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Robert K. Henke for the degree of Master of Science in Nuclear Engineering presented on July 1, 1981

Title: Stochastic Simulation of Sphere Beds and the Effect of Packing Density on the Thermal Conductivity of Sphere Pac Nuclear Fuels

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The establishment of any thermal model of reactor fuel requires a thorough understanding of the behavior of the thermal conductivity. This is especially true in the case of sphere pac fuels where the conductivity is a function of many variables beyond those normally affecting conventional fuels. One of these variables, packing density, is not fully accounted for in present unit cell models of thermal conductivity. In this thesis, a method has been developed whereby the effect of packing density and its importance can be evaluated for any type of unit cell.

The effect of packing density is due to the random orientation of the unit cells in the bed with respect to heat flow. The calculation of the "cell orientation effect" must therefore account for each cell in the packing. This requirement resulted in the development of the RANDPAC code - a Monte Carlo program for simulating the packing of spheres in a cylinder. RANDPAC generates and provides detailed information concerning the location and coordination

of every sphere in a random cylindrical bed. By coupling this information with data pertinent to the characterization of the unit cells in the bed, the effective conductivity of the bed relative to the unit cell conductivity (the cell orientation factor) can be evaluated. This procedure is carried out by the ORIENT code.

Evaluation of the orientation factor for a unit cell currently in use has shown that packing density has a significant effect which cannot be ignored in modeling sphere pac fuels. Additionally, the variation of the orientation factor is seen to be strongly dependent on both cell geometry and the variation of cell geometry with changes in packing factor. Further improvements need to be made to the RANDPAC code to allow these dependencies to be better quantified.

STOCHASTIC SIMULATION OF SPHERE BEDS AND THE EFFECT OF PACKING DENSITY ON THE THERMAL CONDUCTIVITY OF SPHERE PAC NUCLEAR FUELS

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This thesis is dedicated to my parents, Mr. and Mrs. Louis J. Henke. Their love and faith in my abilities has been a constant source of energy and inspiration throughout my education.

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STOCHASTIC SIMULATION OF SPHERE BEDS AND THE EFFECT OF PACKING DENSITY ON THE THERMAL CONDUCTIVITY OF SPHERE PAC NUCLEAR FUELS

I. Introduction

The development of advanced fuels for both fast and thermal reactors has received a great deal of attention in recent years. The potential loss of the reprocessing option in the United States, coupled with widespread concern over the possible diversion of large quantities of fissile material, has initiated a massive effort to extend the lifetime of reactor fuels while maintaining the safeguardability of the nuclear fuel cycle. One fuel concept currently under consideration, sphere pac, originated in the U.S. in the early 1960's. Since that time, a considerable amount of international attention has been devoted to advancing this concept and the techniques associated with its production (1).

Sphere pac fuels have some distinct advantages with respect to the lifetime and fuel cycle considerations mentioned above. To produce a sphere pac fuel rod, microspheres of fuel material are formed by a wet chemistry solution-gelation process and vibrofilled into cladding tubes - procedures which are particularly adaptable to remote processing techniques and, thus, resistant to diversion (2). In addition, strong experimental evidence exists to indicate that fuel-clad mechanical interaction

in a sphere pac fuel rod is much less severe than in a conventional pellet pin (3). This means that sphere pac fuels can be designed for extended burnup without increasing the chance of fuel failure. A considerable amount of work must be done, however, before the sphere pac concept can be applied on a commercial scale.

To avoid the need for an extensive series of complex and costly experiments to characterize the behavior of a new fuel form, a predictive capability is usually established - typically in the form of a computer code. One such program, SPECKLE-I, has been developed by Ades (4) to model the thermal behavior of irradiated sphere pac mixed carbide fuels. Further work on the SPECKLE program is planned which will include the modeling of the mechanical, neutronic, and chemical aspects of sphere pac mixed carbides.

An important consideration in the development of a thermal model for reactor fuels is the proper characterization of the behavior of the thermal conductivity. This is particularly true with sphere pac where the conductivity is not only a function of temperature, burnup, and porosity, but also of fill gas pressure, packing factor, sphere size combinations, etc. Ades developed a two dimensional unit cell approach to the evaluation of the thermal conductivity of a sphere pac fuel. There exists some doubt, however, about the validity of this model, particularly with respect to the effect of packing

density and the orientation of the unit cell relative to the heat flow. The work reported in the following chapters is an attempt to quantify this effect and determine its importance.

The present investigation is divided into two related areas: the development of a method for mathematically simulating randomly packed beds of spheres and the calculation of the conductivity of these random beds given data which characterizes the unit cells within them. These areas are treated in detail in Chapters Two and Three, respectively. The process of the development of a unit cell and the calculation of its effective conductivity have not been included in this work. Of these topics, the former is the subject of a considerable amount of disagreement and the latter is a particularly difficult problem to solve because of gap conductance considerations. Consequently, the methods developed here have been left in a general form applicable to any unit cell.

II. Stochastic Simulation of Sphere Pac Bed

II.1 Modeling Requirements

To study the effects of packing on the properties and behavior of a sphere pac bed, a method of determining the geometric relationships among the spheres of a representative bed must be developed. A computer code, RANDPAC, has been written in the FORTRAN-IV programming language which will provide this information. The program determines the position of each sphere in space, its location relative to the bed boundary, and the identities of the spheres in contact with it. A complete listing of the RANDPAC code may be found in Appendix A.

Cylindrical geometry was chosen as the most appropriate to govern the overall shape of RANDPAC generated beds as it is the most applicable to the full range of thermal and mechanical problems in reactor fuel behavior. Unfortunately, cylindrical geometry is difficult to work with because of its inability to adapt to the simple three dimensional problems found in the method reported here. For this reason, cartesian coordinates were retained as the base coordinate set. This simplifies the bulk of the calculation immensely although it does cause some difficulty in the definition of the circular boundary. In cylindrical coordinates, this boundary is defined as (R_c,θ,Z), where R_c is the boundary radius. In cartesian coordinates this becomes (X,Y,Z), with the requirement that

$$X^2 + Y^2 = R_c^2,$$

R_c defined as above. This can be dealt with, however, and does not significantly affect the mathematics.

An additional problem is that the very nature of a cylindrical boundary introduces defects into arrays of spheres. This means that the packing factor (defined as the fraction of available space occupied by spheres) and the average coordination (the number of spheres likely to be in contact with a sphere not on a boundary) of a cylindrical bed must be less than those of the densest possible packing and will be dependent upon the ratio of boundary radius to sphere radius. These phenomena have been observed experimentally (5,6) and provide the basis for the verification of the RANDPAC code carried out in Section II.3.2. The effect of boundary radius is not expected to be important in most problems of interest, however, as Benenati and Brosilow (7) found packing factor to be strongly dependent on boundary radius only below a R_c/R_{sphere} value of 5.6.

There is currently some disagreement as to the optimal design of sphere pac fuels and fuel rods. An attempt has been made, therefore, to make RANDPAC as general as possible. At present, the code can handle any boundary radius and any number of sphere size fractions. At this time, however, RANDPAC is not capable of adequately treating the problem of infiltration. This phenomenon occurs when a small sphere is able to pass through the

space between three larger spheres in contact with each other. It can easily be shown that the ratio of radii between the largest and smallest size fractions in the bed must be less than 6.464:1 to avoid infiltration. Although this limitation is not a factor in the current study, further development work on RANDPAC will center on this problem in the hope that complete generality of the algorithm can be obtained.

To study the effects of packing factor, it is important to have a method of altering the bed during generation to obtain different packing factors without disturbing the bed's random nature. It has been suggested by Pedersen (8) that this can be done by assigning probabilities to the number of initial contacts a sphere will seek with other spheres and the boundary. In obtaining the densest packing possible, a sphere will always seek three initial contact points. If a sphere occasionally seeks only one or two initial contacts, an additional defect is introduced into the bed and the overall packing factor reduced. In this manner, a wide range of packing factors may be obtained. The concept of controlling initial contacts is reasonable in a physical sense. Sphere beds (and in particular, fuel beds in cladding tubes) are not created by placing spheres one at a time. They are, rather, generated rapidly, commonly under the influence of strong vibration. This makes it entirely possible for a sphere to fail to find three contacts

representing its position of highest contribution to overall packing density since one or more spheres may move to impede its path.

To control the number of initial contacts, it is necessary to define two probabilities, P_{c_1} and P_{c_2}, such that

$$0 < P_{c_1} < P_{c_2} < 1.$$

In the manner in which this method is used in RANDPAC, the values of the probabilities of one, two, and three contacts are, respectively, P_{c_1}, $P_{c_2}-P_{c_1}$, and $1-P_{c_2}$. For obvious reasons, it is impossible to determine these values in advance. For large beds (several thousand spheres or more) they might be obtained by using RANDPAC to perform a parametric study of their effect on the packing factor. Because of the highly statistical nature of the problem this was not possible for the small packings used in this work. Instead, P_{c_1} and P_{c_2} were changed by trial and error until a bed of the desired density was obtained.

The adjustment of the number of initial contacts will always result in the occurrence of one of five situations for a sphere after its placement. These are:

1. one contact with a sphere,
2. two contacts with spheres,
3. one contact with a sphere and one with the boundary,

4. three contacts with spheres, and
5. two contacts with spheres and one with the boundary.

If a sphere is to be properly placed in the bed, exact solutions to these five situations must be determined for any combination of sphere radii. These solutions are developed in detail in Appendix B.

A difficulty in the generation of dense random sphere beds with RANDPAC is that a new sphere will "stick" to the first sphere it contacts. Consequently, a sphere will rarely, if ever, be placed in a position corresponding to its lowest possible potential energy state. To partially remedy this problem, RANDPAC scans the top of the sphere bed and determines an initial position for each new sphere which will result in final placement at or near the lowest potential energy site. While the method used produces acceptable results, room for improvement exists.

A final consideration regarding the random generation of sphere beds is the effect of the method used to initialize the packing (that is, the method used to determine the location of the first few spheres). Susskind, Winsche, and Becker (9) have shown in a series of experiments that order in the first layer of spheres in a bed may propagate along the bed for a considerable distance. The effect of first layer ordering has been investigated and is discussed in Section II.3.3.

The stochastic nature of the bed loading procedure makes a good pseudo-random number generator imperative. The Oregon State University CDC CYBER 70/73 computer system has available within the FORTRAN-IV library a highly efficient pseudo-random number generator of variable seed (initialization constant) which produces values between 0 and 1, exclusive. The choice of seed is left to the user of RANDPAC, but care should be taken to insure that the seed chosen does not produce anomalous results. A discussion of the methods used to validate the CYBER pseudo-random number generator may be found in Section II.3.1.

