Pramāṇa, Vol. 22, No. 1, January 1984, pp. 63–70, © Printed in India.

Thermal conduction in a homogeneous two-phase system

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MS received 14 July 1983; revised 15 December 1983

Abstract. Assuming a regular geometry of dispersed phase (λ_2) an integrated theory for the effective thermal conductivity λ_e of all kind of two-phase materials (including loose materials) is developed. The flux modification is carried out by considering the effective neighbouring interactions in the solution of Poisson's equation. A comparison of calculated λ_e values with the reported experimental results over a wide range of two-phase materials shows a good agreement.

Keywords. Thermal conductivity; Poisson's equation.

1. Introduction

Prediction of the effective thermal conductivity 'λ_e' of two phase materials on the basis of macroscopic structure has been a basic problem of physics dating to Rayleigh (1892). Estimation of λ_e has been carried out using two different approaches. In one approach a homogeneous dispersion of distant spheres of second phase (λ_2) in a continuous phase (λ_1) generating a fixed geometry is considered (Maxwell 1904) for the evaluation of λ_e of two-phase system. A more rigorous mathematical solution (Rayleigh 1892; Meredith and Tobias 1960; Doyle 1978; McPhedran and McKenzi 1978; Bergman 1979) presented much better estimation of λ_e by considering the mutual interactions among the spheres in a cubic array (lattice model). In the second approach λ_e is predicted (Reynolds and Hough 1957; Hashin and Shtrikman 1962; Jeffery 1973; Kumar and Chaudhary 1980; Pande *et al* 1983) by considering a random distribution of dispersed phase material in the continuous phase.

Moreover, the lattice model is applicable to composites only. Its validity for other two-phase homogeneous materials is very much doubtful (Parrott *et al* 1975). In this endeavour we present a geometrical solution for lattice type dispersions and explore the scope of cubic dispersion for the estimation of λ_e of all kind of two phase materials including loose materials and powders as well with the help of a single integrated theory. The flux modifications because of dispersion are evaluated by finding the Green, function solution of Poisson's equation over the microgeometry of dispersion.

2. Model formulation

Consider a regular distribution of spheres of radius a and conductivity λ_2 at an interval R_0 in a continuous phase of conductivity λ_1 to generate a simple cubic lattice. Such a two-phase system along with a line source and sensor along Z axis (figure 1) is placed within a cylindrical container. We wish to find the value of potential and field at the sensor lying at origin in the central cube. Both in the presence and absence of dispersion the source is at a constant potential in steady state. Field will be uniform and radial around the sensor in X-Y plane in the absence of dispersed phase. The modification in flux appears because of the dispersion of the spheres of the second phase in X-Y plane only as the conduction along Z axis is zero. Let us consider such a lattice plane of spheres surrounding the sensor (figure 2). The value E_0 and ϕ_0 of field and potential at the sensor in the absence of second phase is now influenced by the spheres of second phase (λ_2) at the first, second, third and higher neighbouring positions in this plane.

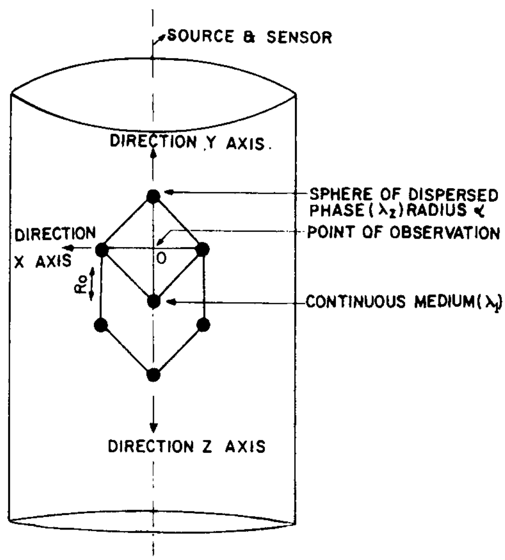

Figure 1. Cylindrical sample container containing the material (two-phase system) with source and sensor.

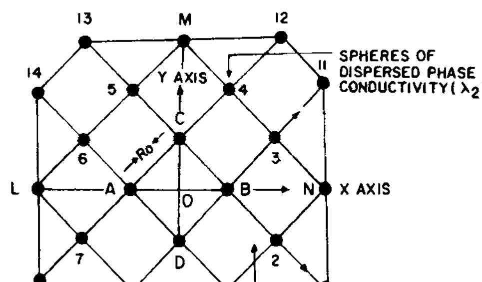

Figure 2. A lattice plane of dispersed spheres around the sensor in X-Y plane.

