The effect of heat source on upper and lower bounds of effective conductivity of anisotropic composites

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ABSTRACT: In the conventional bound theory for transport properties, including heat conductivity, the effect of a heat source has previously not been considered. However, heat sources play an important role in the thermal analysis of any, especially massive engineering structures. Wojnar [1998] defined artificial thermal and heat flux energy expressions, which are shown to be very useful in thermal analyses. Using these energy terms for composite materials with internal heat source, the bounds of the thermal conductivity tensor of two-phase or multi-phase non-homogeneous anisotropic materials are obtained. As a numerical example, the effect of a heat source described in terms of a polynomial in a spherical two-phase composite is studied in detail.

Keywords: Bounds, Heat source, Conductivity, Anisotropy, Thermal Energy

1. INTRODUCTION

The effective properties of a heterogeneous material are often considered as properties of an equivalent homogeneous solid, and there are several methods to describe the effective properties. Among them are the self-consistent method [Hershey; 1954, Hashin-Shtrikman, 1962a; Hill, 1965; Budiansky, 1965; Christensen, 1979; Christensen-Lo, 1979], differential scheme [McLaughlin, 1977; Abudi, 1991], and Mori-Tanaka's method [Mori-Tanaka, 1973; Benveniste, 1986 and 1987 and Abudi, 1991]. In these approaches the effective properties should lie between the bounds of the properties, which can be found by defining appropriate functions and considering special limiting cases related to the problem.

In linear elasticity theory, bounds on the moduli can be obtained by variational methods. To use this approach to obtain the bounds of effective property an appropriate function has to be defined. Also, one set of the appropriate functions is the expressions for potential and complementary energies. Using these energy expressions in the principles of minimum potential energy and minimum complementary energy, one can find the bounds for the strain energy and then the bounds for the elasticity tensor [Hashin, 1962].

Similarly, in the transport problems such as heat transfer, transfer of electricity, magnetic field transfer, and fluid flow processes, defining appropriate functions are useful for finding the bounds for heat and fluid flow conductivities, diffusivity, electric conductivity, dielectric constant, and magnetic permeability. Hashin and Shtrikman [1962a] extended a variational theorem formulated by Brown to find the bounds for magnetic permeability.

Following Gurtin [1972], Wojnar [1998] defined artificial thermal and heat flux energy measures. Then, by finding the bounds for the thermal and heat flux energy measures, he was able to validate the bounds for the effective conductivity of a heterogeneous material.

By generalizing Hashin-Shtrikman variational principle to the coupled problems of piezoelectricity, Hori and Nemat-Nasser [1998] found the upper and lower bounds for the effective moduli.

Recently, Eskandari-Ghadi, Xi and Sture [2003a] found a new bound on the elasticity tensor for the composite material, by modifying the bounds for strain energy for the case when a body force exists in the heterogeneous material.

To the best authors' knowledge, none of the above-mentioned work has considered the effect of heat source on the effective conductivity of composite materials. The effect of heat source on heat conduction is important in practical applications. For many engineering materials, such as concrete, the heat generated by the chemical reactions plays an important role in the performance of concrete structures. The heat of hydration due to the reaction between cement and water can increase the temperature within a concrete structure significantly, which could result in high concentration of thermal stress and severe fracture damage in the structure.

Similar to heat conduction, in the processes of mass transfer and ion penetration, such as moisture diffusion and chloride penetration in concrete, the moisture and chloride react with chemical components of cement and form non-soluble salts. The consumption of moisture and chloride in the reactions can be considered as a sink (a negative source). Therefore, it is also important to consider the effect of source on mass transfer and ion penetration, which are similar mathematically to the effect of heat source on conductivity.

It is the purpose of this paper to evaluate the effect of heat source on the effective heat conductivity. To achieve this goal, following Wojnar [1998], we modify the bounds for the artificial thermal energy and artificial thermal flux energy to consider the effect of heat source on the heterogeneous material. Using these modified artificial energies, the bounds for the effective conductivity are modified in order to consider the effect of heat source.