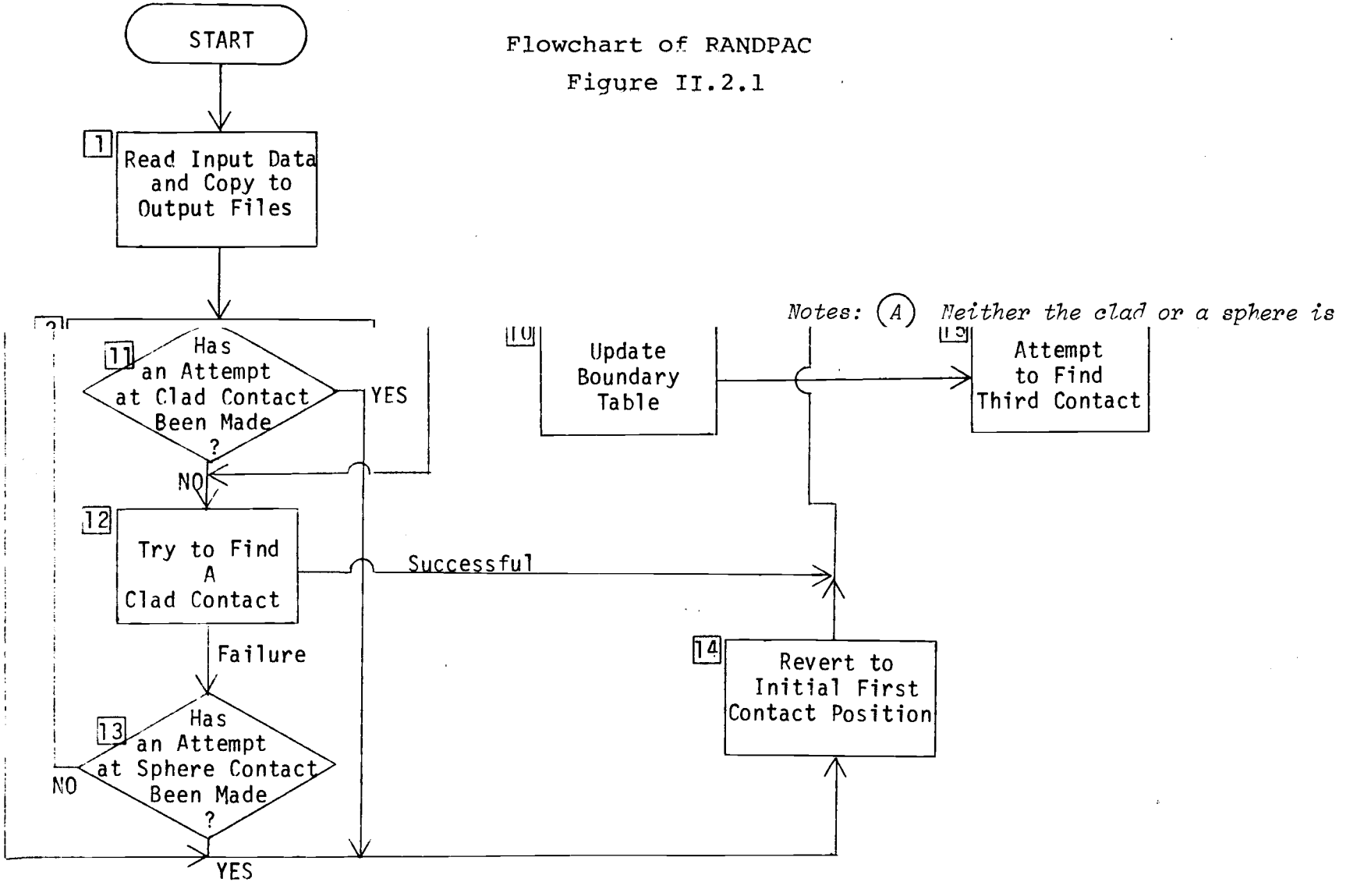
II.2 RANDPAC Computational Method

By the nature of the problem it is designed to treat, RANDPAC is an extensive and complex program. For this reason, the flowsheet (Figure II.2.1) is very simplified and a more detailed description of the algorithm is given below. The number of each step corresponds to the flowbox number in the diagram and the letter corresponds to an individual substep or decision point located within the box.

1. Read the input data and copy it to all output files.
2. Initialize the random number generator.
3. a. Increment the sphere number.
   b. Randomly determine the size fraction of a new sphere.
4. a. Pick initial x, y, and z coordinates for the new sphere such that it does not interact with the clad, is well above the bed surface, and will fall towards the lowest point on the bed surface.
   b. Determine which sphere in the bed the new sphere will contact first if dropped vertically onto the top of the bed and calculate an initial value for z.
   c. If an initial contact is not found, determine a lower boundary z value for the sphere and go to 16.a.

Flowchart of RANDPAC

Figure II.2.1



5.a. Choose the number of contact points (NCP) the sphere will seek.

b. If NCP = 1 go to 16.a.

6.a. Determine all spheres which are local to the present location of the new sphere.

b. If one or more spheres are close enough to establish a second contact, go to 7.a.

c. If the clad is close enough for contact with it to be established, go to 12. If not, go to 14.

7.a. Determine which local sphere is closest and the distance to it.

b. Determine the distance to the clad.

c. If the clad is closer than the closest sphere, go to 12.

8. Search for a second sphere contact at a random angle. If failure occurs, go to 11.a.

9. Update the interaction table. If NCP < 3 go to 16.a.

10. Update the boundary identification table and go to 15.a.

11. If an attempt has already been made to find a clad contact, go to 14.

12. Try to find a clad contact. If successful, go to 16.a.

13. If an attempt has not been made to find a sphere contact, go to 8.

14. Revert to the position defined as the first contact and go to 16.a.

15.a. Attempt to find a contact position with a third sphere and, alternatively, with the clad.

b. Choose at random whether a sphere contact or clad contact is preferable.

c. If a clad contact is both preferable and available, use the contact and go to 16.a.

d. If a sphere contact is both preferable and available, use the contact, update the interaction table, and go to 16.a.

e. If a sphere contact is preferable but not available, use the clad contact position, if available, and go to 16.a.

f. If a clad contact is preferable but not available, use the sphere contact position, if available, and update the interaction vector.

16.a. Set the boundary information table.

b. Write sphere initial contact data to output and to the recovery file.

c. Update the potential energy search table.

d. If all spheres have not been placed, go to 3.a.

17.a. Determine the bed height, upper boundary sphere identities, and packing factor and write to the output files.

b. Write all data generated to the final output file and terminate execution.

A complete listing of RANDPAC and a sample case may be found in Appendices A and C, respectively.

II.3 Model Verification

II.3.1 Qualification of Pseudo-Random Number Generator

The generation of a pseudo-random number (PRN) on the OSU CYBER is done by the repeated manipulation of the bits of a single computer "word." The larger this word is, the more random the values that are generated. Each word used by the OSU CYBER consists of 60 bits. This implies that the CYBER PRN generator should be more or less insensitive to the seed chosen for it. Six seeds have been chosen for use in this investigation. They are:

1. 4565456545654
2. 33669922558811
3. 22558833669911
4. 11559911559911
5. 99887766554411
6. 33221166554477

The methods used to qualify a PRN generator during its development are highly sophisticated and have been the subject of extensive study (10). Two simple approaches, the chi-square test and n-space plotting, will be used to demonstrate that the values produced by the CYBER PRN generator actually possess a high degree of randomness.

The chi-square test is a statistical procedure which examines the discrepancies that exist between the observed and expected frequencies of events (11). To apply this test, the value of chi-squared is determined by the use of the equation:

$$\chi^2 = \sum_{j=1}^{k} \frac{(O_j - E_j)^2}{E_j}$$

where O_j is the observed frequency of the jth event,

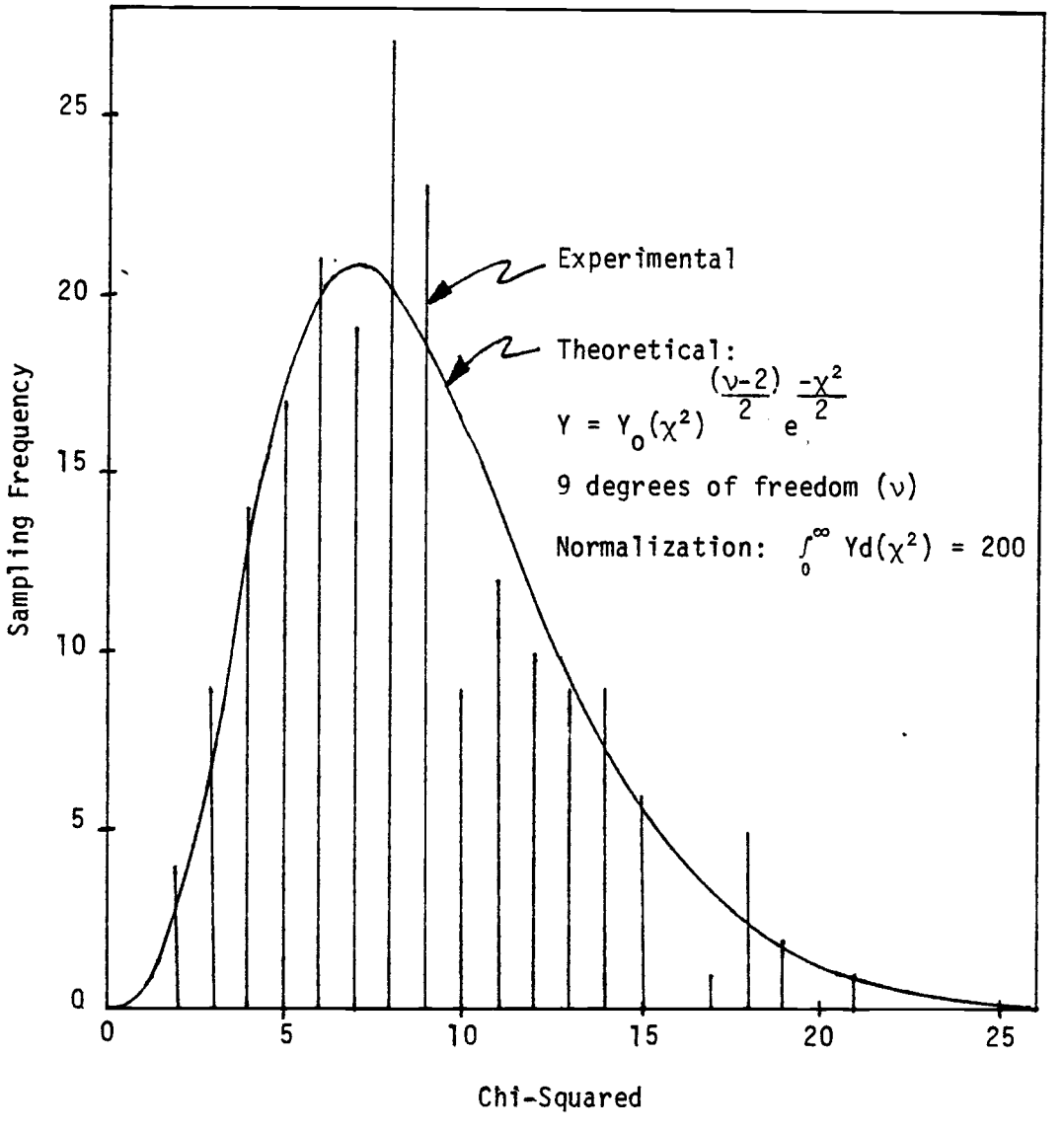
E_j is the expected frequency of that event, and

k is the total number of events.

When the observed and expected frequencies are the same (indicating nonrandom events) the value of chi-squared will be zero. If the events possess some degree of randomness, O_j and E_j will be unequal and chi-squared will be greater than zero. As each PRN is produced, it is "placed" into one of ten "event boxes" corresponding to ten equiprobable value ranges ((0.-.1), (.1-.2), . . ., (.9-1.0)). When enough PRNs have been generated to constitute a reasonable sampling, the frequency of each event is determined and the value of chi-squared calculated. In a similar manner many values of chi-squared are tabulated to determine an overall sampling distribution. For truly random events, this sampling distribution is approximated by

$$Y = Y_o(\chi^2)^{(\nu-2)/2}\ e^{-\chi^2/2}$$

where ν is the number of degrees of freedom (events-1), and Y_o is a normalization constant. By comparing the experimental and theoretical sampling distributions, the deviation from true randomness can be determined. The CYBER PRN generator normally produces quite good results. A typical example of an experimental distribution is shown with the theoretical distribution superimposed (Figure II.3.1.a).

