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Voronoi Cell Properties from Simulated and Real Random Spheres and Points

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Results are reported of a computer-aided study of the properties of Voronoi cells generated from randomly placed impenetrable uniform spheres which saturate a space and of Poisson points in three-dimensional space. An empirical expression is suggested for the volume distribution function and an expression for the probability of the nth nearest neighbor of a Voronoi cell nucleus forming a cell face. Comparison is made with the work of Meijering [*Philips Res. Rep.* **8**:270 (1953)], Finney [*Proc. R. Soc. (London)* **A319**:479, 495 (1970)], Kiang [*Z. Astrophys.* **64**:433 (1966)], and others. Radial distributions, coordination number, and packing density are discussed for the spheres.

KEY WORDS: Voronoi cell; tesselation; Poisson; random spheres; packing density.

INTRODUCTION

The random packing of three-dimensional space has been studied by many investigators[1-20] using physical models and computer simulation. Computer simulations of random assemblies of hard (or elastic) spheres have been used to study the statistical mechanics of fluids.[21,26,36,37] Models for describing the apparently random spacing of stars within galaxies[19] as well as aiding in the understanding of percolation theory,[30] statistical mechanics of microemulsions,[28,29,32] structure of glassy metals,[27] and deformation and microcracking of porous materials[31,33] have been developed using random space dividing processes.

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One of the most promising models of random tesselations of space is the model based on Voronoi cells (also called Dirichlet cells). Voronoi cells are generated by starting with a distribution of points. The distribution of points may represent centers of volumes of physical entities used in any model. The location of the points can be assigned from experimental data or by random processes. For computer simulations, a Poisson distribution of points is often used. In principle the following process can be used to describe the process used to define the cells. Perpendicular bisecting planes are erected to lines connecting all possible pairs of the given points. Out of this rather enormous number of planes, only the portions of those planes that serve to define unique regions about each point are retained. The uniqueness of the region consists in the fact that any location within the region associated with each entity is closer to "its" point center than to any other point center.

Meijering[24] has deduced the following mean values for the Voronoi polyhedra generated by Poisson points: Volume (b^3),[2] number of faces (15.54), number of edges (40.61), number of vertices (27.07), surface area $(5.821b^2)$, and total edge length $(17.50b)$. In addition, Santalo[23] gives a deduced expected mean number of sides per face of 5.226 which has also been experimentally demonstrated by Rahman.[37] The volume probability distribution function is not known for the Voronoi cell volumes generated from a set of Poisson points in space. An evaluation of the variance of the volume probability distribution has been given by Gilbert[25] as $0.178b^2$ for a density of Poisson points of $1/b$.

In this study some additional information about the Voronoi construct of three-dimensional space is reported. The purpose is to describe some additional knowledge of the details of random space filling, i.e., probabilities of high number nearest-neighbor face formation, coordination number information for random equal sphere distributions, a more refined study of the Poisson point cell volume distribution to compare with Kiang's[22] proposed volume distribution, and a determination of the saturation density of sequential random filling of space by uniform spheres, etc. This information, although not necessarily immediately directly applicable to any particular model of material properties, has an intrinsic value in itself in understanding space. For instance, any suggested quantization of space (or phase space) might conceivably be found to bear a relationship to the rather extreme localization brought about by the "regions of influence" defined by Voronoi cells.

[2] The value of b is, of course, completely arbitrary and depends on the choice of scale of spacing (i.e., numerical density) of the Poisson distribution.

