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THERMAL CONDUCTIVITY OF HETEROGENEOUS MIXTURES

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Abstract—A constant density function random number generator was used to predict numerically the effective thermal conductivity of heterogeneous mixtures. The method is an extension of a digital simulation technique originally proposed by Baxley and Couper for suspensions and emulsions. However, the present model has been extended to include the effect of contact areas between particles, the effect of reduced pressure, and radiation heat transfer. The model is applicable to granular materials and powders over a wide range of pressures and temperatures. The model is compared to experimental data for granular materials at pressures ranging from atmospheric to simulated lunar environment (10^{-8} + torr). The model is also compared with models for granular materials at atmospheric pressures existing in the literature. A distinct improvement in the accuracy of calculated results is shown for the proposed model over existing models.

NOMENCLATURE

d, particle diameter [m];
D_p, effective pore size [m];
$(D_p)_c$, effective pore size for conduction [m];
$(D_p)_h$, hydraulic diameter [m];
e, emissivity;
E, Young's modulus [N/m^2];
g^*, temperature jump distance [m];
h_r, coefficient associated with surface microroughness;
k_c, conductivity of continuous phase [kcal/m h K];
k_{cr}, contact conductivity [kcal/m h K];
k_e, effective conductivity [kcal/m h K];
k_g, conductivity of gaseous phase [kcal/m h K];
k_g^*, conductivity of gaseous phase at reduced pressures [kcal/m h K];
k_k, coefficient associated with microgaps at contact areas;
k_r, radiant conductivity [kcal/m h K];
k_s, conductivity of solid [kcal/m h K];
N, grid size;
N_c, number of contact areas per unit volume;
n, coordination number;
P, volume fraction of continuous phase (porosity);
r_c, contact area radius [m];
R_c, contact resistance [kcal/h K]$^{-1}$;
R_L, resistance to heat flow due to contraction of heat flow lines [kcal/h K]$^{-1}$;
R_0, resistance due to oxidizing film [kcal/h K]$^{-1}$;
R_{sp}, resistance due to microroughness of solid particles [kcal/h K]$^{-1}$;
s, molecular diameter [m];
T, temperature [K];
w, overrelaxation factor.

Greek symbols

α, thermal accommodation coefficient;
ρ, density of solid [N/m^3];
λ, molecular mean free path [m];
ν, Poisson's ratio;
σ_b Stefan–Boltzmann constant [kcal/m^2 K^4].

1. INTRODUCTION

CONSIDERABLE effort has been expended over the past sixty years to develop techniques for calculating the effective thermal conductivity of heterogeneous mixtures from the conductivities of the individual components [1].* However, construction of a model which accurately represents heterogeneous materials has proved to be difficult as attested by the number of correlations presented in the literature. The difficulty does not arise from ignorance of the fundamental laws involved but from complications in their application [2]. A detailed solution of the conduction problem would require knowledge of the shape, size, location and conductivity of each particle in the system, together with the interactions between particles. To overcome these difficulties, investigators have generally followed two simplified methods of approach:

1. Ohm's law models—A basic repeated structural unit representative of the heterogeneous mixture is isolated, and equations are derived on the basis of the electrical analogy assuming one dimensional heat transfer.

2. Flux law models—The temperature distribution in the system is determined based on the assumption of

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(a) a regular array of spherical particles, or (b) a random distribution of spherical particles in such small concentrations that there is no field interaction. Temperature gradients are then determined and the effective thermal conductivity is established from the Fourier–Biot law. The flux law models offer the advantage of three dimensional heat flow but present considerable mathematical complexity and generally necessitate significant geometrical simplification. These geometrical simplifications are frequently so extensive that the model generally bears little resemblance to the physical body. Because of the limitations placed by these geometrical simplifications on flux law models increasing interest has turned to Ohm's law models in recent years. Research into the packing structure of granular materials has permitted the models to be developed with considerable geometrical accuracy. Crane and Vachon [3] developed two such models by alternate heat flow assumptions. It was shown that the one dimensional heat flow assumptions of parallel isotherms and uniform heat flux led to calculational results which were respectively high and low. It was explained that these solutions were in fact upper and lower bounds to the exact solution. The range between the upper and lower bounds is shown in Fig. 1. It should be noted that a considerable gap exists between these bounds whenever constituent conductivity ratios are sufficiently large. Moreover, neither bounding equation yields results which are sufficiently close to experimental values for most calculational purposes.

It is therefore concluded that the assumption of one dimensional heat transfer is unsatisfactory for the evaluation of the effective thermal conductivity of such materials. The Ohm's law model approach has therefore been discarded and primary attention turned to numerical solutions as the only alternative to obtain the desired accuracy in solutions.

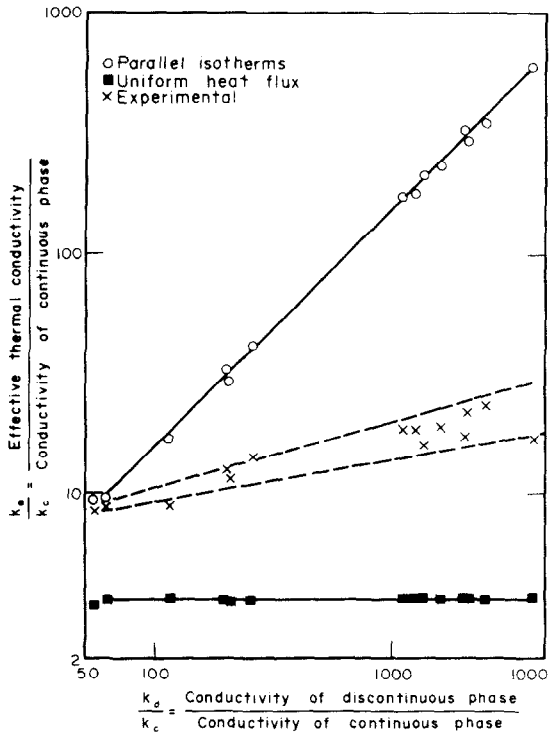

FIG. 1. Comparison of bounding conductivities with experimental data for a porosity of 0.38.

