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A STATISTICAL THERMODYNAMIC THEORY FOR COORDINATION-NUMBER DISTRIBUTION AND EFFECTIVE THERMAL CONDUCTIVITY OF RANDOM PACKED BEDS

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Abstract—The constricted heat flow in packed beds of spherical particles is considered. The clustering of particles about one another is modeled after the statistical thermodynamic approach for the energy-level distribution of degenerate Boltzons. The theory establishes the local coordination number, i.e. total number of contacts on a particle, as the suitable statistical variable and predicts the coordination-number frequency for any specified bulk solid fraction of random packed beds. Heat conduction through particles in contact is then represented analytically by a network of thermal resistance in series and parallel. It is found that the effective lattice conductivity of a random packing of uniform-diameter particles increases monotonically with the bulk solid fraction. Although the theory for conductance and coordination-number distributions has been developed for the general case of random beds with particles of non-uniform diameters, results have been obtained for the case of uniform-diameter particles only. Even for this simple case, the statistical approach exhibits several features superior to the unit-cell methods.

NOMENCLATURE

A, maximum number of satellites around a base sphere;
C, denotes the combination function;
c, numerical constant defined by equation (5);
d, particle diameter;
E, Young's modulus for the constituent material of the particles;
e, thermodynamic discrete energy level;
F, total force on a contact along the line of centers;
g, degeneracy;
g', acceleration due to gravity;
H, numerical constant;
i, local (particle) coordination number; also, summation index for the local coordination number;
j, index for discrete particle species based on range of diameters;
k, thermal conductivity;
m, numerical constant in equation (5);
N, total number of particles in the powder sample, a constant;
P, uniform external pressure;
p, probability frequency;
R, thermal constriction resistances;
r, radius of the circular contact between two spheres;
S, thermodynamic entropy of the powder bed;
T, thermodynamic temperature of the powder bed;
U, thermodynamic internal energy;
V, total volume occupied by the agglomerate sample;
W, thermodynamic probability defined by equation (12);
Z, packed-bed partition function.

Greek symbols

α, Lagrangian multiplier for the number constraint;
β, β', Lagrangian multipliers for the volume constraint;
ν, angle between the direction of loading and the line of centers;
Δ, incremental quantity;
δ, solid fraction;
μ, Poisson's ratio for the constituent material of the particles;
ρ, average density;
Φ, functional form for the local solid fraction in the case of random bed consisting of particles with a size distribution;
ψ, function relating contact force to total particle force in equation (20);
Ω, trihedral solid angle at the center of a base sphere for closely-packed satellites;

Subscripts

c, for lattice or solid conduction;
e, equivalent or effective;
i, i^*, functionally dependent on the coordination numbers for base sphere and satellites, respectively;

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j, j^*, functionally dependent on the base sphere and satellites parameters, respectively;
max, maximum;
min, minimum;
s, for the constituent material of the particles.

1. INTRODUCTION

HEAT transfer in porous media is a subject of growing research interest due to the large-scale industrial use of porous materials. Particular attention here is devoted to stagnant agglomerates of unconsolidated granular particles, also known as fixed or packed beds. The interest in such packings may stem from their excellent thermal insulation characteristics as in the case of cryogenic microsphere insulation [1, 2], or the particularly large effective surface area for solid–void phase interactions leading to high efficiency of filtration, dehydration, mixing, and chemical reaction. The transport processes, whether in the voids or within the solid phase, depend strongly upon the local and the bulk clustering behavior of the particles. The problem of statistical description for the arrangement of either the voids or the solids (particles) therefore takes precedence over the modeling of the actual transport. In the following treatment, the statistical description of the packing of particles is presented in Section 2, while Section 3 is concerned mainly with the solid conduction heat transfer in the packing.

Numerous studies have addressed themselves to packing structures in agglomerates and these have been reviewed in detail by Haughey and Beveridge [3]. With very few exceptions, only packed beds comprising of uniform-diameter spheres have been considered. The macroscopic† (bulk) parameter invariably used for describing the packing state is the bulk solid fraction δ. It has been suggested that, in the case of ordered packings, the parameter δ may be inadequate in uniquely characterizing the packing state [4]. A quantitative treatment demonstrating these limitations for non-random packings has recently been presented [5]. On the hand, for homogeneously random packings, one expects very little deviation from a packing configuration typical of a specified δ. On the microscopic (local) level, this characteristic packing state is generally described by the distribution of the coordination number which is the total number of contacts on any particle. In the literature, there exist very meager experimental data on this distribution as a function of δ [6, 7]. In the absence of more extensive studies, the local and the bulk-mean coordination numbers (respectively, i and I) are often assumed to be the same, the former being considered equal on all particles. Such analyses [8, 9] also assume largely empirical linear relations between I and δ [5, 7]. The prediction of bulk thermophysical properties (e.g. effective lattice conductivity) in these studies is expected to be in some error due to the neglect of the detailed coordination distribution.