METHOD AND RESULTS

Spheres

A previous computer simulation study[35] of the random sequential filling of space with uniform impenetrable spheres of unit diameter has been described. In this study a basic volume of 1000 unit volumes was used and this volume was filled to saturation by successively placing randomly chosen sphere locations. Edge corrections were made by standard replication methods. The study resulted in an estimated saturation density of $0.710 \pm .016$ sphere centers per unit volume. A further study of the completeness of the saturation of the distributions of spheres in the data from this previous work was accomplished by examining (by computer methods) the region in a thin concentric shell about each of the existing spheres for the possible accommodation of any additional sphere placed tangent to the sphere being examined. Any existing void large enough to hold a sphere would necessarily involve an accommodation of a sphere located tangent to one of the spheres defining the walls of the void. For each of the 2079 total spheres in the three arrays of the original study, attempts were made at 529 nearly equally spaced sphere center positions for possible accommodation. In all a total of 42 additional spheres accepting vacancies were found, yielding a final net saturation density of 0.707 sphere centers per unit volume as the best estimate of saturation density of nonoverlapping, randomly placed, and nontouching spheres. The central cores of the three simulation saturation sets (before the location of the 42 arbitrarily filled voids) yielded 709 sphere center locations suitable for a study of Voronoi cell volume distribution under nearly saturation conditions.

Points

In order to obtain the volume distribution for Poisson point generated Voronoi cells a set of 3000 such independent Voronoi cells was generated by the following process: A fixed volume was simulated and within this volume a Poisson distribution of points was laid down by a random number generator setting the Cartesian coordinates of the points. The number of points laid down in the volume in each case was programmed so that the distribution over the 3000 cases would correspond to a normal variation of points per case about a mean value of 1000. For each case, a point near the center of the volume was chosen by random means. The Voronoi cell of this chosen point was evaluated by determining all the nearest neighbors in order about the point and analyzing the structure of the cell.

For the spheres and for the points, a record was kept of the number of faces, vertices, sides per face, nearest-neighbor contribution to face forming, and cell volume. The surface area of each cell was also recorded for the cells generated from points.

Results

Tables I–III show the results of this study on points and spheres, the results of Finney's study on spheres, and Meijering calculated values. The data for the 3000 Poisson points agrees to within one standard deviaiton of the Meijering's means in all categories except for the mean number of faces per cell which falls within 1.5 standard deviations. In addition, the second moment of the observed volume distribution agrees (see below) well with the computer integrated expectation value. Hence the data should serve as a base for determining the empirical volume distribution. The data for the topological parameters in both of the sphere studies indicate significant departures from the values expected for Poisson point-generated parameters. These departures show a definite decrease in faces per cell (and a corresponding decrease in vertices per cell consistent with Euler's condition on edges, faces, and vertices of these types of cells) in both sphere studies, with the greater departure occurring for Finney's more tightly packed spheres. The presence of a sphere at the center of each cell, together with the limiting effect of the increased density of neighboring spheres, might plausibly cause the vertex angles of the cells to be more uniformly obtuse and to thus apparently create fewer faces and vertices as a consequence. Table II and Table III verify that the presence of a sphere at the center of a Voronoi cell inhibits the range of the number of faces and sides, respectively, of the cells.

Packing Densities. The experimental density values (recorded as the fraction of space occupied by the spheres themselves) are given in the last column of Table I. Finney's value was obtained for "lightly touching" spheres where no uniformity of cell structure has been introduced by shaking the steel balls together. His value of 0.6366 represents the saturation density fraction of "touching" randomly placed spheres whose touching is assumed to be sufficient to afford stable support of the spheres for a gravitational field applied in any direction. The corresponding saturation density fraction of 0.370 determined in the present study represents the case of "nontouching" spheres whose random positions preclude the existence of any appreciable number of voids in the sample large enough to accommodate a single additional sphere. Two speculative observations are of interest. The fact that the "nontouching" and the "touching" density fractions

Table I. Descriptive Data on Voronoi Cells

Study	Cases	Faces	Sides/face	Vertices	Area	Density
Meijering study	—	15.54	5.226[a]	27.07	5.821	—
Hanson points	3000	15.63 ± .06	5.23 ± 0.01	27.18 ± 0.12	5.81 ± 0.03	—
Hanson spheres	709	14.96 ± 0.07	5.20 ± 0.01	25.92 ± 0.13	—	0.372 ± 0.008
Finney spheres	5500	14.251 ± 0.015	5.158 ± 0.003	—	—	0.6366 ± 0.0004

[a]Santalo (Ref. 23).

