tag{28}$$

It follows from (18), (19), (23), and (27-28) that $\lambda_0 = \lambda_0' = \lambda_M$. Thus, the lower and upper bounds of (20), (24) coincide:

$$\lambda_c = \lambda_M \frac{\lambda_I(1 + v_I) + \lambda_M v_M}{\lambda_I v_M + \lambda_M(1 + v_I)}.$$

Let us return to the general case of a N-phase matrix with circular fibers. Since the phases are distributed uniformly in V, analogously to (26) we taken the following equalities as a first approximation:

$$\int_{V_\alpha \backslash S} Gd^2y = v_\alpha \int_{V \backslash S} Gd^2y, \quad x_i \in S \subset V,$$

where S is any inclusion. The calculation gives $C_\alpha^{\beta\gamma} = \frac{v_\alpha}{4}\delta_{\alpha\beta}\delta_{\alpha\gamma}$, $\alpha = \overline{1, N-1}$; $\beta, \gamma = 1, N$ (where $V_N$ denotes the matrix phase with the thermal conductivity $\lambda_M$). It follows from (18), (19), (23) that $\lambda_0 = \lambda_0' = \lambda_M$. Thus, in this case as well we obtain

TABLE 1

| $\lambda_c$ | $v$ | | | | |
|---|---|---|---|---|---|
| | 0,1 | 0,3 | 0,5 | 0,7 | 0,9 |
| $\lambda^U$ | 8,487 | 6,058 | 4,194 | 2,717 | 1,518 |
| $\lambda_p^U$ | 7,182 | 5,001 | 3,659 | 2,535 | 1,499 |
| $\lambda_p^L$ | 6,669 | 3,945 | 2,733 | 1,999 | 1,392 |
| $\lambda^L$ | 6,586 | 3,681 | 2,385 | 1,651 | 1,178 |

$$\lambda_c = \lambda_M \frac{2 + M(\lambda_M)}{2 - M(\lambda_M)}.$$

Let us proceed to the case of a two-phase composite with lamellar fibers. Following the same reasoning as above, we obtain:

$$C_I^{II} = \frac{v_I}{4} + \frac{v_I v_M}{4}, \quad -C_I^{IM} = C_I^{MM} = \frac{v_I v_M^2}{4},$$

$$-C_M^{IM} = C_M^{II} = \frac{v_M v_I^2}{4}, \quad C_M^{MM} = \frac{v_M v_I^2}{4} + \frac{v_M}{4}, \quad \lambda_0 = \lambda_I v_M + \lambda_M v_I,$$

$$\lambda_0' = \frac{1}{v_M/\lambda_I + v_I/\lambda_M}, \quad \lambda_p^U \geqslant \lambda_c \geqslant \lambda_p^L,$$

$$\lambda_p^U = \lambda_0 \frac{2 + M(\lambda_0)}{2 - M(\lambda_0)}, \quad \lambda_p^L = \lambda_0' \frac{2 + M(\lambda_0')}{2 - M(\lambda_0')}.$$

Example. Let us examine a two-phase composite with $\lambda_1$ and $\lambda_2$ equal to 1 and 10. The results of calculation of the effective thermal conductivities are shown in Table 1, where $\lambda^L$, $\lambda^U$ are the lower and upper bounds of the Hashin–Shtrikman solution (they coincide with $\lambda_c$ for a polydisperse model, when the matrix has the lowest and highest values of $\lambda$, respectively); v is the volume fraction of the phase having the lowest $\lambda$.

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