3. Theory

Let us consider a position dependent conductivity function $\lambda(\mathbf{R})$ such that

$$\lambda(\mathbf{R}) = \lambda_1 + \delta(\mathbf{R}, \mathbf{r}_i)(\lambda_2 - \lambda_1) \tag{1}$$

where $\delta(\mathbf{R}, \mathbf{r}_i)$ is a kind of step function such that

$$\delta(\mathbf{R}, r_i) = 0 \text{ for } |\mathbf{R} - r_i| > a$$

and

$$= 1 \text{ for } |\mathbf{R} - \mathbf{r}_i| < a$$

where a is the radius of the spheres and $\mathbf{r}_i$ denotes the position of spheres of second phase. The flux $\mathbf{J}$ and potential ϕ at the point $\mathbf{R}$ satisfy

$$\mathbf{J}(R) = -\lambda(\mathbf{R})\nabla\phi(\mathbf{R}) \tag{2}$$

In steady state div $\mathbf{J} \to 0$. Using (1) for $\lambda(\mathbf{R})$ in (2) and applying the steady state condition, we find

$$\nabla^2\phi(\mathbf{R}) = -\frac{1}{\lambda_1}\nabla\cdot[\delta(\mathbf{R}, \mathbf{r}_i)(\lambda_2 - \lambda_1)\{\nabla\phi(\mathbf{R})\}] \tag{3}$$

Using Green's function method the solution of (3) is given as

$$\phi(\mathbf{R}) = \phi_0(\mathbf{R}') + \frac{1}{4\pi\lambda_1}\int_v \frac{1}{|\mathbf{R}' - \mathbf{R}|}\nabla\cdot\{\delta(\mathbf{R}', \mathbf{r}_i)(\lambda_2 - \lambda_1)\nabla\phi(\mathbf{R}')\}\mathrm{d}V \tag{4}$$

The integral in (4) includes the whole volume. On integration by parts the non-vanishing second part in (4) may be written as

$$\phi(\mathbf{R}) = \phi_0(\mathbf{R}') - \frac{1}{4\pi\lambda_1}\int_v \left\{\nabla\left(\frac{1}{|\mathbf{R}' - \mathbf{R}|}\right)\right\}\cdot\{\delta(\mathbf{R}', \mathbf{r}_i)(\lambda_2 - \lambda_1)\nabla\phi(\mathbf{R}')\}\mathrm{d}V \tag{5}$$

As our observation point is the origin where the sensor lies $\mathbf{R} = \mathbf{0}$. Transforming (5) for $\mathbf{R} = \mathbf{0}$ and summing over all the source points $\mathbf{r}_i$, we find the potential at origin 0 as

$$\phi(\mathbf{0}) = \phi_0(\mathbf{r}_i) - \sum_i \frac{\lambda_2 - \lambda_1}{4\pi\lambda_1}\int_v \nabla(1/r_i)\cdot\nabla\phi(\mathbf{r}_i)\mathrm{d}V \tag{6}$$

where $\nabla^2\phi(\mathbf{r}_i) = 0.$

Using the vector relation for $\nabla\cdot\{1/r\,\nabla(\phi)\}$ in (6), transforming the volume integral into surface integral with the help of Gauss's theorem and substituting $\mathbf{E}_0 = \mathbf{E}_0(0) = \mathbf{E}_0(\mathbf{r}_i)$ in a single phase system we find the value of field at the sensor from (6) as

$$\mathbf{E}(0) = \mathbf{E}_0(0) + \sum_i \frac{\lambda_2 - \lambda_1}{4\pi\lambda_1}\int_s \nabla\cdot\left\{\frac{1}{r_i}\nabla\phi(\mathbf{r}_i)\cdot\mathrm{d}\mathbf{s}\right\} \tag{7}$$

It is to be noted that $-\nabla\phi(\mathbf{r}_i)$ appearing within the integral is the field inside the spheres at $\mathbf{r}_i$. As $a \ll |\mathbf{r}_i|$ and in the absence of dispersion the field $\mathbf{E}_0$ is radial, the field $\mathbf{e}(\mathbf{r}_i)$ within the sphere kept in a field $\mathbf{E}_0$ (Phillips and Panofsky 1969) is given as

$$-\nabla\phi(\mathbf{r}_i) = \mathbf{e}(\mathbf{r}_i) = -\frac{3\lambda_1}{\lambda_2 + 2\lambda_1}\mathbf{E}_0\cos\theta \tag{8}$$