Table II. The Frequency of Occurrences of n-Faced Voronoi Polyhedra

Faces per cell	Hanson points		Hanson spheres		Finney spheres
5	1	0.0%	—		—
6	1	0.0%	—		—
7	6	0.2%	—		—
8	10	0.3%	—		—
9	45	1.5%	—		—
10	80	2.7%	3	0.4%	—
11	154	5.1%	15	2.1%	0.2%
12	231	7.7%	41	5.8%	4.3%
13	279	9.3%	84	11.8%	20.5%
14	319	10.6%	136	19.2%	34.9%
15	384	12.8%	171	24.1%	27.3%
16	380	12.7%	117	16.5%	10.7%
17	293	9.8%	87	12.3%	2.1%
18	256	8.5%	38	5.4%	0.1%
19	198	6.6%	15	2.1%	—
20	138	4.6%	2	0.3%	—
21	85	2.8%	—		—
22	60	2.0%	—		—
23	33	1.1%	—		—
24	19	0.6%	—		—
25	16	0.5%	—		—
26	3	0.1%	—		—
27	4	0.1%	—		—
28	4	0.1%	—		—
29		—	—		—
30	1	0.0%	—		—

Table III. The Frequency of Occurrence of n-Sided Faces on Voronoi Polyhedra

Sides per face	Frequency 3000 Hanson points		709 Hanson spheres		5500 Finney spheres
3	6352	13.5%	1124	10.6%	4.8%
4	10741	22.9%	2310	21.8%	18.9%
5	11312	24.1%	2960	27.9%	40.1%
6	8893	19.0%	2454	23.1%	28.9%
7	5398	11.5%	1230	11.6%	6.3%
8	2738	5.8%	399	3.8%	1.0%
9	1030	2.2%	110	1.0%	—
10	313	0.7%	19	0.2%	—
11	85	0.2%	2	0.0%	—
12	30	0.1%	—	—	—
13	3	0.0%	—	—	—
14	1	0.0%	—	—	—
15	—	—	—	—	—

are within standard deviations of $1/e$ and $(1 - 1/e)$, respectively, may suggest a plausible complementarity of the two cases. The second observation is that the observed saturation density of the sphere center points (0.707 centers per unit volume) in the present study is very close to $1/2$ of the value of the accepted maximum possible density of $\sqrt{2}$ centers per unit volume for hexagonal close packing.

Volume Distribution. The value of the mean volume of the cells obtained from the point (or sphere) data and the known value of the Poisson intensity (or saturation density) of distribution are related by a reciprocal averaging relationship. The mean volumes obtained from the Voronoi cell data are within a standard deviation of the values expected from the known densities of distributions of centers for the finite samples involved.

The data from Kiang's[22] study and from this study for the volume distribution of Poisson point-generated Voronoi tesselations are shown in Figs. 1 and 2. The error bars represent standard deviations. The two curves shown represent two approximation functions which may be used to

