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SUMMARY

The effective thermal conductivity k_E of an isotropic composite material is ill-defined unless the geometric arrangement of the phases is sufficiently well specified. Nevertheless, Hashin and Shtrikman have obtained rigorous bounds of practical use provided the component conductivities are sufficiently close. For a two-component system, these bounds are the familiar Maxwell formulae. Effective medium theory gives an estimate of effective conductivity ignoring connectedness; it is the formula of Bruggeman. This appears to provide a further bound for characterising debris beds.

INTRODUCTION

Some of the more commonly used formulae for the effective thermal conductivity of composite materials are referred to in [1] or [2] which provides a comparison with a range of experimental data from many different sources. The often implicit assumption of such semi-empirical formulae is that for a random mixture of materials, there exists an effective thermal conductivity, independent of the details of the material arrangement. We believe that this idea is mistaken; the geometric arrangement of the materials is almost always important. However limiting upper and lower bounds can be specified which can be quite close together. In some circumstances "effective medium theory" can provide a useful estimate. It seems that this approach is relevant to debris beds with an extended spectrum of particle sizes resulting from fragmentation. Since convection and radiation are ignored here, the components of the composite need not be solid; some can be in a (stagnant) fluid state.

UPPER AND LOWER BOUNDS

It is well known that the effective conductivity of composite material must lie between the classical bounds:

$$\langle k \rangle \geq k_E \geq \langle k^{-1} \rangle^{-1} \qquad (1)$$

where $\langle X \rangle$ denotes the average of X. If the only information available about the composite is the volume fraction of the phases, then (1) is the best possible result, for each of the two bounds can clearly be attained; they correspond to the familiar "in-parallel" and "in-series" arrangement of the material.

If it is also known that the composite is randomly arranged and macroscopically isotropic, more restrictive bounds can be obtained. In this

case, Hashin and Shtrikman [3] have shown that

$$k_L + \left\{B/(1-B/3k_L)\right\} \leq k_E \leq k_u + \left\{A/(1-A/3k_u)\right\} \tag{2}$$

where k_u and k_L are the conductivities of the most and least conductive phase respectively and

$$A \equiv \left\langle \left[1/(k(\underline{r}) - k_u) + 1/3k_u\right]^{-1} \right\rangle \tag{3}$$

$$B \equiv \left\langle \left[1/(k(\underline{r}) - k_L) + 1/3k_L\right]^{-1} \right\rangle \tag{4}$$

For the derivation, see the original paper or the clear account by Beran [4], alternatively see [5].

For a two-phase system, a well-known formula (k_{M1}) was obtained by Maxwell [6], applicable when the porosity ε is close to unity. This can be written

$$1/(k_{M1}+2k_1) = \varepsilon/(k_1 + 2k_1) + (1 - \varepsilon)/(k_2 + 2k_1) \tag{5}$$

The dual Maxwell formula (k_{M2}), appropriate when ε is small, is

$$1/(k_{M2} + 2k_2) = \varepsilon/(k_1 + 2k_2) + (1 - \varepsilon)/(k_2 + 2k_2) \tag{6}$$

The Hashin-Shtrikman (H-S) bounds for a two-phase system are *precisely* these well-known Maxwell formulae applied to the whole range of porosity $0 < \varepsilon < 1$. Specifically,

$$k_{M1} \leq k_E \leq k_{M2} \text{ if } k_2 > k_1 \tag{7}$$

$$k_{M2} \leq k_E \leq k_{M1} \text{ if } k_1 > k_2 \tag{8}$$

These bounds are closer than the classical bounds and are the best possible bounds for a two-phase system if no geometric information other than randomness and isotropy is available, as was shown by Hashin and Shtrikman using a simple constructive algorithm. This exemplifies the general principle stressed by Beran [4] and Ziman [7] that the macroscopic properties of a composite can be extremely sensitive to the geometry and topology of the boundary surfaces between the phases. A measure of the usefulness of these bounds is their separation. If Δk_c and Δk_m denote the difference between the classical bounds and between the H-S bounds, evaluated at $\varepsilon = \frac{1}{2}$, then for

$k_1 = 2k_2$,	$\Delta k_c = 0.166(k_1-k_2)$	$\Delta k_M = 0.026(k_1-k_2)$
$= 9k_2$	$= 0.400(k_1-k_2)$	$= 0.199(k_1-k_2)$

It follows that for $k_1/k_2 < 2$ the classical bounds are adequate for

practical purposes, and the H-S bounds similarly for $k_1/k_2 \lesssim 10$ (and correspondingly for $k_1 > k_2$).

EFFECTIVE MEDIUM THEORY

When some of the constituent thermal conductivities differ by more than an order of magnitude, the H-S bounds are sufficiently far apart for a better estimate of k_E to be required. This is only possible if additional geometric information is used.

If k_c is the conductivity of the continuous phase, then in general,

$$k_E = k_c - \sum \varepsilon_i (k_c - k_i) \lambda_i, \qquad (9)$$

where ε_i and k_i are the volume fraction and conductivity of the ith particulate phase and λ_i is the ratio of the mean temperature gradient in the i^{th} phase to the mean overall temperature gradient.