In light of these considerations, major effort in the present work is devoted to the development of a first-principle theoretical model capable of predicting the local coordination-number distribution for any specified δ and particle-size distribution (Section 2). The basic idea behind the present approach is to distribute the particles among different discretized coordination-number levels in a manner analogous to the placement of ideal gas molecules in energy levels. Special attention is given to a rigorous formulation of statistical concepts of degeneracy, distinguishability and equations of constraint for a random bed. It should be pointed out that the idea of applying the principles of statistical thermodynamics as outlined in standard texts [10] to macroscopic systems of practical interest has been successfully explored in the past [11–14].

Several other parameters, besides the preceding coordination distribution, could influence the bulk transport properties of random packed beds. These are mainly the statistical geometrical parameters such as the average number of particles per unit area and length [8, 15, 16], and also the angular distribution of the contacts around a particle [17, 18]. A brief review of such studies is available in the literature [3].

While some statistical methods have been proposed for the prediction of the mechanical [15, 19] and the fluid flow [20, 21] properties of porous media, no statistical treatment has been reported for the conduction heat flow in random packed beds, which is the primary heat-transfer mechanism in opacified evacuated microspheres or for other powder insulations at low temperatures and large compressive loads [1, 2, 22]. The present work for solid conduction can also be applied to the calculation of combined modes of energy transfer in packed beds, since these modes such as solid and gas conduction and radiation can be well approximated independent of one another [8, 23, 24]. The basic model for solid conduction in packed beds is the constriction thermal resistance of a small contact area whose magnitude is determined by the loading and the geometric conditions. The packing structure influences the analysis strongly through the determination of the load distribution and the mode of assembly of the thermal resistors. In idealized ordered packings of uniform-diameter spheres, the problems associated with the characterization of random packing structures are avoided by arranging the particles in regular crystallographic units. Such treatments, though limited to discrete values of solid fraction, yield valuable parametric information concerning the bulk lattice conductivity of a packed bed [5, 25, 26]. However, in order to account for the continuous variation of bulk density in a stratified bed such as the lunar regolith, a random packing approach based on uniform local and bulk coordination has been developed [8]. For the conduction analysis (Section 3), the present work extends this earlier study to include the size distribution of particles and frequency distribution of the local coordination.

† Throughout this paper, the term "macroscopic" indicates evaluation of a quantity for a large statistical sample, while "microscopic" refers to a sample typically of unit-cell dimensions.

2. STATISTICAL THERMODYNAMIC ANALOG FOR PACKED-BED COORDINATION FREQUENCY

General considerations

A stagnant powder bed consisting of an entirely random assemblage of a given number of spherical particles N at a prescribed bulk solid fraction δ is considered. The sample is assumed to be free from the influences of order-generating container boundaries, external force fields including gravity, and inter-particle friction forces. Particles may exhibit a size distribution p_j defined such that

$$N\int_{d_1}^{d_2} p_j\,\mathrm{d}(d_j)$$

gives the total number of particles having diameters between d_1 and d_2. This particle-size distribution depends on several variables, chief among them being the method of granulation and the subsequent sieving techniques. The size distribution is a very useful parameter since it remains invariant with any packing parameter (such as density or the method of packing, etc.) for every statistical sample of the agglomerate. In the strictest sense, the theoretical determination of p_j based on some average bed properties is within the realm of the statistical thermodynamic approach. However, it can be determined with relative ease by using one of the several methods available for this specific purpose [27].

For a macrostate specified by N, p_j and δ (hence the total volume of occupancy V), a very large number of local (i.e. microscopic) arrangements of the spheres in each other's vicinity are possible. For a complete description of these microscopic arrangements, the position coordinates for the center of every particle and its diameter d_j should be known. Based on such a description every particle can be associated with a total volume of occupancy, where the term "total" indicates both solid and void phases. This volume is a measure of the local solid fraction and depends on the coordinates and the sizes of the base sphere as well as the satellites, both in near and actual contact. As in the case of uniform-diameter beds [7], the local volume should be obtained on the basis of characteristic spherical envelope concentric with the base particle and usually of a radius equal to the base-sphere diameter. These considerations also apply for the alternate representation followed in the present treatment. According to this, the particle total volume for i contacts between a base sphere of diameter $d_j \pm \Delta d_j/2$ and satellites whose diameters can each have a variation of $\pm \Delta d_{j*}/2$ about a distinct d_{j*} is denoted by V_{ijj*} (i, d_j, d_{j*}). The dependence of V_{ijj*} on i^*, the coordination of the satellites, on the angular location around the base sphere, and on the number and position of the near contacts is considered too weak to be significant. For the case of uniform particles at least, such an assumption appears to be fairly valid [7]. The dependence of V_{ijj*} simultaneously on the parameters of the base sphere and the satellites shows that the particles cannot be treated as independent of each other as the ideal gas molecules. As seen in the treatment of moderately dense gases [10], the statistical description of such interacting particles is exceedingly complex. In the present model, it is therefore assumed that the expected value of V_{ijj*} for i contacts on a particle of diameter $d_j \pm \Delta d_j/2$ with satellites of any possible combination of diameters can be used as the particle total volume V_{ij}. By virtue of this averaging, V_{ij} is independent of the satellite parameters. For the purpose of this analysis, therefore, the particles of the packed bed consist of N independent spheres obeying the size distribution p_j and each associated with a total volume V_{ij}.