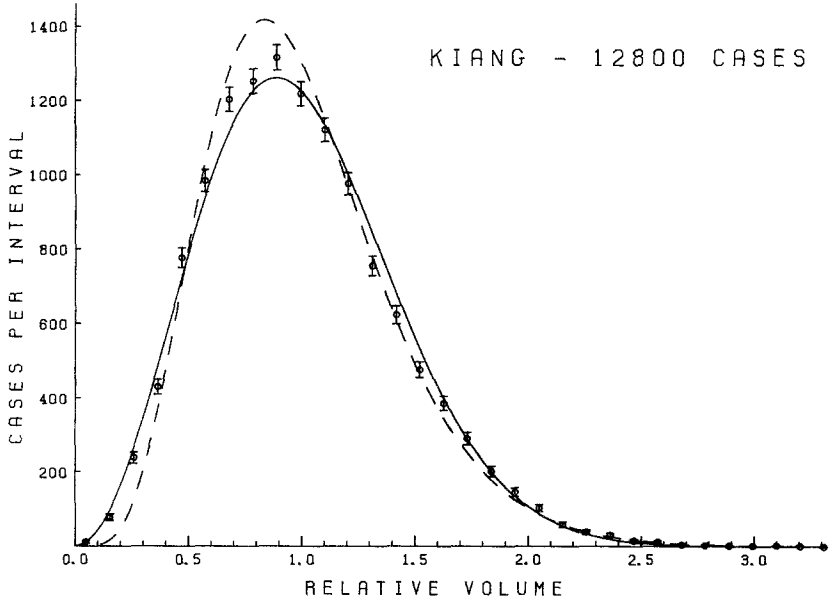

Fig. 1. The relative volume distribution data for the Voronoi tesselations generated by Kiang's study (Ref. 19) of 12800 Poisson points. The x-axis represents the ratio of the volumes of the tesselation cells to the mean volume. The bars denote standard deviations. The solid curve represents the Maxwell expression and the broken curve represents Kiang's suggested function.

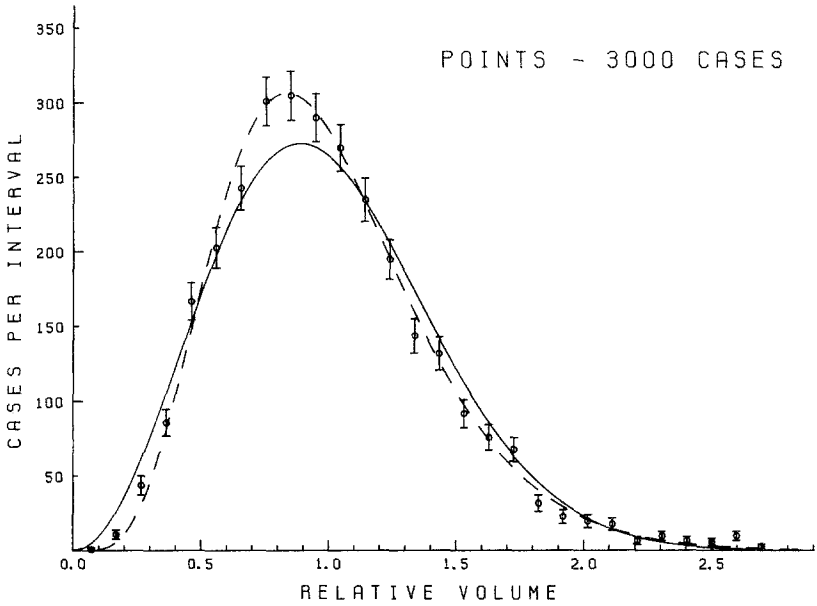

Fig. 2. The relative volume distribution data for the Voronoi tesselations generated by this study of 3000 Poisson points. The x axis represents the ratio of the volumes of the tesselation cells to the mean volume. Intervals are 0.0972 on centers. Symbols are the same as Fig. 1.

represent the volumes in modeling work. The function represented by the broken curve is suggested by Kiang:

$$P_{x,x+dx} = \frac{6}{\Gamma(6)} (6x)^5 e^{-6x}\, dx$$

where the relative volume, x = volume/(mean volume), and $P_{x,x+dx}$ represents the probability of a cell's relative volume lying between x and $x + dx$.