II. NUMERICAL DEVELOPMENT

The basic geometry for the numerical model is shown in Fig. 2a. The two opposing faces of the cube are isothermal, and the other four faces are insulated, so that application of a constant temperature potential gives rise to a net conduction heat transfer in one direction. The technique to determine the effective thermal conductivity of such a system requires that the temperature distribution in the unit cube first be obtained. Once this has been accomplished, the heat flow rate can be determined through the temperature gradient and an effective thermal conductivity can be assigned to the material by the Fourier–Biot law.

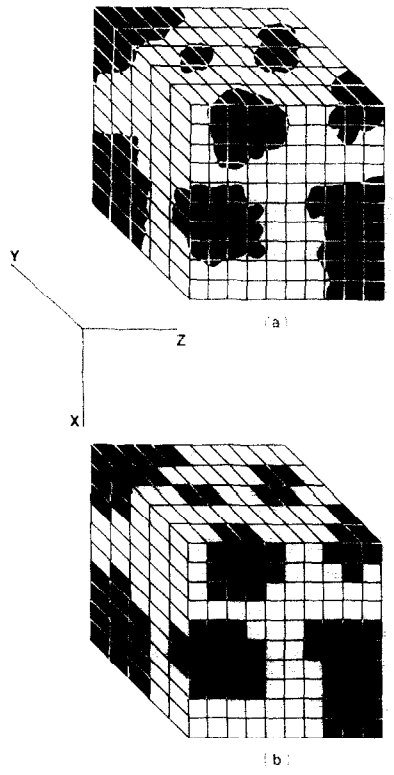

FIG. 2. Equivalent geometries for unit cube.

1. *System synthesis*

A representative unit cube of a granular material is shown in Fig. 2(a). The unit cube is subdivided into small regular cubicles such that each cubicle is totally occupied by one of the phases present. Effectively, any irregular shaped particle can be built to any degree of approximation by arranging a number of cubicles according to a predetermined format [2], as indicated in Fig. 2(b). These particles can then be placed in the unit cube according to a specified statistical distribution. This way, the basic assumption of a

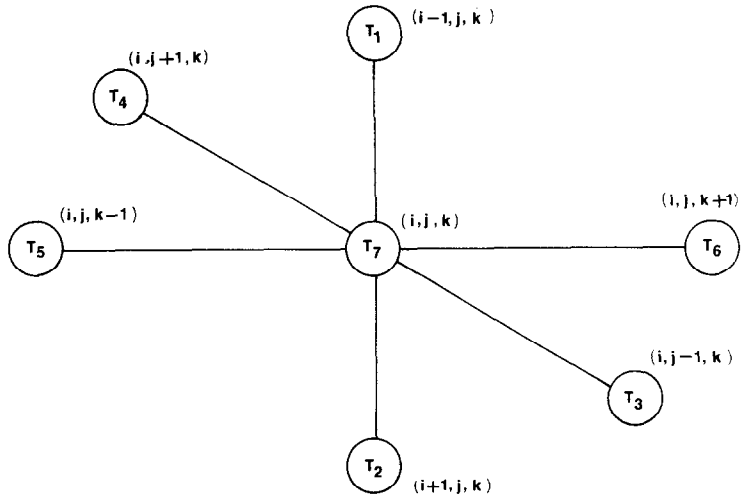

FIG. 3. Heat balance basic nodal orientation.

regularly repeated elementary cell of spatial configuration, common to most previous models, is avoided.

The representative cube will be constructed from cubicles of the continuous and discontinuous phases. The discontinuous phase, as distinct from the continuous phase, will be characterized by a distributed contact resistance between like cubicles. This would be typical of solid particles within the granular system.

The method of placing continuous phase cubicles in the unit cube, is based on the assumption that the granular material can be considered as a random mixture of the two phases. In order to place a continuous phase cubicle in the system, three random numbers are generated by a 0–1 constant density function random number generator, and these random numbers are associated with three coordinates, defining the position of a cubicle in the system. If the cubicle thus defined is already occupied by the continuous phase another triplet of random numbers is generated. This process continues until the total number of continuous phase cubicles is equal to the continuous phase solid fraction of the granular system times the total number of cubicles in the unit cube. The geometry of the system thus defined represents a random mixture of two phases such that the probability that a particular cubicle is occupied by the continuous phase is equal to the volume fraction of the continuous phase.

The geometry of the model has been based on the assumption that irregular packed beds can be considered as a random mixture of the two phases. It has been shown [4–6] that for granular materials in which the particle sizes are not much different, and in which the particles can be approximated by spheres, this is a valid assumption. For packed beds consisting of irregularly shaped particles, no generalized conclusions have been reached concerning the distribution of local properties. However, it has been shown that the geometry of packed beds of irregularly shaped particles does not satisfy the randomness criteria when the particle size distribution is narrow [6]. Therefore, it is possible that the geometry of certain classes of granular materials differ from that assumed.