We seek a formula appropriate for a debris bed which has a wide spectrum of particle sizes, such as the log-normal distribution predicted by Kolmogorov [8] in 1941 for fragmented debris. For such a size distribution we argue that λ_i can be usefully approximated by considering single spheres of particulate in a uniform medium with smeared conductivity k_E. This leads to

$$\lambda_i = 3k_E/(2k_E + k_i) \qquad (10)$$

One would expect this approximation to be better for a wide spectrum of particle sizes than for roughly equally sized particles: for in the former case a particle of any scale other than the smallest will be in contact with many others and will perceive a much more uniform immediate environment.

Equations (9) and (10) can be combined to give

$$\frac{1}{k_E+2k_E} = \frac{\varepsilon_c}{k_c+2k_E} + \sum \frac{\varepsilon_i}{k_i+2k_E}, \qquad (11)$$

which has the same structure as the 'in-series' classical formula, but with each k augmented by an effective medium contribution (cf.eqs.(5)& (6). This formula is equivalent to the theory of Bruggeman [9] which implies an additional approximation of the form (10) for the continuous phase. Thus all phases are treated equally and the connectedness of the continuous phase ignored. This is plausibly so in a debris bed with a broad spectrum of particle sizes, because the filling of the necks with smaller particles drastically reduces the significance of the connectedness. Below we denote the Bruggeman estimate by k_B. It roughly bisects the region between the HS bounds. For real debris beds

the difference in thermal resistance between necks in the continuous phase and particle contacts introduces an asymmetry between the phases. Hence we expect for two components that if $k_p < k_c$, then $k_B \leq k_E \leq k_{M1}$; whereas if $k_p > k_c$, then $k_B \geq k_E \geq k_{M1}$.

ILLUSTRATIVE CALCULATIONS

We begin with a three-phase example. Consider a bed composed of UO_2($k=k_c/20$) and steel ($k=k_c/3$) particles in a liquid sodium matrix ($k=k_c$). For simplicity let the volume fractions be equal i.e. $\varepsilon_i=1/3=\varepsilon_c$. Then the classical bounds are $0.46 > k_E/k_c > 0.17$; the H-S bounds are $0.4 > k_E/k_c > 0.22$; the Bruggeman formula gives $k_B/k_c = 0.29$. This formula applies for an unstratified, random isotropic bed with a wide particle spectrum.

Figures 1 to 4 show some illustrative examples for two-phase systems. For fig.1, $k_p/k_c=6$, illustrative of UO_2 and water; for fig.2, $k_p/k_c=1/7$, illustrative of a UO_2/stainless steel cermet. In cases such as these the HS bounds are so close together that it is unlikely that they could be reliably improved upon. Fig.3 shows the case $k_p/k_c=40$, illustrative of UO_2 and sodium vapour; in Fig.4, $k_p/k_c=1/20$, illustrative of UO_2 and liquid sodium. Note that the Bruggeman estimate asymptotes at large and small porosity to the Maxwell formulae, appropriate on physical grounds.

DISCUSSION

For isotropic media, equation (9) is valid and the differences in the many formulae in the literature depend on the choice made for λ_i. However, the H-S bounds do apply and any formula which fails to fall between these bounds must be rejected.

The Kampf and Karsten (KK) formula [10] is widely used in debris bed studies (e.g.[11]), and is based on a semi-empirical rectangular series-parallel model. If the particulate phase is more conductive, then the KK formula falls outside the HS bounds and so is inappropriate (see Fig.3). Secondly, when very little porosity is present the KK formula is erroneous; it tends to the wrong Maxwell bound.(See Fig.4). For a highly conducting coolant, KK falls slightly below the upper H-S bound and is quite close for $0.3 < \varepsilon < 0.7$; it should not be used where it falls below k_B.

The Schulz estimate [12] for spherical particles approximates to the Bruggeman formula for high porosities; it always satisfies the H-S bounds and lies on the expected side of k_B. It is a more robust formula

than KK.

This paper has been concerned with isotropic media, but the approaches considered here are capable of generalisation to allow for anisotropy, such as channelled beds.

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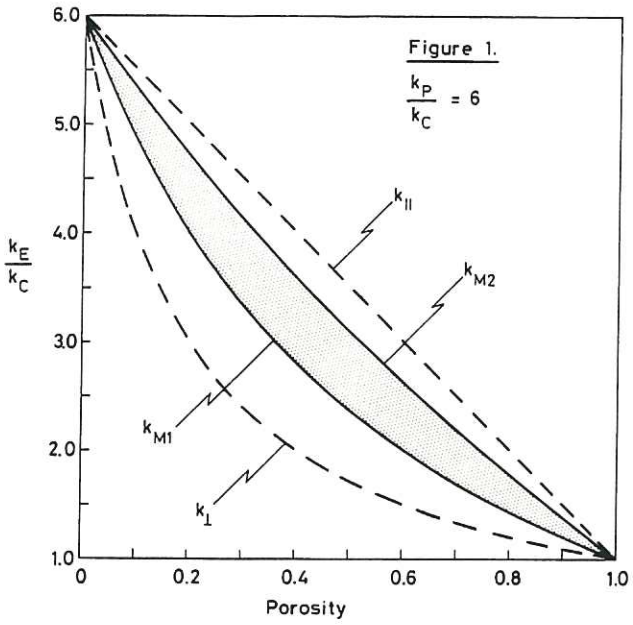