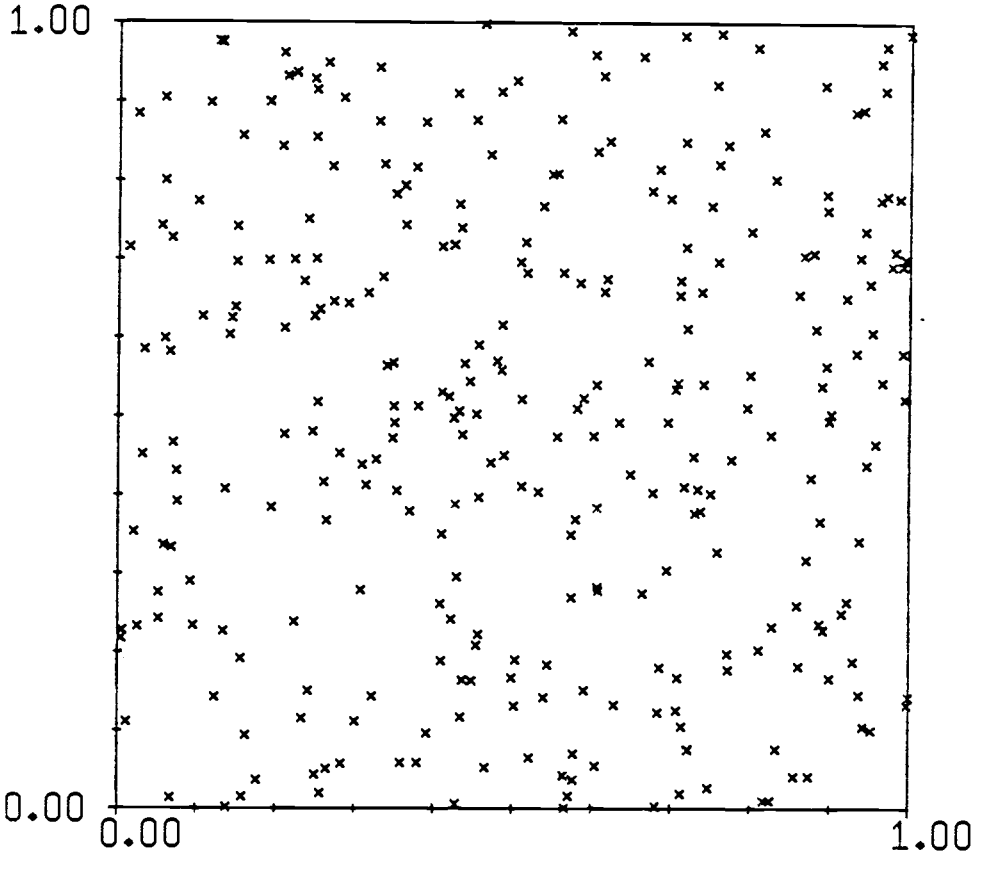


Experimental and Theoretical χ^2
Sampling Distributions

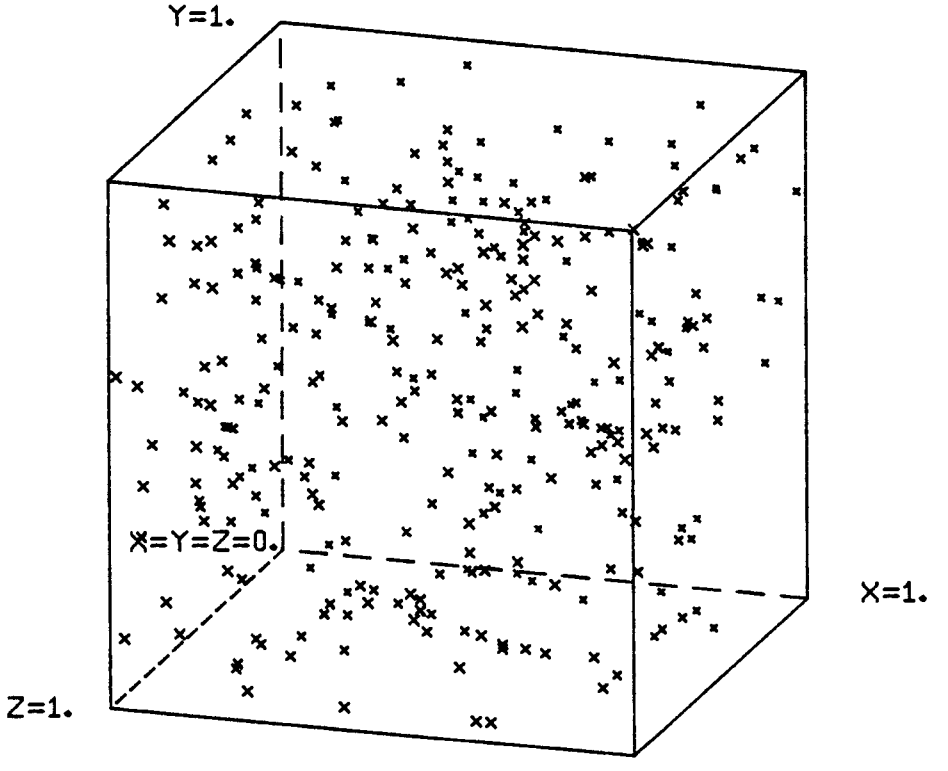
Figure II.3.1a

N-space plotting is a simple method of directly observing peculiarities in a PRN generator. In this test, many pairs, triplets, or "n-tuples" of consecutive PRNs are taken as the coordinates of a point in space and plotted. If the points form any significant "clumps," "holes," or "crystals" (regular arrays), the generator is not producing acceptable results. For obvious reasons it is only possible to actually create plots in two and three space. "Plotting" in higher ordered spaces is treated by interval tabulation methods similar to those used in the chi-squared test. The examples shown (Figures II.3.1b and II.3.1c) are typical of the results obtained from the CYBER PRN generator. When no obvious defects are observed it can be stated with reasonable assurance that this test has been completed successfully.

In summary, the CYBER PRN generator has not been found to produce anomalous results for the tests performed although these tests constitute only the most cursory of examinations. It can be safely stated that it is impossible to assure the adaptability of a sequence of pseudo-random numbers to a specific use with a finite series of tests. That is, for any set of tests, a sequence of numbers will exist which appears acceptable but which cannot be put to a particular use (10,12). This is an important concept which should be considered whenever a stochastic or Monte Carlo type simulation is performed. Fortunately, the nature of the bed packing problem



Distribution of Random Pairs
Figure II.3.1b



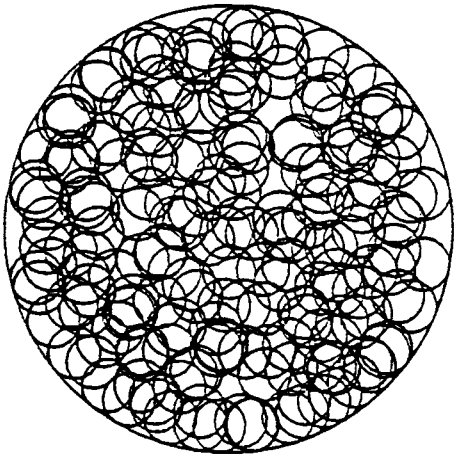
Distribution of Random Triples
Figure II.3.1c

contains a certain amount of order (the existence of the boundaries, for example) which renders it relatively insensitive to PRN generator anomalies.

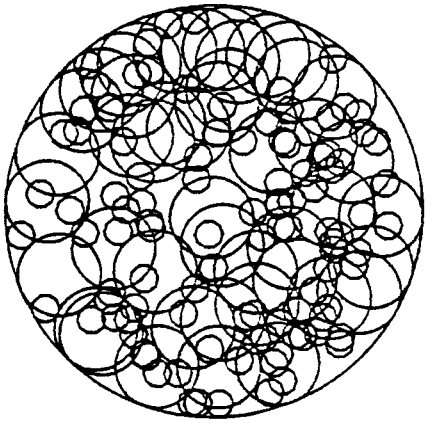
II.3.2 Verification of RANDPAC

An important step in the development of any model is the assessment of that model's accuracy. When the model is a computer algorithm, this evaluation is usually carried out by simulating some well defined event and comparing the code prediction to an analytic solution or existing experimental data. Initially, the performance of RANDPAC will be considered in a qualitative manner by simple observation of the characteristics of the randomly generated bed. Finally, a quantitative verification will be carried out using the body of information that has been acquired over the years by investigators with interests ranging from pebble bed nuclear reactors to fluidized bed combustion. Unfortunately, all of the experimental data available is derived from assemblies containing spheres of a single size. Despite this, a few two size fraction RANDPAC beds have been examined qualitatively and are discussed in parallel with the single size fraction beds.

The qualitative analysis of RANDPAC is performed by examining a large number of random beds in three ways. The first of these is a simple check to see that no obvious anomalies (i.e., spheres "floating" without supporting contacts or spheres overlapping each other or the clad) exist. Of the 41 beds examined, none were found to be defective in this respect. The second procedure involves plotting an axial view of the sphere bed as seen from above the upper bed boundary (e.g., Figure II.3.2a,b).



One Size Fraction Bed
Figure II.3.2a

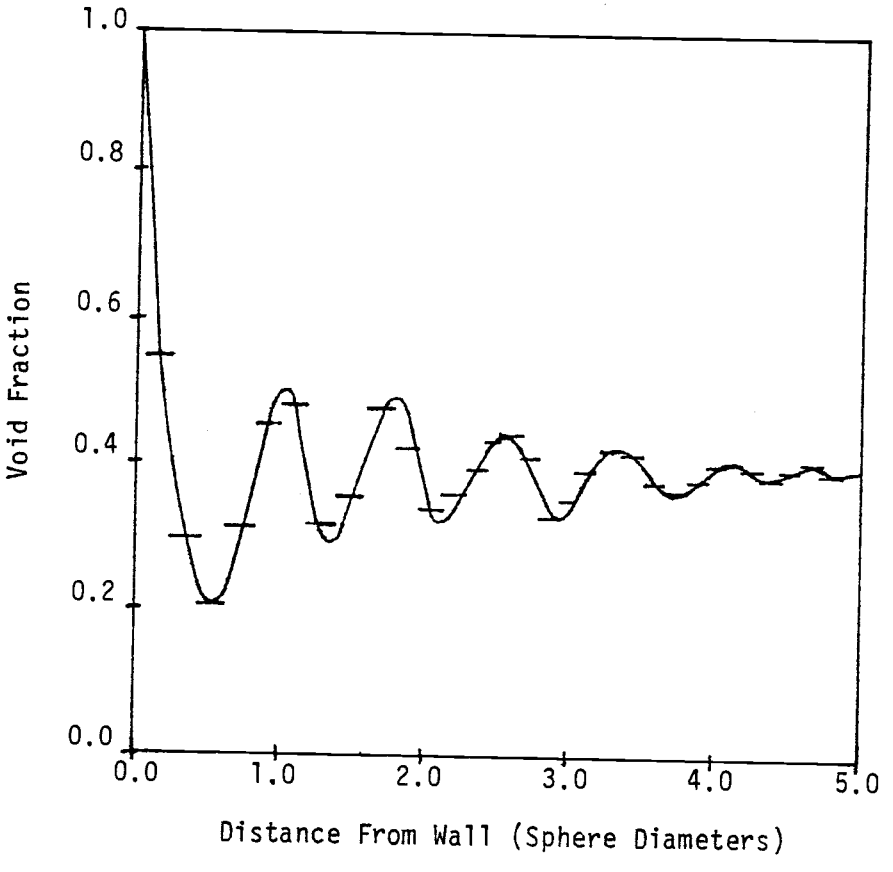


Two Size Fraction Bed
Figure II.3.2b

By inspecting these plots for excessively large voids or extreme ordering within the bed, it is easy to spot potential trouble spots within the algorithm. The beds examined during the verification process yielded only one obviously anomalous packing. This case was not considered serious, however, as it involved excessive ordering of a single size fraction within a tube whose diameter was equal to only three sphere diameters.