Equations of constraint

The number constraint simply states that in the absence of any comminution, a constant mass bed contains the same number of particles in any diameter range. Denoting by N_{ij} and p_{ij} the number and the frequency distribution of particles having coordination of i and diameters between $d_j \pm \Delta d_j/2$, it is seen

$$\sum_i N_{ij} = N_j = \text{constant for every } j. \tag{1}$$

For a continuous distribution of diameter, equation (1) is easily expressed as:

$$\sum_i \int_{d_j-(\Delta d_j/2)}^{d_j+(\Delta d_j/2)} p_{ij}\,\mathrm{d}(d_j) = \int_{d_j-(\Delta d_j/2)}^{d_j+(\Delta d_j/2)} p_j\,\mathrm{d}(d_j)$$

or

$$\sum_i p_{ij} = p_j = \text{constant for every } j. \tag{1a}$$

It is seen that equations (1) and (1a) are each j equations of number constraint.

The volume constraint states that a constant mass bed at a prescribed δ has a fixed total volume of occupancy V. Since volume is an extensive property, this yields:

$$\sum_i \sum_j N_{ij}V_{ij} = V = \frac{\pi}{6\delta}\sum_i \sum_j N_{ij}d_j^3 = \frac{\pi}{6\delta}\sum_j N_j d_j^3. \tag{2}$$

Define a local solid fraction δ_{ij} such that

$$\delta_{ij} = \pi d_j^3/6V_{ij}.$$

Equation (2) can now be written as

$$\sum_i \sum_j N_{ij}\frac{d_j^3}{\delta_{ij}} = \frac{1}{\delta}\sum_j N_j d_j^3. \tag{2a}$$

In the integral form, equation (2a) reduces to

$$\sum_i \int_{d_{\min}}^{d_{\max}} \frac{d_j^3}{\delta_{ij}} p_{ij}\,\mathrm{d}(d_j) = \frac{1}{\delta}\int_{d_{\min}}^{d_{\max}} d_j^3 p_j\,\mathrm{d}(d_j). \tag{2b}$$

It is observed that there is only a single equation of volume constraint, i.e. equation (2a) or (2b). For agglomerates of uniform-diameter particles, $N_{ij} = N_i$, $V_{ij} = V_i$, $d_j = d$, and $\delta_{ij} = \delta_i$. Equations (1) and (2a) then assume the following simple forms:

$$\sum_i N_i = N, \tag{3}$$

$$\sum_i \frac{N_i}{\delta_i} = \frac{N}{\delta}. \tag{4}$$

It is seen that for the case of uniform-diameter particles, the particle solid fraction depends on the

particle coordination only. Based on unit-cell results [5], the functional nature of this dependence should be of the form:

$$i = c\delta_i^m \tag{5}$$

where i and m are numerical constants. Therefore, equation (4) can be further written as

$$\sum_i i^{(-1/m)} N_i = N/[\delta c^{(1/m)}]. \tag{6}$$

For packed beds with a size distribution, the local solid fraction will depend both on the local coordination as well as the size distribution p_j. One can then express in general, $\delta_{ij} = \Phi(i, d_j)$. Equation (2b) for the variable size case can be written as:

$$\sum_i \int_{d_{\min}}^{d_{\max}} \frac{d_j^3}{\Phi(i, d_j)} p_{ij}\, \mathrm{d}(d_j) = \frac{1}{\delta} \int_{d_{\min}}^{d_{\max}} d_j^3 p_j\, \mathrm{d}(d_j). \tag{7}$$

Difficulties are anticipated in quantitative use of equation (7) since the nature of the function Φ is not explicitly known.