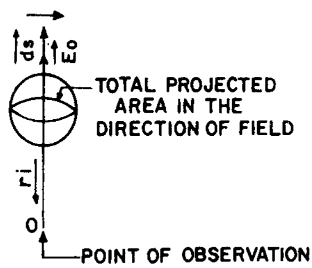

Figure 3. Projection area of a sphere in field direction.

substituting (8) in (7) we find,

$$\mathbf{E}(0) = \mathbf{E}_0 + \sum_i \frac{3(\lambda_2 - \lambda_1)\mathbf{E}_i}{4\pi(\lambda_2 + 2\lambda_1)} \int_s \nabla\left(\frac{1}{r_i}\right) \cdot \mathbf{ds} \tag{9}$$

Here $\mathbf{E}_0$, $\mathbf{r}_i$ and $\mathbf{ds}$ are in the same direction. The negative sign in (8) indicates that $\mathbf{e}(\mathbf{r}_i)$ is opposite to $\mathbf{r}_i$ (figure 3). Using these considerations in (9) we find

$$\mathbf{E}(0) = \mathbf{E}_0 - \sum_i 3(\lambda_2 - \lambda_1)/4\pi(\lambda_2 + 2\lambda_1) \int_s \mathrm{d}s \cos\theta / r_i^2 \tag{10}$$

3.1 *The effect of first neighbours*

The spheres A, B, C and D are the first neighbours at $|\mathbf{r}_i| = (2)^{-1/2} R_0$ (figure 2). Since $\theta = 0$, in radial direction ($a \ll r_i$) the field modification term by these spheres may now be written from (10) as $\delta\mathbf{E}_1$ where

$$\delta\mathbf{E}_1 = -6\frac{(\lambda_2 - \lambda_1)}{(\lambda_2 + 2\lambda_1)}(a^2/R_0^2)\mathbf{E}_0 \tag{11}$$

3.1*a* *Effect of second neighbours:* The spheres 1 to 8 (figure 2) are the second neighbours with $|\mathbf{r}_i| = (5/2)^{1/2} R_0$. The summation carried through (10) over these spheres gives the other field modification $\delta\mathbf{E}_2$ where

$$\delta\mathbf{E}_2 = -(12/5)(\lambda_2 - \lambda_1/\lambda_2 + 2\lambda_1)(a^2/R_0^2)\mathbf{E}_0 \tag{12}$$

3.1*b* *Effect of third neighbours:* The third neighbouring spheres L, M, N and P occupy the position at $|\mathbf{r}_i| = (9/2)^{1/2} R_0$. The summation (10) over these spheres yields an additional field $\delta\mathbf{E}_3$ at 0 as

$$\delta\mathbf{E}_3 = -(2/3)(\lambda_2 - \lambda_1/\lambda_2 + 2\lambda_1)(a^2/R_0^2)\mathbf{E}_0 \tag{13}$$

3.1*c* *Effect of fourth neighbours:* The spheres numbered 9 to 16 are fourth neighbours at $|\mathbf{r}_i| = (13/2)^{1/2} R_0$. The field modification by these spheres as calculated by (10) is $\delta\mathbf{E}_4$ given as

$$\delta\mathbf{E}_4 = -(12/13)(\lambda_2 - \lambda_1/\lambda_2 + 2\lambda_1)(a^2/R_0^2)\mathbf{E}_0 \tag{14}$$

3.2 *The effective thermal conductivity:*

In (2) $\mathbf{J}(\mathbf{R})$ and $\lambda(\mathbf{R})$ represent the flux and conductivity at $\mathbf{R}$ in a single phase medium when there is no dispersion. Let after making the dispersion of second phase the change in conductivity and field at **R** be $\delta\lambda(\mathbf{R})$ and $\delta\mathbf{E}(\mathbf{R})$. This change appears from (2) as

$$\delta\mathbf{J}(\mathbf{R}) = \delta\lambda(\mathbf{R})\,\mathbf{E}(\mathbf{R}) + \lambda(\mathbf{R})\,\delta\mathbf{E}(\mathbf{R}) \tag{15}$$

As the source is at a constant potential the ensemble average $\langle \delta J \rangle$ is zero. Thus from (15) we find,

$$\frac{\langle \delta\lambda(\mathbf{R}) \rangle}{\langle \lambda(\mathbf{R}) \rangle} = -\frac{\langle \delta\mathbf{E}(\mathbf{R}) \rangle}{\langle \mathbf{E}(\mathbf{R}) \rangle} \tag{16}$$