2. PROBLEM STATEMENT

We define the region (of a composite material) in Euclidian space $\mathscr{E}$ and denote it by B and its boundary by ∂B. The entire region and its boundary are denoted by $\overline{B}$. So, B, ∂B and $\overline{B} \subset \mathscr{E}$. The vector space associated with $\mathscr{E}$ is again described by $\mathscr{E}$. So, the points and vectors are in $\mathscr{E}$. In this paper, the vectors and second order tensors are shown by lower case bold letters and capital letters in bold, respectively. The scalar terms are described by either lower or capital italic letters.

We denote the temperature variation from a reference temperature as θ and its gradient, $\nabla\theta$, as $\boldsymbol{\eta}$:

$$\boldsymbol{\eta} = \nabla\theta \tag{1}$$

Thus, $\boldsymbol{\eta}$ is a vector. Using (1) Fourier's law takes the following form:

$$\mathbf{q} = -\mathbf{K}\boldsymbol{\eta} \tag{2}$$

Where $\mathbf{q}$ is the heat flux and $\mathbf{K}$ is the thermal conductivity tensor. $\mathbf{K}$ is symmetric and positive definite tensor. Since $\mathbf{K}$ is positive definite, its eigenvalues are positive, and thus it is invertible. We denote its inverse tensor by $\mathbf{R}$, which is the thermal resistivity tensor, and which clearly is a symmetric and positive definite tensor. If the heat source is described by r_θ, then the stationary heat conduction equation (equilibrium heat equation, takes the form:

$$\operatorname{div}\mathbf{q} + r_\theta = 0 \tag{3}$$

We divide the boundary of B into two parts in such a way $\partial B = \partial_1 B \bigcup \partial_2 B$ and $\phi = \partial_1 B \bigcap \partial_2 B$, where ϕ is the empty set. Here $\partial_1 B$ and $\partial_2 B$ are respectively the parts of ∂B, where the temperature and heat flux are known:

$$\theta = \hat{\theta} \qquad \text{on } \partial_1 B \tag{4}$$

$$\mathbf{q}\,.\,\mathbf{n} = \hat{q}_n \qquad \text{on } \partial_2 B \tag{5}$$

Here $\hat{\theta}$ and $\hat{q}_n$ are prescribed functions. $\mathbf{n}$ is the unit vector normal to ∂B. The ordered pair $(r_\theta, \hat{q}_n)$ is describes by the external thermal load.

If $\partial_2 B$ is empty, then the boundary value problem (1) to (4) is the 1st type or temperature boundary value problem (TBVP). If $\partial_1 B$ is empty, then the boundary value problem (1), (2), (3) and (5) is the 2nd type or flux boundary value problem (FBVP). If neither $\partial_1 B$ nor $\partial_2 B$ is empty, then the boundary value problem (1) to (5) is a mixed boundary value problem (MBVP).

Definitions:

The scalar field θ is said to be an *admissible temperature field* within $\overline{B}$ provided θ is of class C^2 on B and θ and $\nabla\theta$ are continuous within $\overline{B}$. Similarly, the vector field $\mathbf{q}$ is an *admissible flux field* in $\overline{B}$ if $\mathbf{q}$ is of class C^1 within B, and $\mathbf{q}$ and div $\mathbf{q}$ are continuous within $\overline{B}$. $\boldsymbol{\eta}$ is an *admissible temperature gradient,* if it is continuous within $\overline{B}$. The ordered triple $s = (\theta, \boldsymbol{\eta}, \mathbf{q})$ is named by *admissible thermal state* provided θ, $\boldsymbol{\eta}$ and $\mathbf{q}$ are admissible functions. So, in an admissible thermal state there is not a necessary relationship between θ, $\boldsymbol{\eta}$ and $\mathbf{q}$. The admissible thermal state is related to the system $(r_\theta, \hat{q}_n)$ provided equations (1), (2) and (3) are satisfied. In this case, we say $s = (\theta, \boldsymbol{\eta}, \mathbf{q})$ is an *admissible thermal state corresponding to* $(r_\theta, \hat{q}_n)$ or simply *thermal state*.