Distinguishability

Whereas in the case of the ideal gases the arrangement of molecules is considered in different energy levels, for the powder beds the particles are classified according to their local solid fraction and hence local coordination. Since the particles in different diameter groups (different j) have differing functional behavior for V_{ij} and δ_{ij}, the packed bed may be regarded similar to a mixture of j species of independent particles. Further it is seen that the particles are distinguishable by virtue of their physical locations in the powder matrix. This follows since the position coordinates enter in any complete microscopic description and therefore influence the local solid fraction levels also. An analogous situation occurs in the statistical treatment of solids [10] where the atoms in crystal lattices are considered distinguishable for similar reasons.

Degeneracy

Before a proper statistical description can be formulated for the agglomerate, it is important to determine if the coordination levels are degenerate. Degeneracy, as applied to the case of packed beds, is the statistical weight associated with the occupancy of any particular local solid fraction level. Qualitatively, one expects very large and very small coordination to be relatively less likely for contacts between particles of any size. Relatively large values of i should be more typical of large d_j and small d_{j*} while low values should occur for small d_j and large d_{j*}. Qualitatively therefore it appears that the coordination levels must be considered degenerate. It is further observed that around a base sphere of diameter d_j, only a fixed maximum number of spheres of uniform diameter d_{j*} can be placed. This number A_{jj*} (d_j, d_{j*}) is approximately given by

$$A_{jj*} \approx 4\pi/\Omega_{jj*} \tag{8}$$

where Ω_{jj*} is the trihedral solid angle at the vertex of a tetrahedron, the base of which is an equilateral triangle of side d_{j*} and the median is of height $\frac{1}{2}(d_j + d_{j*})$. In general, equation (8) slightly overestimates A_{jj*} by assuming a completely close-packed arrangement among the satellites. This is exact only in special cases such as when $d_j = d_{j*}$ or $d_j = d_{j*}(\sqrt{3/2} - 1)$. The latter case occurs when the base sphere fits exactly in the cavity between four equal contacting spheres. In any case, the approximation introduced in equation (8) for non-uniform particles is of minor consequence since in that case the equation needs further modification for the size variation among the satellites. This is incorporated by assuming that the frequency distribution for the diameters of the satellite spheres for any base sphere is the same as their particle size distribution. Such an assumption is evidently the most reasonable one for random beds where stratification according to particle sizes is ignored. The expected maximum number of contacts is therefore

$$A_j = \int_{d_{\min}}^{d_{\max}} A_{jj*} p_{j*}\, \mathrm{d}(d_{j*}) \tag{9}$$

where $p_{j*} = p_j$. To model degeneracy incorporating the qualitative considerations discussed earlier, a coordination number equal to A_j is assumed to be unique and therefore the degeneracy g_{A_j} is assigned a value of unity. The degeneracy for numbers other than A_j can be obtained by assuming the i contacts to be formed by spheres occupying these A_j slots. Positions causing the particles to be shared simultaneously among two or more slots are not permitted since in the absence of such a restriction g_{A_j} becomes non-unique. The statistical averaging in equation (9) also ignores the possibility (admittedly having only minor weight) of satellites which subtend partially or wholly shared solid angles at the center of the base sphere. With these restrictions in mind, it is seen that the degeneracy associated with i contacts on a particle is simply the number of different ways i slots can be picked out of a total of A_j slots without regard to the order of the choice. Hence in the notation of combination functions:

$$g_{ij} = C_i^{A_j} \equiv \frac{A_j!}{i!(A_j - i)!}. \tag{10}$$

It is noted that this combinational form of the degeneracy function does not belong in the class of the simple degeneracy relations of the type $g_i \sim i^{\text{constant}}$ as addressed by the treatment of Lienhard *et al.* [11–13]. For the case of uniform-diameter particles, $A_{jj*} = A_j = 12$. Substituting in equation (10) there obtains:

$$g_{ij} = g_i = \frac{12!}{i!(12 - i)!}. \tag{11}$$

Limits of i *and* j

The index i is assumed to vary between 1 and A_j. Actually both the lowest and the largest coordination in a real bed will be higher than these two limits. However, if $i > A_j$, the degeneracy in equation (10) is not well-defined. This discrepancy is due to the fact that an expected average maximum is used in obtain-

ing that expression. Similarly, such a low coordination as unity can occur in real beds only when effects due to inter-particulate friction forces or non-sphericity are present. It is however noted that a coordination as low as three has been observed in an experimental investigation of equal particles [6]. The important fact to note is that neither the truncation of the higher values of i nor extension at the lower end should affect the final results significantly since both these extremes have negligible statistical weight [6].

The minimum value of j is unity for the case of equal particles. An agglomerate with size distribution can be considered a mixture of as many species as we can obtain distinct constitutive equations for δ_{ij}, A_{jj}, etc. It is however essential to the statistical analysis that each of these species contains a large number of particles N_j.