Using the properties of two phase medium (Hori 1973) we find,

$$\begin{aligned} \langle \delta\lambda(\mathbf{R}) \rangle &= \lambda_e - \lambda_1 \\ \langle \lambda(\mathbf{R}) \rangle &= \lambda_1 \\ \langle \delta\mathbf{E}(\mathbf{R}) \rangle &= \langle \mathbf{E}(0) - \mathbf{E}_0 \rangle \\ \langle \mathbf{E}(\mathbf{R}) \rangle &= \mathbf{E}_0 \end{aligned} \tag{17}$$

With these substitutions in (16) we find

$$\lambda_e = \lambda_1 \left\{ 1 + \frac{\langle \mathbf{E}_0 - \mathbf{E}(0) \rangle}{\mathbf{E}_0} \right\} \tag{18}$$

3.3 *Porosity determination*

In the two phase system under consideration there is a dispersion of one sphere per cube. The volume fraction ψ of the dispersed phase is thus given as

$$\psi = (4\pi/3)(a^3/R_0^3) \tag{19}$$

Case I when $(\lambda_2/\lambda_1) \rightarrow \infty$:

In this case the estimation of λ_e requires the consideration of higher neighbouring interactions. Considering upto fourth neighbours one finds λ_e through (11), (12), (13), (14), (18) and (19) as

$$\lambda_e = \lambda_1 \{1 + 3\cdot 844(\psi)^{2/3}\} \tag{20}$$

Case II when $(\lambda_2/\lambda_1) \rightarrow 0$:

As the conductivity of dispersed phase is too low in this case the mutual interactions upto first neighbours are only important. The λ_e value is obtained through (11), (18) and (19) as

$$\lambda_e = \lambda_1 \{1 - 1\cdot 545(\psi)^{2/3}\} \tag{21}$$

Case III when $(\lambda_2/\lambda_1) \approx 1$:

Here the interactions upto first neighbours are only important like case II. The λ_e is evaluated through (11), (18) and (19) as

$$\lambda_e = \lambda_1 \{1 + 2\cdot 307(\lambda_2 - \lambda_1/\lambda_2 + 2\lambda_1)(\psi)^{2/3}\} \tag{22}$$

Moreover when dispersion is very dilute the influence of individual sphere is only important. Substituting $i = 1$, $|\mathbf{r}_i| = R_0/2$ and $\mathbf{E}(\mathbf{r}_i)$ from (8) in (10) one finds λ_e

through (10), (18) and (19) as

$$\lambda_e = \lambda_1\{1 + 1\cdot545(\lambda_2 - \lambda_1/\lambda_2 + 2\lambda_1)(\psi)^{2/3}\} \tag{23}$$

4. Comparison with experimental results and discussion

The expressions (20) to (23) derived for the estimation of λ_e in the present endeavour may be used as general expressions as these depend upon the averaged quantitionlike λ_1, λ_2 and ψ. In table 1 the calculated λ_e values through (20) to (23) for a variety oı two phase materials, whose (λ_2/λ_1) is too high, moderate and too low, are compared with reported experimental results and with those given by Maxwell's expression. In addition a comparison for λ_e using Rayleigh, Tobias, Maxwell and present relations is also presented in table 2 for the systems whose (λ_2/λ_1) tends to infinity.

In the estimation of λ_e for systems whose $(\lambda_2/\lambda_1) > 10^3$ [system 1, table 1], Maxwell's expression and expression (20) both underestimate the λ_e values by 19·6 and

Table 1. Comparison of calculated and measured λ_e values in $WM^{-1}K^{-1}$ for various two phase systems.