Calculations for the unit cube size, pore size, etc. have been based on a characteristic particle size. For packed beds in which the particle size distribution is narrow, it has been assumed by all models in this study that the characteristic particle size is equal to the mean volume diameter [7]. However, no set method exists in the literature for calculating the characteristic particle size for beds having a broad particle size distribution. Further, as indicated in [1], the mean volume diameter is not a satisfactory description of the characteristic particle size for such beds.

The geometrical parameters utilized in the development of the models such as pore size, coordination number, etc. and the equations for contact resistance have been based on equations given in the literature for randomly packed beds of equal sized spheres. It follows that none of the models presented in this study is applicable in the case of heterogeneous mixtures containing highly irregular shaped particles such as Rashing rings, Berl saddles, etc.

2. *Determination of the actual temperature distribution*

Heat transfer to a single cubicle under steady state conditions with no internal heat generation is given by the equation

$$\nabla \cdot (k \cdot \nabla T) = 0.$$

The finite difference form of this equation can be obtained assuming that each cubicle may be lumped as a uniform isothermal node surrounded by six adjacent nodes as shown in Fig. 3.

The resulting equation is

$$\sum_{i=1}^{6} k_{i7}(T_i - T_7)\frac{A}{L} = 0 \qquad (1)$$

where k_{i7} is the effective thermal conductivity between adjacent nodes as given by simple series model $[K_{ij} = 2K_iK_j/(K_i+K_j)]$ [5].

Application of equation (1) to all cubicles results in N^3 simultaneous linear equations. The coefficients of this system of equations are functions of the average

working conductivities and the unknowns are the node temperatures.

One method of solving this system of equations is the technique of relaxation. To reduce convergence time an over-relaxation technique has been employed [8]. Assuming an arbitrary initial temperature distribution, repetitive application of the equation

$$T^{n+1} = T^n + \frac{w}{\sum_{i=1}^{i=6} k_{i7}} \left| \sum_{i=1}^{i=6} k_{i7}(T_i - T_7) \right| \quad (2)$$

will quickly result in the appropriate steady state temperature profile. Here w is an over-relaxation factor and is generally assigned a value $1 < w < 2$ [9]. In the present study w was found to be $(1.1 < w < 1.5)$.

A reasonable selection for the initial temperature field is to assume that planes of nodes normal to the direction of the heat flow are isothermal, and the temperature of each plane is proportional to its distance from the surface of the cube. Also, the imposed boundary conditions dictate that the temperatures of the nodes on the front and back faces, which are normal to the direction of the heat flow, remain constant, and the heat flow away from nodes associated with the other four faces is zero. Application of equation (2) coupled with the assumed initial temperature distribution and the boundary conditions, gives the actual temperature distribution in the unit cube. In the calculations, the iteration process cut-off point is selected so that the sum of the absolute values of the thermal residues is less than or equal to 1.0.

3. *Determination of the average working thermal conductivities*

At this point it should be noted that the working thermal conductivities thus defined require that the adjacent cubicles are in perfect contact with each other. However, physical granular systems contain randomly distributed and oriented contact areas between neighboring particles that provide additional resistance to the heat flow from one particle to the other. Further, when the voids between particles are evacuated, these contact areas provide the only path of heat transfer, other than radiation heat transfer, from one particle to the other. Consequently, failure to account for these contact areas induces large errors in the calculation of the effective thermal conductivity of granular materials, especially when the ratio of the constituent conductivities is high. In order to incorporate the effect that these contact areas have on the flow of heat in the physical model presented, it is necessary to associate a constant conductivity with each contact area and to know the number of these contact points in the unit cube. A number of expressions have been reported in the literature relating the contact resistance to the contact area between two particles (a complete review of these expressions is found in [1]). In the present calculations, the expressions given by Luikov [10] have been used, being in good agreement with experiments.

Luikov [10] states that the contact resistance consists of three components. In addition to the contraction of the heat flow lines, the effect of the microroughness of real particles should be included in the estimation of the contact resistance, together with the effect of any oxidizing film covering the particles: However, in general the resistance due to oxide films is neglected. Therefore the total contact resistance is

$$R_c = R_L + R_{sp}. \quad (3)$$

The following expressions were given by Luikov [10] for these resistances as

$$R_L = \frac{1}{2r_c K_s} \quad \text{and} \quad R_{sp} = \frac{h_r k_k}{\Pi r_c^2 K_s} \quad (4)$$

where R_L is due to the contraction of heat flow lines and R_{sp} is due to microroughness thermal effect. The h_r and k_k are experimentally determined coefficients depending on the height of the microroughnesses and the degree of adhesion respectively. Luikov [10] lists the recommended values for these coefficients for a number of granular material classes. The radius of contact area r_c, between two particles is given as

$$r_c = 0.465d \left| \frac{(1-\nu)\rho H}{E(1-P)} \right|^{1/3} \quad (5)$$

where H is the height of the bed (in this study H is taken as the height of the unit cube). The thermal conductivity at the contact areas can be related to the contact resistance by:

$$k_{cr} = \frac{1}{R_c d}. \quad (6)$$

The heat flux through contact areas depends on the number of contacts each particle has with its neighbors, or the coordination number n [11]. Various correlations have been proposed [4, 12–14] to represent the coordination number as a function of the porosity as shown in Fig. 4. The authors have selected the relation proposed by Haughey and Beveridge [4, 11] for the coordination number, which is

$$n = 22.47 - 39.39P. \quad (7)$$

This equation is represented by curve 3 and may be seen to closely represent the available data.