An interesting result of this exercise is the observation of the low density region adjacent to the bed boundary. This effect has been observed experimentally and is a result of the ordering effect of the wall (7,13). Careful measurements in single size fraction beds have shown that void fraction variation takes the form of a damped sinusoid which peaks at the boundary, decays completely within a distance of about five sphere diameters (Figure II.3.2c), and is largely independent of the wall geometry. The obvious consequence of this phenomenon is that a bed property such as thermal conductivity may change radically near a boundary.

The third and final qualitative method used to check RANDPAC is an evaluation of the logic used to minimize the potential energy of each sphere as it is placed in the bed. As mentioned previously, RANDPAC produces acceptable though not ideal results in this respect. By plotting the elevation of each sphere in the order of placement, the performance of the algorithm can be

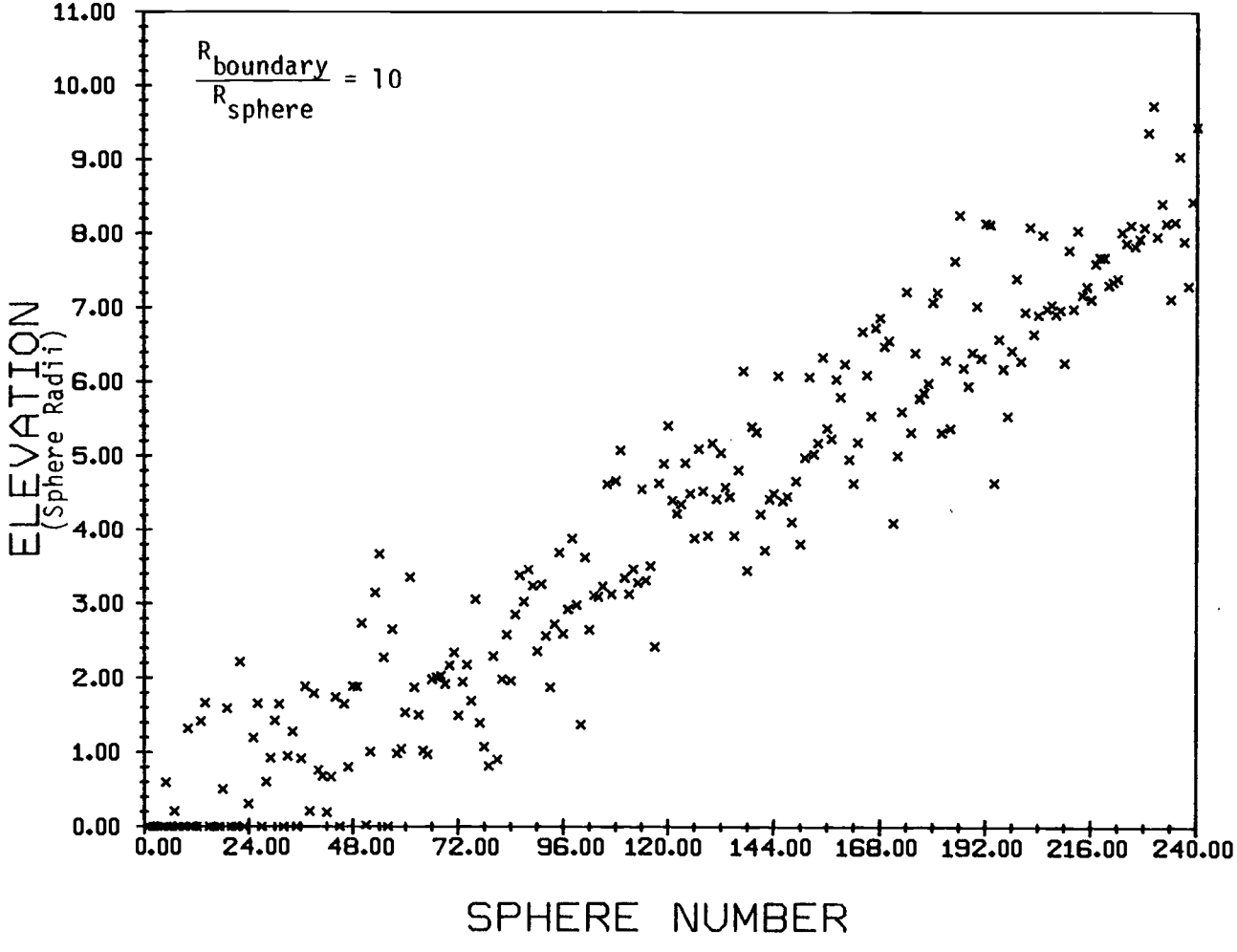


Void Fraction Variation
Near the Boundary of a Semi-Infinite Bed of Spheres (7)

Figure II.3.2c

observed. In a single size fraction packing, each sphere would ideally be placed slightly higher than the last resulting in a continuously increasing plot of sphere position. In practice, RANDPAC produces a "noisy" elevation plot (Figure II.3.2d) which shows the right basic behavior but exhibits an average scatter of about one sphere radius. In a multiple size fraction bed, the noise is more pronounced and in part physical. If it can be eliminated in the single fraction beds it should also be lessened in the more complicated packings, however. A few attempts have been made by previous investigators at minimizing this scatter or actually achieving ideal packing. Clancy (14), for example, achieved minimum potential energy for each sphere by keeping track of all sites on the surface of the bed which a newly placed sphere might occupy and choosing the lowest elevation available. Unfortunately, this approach would be difficult to apply in RANDPAC because it must treat spheres whose sizes are determined in a random fashion while Clancy generated beds of uniform spheres. With more than one size fraction, a potential site for a large sphere may not be a potential site for a smaller sphere and vice-versa, making the once simple bookkeeping procedure much more complex.

The quantitative analysis of randomly generated sphere beds falls into two categories: the study of sphere coordination and the study of bed density. The



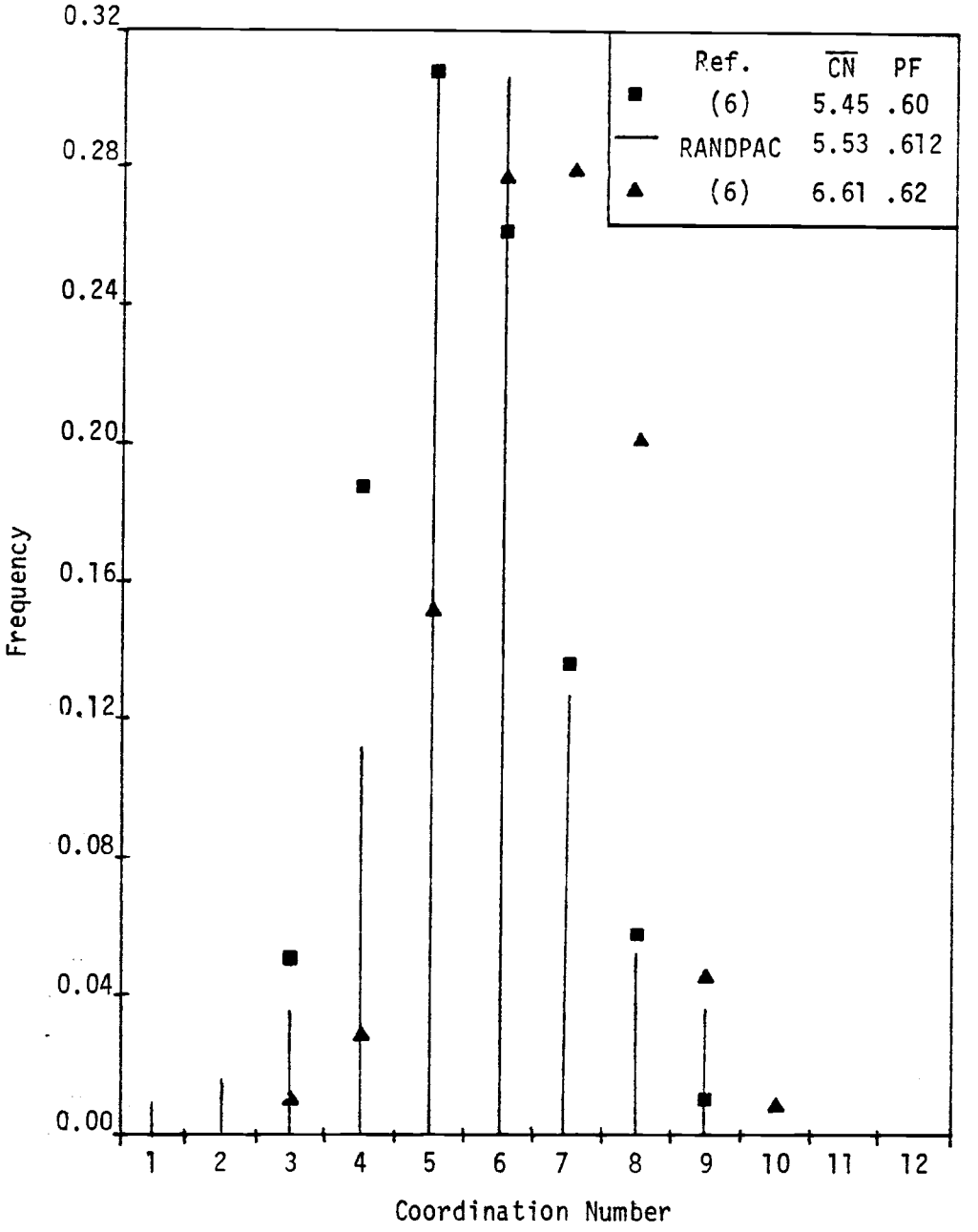
Elevations of Spheres in Order of Placement

Figure II.3.2d

former involves an examination of the average number of contacts a sphere has and the statistical distribution of those contacts, while the latter entails an investigation of packing factor with respect to boundary radius. Both of these procedures are well supported by experimental data and are commonly used in evaluations of this type.

RANDPAC maintains a table of contacts between spheres as part of its solution process making coordination data readily available. The acquisition of experimental coordination data for a packed bed of spheres is also a relatively simple process. Bernal and Mason (6) accomplished this by soaking a packed bed in paint, allowing it to stand, and then draining off the excess. After drying, the spheres were broken apart and the number of contact points counted. In both cases only spheres not immediately adjacent to the boundary were considered. The result of this procedure is a frequency distribution of coordination number for two experimental packings described as "random loose packed" and "random close packed" and a RANDPAC bed of similar density (Figure II.3.2e). These results appear to be in quite good agreement.