Development of the equilibrium particle distribution

The preceding treatment indicates that the particles of the agglomerate are distributed among coordination levels according to Maxwell–Boltzmann statistics. As in the case of a mixture of independent ideal gases, the thermodynamic probability of a macrostate as prescribed by the constraint equations (1) and (2a) is

$$W = \prod_j W_j = \prod_j \prod_i \frac{(g_{ij})^{N_{ij}}}{N_{ij}!}. \tag{12}$$

Analogous to the conventional definition of thermodynamic probability, W_j is the number of different ways of distributing N_j Boltzons in i coordination levels each with a degeneracy g_{ij}. It is noted that in the packed-bed formulation, only a finite number of coordination levels occur unlike the correspondingly infinite number of energy levels for the case of ideal gases. The distribution of N_{ij} which maximizes W and hence $\ln W$ is considered so much more likely (i.e. $W_{\max} \gg$ and other W) that any other distribution is virtually impossible. The "equilibrium" distribution is obtained by setting $d \ln W = 0$ and solving this equation together with the constraint equations (1) and (2a). Using the method of Lagrangian multipliers (denoted as α_j and β') there obtains [10]:

$$N_{ij} = g_{ij} \exp[-\alpha_j - \beta'(d_j^3/\delta_{ij})]. \tag{13}$$

The multiplier α_j is easily eliminated by the use of equation (1) as

$$N_{ij}/N_j = p_{ij}/p_j = g_{ij} \exp[-\beta'(d_j^3/\delta_{ij})]/Z_i \tag{14}$$

where the species partition function Z_j is defined as

$$Z_j = \sum_i g_{ij} \exp[-\beta'(d_j^3/\delta_{ij})]. \tag{15}$$

Equations (14) and (15) can be further written by substituting $\Phi(i, d_j)$ for δ_{ij} as discussed earlier. For the uniform-diameter case, based on the constraint equations (3), (6) and on the single-species behavior, the above analysis results in the following expression for the coordination number distribution:

$$N_i/N = g_i \exp[-\beta i^{(-1/m)}]/z \tag{16}$$

where Z for uniform particles is seen to be $\sum_i g_i \exp[-\beta i^{(-1/m)}]$. It is seen that the Lagrangian multiplier β for the uniform-diameter case is based on the special constraint equation (6) and is dimensionally different from β'. Substituting equation (16) into equation (6), there obtains:

$$\frac{1}{\delta} = c^{(1/m)} \frac{\sum_i g_i i^{(-1/m)} \exp[-\beta i^{(-1/m)}]}{\sum_i g_i \exp[-\beta i^{(-1/m)}]} \tag{17}$$

where g_i for uniform-diameter particles is obtained from equation (11). Equation (17) is an implicit relation between the bulk solid fraction δ and the multiplier β for a specified value of the constant c.

Comparing with the ideal gas case, the thermodynamic analog of the packed bed is seen to be: the total internal energy $U \equiv$ total volume V, the discrete energy levels $e_i \equiv [i^{(-1/m)}]$. The entropy can similarly be defined as the measure of disorder and obtained from $S = H \ln W$ where H is a constant. Following the conventional definition, the thermodynamic temperature T for a packed bed can be shown as $[\beta h]^{-1}$.

Results and discussion

A set of β and the corresponding δ values is obtained by performing the summation in equation (17) on a digital computer and using for c and m respectively 11.6 and 1 as recommended by the results of a discrete analysis [5] of uniform-diameter particles in the range of the statistical solid fractions (δ between 0.56 and 0.65). It is seen from Fig. 1 that β is positive and increases with the increasing solid fraction. Once β is determined for a known solid fraction, the coordination frequency is simply that given by equation (16). Figure 2 compares the theoretical predictions of N_i/N with the experimental data [6] for two different values of δ. The lower of these corresponds to a loose or

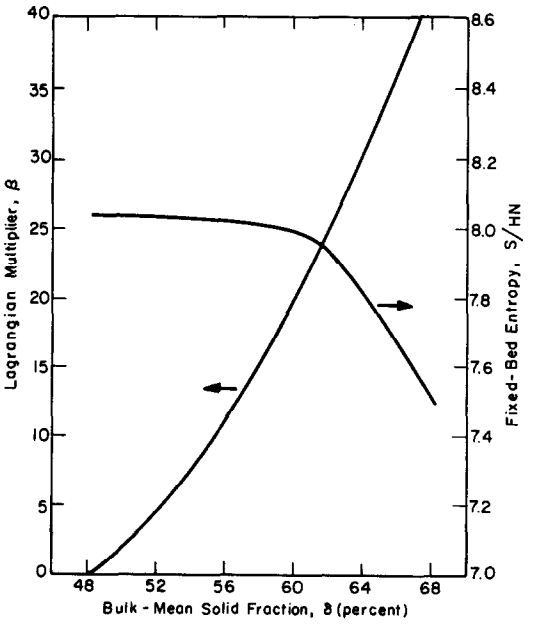

FIG. 1. Lagrangian multiplier β and fixed-bed entropy S/HN for different solid fraction δ.

gently-settled powder bed while the higher one is for dense random packings. The theory and the experiment are in excellent agreement in several aspects such as the location of the maximum (i.e. the mode of the distribution), the relative shift in the mode with change of the bulk solid fraction, and the general two-parameter asymmetric shape of the distribution.