The number of contact points in the cube, N_c, can be determined as a function of the unit cube size, a characteristic particle size obtained from sieve analysis of the granular material, and the coordination number. As indicated in [7], the characteristic volume of each particle is $\varepsilon_v d^3$, where ε_v is an experimentally determined volumetric parameter that depends on the particle shape, and d is a characteristic particle size obtained from the sieve data. It follows then that the number of particles per unit volume is $(1-P)/\varepsilon_v d^3$. For spherical particles ε_v is equal to $\pi/6$. Combining this expression with equation 7 yields the number of contact points in a unit cube for spherical particles:

$$N_c = \frac{12.54(0.571 - P)(1-P)}{d^3} \quad (8)$$

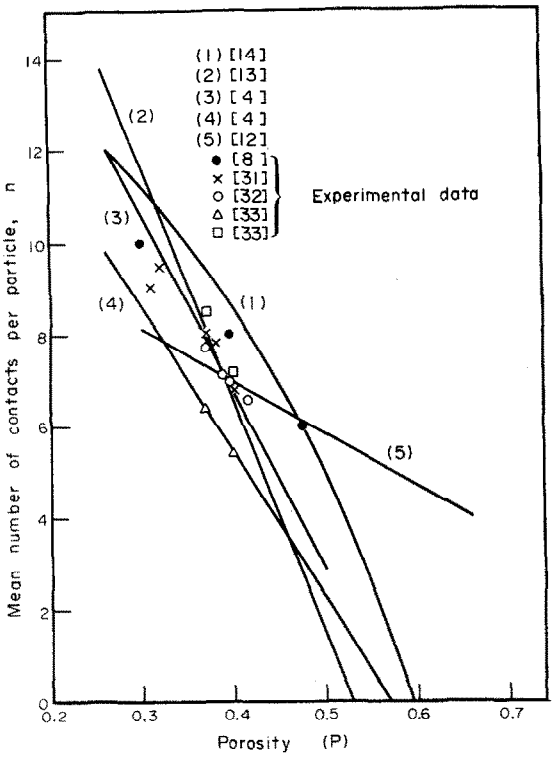

FIG. 4. Co-ordination number.

To complete the determination of the working thermal conductivities, it is necessary to randomly distribute N_c contact conductivities between adjacent cubicles occupied by the discontinuous phase. Again a triplet of random numbers is generated and is associated with three coordinates, defining the position of a cubicle in the system. If the cubicle is occupied by the discontinuous phase, the composition of its neighbors is determined, and the working conductivity between the first pair of solid cubicles is replaced by k_{cr}. The process is repeated until N_c such replacements have been executed. A point of importance is that since contact points at the boundaries of the unit cube should also be included, it is necessary to determine the composition of the cubicles surrounding the six faces of the unit cube.

4. *Determination of the heat flows and the effective thermal conductivity*

After the steady-state temperature field has been determined, three orthogonal heat flux vectors can be defined at each node. However, since the net heat flow is in one direction only, this is the rate of heat flow on which the effective thermal conductivity should be based. To find the rate of heat flow Q, the net heat flow between all nodes in any two successive planes are summed. This process is repeated for all successive planes, and Q is taken as the average value of these sums. The averaging process of Q is found to be a necessary procedure in order to minimize the errors resulting from round-off and numerical errors of the solution. The effective thermal conductivity of the granular material, as defined by the Fourier–Biot law, is given by:

$$k_e = \frac{Q}{N\Delta T} \tag{9}$$

where ΔT is the difference between the temperatures of the back and front faces of the unit cube that are normal to the net heat flow direction.

III. LOW PRESSURE EFFECTS

Figure 5 shows a typical pressure dependence of the effective thermal conductivity of a gas–powder mixture. At higher pressures the thermal conductivity of the mixture is independent of pressure. At lower pressures when the mean free path of the gas molecules approaches the characteristic length of the gas space, the effective conductivity becomes pressure dependent, as indicated by the portion between A and B. Further reduction of the pressure does not result in any appreciable changes in the effective conductivity, since in this region the dominant modes of heat transfer are conduction through the contact areas between particles and radiation.

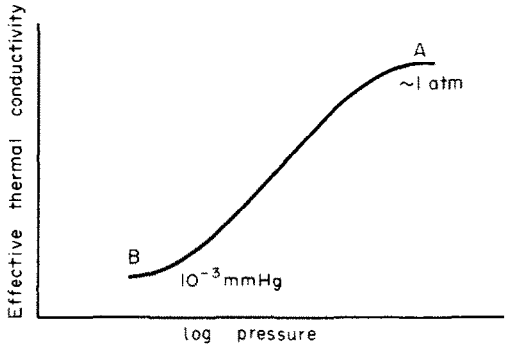

FIG. 5. Pressure dependence of effective thermal conductivity.