An admissible thermal state is a *kinematically admissible thermal state,* if equations (1) and (2) are satisfied and θ satisfies the thermal boundary condition (4). We say $\mathbf{q}$ is a *stationary admissible heat flux,* if it satisfies the stationary heat conduction equation and the flux boundary condition (5). An admissible thermal state, $s=(\theta,\boldsymbol{\eta},\mathbf{q})$ is a *stationary admissible thermal state*, if $\mathbf{q}$ is a stationary admissible heat flux. It is clear that if a state is both kinematically and stationary admissible thermal state then it is the solution of MBVP. We state that two states $s=(\theta,\boldsymbol{\eta},\mathbf{q})$ and $s'=(\theta',\boldsymbol{\eta}',\mathbf{q}')$ are equal modulo a constant temperature, if

$$(\theta,\boldsymbol{\eta},\mathbf{q})=(\theta'+\theta_0,\boldsymbol{\eta}',\mathbf{q}') \tag{6}$$

Where θ_0 is constant.

After Wojnar[1], we say $U_k(\boldsymbol{\eta})$ is an *artificial thermal energy* corresponding to an admissible temperature gradient field $\boldsymbol{\eta}$ on B if:

$$U_{\mathbf{K}}(\boldsymbol{\eta})=\frac{1}{2}\int_B \boldsymbol{\eta}\,.\,\mathbf{K}\boldsymbol{\eta}\,dV \tag{7}$$

The *artificial heat flux energy* is defined as:

$$U_{\mathbf{R}}(\mathbf{q})=\frac{1}{2}\int_B \mathbf{q}\,.\,\mathbf{R}\,\mathbf{q}\,dV \tag{8}$$

Where $\boldsymbol{.}$ denotes the usual inner product of vectors.

3. BOUNDS FOR ENERGIES

By the above mentioned definitions and the theorems appeared in Wojnar [1998], the following theorem is readily proved [Eskandari-Ghadi, Xi & Sture, 2003b]:

Theorem (Upper and Lower bounds for the artificial thermal energy): Let U_1 be the artificial thermal energy corresponding to TBVP. Then

$$-U_{\mathbf{R}}(\mathbf{q}')-\int_B \theta\, r_\theta\, dV-\int_{\partial B}\hat{\theta}\, q'_n\, dA \le U_1 \le U_{\mathbf{K}}(\tilde{\boldsymbol{\eta}})+\int_B r_\theta(\tilde{\theta}-\theta)\,dV \tag{9}$$

Where $\tilde{\theta}$ is a thermally admissible temperature and $\tilde{\boldsymbol{\eta}}$ is the related field. $\mathbf{q}'$ is a stationary admissible heat flux field and $q'_n=\mathbf{q}'.\mathbf{n}$ is the corresponding heat flux in the $\mathbf{n}$ direction.

[1] Wojnar denoted $U_{\mathbf{K}}(\boldsymbol{\eta})$ as the thermal energy and he, showed the unit of this function is WK rather than J.