System	λ_2/λ_1		λ_e using Maxwell's expression	λ_e using Present expression	λ_e Reported
Resin and copper powder 46 μM (De Araujo and Rosenberg 1976)	1965	0·132	0·291	0·367	0·350
		0·206	0·355	0·425	0·420
		0·301	0·458	0·545	0·600
Resin and stainless steel spheres at 20°K (De Araujo and Rosenberg 1976)	23·83	0·093	0·108	0·120	0·112
		0·195	0·138	0·143	0·140
		0·304	0·178	0·192	0·185
Uranium oxide and molybdenum (Gilcherist *et al* 1975)	14·40	0·217	13·32	15·54	15·70
		0·282	15·35	19·78	18·30
Uranium oxide and sodium (Huetz, 1972)	10·00	0·25	15·23	17·76	17·00
		0·50	25·20	33·87	32·60
		0·75	43·71	54·60	54·10
Silicon rubber and glass beads (Hayashi *et al* 1976)	5·2	0·089	0·221	0·226	0·231
		0·198	0·278	0·291	0·283
		0·306	0·330	0·322	0·325
Petrol-water system (Knudson and Wand 1958)	3·63	0·20	0·197	0·208	0·205
Foresterite and magnesia (Kingrey 1959)	$16·7 \times 10^{-2}$	0·132	2·57	2·39	2·48
Zirconium oxide and air (Waterman and Goldsmith 1961)	$1·73 \times 10^{-2}$	0·09	1·50	1·34	1·35
Rajasthan Desert sand (Kumar and Chaudhary 1980)	$7·74 \times 10^{-3}$	0·4297	1·638	0·312	0·302
		0·4394	1·606	0·269	0·312
Uranium oxide and air (Waterman and Goldsmith 1961)	3×10^{-3}	0·100	8·00	6·44	7·56
		0·267	5·80	4·71	5·66
		0·450	4·04	2·90	2·90

Table 2. Comparison of calculated values of λ_e in $WM^{-1}K^{-1}$ by other expressions based on flux laws for systems whose $(\lambda_2/\lambda_1) \rightarrow \infty$.

λ_1		λ_e using Maxwell's expression	λ_e using Rayleigh's* expression	λ_e using Meredith and Tobias's expression	λ_e using present expression
1	0·1	1·3334	1·3401	1·3407	1·8280
	0·2	1·7439	1·7456	1·7508	2·3150
	0·3	2·2510	2·2595	2·2773	2·7230
	0·4	2·8720	2·9016	2·9423	3·0870

* Rayleigh's relation:

$$\lambda_e = \lambda_1 \left\{ \frac{1 - 2k\psi + kf(\lambda_2, \lambda_1 \cdot \psi)}{1 + k\psi + kf(\lambda_2, \lambda_1, \psi)} \right\}$$

where $f(\lambda_2, \lambda_1, \psi) = 1{\cdot}65\{(\lambda_2 - \lambda_1)(\lambda_2 + 4\lambda_1/3)^{-1} \times \psi^{10/3}\}$

and $k = (\lambda_1 - \lambda_2)/(\lambda_2 + 2\lambda_1)$

Meredith *et al* relation:

$$\lambda_e = \lambda_1 \left\{ \frac{1 - 2\psi k + 0{\cdot}409k(6\lambda_1 + 3\lambda_2/4\lambda_1 + 3\lambda_2)\psi^{7/3} - 2{\cdot}133k\psi^{10/7}(3\lambda_1 - 3\lambda_2/4\lambda_1 + 3\lambda_2}{1 + \psi k + 0{\cdot}409k(6\lambda_1 + 3\lambda_2/4\lambda_1 + 3\lambda_2)\psi^{7/3} + 0{\cdot}906k\psi^{10/3}(3\lambda_1 - 3\lambda_2/4\lambda_1 + 3\lambda_2)} \right\}$$

where k is same as above·

Maxwell's relation:

$$\lambda_e = \lambda_1 \left\{ \frac{1 - 2\psi k}{1 + \psi k} \right\}$$

2·4% respectively. When $(\lambda_2/\lambda_1) > 1$ [systems 2 to 6, table 1] evaluation of λ_e is done using (22). Maxwell's relation underestimates the λ_e values by 12·9, 19·6, 18·8, 1·2 and 3·9% while (22) overestimates these by 4·1, 3·9, 2·4, 0 and 1·5% respectively.

In systems whose $(\lambda_2/\lambda_1) < 1$ [systems 7 to 10, table 1] expression (21) for systems 9 and 10 and (22) for systems 7 and 8 are used to estimate the values of λ_e. Maxwell's expression overestimates the λ_e values by 11, 13·6, 16·3 and 434·0 percent while the proposed expressions underestimates the same by 0·7, 3·6, 16·3 and 11·5 respectively.

In table 2 (20) yields larger values for λ_e (as required) as ψ increases than those given by Rayleigh, Tobias and Maxwell's expressions.

This comparison suggests that the proposed expressions satisfactorily estimate the λ_e of various kind of two phase materials although these are derived for a restricted geometry.

Acknowledgements

The authors are thankful to Dr P V Bakore and Dr N S Saxena for valuable suggestions. One of them (RNP) is grateful to UGC, New Delhi for the award of a teacher fellowship.

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