1. *Gaseous conductivity*

Thermal conduction in rarefied gases was first analyzed in the pioneer works of Smoluchowski and Knudsen, as indicated by Kennard [15]. Kennard's equation for the effective conductivity, k_g^*, of a gas between two parallel plates of the same material, separated by a relative small distance, D_p, is:

$$k_g^* = \frac{k_g}{1+2\dfrac{g^*}{D_p}} \tag{10}$$

where g^* is the temperature jump distance at one of the plates, given by:

$$g^* = \frac{2-\alpha}{\alpha}\frac{2\gamma}{\gamma+1}\frac{1}{Pr}\lambda \tag{11}$$

where α is the thermal accommodation coefficient, γ is the ratio of the specific heats of the gas, Pr is the Prandtl number and λ is the mean free path of the gas molecules. Equations (10) and (11) indicate that k_g^* decreases with respect to k_g when λ/D_p increases.

The principal difficulty in applying this equation lies in evaluating the thermal accommodation coefficient,

α, and the effective pore length, D_p. As indicated in [16], several attempts have been made to predict the accommodation coefficient analytically, but they have not proved particularly successful. Furthermore, the accommodation coefficient is strongly influenced by parameters describing the solid surface (i.e. smoothness, impurities, etc. not reported in experimental work on the conductivity of granular materials), and experimentally determined values of α are not available for solids other than pure metals and alloys [13]. For this reason, most investigators of the effective conductivity of heterogeneous mixtures have either set $\alpha = 1$, effectively assuming that the solid surface is so irregular that most of the molecules strike it a number of times before escaping, or they have included α in an experimentally determined coefficient.

Deissler and Boegli [17] found from experimental data on magnesium oxide in air that the pressure at which the effective conductivity begins to vary with pressure (breakaway pressure) is 15 psia at 340°F. From this they evaluated the Knudsen number ($Kn = \lambda/d$), based on the mean particle size, to be 0.00072. Finally, arguing that Kn at the breakaway pressure must be independent of the gas, powder, temperature and pressure, they found that the breakaway pressure in the English system of units is given by:

$$P_b = 1770 \times 10^{-24} \frac{T}{s^2 d} \tag{12}$$

where T is the temperature and s is the molecular diameter of the gas. Equation (12) seems to correlate their experimental data with good accuracy. It is of particular importance that the value of the Knudsen number corresponding to the breakaway pressure is much less than unity, indicating that most of the heat transfer through a powder takes place in the immediate vicinity of the contact areas. Effectively, this means that the dimensions effective in transferring heat in the voids are much less than the effective geometric length of the void.

2. *Effective pore size*

The equation for k_g^* has been expressed in terms of an effective distance between particle surfaces D_p, called the effective pore size. In the case of k_g^*, this is the mean distance gas molecules travel from the surface of one particle to that of another, when the molecular mean free path is large. It follows that this parameter is significant both for the geometric characterization of the granular material, as well as for the heat-transfer process.

Haughey and Beveridge [4] investigated both analytically and experimentally the case of randomly packed beds of equal-sized spheres for loose packed ($P = 0.3812$–0.4), poured packed ($P = 0.364$) and close packed ($P = 0.3587$) beds. They then generalized their results for a wide range of porosities. The reported expressions for the mean void hydraulic diameter is as follows:

$$(D_p)_h = \tfrac{2}{3} dP/(1-P). \tag{13}$$

It has been noted, however, that for powders under reduced pressures most of the heat transfer through the voids takes place in the vicinity of the contact areas. This means that the dimensions effective in conducting heat through the voids are much less than the effective geometric length of the void. To account for this phenomenon the correlation for the effective thermal conductivity is correlated to the experimentally determined values for the breakaway pressure. Effectively, the pressure at which the effective thermal conductivity of a granular material is reduced by 5% was determined from a number of experimental data in the region A of Fig. 5. Subsequently, the value of k_g^*/k_g required to attain this decrease in k_e was calculated, and from equation (10) the corresponding value of (D_p) was determined. The experimental data were taken from [12, 17–22]. The least squares fit of $(D_p)_c/d$ as a function of P is:

$$\frac{(D_p)_c}{d} = \frac{0.2177P - 0.051}{1-P}, \quad 0.3 < P < 0.7 \tag{14}$$

3. *Radiation heat transfer in granular materials*

Thermal radiation is known to be a significant mode of heat transfer in evacuated granular materials, or in powders at elevated temperatures. However, due to the scarcity of information about absorption and scattering of radiation in granular materials, only approximate methods have been developed for the inclusion of radiation as a mode of heat transfer in granular materials.

Summarizing the methods of predicting radiant heat transfer in granular materials, developed in the literature, it is seen that they can be classified into groups (a) those assuming the heterogeneous mixture can be approximated by a pseudohomogeneous material, and (b) those based on regular geometric arrangements that permit an algebraic formulation of the radiation process. Although the first class provides the best approximation to the interaction between pure conduction and pure radiation heat transfer, lack of experimental work on radiative properties of heterogeneous mixtures necessitates the application of the second method. Russell [23], Wesselink [24], Jacob [25], Argo and Smith [26], and Chen and Churchill [27] assumed that with respect to radiation a mixture can be treated as alternating solid and gas perpendicular to the heat flow. In each of these cases the effective radiant conductivity is given by

$$K_r = \frac{4\sigma_b e D_p T^3}{2-e} \tag{15}$$

where each of the investigators have assumed different relations between D_p and the porosity of the material. Equation (15) has been adapted for use in the present proposed model. The emissivity e is generally a function of bed temperature and is obtained experimentally

IV. COMPARISON OF CALCULATED EFFECTIVE CONDUCTIVITY TO EXPERIMENTAL DATA

The effective thermal conductivity has been calculated and compared to experimentally determined

values for a number of granular materials at atmospheric pressures.* The range of porosities and ratio of constituent conductivities is 0.31–0.59 and 1.67–2444.4 respectively so that a broad range of conditions are included. For all these cases the conductivities of the constituents were assumed to be constant or independent of temperature distribution in the unit cube. For the model described in this paper, the effective conductivity in each case was determined by considering five or more random placements of the continuous phase in a unit cube, and finding the average of the calculated values. The variance of the calculated values was less than 0.1 for 78 cases and its highest value was 0.587. Whenever the variance was exceedingly high, more random placements were considered, so that a more representative average could be obtained for the effective thermal conductivity. For 1728 cubicles (1440 nodes) with over-relaxation $W = 1.5$ the program takes approximately a minute (about 50 iterations) on an IBM-370 computer. A listing of the computer program is found in [1].