It was noticed that the surprisingly good fit with the experimental data was achieved by using a Maxwell speed distribution function to represent the data. No a priori reason can be cited for expecting a match between the speed distribution function of Maxwell and the volumes distribution of Voronoi tesselations other than a vague similarity in the nature of the randomness of the vectors describing velocities in Maxwell's case and normals to the faces of the cells of the tesselations in the Voronoi case. The Maxwellian expression for the probability of the relative speed of an atom lying between x and $x + dx$ is given by

$$P_{x,x+dx} = \frac{32}{\pi^2} e^{-(4/\pi)x^2}\, dx$$

This expression is derivable from the geometric properties of three-dimensional space alone[34] and is represented by the full curve in the figures. Boltzmann's constant k and the absolute temperature T usually associated with the Maxwellian distribution function are related to thermodynamical reasoning and play no role in the above equation. In any event, the expression fits the data quite well if one simply allows x to represent the relative volume of the cells. The relationship becomes then

$$n = \frac{32N}{\pi^2}\left(\frac{v}{\bar{v}}\right)^2 e^{-(4/\pi)(v/\bar{v})^2}\frac{dv}{\bar{v}}$$

where n is the expected number of observations in any interval of width $(dv/\bar{v})$ and N is the total number of cases observed. The Maxwell curve is shown by the full line in Figs. 1 and 2.

It appears from Kiang's data in Fig. 1 that both curves are only approximate representations of the empirical distribution function for Voronoi tessellations. Near the peak of the curves and at smaller volumes, the Maxwell expression fits Kiang's data best while Kiang's expression gives a better fit in the range of relative volumes from 1.0 to 2.0. In the case of the present study shown in Fig. 2, however, Kiang's expression is clearly superior. A chi-square distribution test ranks the Kiang function fit near the 80 percentile (i.e., 80% of data would exhibit a better fit). The lack of positive fit of the Maxwell expression, however, became apparent in the study when approximately 3000 cases were analyzed. Either function might be useful in models that depend on the properties of Voronoi tesselations.

An evaluation of the second moments of the two above functions as well as the moments of the data and of the expected second moment of the point generated cells was made. The second moment of both functions can be calculated to any desired degree of precision. A value of 1.178097 . . . for Maxwell and a value of 1.166667 for Kiang is obtained. Gilbert[25] gives 1.178 as the second moment value obtained by numerical integration of the expectations implied in the Voronoi construct. Gilbert's numerical integration value and the precisely known value of the second moment for the Maxwellian expression are so nearly the same that a repetition of Gilbert's method was performed to gain greater numerical precision. The results of this computer integration gave a value of the second moment of 1.178817. Hence, this confirms that the Maxwell function definitely is not a true representation of Voronoi cell volume distributions. Nevertheless, it may serve as a useful tool in applied modeling. The data for relatively large volumes are not sufficient to distinguish which curve is better. Estimates of possible systematic errors inherent in the "graininess" contributed by the pseudorandom number generator used and the finiteness of the computer do not seem large enough to account for the discrepancy between the data

and either of the suggested expressions. The experimental value of the second moment calculated for Kiang's data is 1.168 and for the Poisson points of this study the value obtained is 1.179.

Figure 3 shows the data for the computer-simulated filling of space by equal spheres together with the Maxwell and Kiang curves. Both expressions have been modified to include a "smallest volume," v_0, so that x becomes

$$x = \frac{v - v_0}{\bar{v} - v_0}$$

The value of v_0 which best fits the data in a "least-squares" sense was $v_0 = 0.694$. Figure 4 shows corresponding data for Finney's 5500 actual spheres whose measured center positions were used as Voronoi tesselation centers. A "least-squares" determined value of $v_0 = 0.900$ was used in representing the Finney data. No significance is readily apparent for these