It should be mentioned at this point that the calculation of packing factor for the RANDPAC simulation is somewhat different here than elsewhere. The beds created by Bernal and Mason were roughly spherical and contained several thousand spheres, making the central portion of the bed (used in the coordination study) appear to be

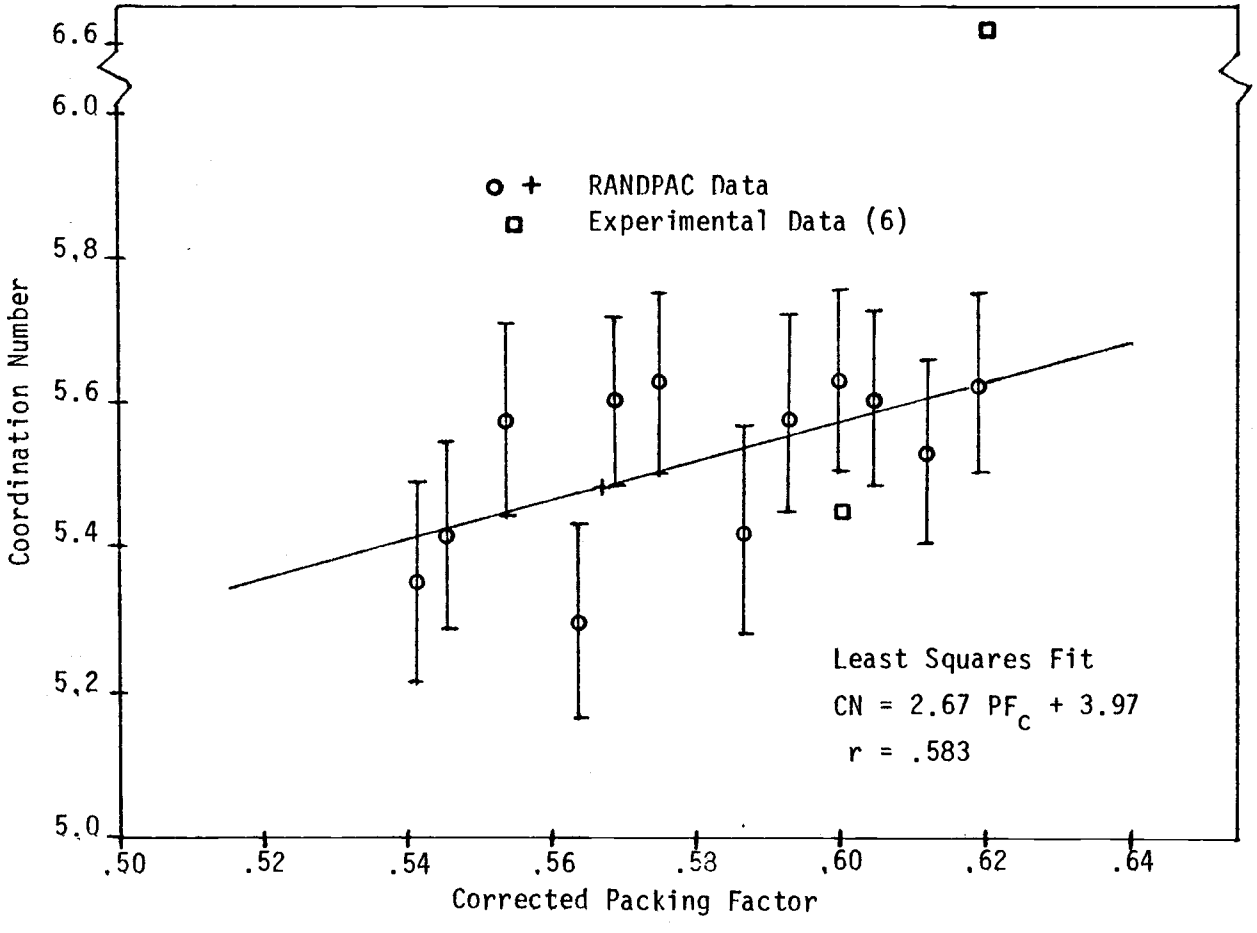


Coordination Number Frequency

Figure II.3.2e

part of an infinitely large packing. In an attempt to mitigate the wall effect in the small radius RANDPAC beds, all of the mass and volume less than one sphere radius from the cylindrical boundary was neglected in the density calculation. A strong argument for this procedure, which seems to produce adequate results, may be made by referring to the appearance of a bed as seen from above (Figure II.3.2a).

There appears to be a definite, though not strong, linear correlation between the corrected packing factor and the average coordination number (correlation coefficient, r = .583, Figure II.3.2f). Although the value for Bernal and Mason's random loose packing agrees quite well with the RANDPAC data, there is a large discrepancy (approximately one contact) between the experimental value for random dense packing and the RANDPAC generated correlation. This is probably caused by two separate factors: the inefficiencies inherent in the minimum potential energy algorithm and the fact that RANDPAC counts only true contacts while the experimental method indicates contact between spheres which may be separated by as much as five percent of the sphere radius. At the present time this does not appear to be an important consideration. It may gain significance, however, when more detailed analyses of sphere bed behavior are performed in the future.

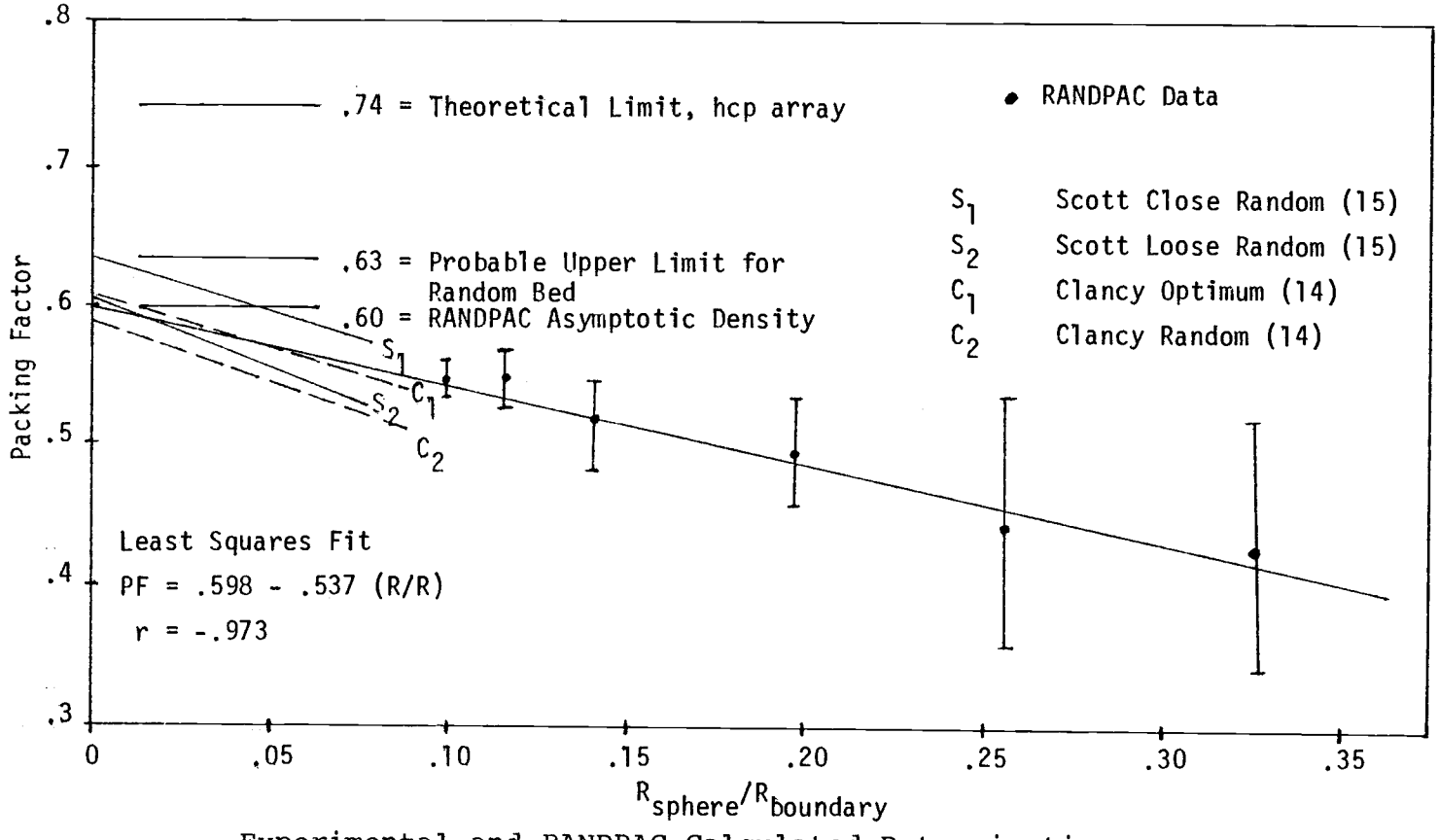


RANDPAC Calculated Dependence of Coordination Number on Packing Factor

Figure II.3.2f

The study of the effect of bed radius on packing factor generally centers on the determination of the "asymptotic" density (the density, uncorrected for wall effects, as the boundary radius become infinite). This is determined by plotting the packing factor as a function of the ratio of sphere radius to boundary radius (Figure II.3.2g). Unfortunately, restrictions on the amount of core memory available on the OSU CYBER made it impossible to treat the very large radius beds examined experimentally by Scott (15) and numerically by Clancy (14). It is significant, however, that the strong linear correlation ($r = -.973$) of the small radius RANDPAC beds produces a least squares fit which passes among all of the Scott and Clancy data when extrapolated to large boundary radius. This is a very good indication that RANDPAC is modeling the effect of boundary radius on packing density accurately. The extrapolation to infinite radius also produces a good result, showing that RANDPAC beds are very similar to what is commonly called random loose packed. This is consistent with the information presented earlier concerning coordination number frequency.

In conclusion, RANDPAC appears to simulate loosely packed random beds fairly accurately. This is a positive indication that these packings may be used in sphere bed properties modeling without inducing artificial behavior. Most packing densities of current interest are above that currently available from RANDPAC as they lie in the range



Experimental and RANDPAC Calculated Determinations of Asymptotic Density

Figure II.3.2g

of random dense packing. This problem should be alleviated, however, with the improvement of the minimum potential energy algorithm.

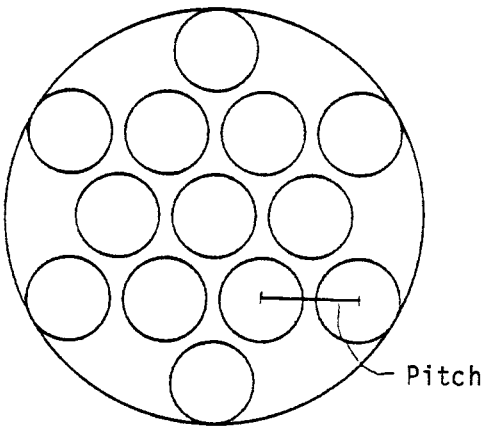
II.3.3 The Placement of Initial Spheres in Random Beds

As mentioned earlier, the placement of the initial spheres in a bed may have a significant effect on the ultimate bed structure. The purpose of investigating this phenomenon with RANDPAC has, therefore, two goals. First, it must be determined if the present method of choosing bottom boundary sphere coordinates at random is adequate. The second goal is to observe the effect of different types of ordering on packing density relative to each other and to random initialization. This analysis will include an examination of the ability of ordering to propagate along the length of the bed.