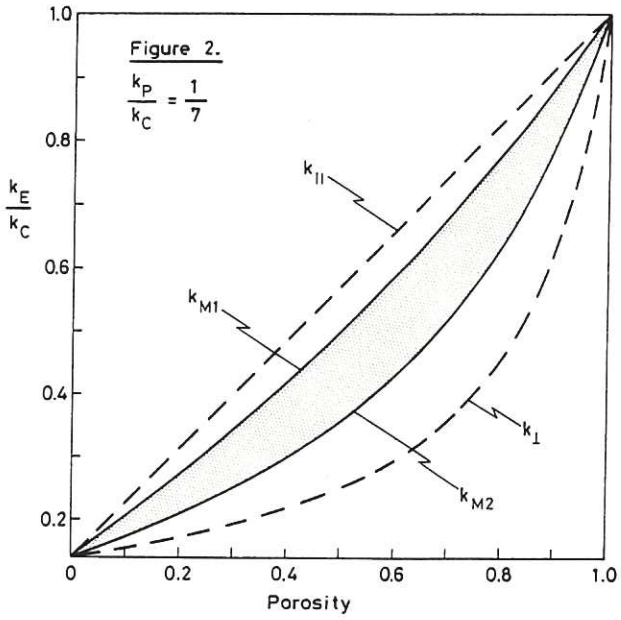

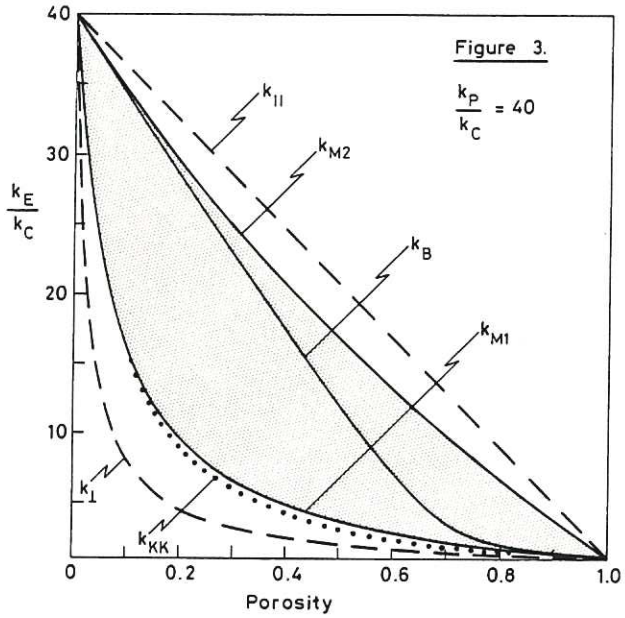

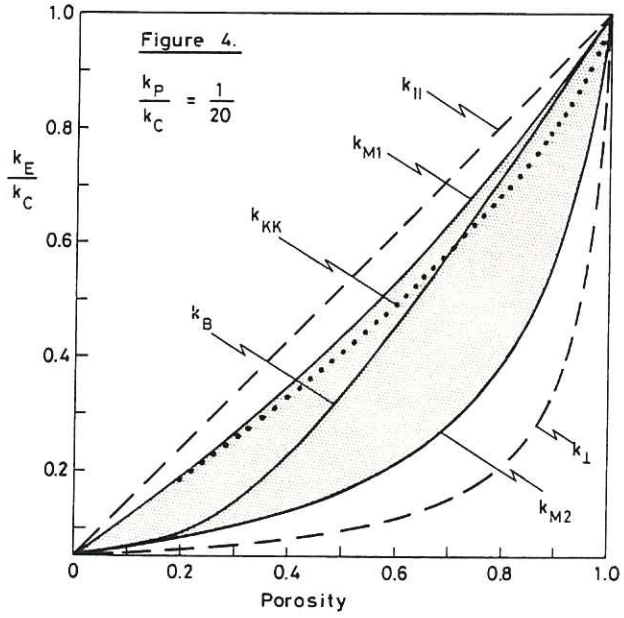

Key to figures:

k_{II} : Classical upper bound, eq.(1).
$k_\perp$: Classical lower bound, eq.(2).
k_{M1} : Maxwell formula, eq.(5).
k_{M2} : Dual Maxwell formula, eq.(6).
k_B : Bruggeman formula, Eq.(11).
k_{KK} : Kampf-Karsten formula, ref.[10].
k_E : Effective thermal conductivity.
k_p : Thermal conductivity of particles.
k_c : Thermal conductivity of continuous phase.
Porosity: Volume fraction of continuous phase.

H–S bounds