4. BOUNDS FOR EFFECTIVE CONDUCTIVITY

In this section, the previous bounds for conductivity are modified to consider the effect of a heat source. To do this, we start by defining the mean values of flux and the gradient of temperature as

$$\overline{\mathbf{q}}=\frac{1}{V}\int_B \mathbf{q}\,dV \tag{10}$$

$$\overline{\boldsymbol{\eta}}=\frac{1}{V}\int_B \boldsymbol{\eta}\,dV \tag{11}$$

The effective conductivity for these two terms is defined by

$$\frac{1}{V}\int_B \boldsymbol{\eta}\,.\,\mathbf{K}\,\boldsymbol{\eta}\,dV=\overline{\boldsymbol{\eta}}\,.\,\mathbf{K}^{(e)}\,\overline{\boldsymbol{\eta}} \tag{12}$$

We show the effective resistivity by $\mathbf{R}^{(e)}$:

$$\frac{1}{V}\int_B \mathbf{q}\,.\,\mathbf{R}\,\mathbf{q}\,dV=\overline{\mathbf{q}}\,.\,\mathbf{R}^{(e)}\,\overline{\mathbf{q}} \tag{13}$$

Using (12) and (13), one can write

$$U_{\mathbf{K}}=\frac{1}{2}\int_B \boldsymbol{\eta}\,.\,\mathbf{K}\,\boldsymbol{\eta}\,dV=\frac{1}{2}V\,\overline{\boldsymbol{\eta}}\,.\,\mathbf{K}^{(e)}\,\overline{\boldsymbol{\eta}} \tag{14}$$

$$U_{\mathbf{R}}=\frac{1}{2}\int_B \mathbf{q}\,.\,\mathbf{R}\,\mathbf{q}\,dV=\frac{1}{2}V\,\overline{\mathbf{q}}\,.\,\mathbf{R}^{(e)}\,\overline{\mathbf{q}} \tag{15}$$

On the other hand, by using the above-mentioned theorem and theorems in [Eskandari-Ghadi, Xi & Sture, 2003b], we can develop the inequalities

$$U_1 \le U_k(\tilde{\boldsymbol{\eta}})+\int_B r_\theta(\tilde{\theta}-\theta)\,dV \tag{16}$$

$$U_2 \le U_R(\mathbf{q}') \tag{17}$$

where $\tilde{\theta}$ is an admissible temperature and $\tilde{\boldsymbol{\eta}}$ is its gradient. $\mathbf{q}'$ is a stationary admissible heat flux. So, if we identify $\tilde{\boldsymbol{\eta}}$ with $\overline{\boldsymbol{\eta}}$ and $\mathbf{q}'$ with $\overline{\mathbf{q}}$, then (16) and (17) imply

$$\frac{1}{2}V\,\overline{\boldsymbol{\eta}}\,.\,\mathbf{K}^{(e)}\,\overline{\boldsymbol{\eta}} \le \frac{1}{2}\overline{\boldsymbol{\eta}}\,.\left(\int_B \mathbf{K}\,dV\right)\overline{\boldsymbol{\eta}}+\int_B r_\theta(\overline{\theta}-\theta)\,dV \tag{18}$$

$$V\,\overline{\mathbf{q}}\,.\,\mathbf{R}^{(e)}\,\overline{\mathbf{q}}=\overline{\mathbf{q}}\,.\left(\int_B \mathbf{R}\;\; dV\right)\overline{\mathbf{q}} \tag{19}$$

Of course, in inequality (18), $\overline{\theta}$ is the average of θ. Equation (18) shows that the upper bound for the effective conductivity tensor, $\mathbf{K}^{(e)}$, which may be anisotropic, depends on the conductivity at each point of the material and heat source.

Assuming that the material is non-homogeneous but isotropic, we reach

$$\mathbf{K} = K\,\mathbf{I}, \qquad \mathbf{K}^{(e)} = K^{(e)}\,\mathbf{I} \tag{20}$$

$$\mathbf{R} = R\,\mathbf{I}, \qquad \mathbf{R}^{(e)} = R^{(e)}\,\mathbf{I} \tag{21}$$

Then, by defining $\bar{\eta}^2 = \boldsymbol{\eta}.\boldsymbol{\eta}$, from (18)

$$K^{(e)} \le \frac{1}{V}\left(\int_B K\,dV\right) + \frac{2}{V\bar{\eta}^2}\int_B r_\theta(\bar{\theta}-\theta)\,dV \tag{22}$$