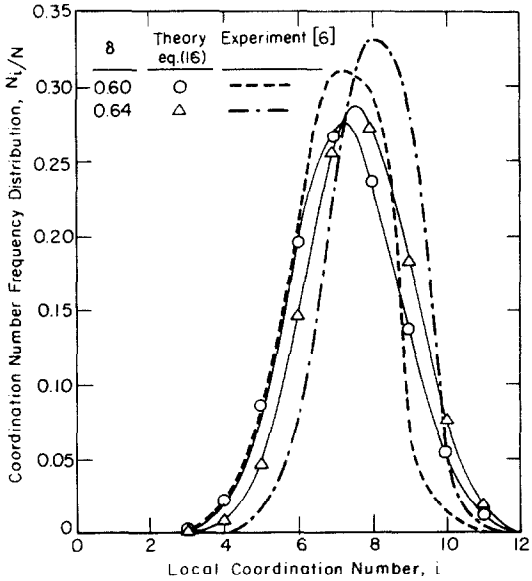

FIG. 2. Comparison between the theoretical and experimental frequency distributions of coordination numbers for uniform-sized particles.

The error in the prediction of the maximum frequency is less than 14% of the experimental value for either of the densities compared in Fig. 2. Despite various idealizations, the statistical analog thus describes the coordination distribution of uniform-diameter particles quite adequately. For the more general case of beds with a particle-size distribution, computations based on equation (14) cannot be carried out explicitly since the nature of the function $\phi(i, d_j)$ is not known. The function S/HN is also plotted in Fig. 1. It is shown that denser beds are more ordered (less entropy). Physically this is reasonable since denser beds are expected to offer less latitude in particle arrangements.

3. PREDICTION OF THE LATTICE CONDUCTIVITY OF A RANDOM PACKED BED

Analytical considerations

To analyze the thermal conductivity, it is now assumed that the random bed under consideration is subjected to a unidirectional external compressive load or to loading due to particle self-weight. The non-randomness caused by the application of a directional force-field is ignored. The density change that accrues from the application of the load is incorporated simply by considering all the parameters to be based on the final "equilibrium" bulk-mean density. The behavior of the bulk-mean density with the applied load is assumed to be known beforehand, either empirically or otherwise.

The contact radius for an elastic frictionless contact between two smooth solid spheres of the same material but different diameters is obtained from the well-known Hertz relation [28] as:

$$r_{jj*} = \left[\frac{3}{4}\frac{1-\mu^2}{E} F \frac{d_j d_{j*}}{d_j + d_{j*}}\right]^{1/3} \tag{18}$$

For a packed bed of particles such as microspheres, either under moderate loads or under self-loading, it is seen that the contact radii are on the order of 10^{-2} μm. Since particles are invariably larger than a few microns, the ratio of contact radius to particle diameter is much smaller than unity. For solid or ultra-thick microspheres, it follows that the constricted heat flow through the contact area can be closely approximated by that through a contact on a semi-infinite body [25, 26, 28]. Therefore, the Holm formula yields the correct contact resistance even in the presence of a particle size distribution. Accordingly

$$R_{jj*} = \frac{0.5}{k_s r_{jj*}}. \tag{19}$$

In the case of a uniform external load P, the total force on any unit section through the powder and perpendicular to the direction of loading is constant. For the self-loading case, however, the force due to "hydrostatic" pressure at a particular depth z in the bed ($P = \rho g' z$) increases with this depth. In either case, the present treatment assumes that the total force at a cross-section manifests as a uniform pressure on the solid areas in a cross-sectional slice perpendicular to the direction of loading. In both the cases the bulk density can vary with the depth. Considering the fact that for a random bed the bulk area and volume solid fractions are equal [16], the uniform pressure on the solids P_s equals P/δ. The expected solid area of a random cross-sectional slice through a particle of diameter d_j has been shown equal to $\pi d_j^2/6$ [8, 15]. Therefore the load at any frictionless contact is simply

$$F = \frac{\pi}{6}\frac{P d_j^2}{\delta}\psi(i, \gamma) \tag{20}$$

where $\psi(i, \gamma)$ is a function of the particle coordination number i and γ with γ being the angular location of the contact with reference to the direction of loading. The precise functional nature of $\psi(i, \gamma)$ evidently depends on the complex static force balance on the base sphere.