For comparative purposes the effective conductivity predicted by a number of selected models was also determined. Table 1 summarizes the results of an analysis of the percentage error between experimentally determined thermal conductivity and the conductivity predicted by all selected models. It should be noted that the model of this study predicts the experimental thermal conductivities with a mean of 15.8%, an error variance of 1.63, and is biased below the experimental values by 5.78%. This is somewhat better than the Krupiczka model, for which a mean error of 17.48% with a variance 2.63 has been calculated. This is significant in that the Krupiczka model [29] is a semi-empirical model based on an interpolation or extrapolation between or beyond square packings of sphere or cylinders. Moreover, the Krupiczka model is somewhat limited in that it is based on a limited range of porosities under continuous conditions where temperatures are sufficiently low that thermal radiation is negligible. The mean error of all other models is in the range 30.12–42.2%; all result in considerably larger error than the proposed numerical model. A graphical representation of the effective thermal conductivity predicted by the model described in this study is shown in Fig. 6.

Table 1. Average error, bias and variance between predicted and experimental thermal conductivities

Model	Average error %	Average bias %	Variance of % error
This study	−5.78	15.8	1.63
Maxwell [40]	−40.59	41.1	4.99
Rayleigh [41]	−42.05	42.2	4.96
Meredith & Tobias [42]	−22.46	31.34	3.56
Russell [23]	−32.65	34.37	4.90
Jefferson [43]	13.80	37.59	38.58
Krupiczka [29]	6.76	17.48	2.63
Lichtenecker [44]	−40.52	40.82	4.93
Woodside & Messmer [34]	19.10	30.12	6.68
Fig. 6	−15.9	15.9	8.7
Fig. 7	−20.8	20.8	2.1
Fig. 8	−39.4	39.4	7.5
Fig. 9	−9.4	19.4	2.4
Fig. 10	11.8	18.5	1.2
Fig. 11	−17.6	17.6	1.1

*A table containing 92 study cases is found in [1,28], together with thermal-mechanical properties of the solid phase used in the calculation.

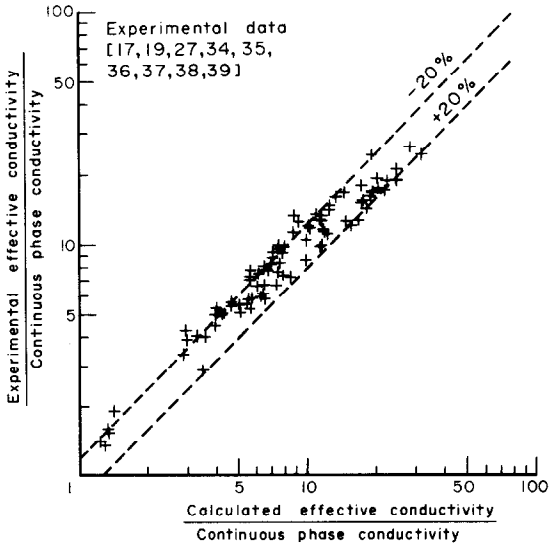

FIG. 6. Comparison of experimental and model predicted thermal conductivities.

In Fig. 7 the calculated effective thermal conductivity is evaluated for data with very high constituent conductivity ratios. Experimental data [30] for particulate basalt in a simulated lunar environment

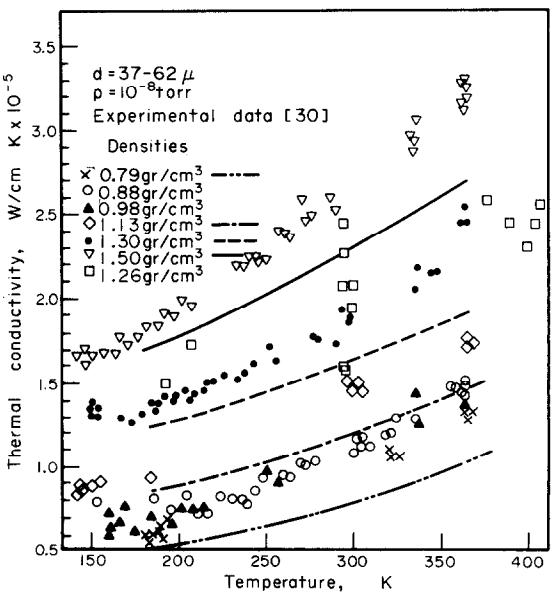

FIG. 7. Experimental and calculated conductivity of particulate basalt in simulated lunar environment.