And from (19)

$$R^e \le \frac{1}{V}\left(\int_B \mathbf{R}\,dV\right) \tag{23}$$

Considering K as the inverse of R, inequalities (22) and (23) are combined as

$$\begin{aligned}\left(\frac{1}{V}\int_B \frac{1}{K}\,dV\right)^{-1} &\le K^{(e)} \\ &\le \frac{1}{V}\left(\int_B K\,dV\right) + \frac{2}{V\bar{\eta}^2}\int_B r_\theta(\bar{\theta}-\theta)\,dV\end{aligned} \tag{24}$$

These derivations provide general theories for upper and lower bounds of effective conductivity of composite materials.

5. ANALYSIS

In this section, we provide an example to examine the effects of heat source on the bounds of effective conductivity of a composite comprising of to isotropic phases. This example shows useful results on basic trends of the bounds when heat source varies in the composite materials.

We consider B as a spherical domain containing two different phases (Fig. 1). Phase 1 is a sphere of inner radius a and outer radius b, and Phase 2 is a sphere of radius a, which is inside Phase 1. The conductivities of Phase 1 and Phase 2 are $K^{(1)}$ and $K^{(2)}$, respectively. The heat sources are assumed as $r_\theta^{(1)} = \delta^{(1)}(r/a)^n$ and $r_\theta^{(2)} = \delta^{(2)}(r/a)^n$ in each phase, where n is a non-negative real number; $\delta^{(1)}$ and $\delta^{(2)}$ are constants representing the magnitudes of the heat source of Phase 1 and Phase 2; and r is the spherical radial coordinate. In these circumstances, the stationary heat conduction equation takes the form

$$\nabla^2\theta^{(i)} = -\frac{\delta^{(i)}}{K^{(i)}}(r/a)^n, \quad (i = 1, 2) \tag{25}$$

Considering spherical symmetry, the total solution of this equation is

$$\theta^{(i)}(r) = \frac{A^{(i)}}{r} + B^{(i)} + \frac{\delta^{(i)}}{K^{(i)}}\frac{r^n}{a^n}\frac{r^2}{(n+2)(n+3)}, \quad (i = 1, 2) \tag{26}$$

Where $A^{(i)}$ and $B^{(i)}$ are constants. Regarding the limiting value for temperature at r = 0, $A^{(2)}$ vanishes. The remaining constants are determined by satisfying the continuity conditions at $r = a$ and the boundary condition at $r = b$. We consider the following boundary condition:

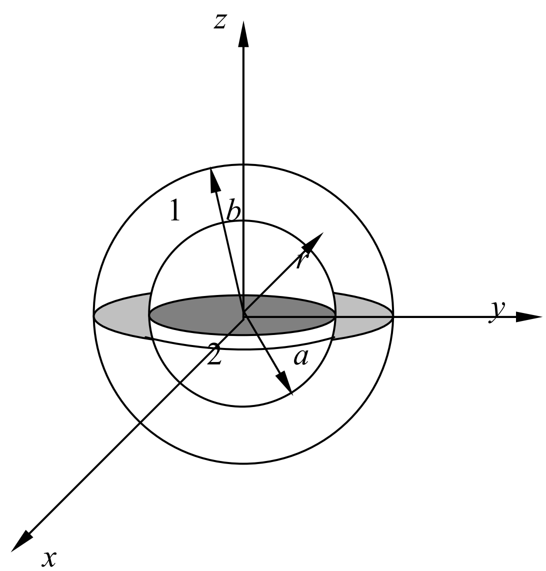

Fig. 1 A spherical composite element contains an inclusion of radios a and thermal conductivity $K^{(1)}$, and a matrix of inner radios a and outer radios b with conductivity $K^{(2)}$