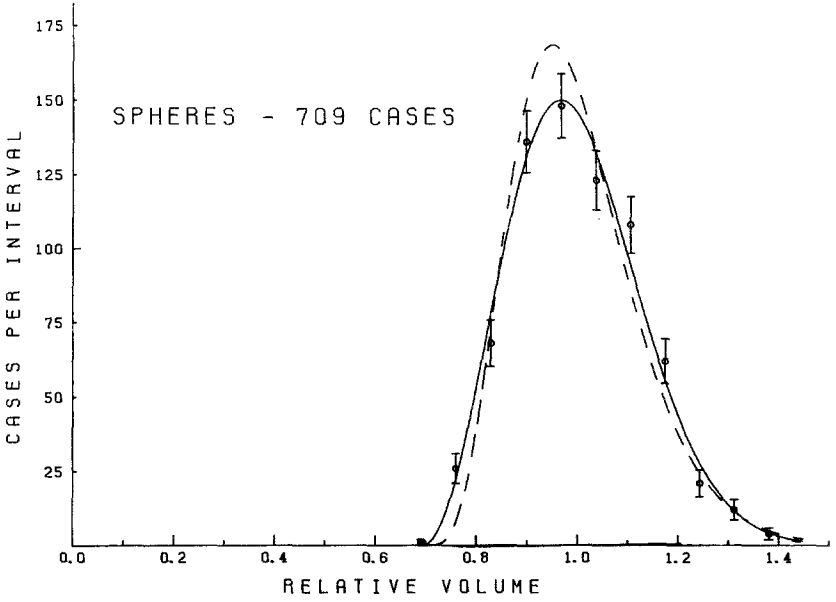

Fig. 3. The relative volume distribution data for the Voronoi tesselations generated by 709 computer simulated nonoverlapping and nontouching spheres whose random locations were serially chosen by a random generator until a replicated region was saturated. The x axis represents the ratio $(v - v_0)/(\bar{v} - v_0)$, where $\bar{v}$ is the mean volume of the tesselation cells and v_0 is an arbitrary constant chosen to give the best fit. The bars denote standard deviations. The solid curve represents a modified Maxwell expression and the broken curve represents Kiang's modified function.

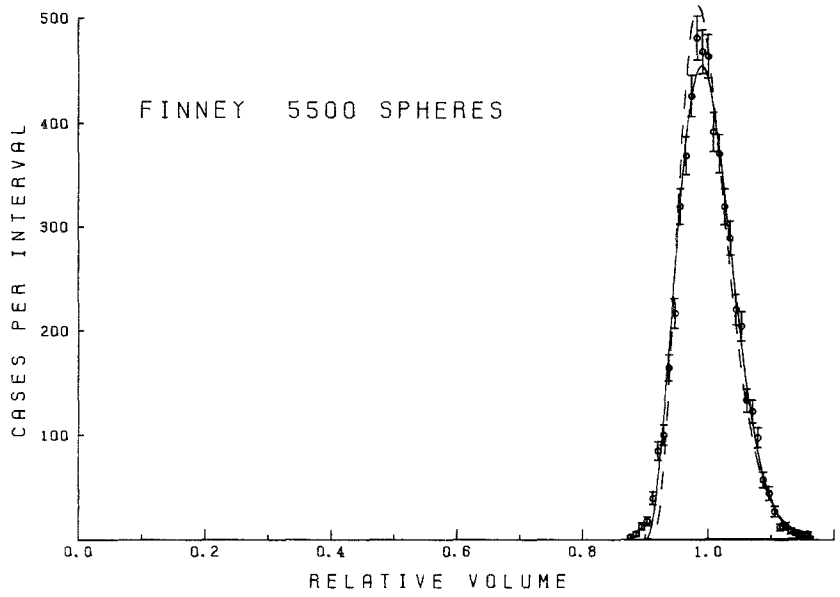

Fig. 4. The relative volume distribution data for the Voronoi tesselations generated by Finney's study (Ref. 11) of 5500 steel spheres. The x axis represents the ratio $(v - v_0)/(\bar{v} - v_0)$, where $\bar{v}$ is the mean volume of the tesselation cells and v_0 is an arbitrary constant chosen to give the best fit. The bars denote standard deviations. The solid curve represents the modified Maxwell expression and the broken curve represents Kiang's modified function.

values of v_0. The resulting volume distribution data are remarkably well represented by the Maxwell curve. As expected, both Fig. 3 and Fig. 4 show narrower peaks than Fig. 1 and Fig. 2 because the "saturation" effects of the volume occupied by the spheres themselves. There is less space to be randomly divided among the cells.