Combining equations (18) (20)

$$R_{jj*} = \frac{1}{k_s}\left[\frac{1-\mu^2}{E}\frac{\pi P \psi}{\delta}\frac{d_j^2 d_{j*}}{(d_j + d_{j*})}\right]^{1/3} \tag{21}$$

It is further noted that an average area equal to $(\pi d_j^2/3i\delta_{ij})$ and an average layer height equal to $(1/2)(d_j + d_{j*})\cos\gamma$ are associated with the resistance R_{jj*}. The equivalent thermal resistance per unit bulk area and length is therefore seen to be

$$(R_e)_{i,j,\gamma} = \frac{2\pi d_j^2 R_{jj*}}{3\delta_{ij} i (d_j + d_{j*})\cos\gamma} \tag{22}$$

Hence the effective lattice conductivity for base particles of diameter d_j with coordination number i and

contact at angle γ is

$$(k_c)_{i,j,\gamma} = (R_e)^{-1}_{i,j,\gamma} = \frac{3\delta_{ij} i (d_j + d_{j*}) k_s \cos\gamma}{2\pi d_j^2 \left[\dfrac{(1-\mu^2)\pi P \psi d_j^3 d_{j*}}{E\delta(d_j + d_{j*})}\right]^{-1/3}}. \quad (23)$$

The effective lattice conductivity for particles of all sizes and coordination numbers and of equi-probability of contact angular distribution is therefore given by:

$$k_c = \frac{2}{\pi} \sum_i \sum_j \left(\frac{N_{ij}}{N}\right) \int_0^{\pi/2} (k_c)_{i,j,\gamma} \, d\gamma. \quad (24)$$

Substituting from equation (14) for (N_{ij}/N), there results:

$$k_c = \frac{2}{\pi} \sum_i \int_{d_j} \int_0^{\pi/2} \frac{g_{ij}}{z_j} \exp[-\beta' d_j^3 / \Phi(i, d_j)] p_j \times (k_c)_{i,j,\gamma} \, d(d_j) \, d\gamma. \quad (25)$$

For the case of uniform-diameter particles, $d_j = d_{j*} \equiv d$, $\delta_{ij} \equiv \delta_i$ and $N_{ij} \equiv N_i$. Based on $\psi = 2/i \cos\gamma$ and equation (16) for N_i/N there follows:

$$\frac{k_c}{k_s \left[\dfrac{(1-\mu^2)P}{E}\right]^{1/3}} = \frac{0.65\,\delta^{-1/3}}{Z} \sum_i g_i \delta_i i^{2/3} \exp[-\beta i^{(-1/m)}] \quad (26)$$

where β is known for any bulk density from Fig. 1.

Results and discussion

The variation of the non-dimensional lattice conductivity based on the present theory has been obtained by numerical summation of equation (26) on a digital computer and is presented in Fig. 3 along with the discrete points obtained from the lattice-defect analysis. The statistical results cover the range from a lower critical solid fraction of about 0.48 to an upper closest-packed bed of solid fraction 0.74. The calculations assume c and m values equal to 11.6 and 1 in equation (5) up to a solid fraction of 0.68 [5, 9].

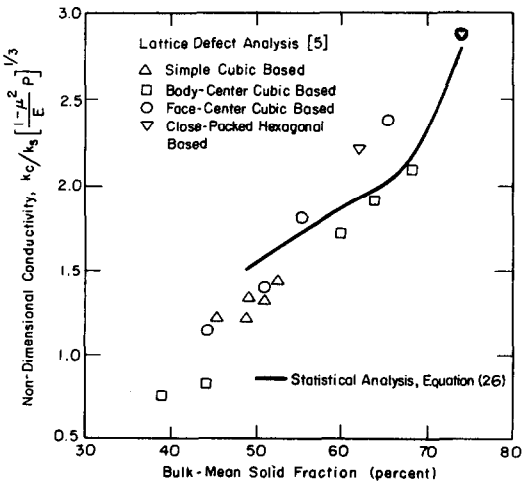

FIG. 3. Theoretical lattice conductance as a function of solid fraction.

However, these values do not characterize the closest-packing state adequately [9]. Corresponding to this solid fraction, equation (26) simply uses $\delta = \delta_1 = 0.74$ and $i = I - 12$. Also for this unique state, $N_i/N = 1$.