$$\theta^{(1)} = 0 \qquad \text{at } r = b \tag{27}$$

In this way, we obtain

$$A^{(1)} = \frac{\delta^{(1)} - \delta^{(2)}}{K^{(1)}}\frac{a^3}{n+3} \tag{28}$$

$$B^{(1)} = -\frac{\delta^{(1)}}{K^{(1)}}\frac{b^n}{a^n}\frac{b^2}{(n+2)(n+3)} - \frac{\delta^{(1)} - \delta^{(2)}}{K^{(1)}}\frac{1}{n+3}\frac{a^3}{b} \tag{29}$$

$$\begin{aligned}B^{(2)} = &\frac{\delta^{(1)} - \delta^{(2)}}{K^{(1)}}\frac{a^2}{n+3}\left(1-\frac{a}{b}\right) \\ &+ \frac{\delta^{(1)}}{K^{(1)}}\frac{a^2 - (b/a)^n b^2}{(n+2)(n+3)} - \frac{\delta^{(2)}}{K^{(2)}}\frac{a^2}{(n+2)(n+3)}\end{aligned} \tag{30}$$

Substituting $A^{(1)}, B^{(1)}$ and $B^{(2)}$ from (28) to (30) into (26) gives the temperature in each phase.

Then, the mean value of the temperature (volumetric average) is

$$\bar{\theta} = \frac{3}{b^3}\left[\frac{1}{3}(B^{(2)} - B^{(1)})a^3 + \frac{1}{3}B^{(1)}b^3 + \frac{1}{2}A^{(1)}(b^2 - a^2) + \frac{1}{(n+2)(n+3)(n+5)}\right.$$
$$\left.[\frac{\delta^{(2)}}{K^{(2)}}a^5 + \frac{\delta^{(1)}}{K^{(1)}}\frac{b^{n+5} - a^{n+5}}{a^n}]\right] \qquad (31)$$

Substituting the heat sources, temperatures from (26), $\bar{\theta}$ from (31), the upper bound of the effective conductivity is

$$\frac{K_u^{(e)}}{K^{(1)}} = c_1 + c_2\frac{K^{(2)}}{K^{(1)}} + \frac{6}{b^3\,\bar{\eta}^2 K^{(1)}}\left[\int_0^a r_\theta^{(2)}(\theta^{(2)} - \bar{\theta})r^2dr + \int_a^b r_\theta^{(1)}(\theta^{(1)} - \bar{\theta})r^2dr\right] \qquad (32)$$

where

$$\bar{\eta} = \frac{3}{b^3}\left[-A^{(1)}(b-a) + \frac{1}{(n+3)(n+4)}[\frac{\delta^{(2)}}{K^{(2)}}a^4 + \frac{\delta^{(1)}}{K^{(1)}}\frac{b^{n+4} - a^{n+4}}{a^n}]\right] \qquad (33)$$

Based on equation (32), a numerical evaluation of $K_u^{(e)}/K^{(1)}$ is obtained. Table (1) shows a comparison between the Voigt model and the present study, when $K^{(1)}/K^{(2)} = 10$, n = 0, $\delta^{(1)} = 1.0$ and $\delta^{(2)} = 1.0$. It is observed that within the selected accuracy both bounds coincide, which means that based on this example, for a constant heat source the bound obtained in this study is exactly the same as the Voigt bound.

Table 1 Comparison of the upper bound for effective conductivity based on Voigt model and the present study when n = 0, $\delta^{(1)} = 1.0$ and $\delta^{(2)} = 1.0$

c_2	Upper bound for conductivity due to present study when n = 0, $\delta^{(1)} = 1.0$ and $\delta^{(2)} = 1.0$	Upper bound for conductivity based on Voigt (parallel) model
0.00000	1.00000	1.00000
0.00241	0.99783	0.99783
0.01680	0.98489	0.98488
0.05403	0.95138	0.95137
0.12500	0.88750	0.88750
0.24059	0.78347	0.78347
0.41167	0.62950	0.62950
0.64913	0.41578	0.41578
0.96386	0.13253	0.13253