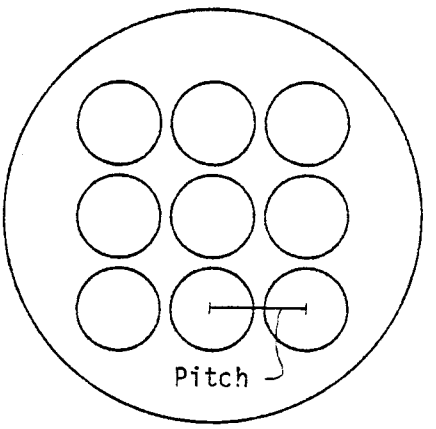
Two basic types of ordering were treated: hexagonal and square (Figure II.3.3a). By varying the sphere-sphere pitch (center to center distance), several patterns were developed which were used to initialize the packings. All packings were of equal size and dimension and spheres were of unit radius. The results of the analysis are as follows:

Shape	Pitch	Packing Factor
hexagonal	2.00	.485
hexagonal	2.31	.451
hexagonal	2.60	.391
hexagonal	3.00	.413
square	2.00	.466
square	2.25	.394
square	2.45	.412
random	----	.494

There is, at best, a very weak correlation to this data (Figure II.3.3b). One fact is evident, however: random initialization produces the highest packing density and



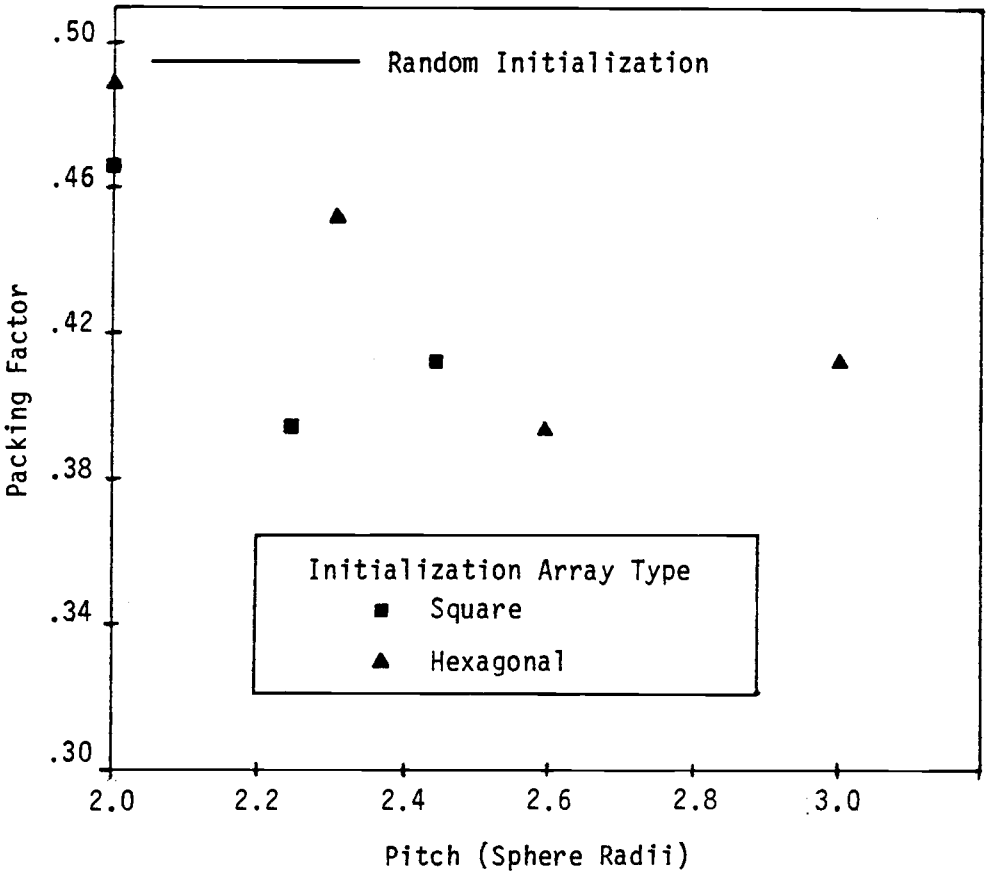
HEXAGONAL



SQUARE

Typical Placement of First Layer Spheres
in Ordering Studies

Figure II.3.3a

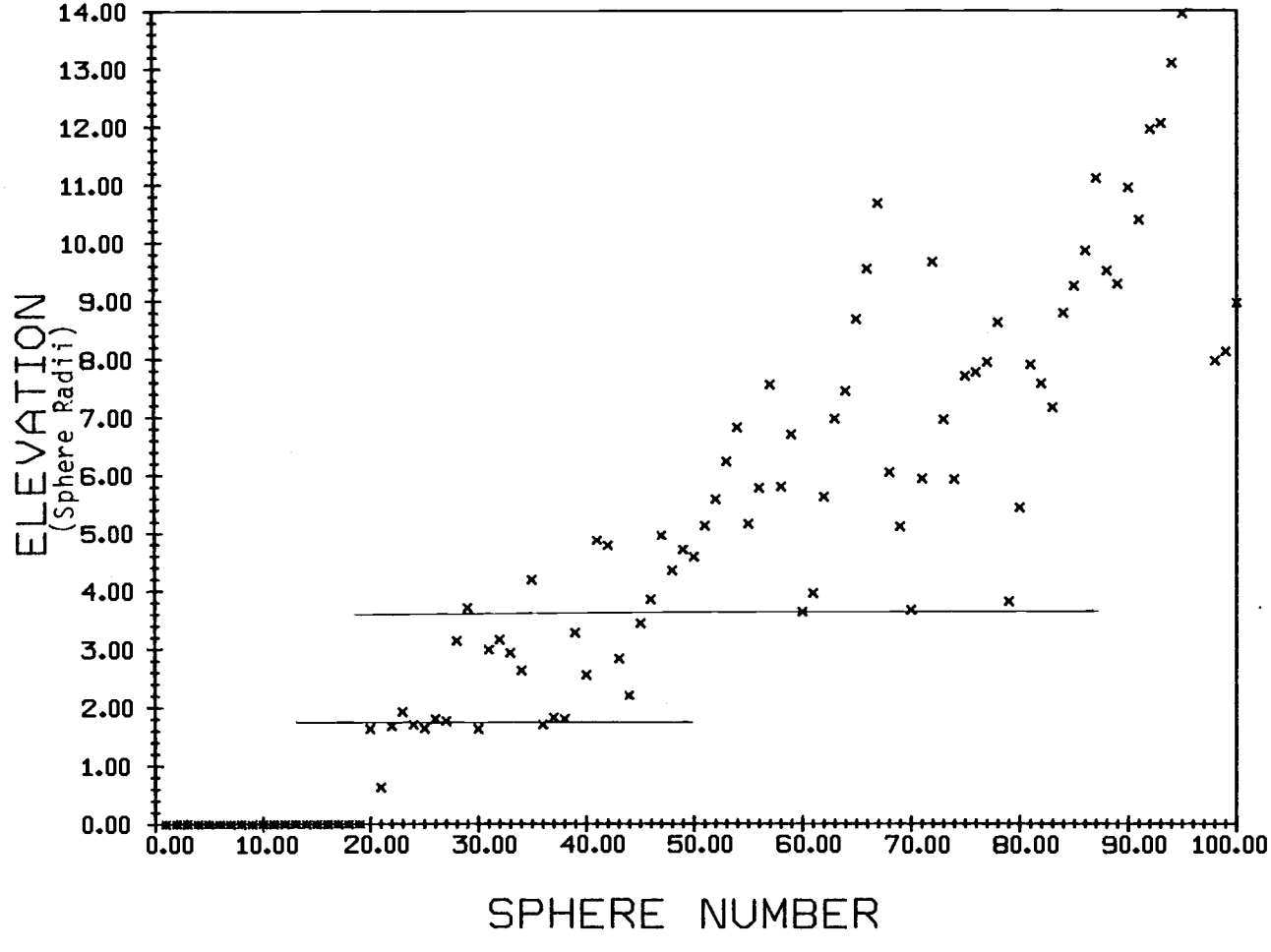


Effect of Initialization of Bed on Packing Factor
Figure II.3.3b

square array initialization produces the lowest density, hexagonal being consistently intermediate. This is a reasonable result in that a hexagon is a somewhat better approximation to a circle than a square is. The overall lowering of the packing fraction may have a combination of physical and nonphysical causes, however. Observations of the generated beds indicate that the ordering of the first layer causes high voidage to occur at the bottom of the bed near the circular boundary - an effect felt the most when the ordering is rectangular. The nonphysical cause would again seem to be related to the inefficiencies in the algorithm used to minimize each sphere's potential energy. At the present stage of development, ideal sites are often overlooked resulting in a lower bed density. The ultimate significance of the observed behavior is problematic, however, as the majority of the experimental work has involved arrays of spheres in square tubes (9).

The propagation of ordering through the bed can be observed by inspecting elevation plots of the type discussed in Section II.3.2. A plot for a hexagonally initialized bed (pitch = 2.0) shows weakly defined "energy levels" at approximately 1.7 and 3.5 sphere radii elevation (Figure II.3.3c). Above this point no ordering is evident, implying that the effect of the first layer of spheres quickly dies out.

In summary, the most efficient means of initializing a sphere bed would appear to be by the random placement of



Propagation of Order in a Cylindrical Sphere Bed

Figure II.3.3c

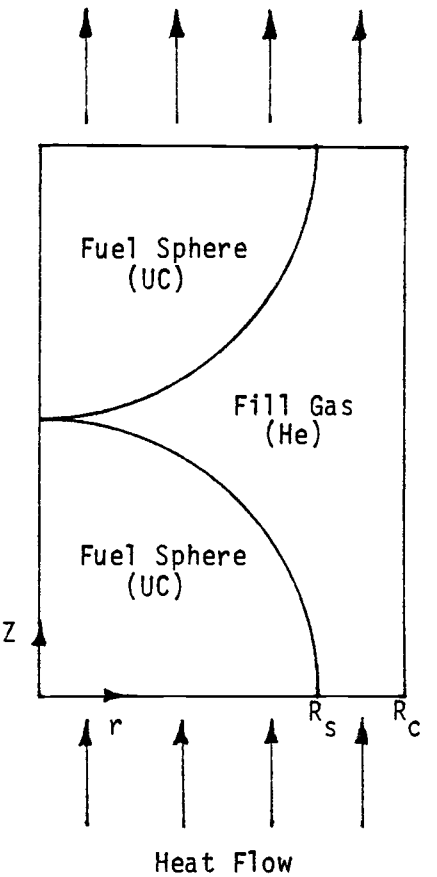
spheres. This seems to consistently produce the highest packing density. It would be very useful to conduct a series of experiments with circular boundaries, however, which could validate the RANDPAC predicted inability of order to propagate along a cylinder.