Radial Distribution of Spheres. Figure 5 shows a plot of the radial distribution of the centers of the spheres in the saturation of space simulation study. A splitting in the second peak is observed in other studies[2,5,10,11] of touching spheres. A suggestion of a split in the second peak at a radius of 2.0 diameters is apparent in Fig. 5 even though the spheres in this case are not touching.

Coordination Number. Figure 6 shows a plot of the local average density around the cells in the saturation of space by spheres study. An insert in the figure shows the details of the slope of the local numerical

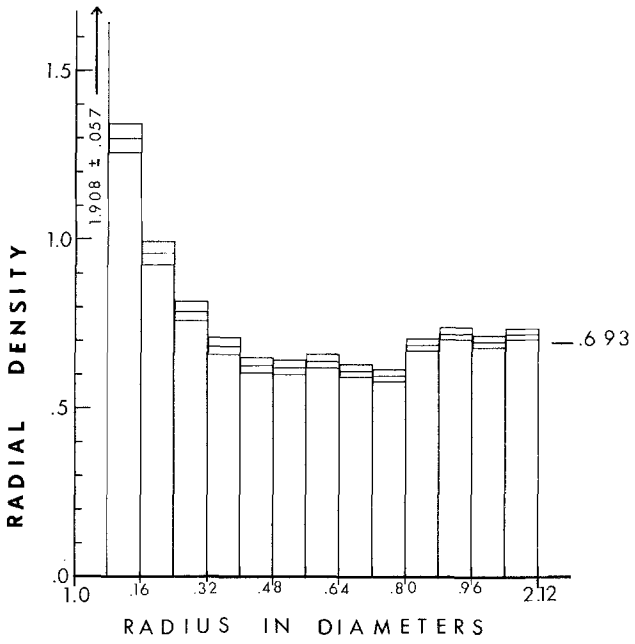

Fig. 5. The observed radial distribution of densities of the centers of simulated spheres (sphere centers/unit volume) about 1067 sphere centers from Ref. 35. Radial intervals are 0.16 sphere diameter. Standard deviations are indicated for each interval. The value of 0.693 represents the mean density of the data shown.

density of spheres centers. It is readily seen that the slope changes at $n = 8$. Hence, the first eight nearest neighbors bear a special relation to any sphere in a "saturated" configuration. This information agrees with the observation of Finney[11] and may be of value in "hard sphere" models of the transition region between the liquid and gas phases of matter.

Nearest-Neighbor Use. Figure 7 shows the data on the probability of use of the nearest neighbors of a point or sphere center in forming a face of a Voronoi cell. Standard deviation bars are displayed for the data. The solid curve is a plot of the arbitrarily selected function

$$P_n = \exp\left[- K(n-1)^{3/2} \right]$$

where P_n represents the probability of use of the nth neighbor. No a priori reasoning suggest this functional form but it does seem to represent the data for Poisson points as centers of Voronoi cells quite well when K is selected so that the integrated sum of the expression for all n agrees with the Meijering value of 15.54 for the average number of faces. The value of K obtained is 0.01471. Chi-square tests of the fit for the 3000 cases of