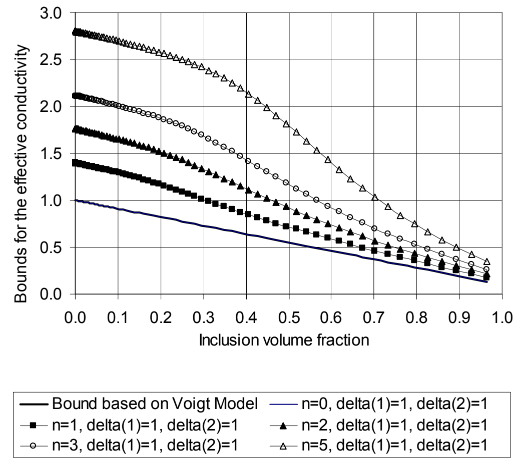

Fig. 2 Bounds for effective conductivity with the effect of heat source for $n = 0$ and different values $\delta^{(1)}$ and $\delta^{(2)}$, when $K^{(1)}/K^{(2)} = 10$.

Fig. (2) shows the upper bounds of effective conductivity for different values of $\delta^{(1)}$ and $\delta^{(2)}$ with n = 0. In these cases, the heat sources are constants (n = 0), but different constants within Phase 1 and Phase 2. One can see that, at a fixed volume fraction of Phase 2, the upper bound of effective conductivity decreases with increasing $\delta^{(2)}$, if $\delta^{(1)}$ is held constant, and the upper bound increases with increasing $\delta^{(1)}$, if $\delta^{(2)}$ is held constant. In another words, the upper bound of the effective conductivity is a function of the ratio of the heat sources, $\delta^{(1)}/\delta^{(2)}$ in constituent phases. It increases if this ratio increases and it decreases if the ratio $\delta^{(1)}/\delta^{(2)}$ decreases.

Fig. (3) shows the upper bounds of the effective conductivity for different values of n with $\delta^{(1)} = \delta^{(2)}$. One can see that the upper bound increases when n increases.

6. CONCLUSIONS

1. Using the principle of minimum artificial potential energy and complementary energy defined by Wojnar [1998], the bounds for effective conductivity were modified to consider the effect of a heat source.

2. Within the framework of this article, the heat source does not have any effect on the lower bound for effective thermal conductivity. The heat source affects only the upper bound.

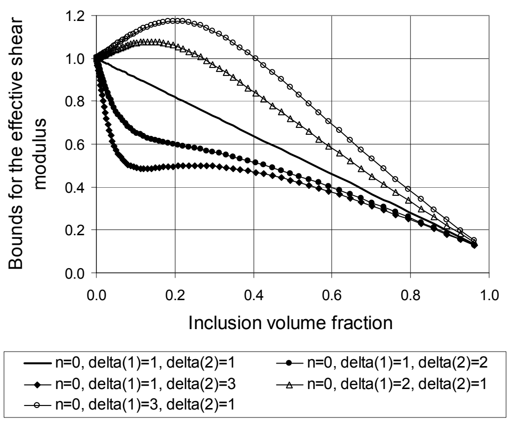

Fig. 3 Bounds for effective conductivity with the effect of heat source for different values of n, when $\delta^{(1)} = \delta^{(2)} = 1$ and $K^{(1)}/K^{(2)} = 10$.

3. A polynomial-described heat source was used as a numerical example. The upper bound of the effective conductivity with heat source is usually above the Voigt bound, if the coefficients of the heat source in the inclusion (phase 2) and matrix (phase 1) are the same; while its lower bound does not change. But, when the heat source in the inclusion (phase 2) is higher than the heat source in the matrix, the upper bound could be significantly below the Voigt bound.
4. The results for the effect of heat source on conductivity of composites can also be used for evaluating the effect of source (and sink) on effective permeability and diffusivity of composites.

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