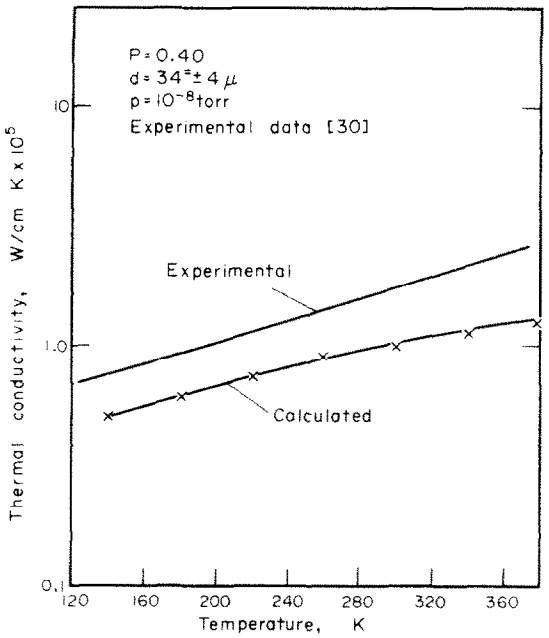

FIG. 8. Experimental and calculated thermal conductivity of particulate glass in simulated lunar environment.

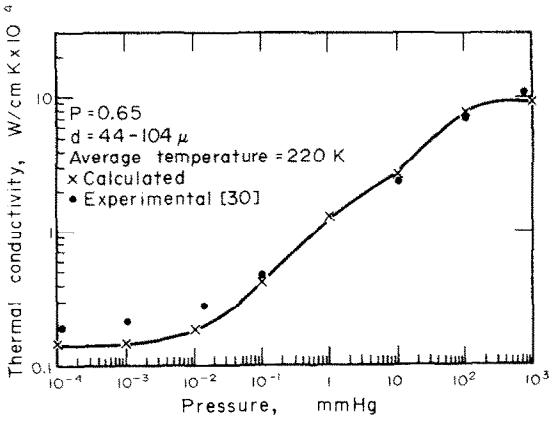

FIG. 9. Experimental and calculated thermal conductivity of particulate basalt in air.

is shown together with the calculated effective conductivities. The calculated conductivities are noted to be lower than the experimental; probably this is due to two factors. First, the semi-empirical equation for the contact resistance used in this study probably predicts low values for the contact conductivity. Evidence to this effect is that calculated conductivities at low pressures, in which case heat transfer from particle to particle is dominant mode, are generally low. A second source of error is failure to include radiation heat transfer as a photon diffusion process. Evidence to this effect is that the discrepancy between calculated and experimental values generally increases with temperature. Nevertheless, it is seen that the model predicts fairly well the increase in slope with decreasing porosity, and the increase in slope with temperature, due to the increase of the relative influence of radiant heat transfer with decreasing porosity and increasing temperature. The maximum error of the calculated thermal conductivities is 23.7% and the mean error is 15.9%.

In Fig. 8 the calculated effective thermal conductivity is compared to experimental data obtained by Fountain and West [30] for particulate basalt in a simulated martian environment. In this case the gaseous conductivity and the radiant conductivity are of the order of magnitude 3×10^{-5} and 10^{-7} W/cm K respectively. Consequently, radiation can be neglected. Again the predicted values are lower than the experimental, and the maximum error and mean error are 25.2% and 20.8% respectively. The slight increase of the effective thermal conductivity with temperature is due to the simultaneous increase of the conductivity of the solid and gaseous phases with temperature, and not to radiation heat transfer.

The experimental and calculated thermal conductivities of particulate basalt in air, lead shot in air, and glass beads in air are compared in Figs. 9, 10 and 11 respectively, as a function of pressure. It is observed that the model predicted values are generally in good agreement with the experimental values, although somewhat lower conductivities are predicted at low pressures. The relatively good agreement is attributed

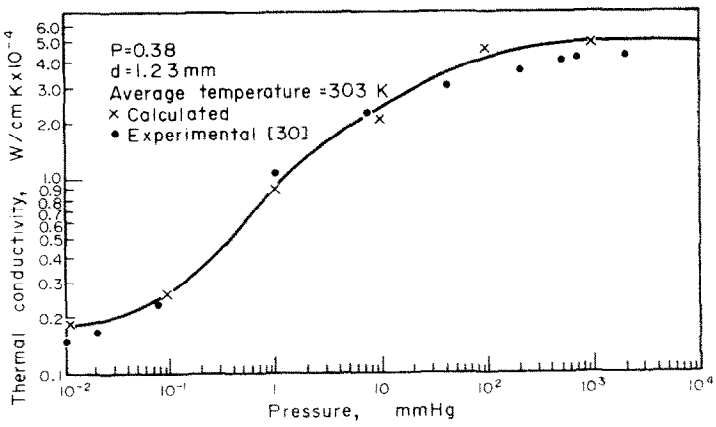

FIG. 10. Experimental and calculated thermal conductivity of lead shot in air.

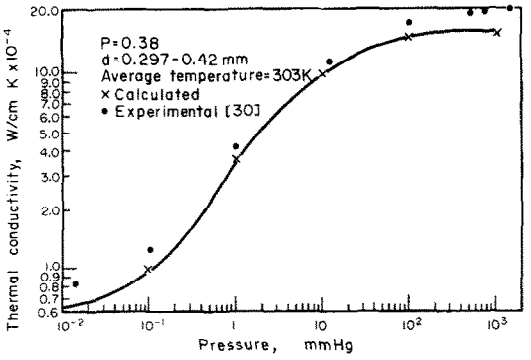

FIG. 11. Experimental and calculated thermal conductivity of glass beads in air.

to the choice of equation (19) for the effective pore size associated with the conduction heat transfer in the voids. The maximum and mean errors corresponding to Figs. 9, 10 and 11 are 28.4 and 19.4, 37 and 18.5, 23 and 17.6 respectively.