III. Evaluating the Effective Thermal Conductivity of Sphere Pac Beds

III.1 The Unit Cell and the Idea of Effective Conductivity

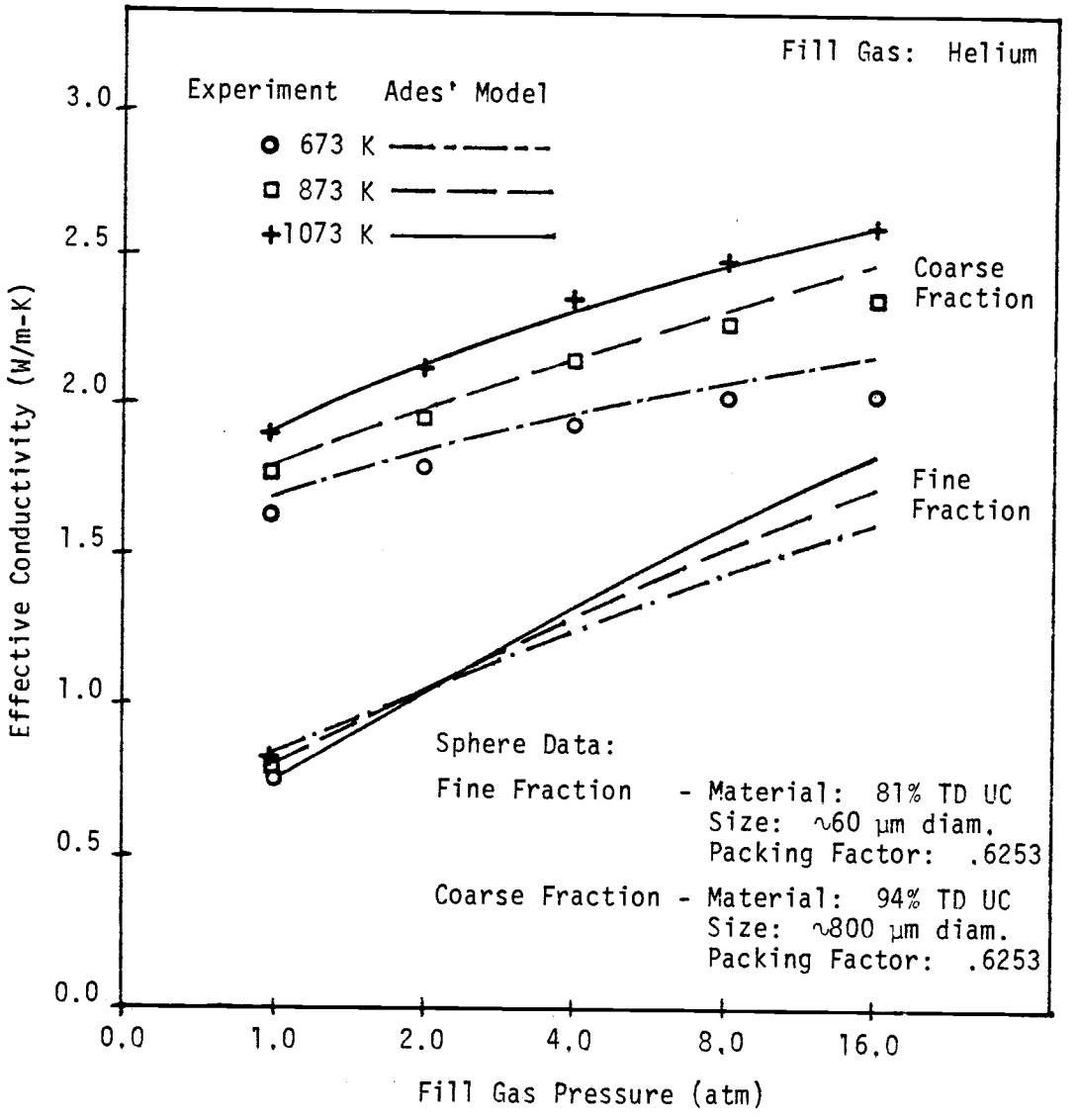
Conventional treatments of particle bed conductivity often involve some sort of "unit cell" approach. That is, the microscopic structure of the bed is examined for some repetitive feature which is fundamental to the macroscopic behavior of the bed. A recent attempt to evaluate the conductivity of sphere pac nuclear fuels by Ades (4) employs a model consisting of two hemispheres in contact surrounded by a gas to represent the basic unit of a random sphere bed (Figure III.1a). The conductivity of this cell is taken to be representative of the bed itself.

While Ades' results compare quite favorably with experimental data (Figure III.1b), there is some question as to the acceptability of equating the cell conductivity to that of the bed. This approach should only be valid if all of the heat flow is parallel to the cell axis, as would be true if the bed had a simple cubic structure (Figure III.1c). In a random bed the unit cells are oriented in all directions with respect to the heat flow. This in effect decreases their contribution to the overall bed conductivity. It is this "cell orientation effect" which is being considered here.



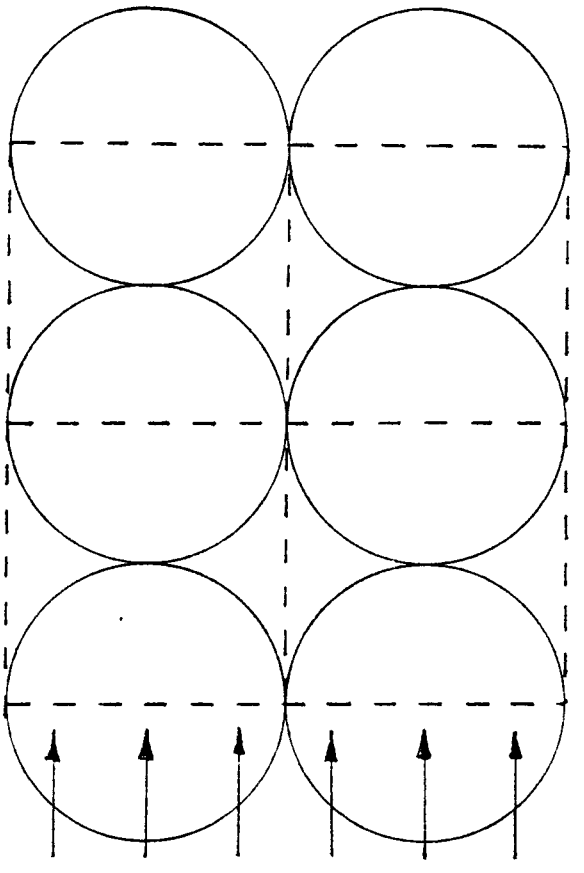
Ades' Unit Cell for
Single Size Fraction Sphere Pac Nuclear Fuel (4)

Figure III.1a



Comparison of Experimental and Predicted Values of Thermal Conductivity for Sphere Pac Nuclear Fuel (Ades' Model)

Figure III.1b



Ades' Unit Cells in the
Valid Simple Cubic Orientation

Figure III.1c

The concept of the cell orientation effect makes it important to understand the idea of effective conductivity and how it is defined for both a unit cell and a sphere bed. The effective conductivity of a system may be thought of as the conductivity of some imaginary material which, in replacing the original system constituents, conducts the same amount of heat across the same temperature difference. For the unit cell, the effective conductivity is determined by a detailed examination of the conduction of heat through the cell constituents (the fuel hemispheres and surrounding gas in the case of Ades' cell). For a sphere bed, however, effective conductivity is based on heat transfer through a three dimensional network of one or more types of interconnected unit cells. The calculation of the effective resistance of a network of electrical resistances is strongly analogous to this, the thermal resistance of each link in the sphere bed being based on the effective conductivity of the cell it corresponds to.

It is not the intention of the current investigation to treat the modeling of the unit cell in detail. In a sphere pac nuclear fuel, the gas gaps between the microspheres are typically on the order of a few microns. Heat transfer in this regime is very complex and, while it has received a great deal of attention (17,18,19), is not fully understood. However to demonstrate the method, the present work assumes the existence of a unit

cell whose dimensions and effective conductivity are known and will be restricted to the examination of the cell orientation effect discussed earlier. A FORTRAN-IV computer program called ORIENT has been written which will evaluate the effective conductivity of a sphere bed made up of a single type of unit cell (that is, a bed made up of uniform spheres). It would not be difficult to generalize this code to multiple size fraction packings consisting of many different unit cells, however. This is discussed in Section III.2.

III.2 Modeling the Effective Conductivity of a Sphere Bed

Fourier's Law of Conduction,

$$q'' = -k \vec{\nabla} T, \qquad \text{III.2.1}$$

implies that the conductivity of a material can be determined by a knowledge of the heat flux, q", resulting from the temperature gradient, $\vec{\nabla} T$. To determine the heat flux, however, the temperature field must first be evaluated. As mentioned in Section III.1, the bed can be looked upon as a three dimensional network of unit cells whose dimensions and effective conductivities are well characterized. By treating each cell as a one dimensional conductor of heat whose conductivity is determined for a specific temperature, III.2.1 can be written as

$$\frac{q}{A_e} = -k \frac{(T_a - T_b)}{L}, \qquad \text{III.2.2}$$

where q is the heat flow,

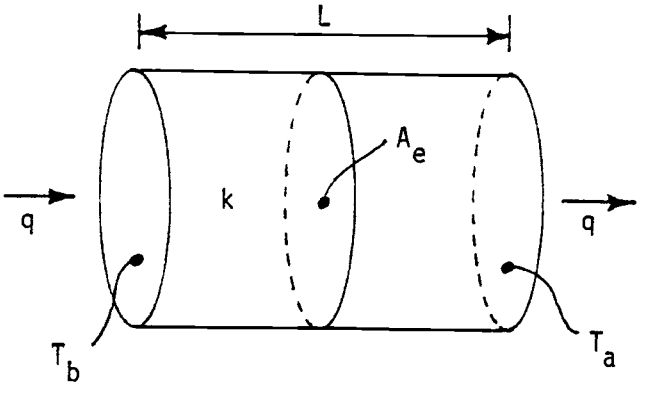
A_e is the effective heat transfer area of the cell,

L is the length of the unit cell,

k is the effective conductivity, and

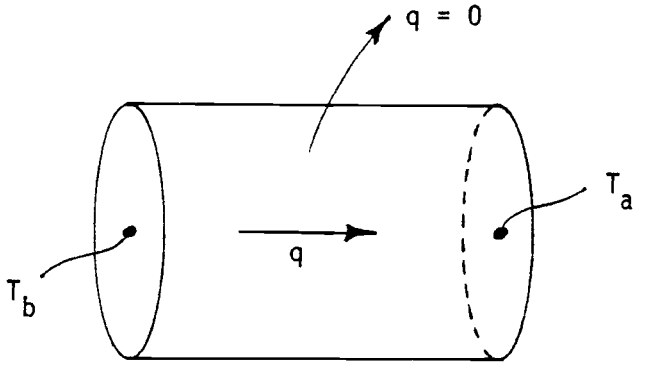
$(T_a - T_b)$ is the temperature drop across the cell (Figure III.2a).

Rearranging this and defining the quantity $(L/(kA_e))$ as the thermal resistance to heat flow, R, results in the



Important Parameters of a
One Dimensional Heat Conductor

Figure III.2a



Boundary Conditions on a Cylindrical Sphere Bed
to Force Pseudo-One Dimensional Heat Flow

Figure III.2b

relationship $$q = \frac{(T_a - T_b)}{R} \qquad \text{III.2.3}$$

The analogy to the electrical conduction problem is obvious. At steady state, the total heat entering and leaving any sphere must equal zero. Since all heat transfer paths considered here are unit cells, this zero net heat flow condition can be expressed by summing Equation III.2.3 over all of the cells involved:

$$\sum_{i=1}^{N_j} q_i = \sum_{i=1}^{N_j} \frac{(T_i - T_j)}{R_i} = 0, \qquad \text{III.2.4}$$

where N_j is the total number of unit cells sphere j contributes to, and

R_i is the resistance of the ith unit cell.