The statistical analysis is seen to be in excellent agreement with the discrete unit-cell analysis for the case of uniform-diameter particles [5]. By providing conductance continuously for any specified bulk density, the statistical treatment is a definite improvement over the unit-cell method. However, the most significant advantage of the present statistical approach lies probably in its ability to predict both the coordination-number distribution and the thermal conductance of packed beds with varying particle size. Computational work for this case is currently in progress.

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UNE THEORIE DE THERMODYNAMIQUE STATISTIQUE POUR LA DISTRIBUTION EN NOMBRE DE COORDINATION ET LA CONDUCTIVITE THERMIQUE EFFECTIVE DES LITS FIXES

Résumé—On considère le transfert thermique dans les lits fixes de particules sphériques. Le groupement de particules autour d'une autre est modélisé à partir de la thermodynamique statistique pour la distribution des niveaux d'énergie de Boltzons dégénérés. La théorie établit le nombre de coordination local c'est à dire le nombre total de contacts d'une particule, comme étant la variable statistique convenable et elle prédit la fréquence du nombre de coordination pour des lits fixes en désordre. La conduction thermique à travers les particules en contact est représentée analytiquement par un réseau de résistances thermiques en série et en parallèle. On trouve que la conductivité de structure, de particules de diamètre constant et disposées au hasard, croit monotoniquement avec la fraction de solide. Bien que la théorie ait été développée dans le cas général de lits en désordre avec des particules de diamètre non uniforme, on a obtenu des résultats dans le cas de particules de diamètre uniforme. Même dans ce cas simple, l'approche statistique montre plus de richesse que les méthodes à cellule unitaire.

EINE THEORIE DER STATISTISCHEN THERMODYNAMIK ZUR VERTEILUNG DER KOORDINATIONSZAHL UND EFFEKTIVEN WÄRMELEITFÄHIGKEIT VON BELIEBIG GEPACKTEN SCHÜTTUNGEN (ZUFALLSSCHÜTTUNGEN)

Zusammenfassung—Es wird der eingeschnürte Wärmestrom in Schüttungen von sphärischen Körpern betrachtet. Die Lage der Partikel zueinander wird dargestellt entsprechend der Behandlung der Energieniveauverteilung von degenerierten Boltzmann-Teilchen in der statistischen Thermodyanmik. Die Theorie führt die örtliche Koordinationszahl, d.h. Gesamtzahl aller Kontakte an einem Partikel, als die geeignete statistische Variable ein und gestattet die Bestimmung der Häufigkeit der Koordinationszahl für jeden bestimmten Feststoffanteil von Zufallsschüttungen. Die Wärmeleitung durch Partikel, die sich berühren, wird analytisch dargestellt durch ein Netzwerk von Wärmeleitwiderständen, die in Reihe und parallel geschaltet sind. Es wurde festgestellt, daß die effektive Gitterleitfähigkeit von Zufallsschüttungen von Partikeln gleichen Durchmessers monoton mit dem Feststoffanteil wächst. Obgleich die Theorie für die Leitfähigkeit und die Verteilung der Koordinationszahl für den allgemeinen Fall von Zufallsschüttungen von Partikeln ungleichen Durchmessers entwickelt wurde, konnten Ergebnisse nur für den Fall einheitlichen Durchmessers erzielt werden. Selbst für diesen einfachen Fall weist die statistische Behandlung mehrere Eigenschaften auf, die den Methoden der Elementarzellen überlegen sind.

СТАТИСТИЧЕСКАЯ ТЕРМОДИНАМИЧЕСКАЯ ТЕОРИЯ РАСПРЕДЕЛЕНИЯ КООРДИНАЦИОННОГО ЧИСЛА И ЭФФЕКТИВНОЙ ТЕПЛОПРОВОДНОСТИ СЛОЕВ С БЕСПОРЯДОЧНОЙ УКЛАДКОЙ ЧАСТИЦ

Аннотация — Рассматривается обжатый тепловой поток в плотных слоях сферических частиц. Взаимная группировка частиц моделируется на основе статистического термодинамического подхода к распределению энергетического уровня вырожденных больцонов. В теорию вводится локальное координационное число, т. е. полное число контактов отдельной частицы в качестве удобной статистической переменной, и расчитывается частота координационного числа для любого относительного объема твердой фазы слоев с беспорядочной упаковкой частиц. Теплопроводность через контактирующие частицы представлена аналитически с помощью сетки последовательных и параллельных теплосопротивлений. Найдено, что эффективная проводимость сетки беспорядочных частиц одинакового диаметра монотонно увеличивается с ростом относительного объема частиц. Хотя теория теплопроводности и распределения координационного числа развита в общем случае для слоев беспорядочной упаковки частиц разных диаметров, конкретные результаты получены только для частиц одинакового диаметра. Статистический метод имеет некоторые преимущества по сравнению с методами одной ячейки даже для данного простого случая.