Table 1 summarizes the mean error and the variance of percentage error for all low pressure cases.

Summarizing the comparisons between calculated and experimental thermal conductivities, it is seen that the performance of the model described in this paper is sufficiently good for granular materials at atmospheric pressures. For granular materials at low pressures, the predicted thermal conductivities are generally low, but the change of the thermal conductivity with temperature and pressure is in good agreement with the changes observed in the experimental values.

The major sources of error in the calculated effective thermal conductivity values are as follows:

1. Low values for the contact conductivity predicted by $k_{cr} = 1/R_c d$.
2. Failure to account for the pure radiation process.
3. Incomplete description of particle and pore size and shape distribution by the random placement method.
4. Deviation of the actual distribution of two phases from the assumed random distribution.
5. The approximation inherent in the determination of the number of points between particles (coordination number).
6. The inexactness in estimation of the void conductivity at low pressure.

Detailed discussion of these major points is found in [1] together with recommendations for their remedy. NTIS No. N7419579.)

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APPENDIX

The model was encoded into a computer program [1] as explained. An example case is presented to give some appreciation for the program.

Case description: stainless steel spherical particles (1.7678×10^{-4} m in diameter) in helium at a temperature of 366 K and pressure greater than 2.75 atm [17].

Physical properties: $Kd = 17.85$ kcal/m hr K; $Kc = 0.156$ kcal/m hr K; $P = 0.5, 20.70 \times 10^{-10}$ N/M^2; $\nu = 0.31$; $H = 2.5 \times 10^{-2}$ m; $\delta = 7.86 \times 10^{-4}$ N/M^3; $hr/d = 4 \times 10^{-3}$; $K_r = 1.5$ g; $e = 0.93$.

Computer: $8 \times 8 \times 8$ nodes.

Input conditions: over-relaxation factor, $w = 1.2$.

Computer Program.

Iterations: 65.

Results: calculated 1.155 kcal/m hr K; experimental 1.174 kcal/m hr K [17].

CONDUCTIVITE THERMIQUE DE MELANGES HETEROGENES

Résumé—Une fonction aléatoire génératrice à densité constante est utilisée pour prédire numériquement la conductivité thermique effective des mélanges hétérogènes. La méthode est une extension de la technique de simulation digitale proposée par Baxley et Couper pour des suspensions et des émulsions. Néanmoins le modèle a été élargi pour inclure l'effet des aires de contact entre particules, l'effet de la pression réduite et du transfert par rayonnement thermique. Le modèle est applicable aux matériaux granulaires et aux poudres dans un large domaine de pression et de températures. Le modèle est comparé aux résultats expérimentaux pour des matériaux granulaires à des pressions s'étendant de la pression atmosphérique à l'environnement lunaire (10^{-8} torr). Le modèle est comparé à ceux qui existent pour les matériaux granulaires à pression atmosphérique. On note une amélioration du modèle proposé par rapport aux autres.

WÄRMELEITUNG VON HETEROGENEN MISCHUNGEN

Zusammenfassung—Ein Zufallszahlengenerator für konstante Dichtefunktionen wurde benutzt, um die effektive Wärmeleitfähigkeit von heterogenen Mischungen numerisch zu berechnen. Die Methode ist eine Erweiterung der digitalen Simulationstechnik, vorgeschlagen von Baxley und Couper für Suspensionen und Emulsionen. Das hier beschriebene Modell wurde jedoch so erweitert, daß nun der Einfluß der Kontaktflächen zwischen den Partikeln, der Effekt des verminderten Druckes und der Strahlungsaustausch berücksichtigt wird. Das Modell ist anwendbar auf körnige Materialien und Pulver über einen weiten Bereich von Druck und Temperatur. Die numerischen Ergebnisse wurden mit experimentellen Daten für Granulate vom Atmosphärendruck bis zur simulierten Mond-Umgebung (10^{-8} Torr) verglichen. Außerdem wird das Modell mit Modellen für körnige Materialien unter Atmosphärendruck aus der Literatur verglichen. Im Vergleich zu den bestehenden Modellen wird eine deutliche Verbesserung in der Genauigkeit der berechneten Ergebnisse für das vorgeschlagene Modell gezeigt.

ТЕПЛОПРОВОДНОСТЬ ГЕТЕРОГЕННЫХ СМЕСЕЙ

Аннотация — Генератор случайных чисел с постоянной плотностью распределения вероятности используется для численного расчета эффективной теплопроводности гетерогенных смесей. Данный метод является обобщением метода цифрового моделирования, предложенного Бэксли и Купером для анализа суспензий и эмульсий. В модели учитывается поверхность контакта между частицами, приведенное давление и лучистый теплообмен. Модель можно использовать для исследования зернистых материалов и порошков в широком диапазоне давлений и температур. Проведено сравнение полученных результатов с экспериментальными данными для зернистых материалов при давлениях от атмосферного до 10^{-8} + торр, которые моделируют условия на лунной поверхности. Проведено также сравнение предлагаемой модели с другими описанными в литературе моделями для зернистых материалов при атмосферных давлениях. Показано, что предлагаемая модель позволяет получить гораздо более точные результаты.