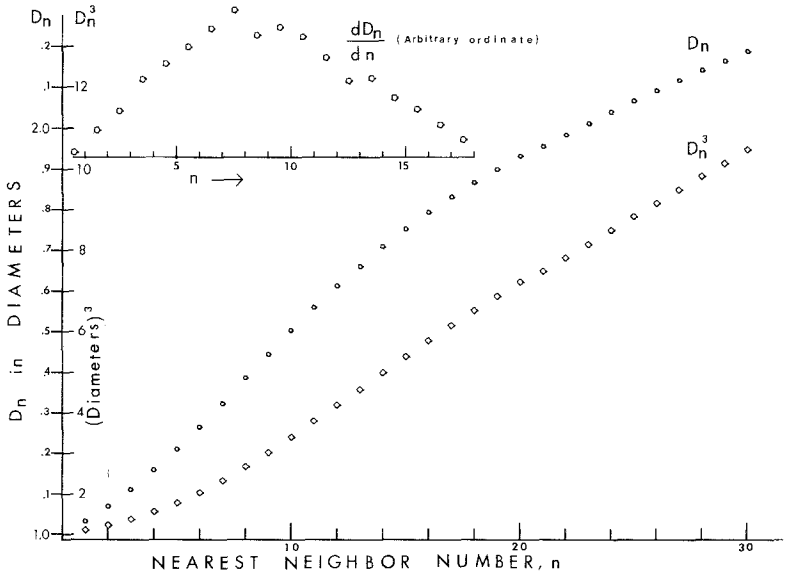

Fig. 6. Mean center-to-center distances D_n and D_n^3 of Nth nearest neighbors for 1067 spheres from Ref. 32. Insert shows slope of D_n curve for first 15 nearest neighbors. Change of slope at $N = 8$ indicates effective coordination number of 8.

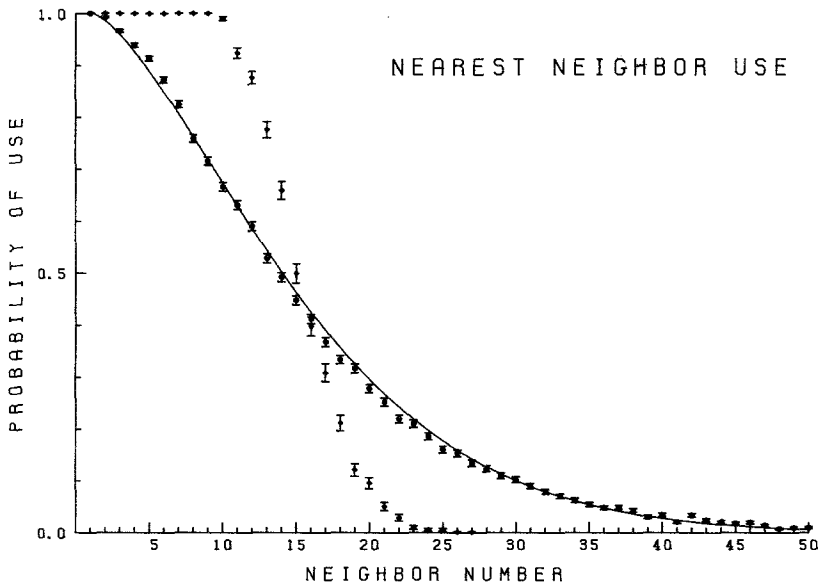

Fig. 7. Nearest-neighbor probabilities of forming a Voronoi cell face for first 50 nearest neighbors. Solid curve data points are for Poisson point generated cells. Independent points are for saturation sphere study data (Ref. 32). Solid curve is arbitrary function described in text.

Poisson points show a definite lack of fit for this expression, especially in the range of the second to the seventh nearest neighbor. Nevertheless, the expression may be of value for modeling purposes. Out of the (3000)(15.54) faces observed in the point study, two faces were found at the 95th and 98th nearest neighbor. Note of interest: The expression for P_n taken together with the general dependence of the location of the nth neighbor as being determined by the cube of the neighbor's radial coordinate establishes a "sphere of influence" about each nucleus of a Voronoi cell that is attenuated as $\exp(-\text{const}\, r^{9/2})$. That is, the probability of inclusion ("inside" a face along line of centers) decreases in an especially rapid fashion.

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