If this equation is written down for every sphere in the bed, the result is a system of j linear equations in j unknowns (the temperatures T_j) where j is the number of spheres in the bed. If we make the assumption that all of the unit cells in the bed are identical, III.2.4 reduces to

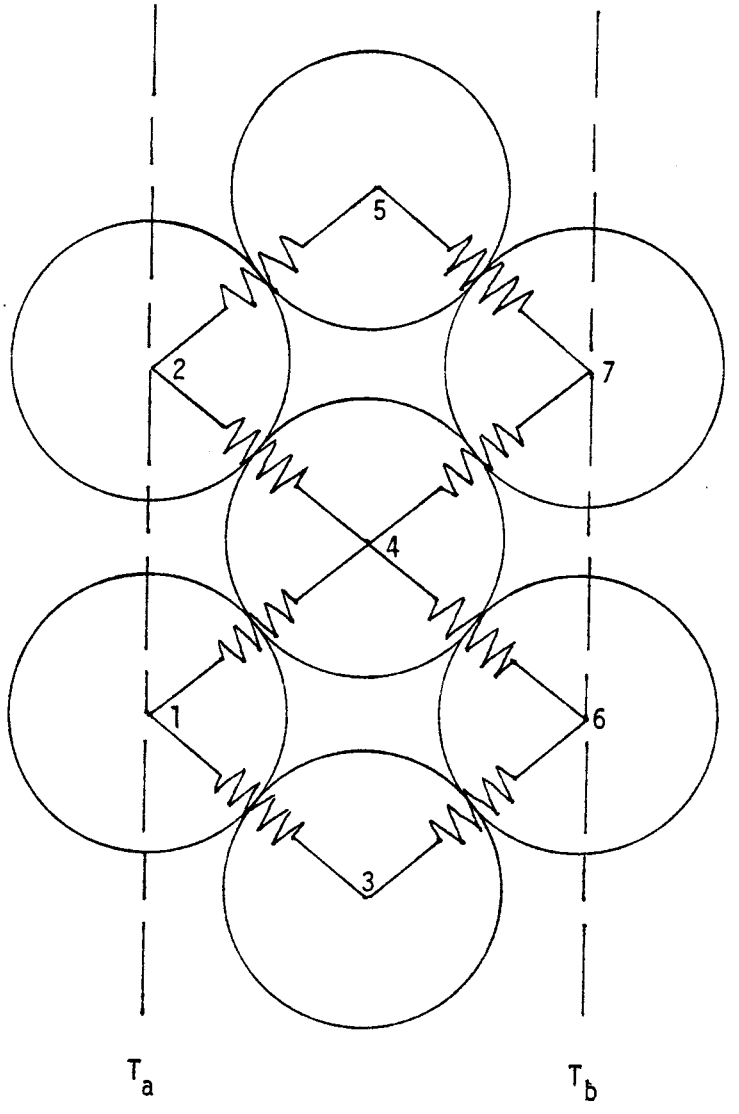
$$\sum_{i=1}^{N_j} (T_i - T_j) = 0. \qquad \text{III.2.5}$$

ORIENT solves the system of equations represented by III.2.5 to determine the temperature distribution within the sphere bed. To generalize the program to multiple size fraction beds would require a knowledge of the basic parameters of all possible unit cells and the solution of

III.2.4. Note that Equation III.2.5 is similar to the finite difference formulation of Laplace's Equation. The result of this similarity is that it is necessary to specify conditions on the bed boundaries to obtain a meaningful solution.

To evaluate the effective conductivity of the bed from Equation III.2.2 (where k, A_e, and L now represent bed parameters), the heat flow must be pseudo-one dimensional. That is, all heat must flow in one end of the bed and out of the other. This is easily achieved by specifying constant temperatures on the end planar boundaries of the bed and an adiabatic condition on the cylindrical surface (Figure III.2b). The latter condition requires no modification to the system of equations represented by III.2.5. The former, however, requires that all spheres considered part of the planar boundaries be identified and their temperatures fixed appropriately. The resultant problem is now identical to one of heat flow through an infinite wall. For the simple example shown (Figure III.2c) the system of equations can be written down in the following matrix form:

$$\begin{bmatrix} 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & -N_3 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & -N_4 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 & -N_5 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 \end{bmatrix} \begin{Bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \\ T_7 \end{Bmatrix} = \begin{Bmatrix} N_1 T_a \\ N_2 T_a \\ 0 \\ 0 \\ 0 \\ N_6 T_b \\ N_7 T_b \end{Bmatrix} \qquad \text{III.2.6}$$



A Sphere Bed as a Network of Resistances
Figure III.2c

For a random bed containing many spheres, the coefficient matrix will be very large, sparse, and asymmetrical. Consequently, solution by direct inversion will be very intensive in terms of computing time and core memory. These problems can be avoided with an iterative solution technique, however. The method used here is a successive overrelaxation procedure using Gauss-Seidel replacement (20). Initially, a linearly varying temperature is assumed throughout the bed. Then, for each of the j spheres the following equation is evaluated:

$$T_i = T_i^*(1-\alpha) + \frac{\alpha}{N_j} \sum_{i=1}^{N_j} T_k^*, \qquad \text{III.2.7}$$

where T_i^* and T_k^* are the most recent temperature estimates for spheres i and k, and

α is the overrelaxation parameter (determined by trial and error to have an optimal value of 1.48 for systems typically encountered in this work.

Once new estimates of temperature have been obtained for each sphere, the maximum fractional error between the new and previous estimates is determined by evaluating

$$\underset{j}{\text{MAX}} \left| \frac{T_j - T_j^*}{T_j^*} \right|. \qquad \text{III.2.8}$$

When this value is acceptably small (typically on the order of .0000001), the solution is assumed to be converged and the temperature field fully determined.

The final step in the determination of the effective conductivity is the evaluation of the total heat flux across the end of the bed. This is found by summing the heat transfer from one of the two sets of fixed temperature boundary spheres and dividing by the effective bed area:

$$q''_{tot} = \frac{1}{A_e} \sum_{j=1}^{N_s} \sum_{i=1}^{N_j} \frac{(T_i - T_j)}{R_i}, \qquad \text{III.2.9}$$

where q''_{tot} is the total heat flux across the surface,

N_s is the number of spheres on the surface, and

N_j is the number of unit cells sphere j is part of.

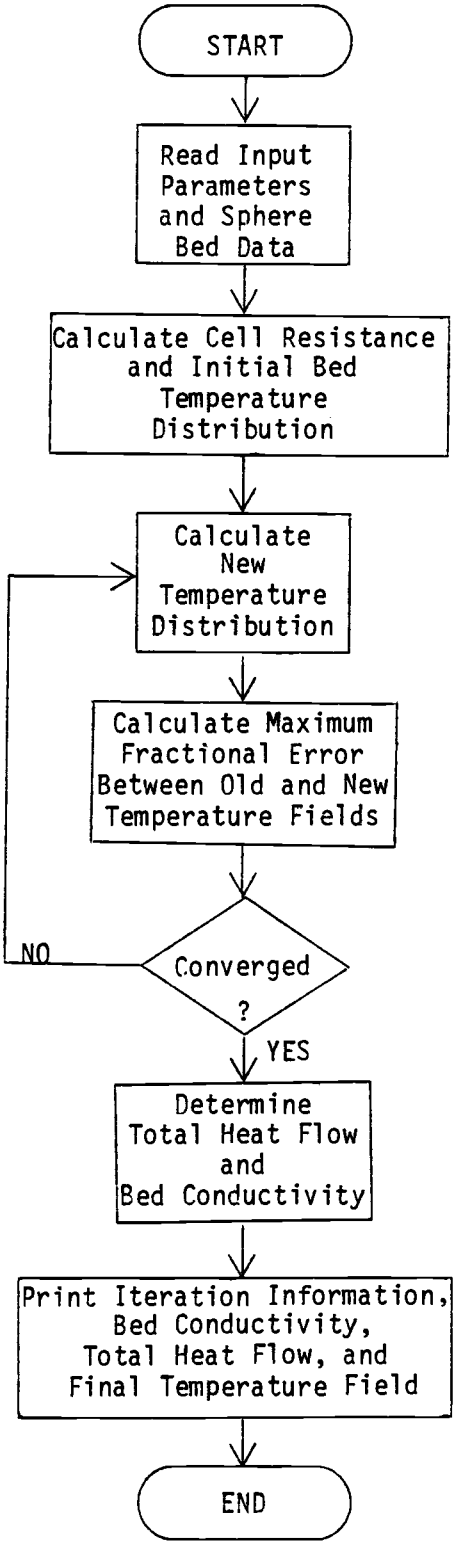
This total heat flux, combined with knowledge of the bed length and boundary temperatures, can now be used to evaluate the effective conductivity of the bed by rearranging III.2.2:

$$k = \frac{q''_{tot} L}{(T_b - T_a)}, \qquad \text{III.2.10}$$

A detailed verification of ORIENT was not undertaken. However, several simple checks involving comparison of the heat flow in and out of the bed and evaluation of Equation III.2.5 for a few randomly selected spheres using the converged temperature distribution revealed no flaws in either the method or the program.

III.3 Flowchart of ORIENT

The following flowchart (Figure III.3) is self explanatory and not discussed in detail here. A complete list of the code and a sample case may be found in Appendices D and E, respectively.



Flowchart of ORIENT

Figure III.3

III.4 The Effect of Packing Factor on Conductivity

The development of the RANDPAC and ORIENT codes represent a significant opportunity to study in detail the thermal behavior of sphere beds. Of specific interest, however, is the effect of packing factor on thermal conductivity. This could, in part, be determined by experimentally measuring the thermal conductivities of beds of various packing densities. Unfortunately, the observed behavior would only be a second order effect. The first order contribution, which cannot easily be separated, is related to the overall increase in distance (due to the random orientation of the spheres) heat must travel when moving between two points in the bed. Separation of this effect requires a knowledge of the absolute magnitude of the conductivity of the very small "straight" heat transfer paths within the bed - the unit cells of Section III.1. In a sphere pac nuclear fuel, the dimensions of these cells are on the order of tens to hundreds of microns making any accurate quantitative determination of the thermal interaction between two spheres impractical. The RANDPAC and ORIENT codes provide a solution to this problem. Random beds of almost any experimentally achievable density may be generated with RANDPAC and analyzed with ORIENT. The cell conductivity used in the latter program is useful in determining intermediate results (such as the absolute heat transfer across the bed being studied) but in reality, has no effect on the

calculation of the bed conductivity. That is, the ratio of the cell conductivity to the bed conductivity is constant for a given packing factor. By simply assuming a cell conductivity of unity, the effect of packing density on the bed conductivity can be determined directly. Appendix E shows an example of this procedure.

As mentioned previously, no specific unit cell is being investigated in this work. Every approach to the unit cell will result in a unique value of cell thermal resistance due to variations in heat transfer area and length, material properties, gap treatment, etc. This, in turn, affects the total heat transfer and the calculation of the effective bed conductivity. An instructive example, however, is the application of this procedure to the unit cell developed by Ades (Figure III.1a). The radius of Ades' cell is calculated from:

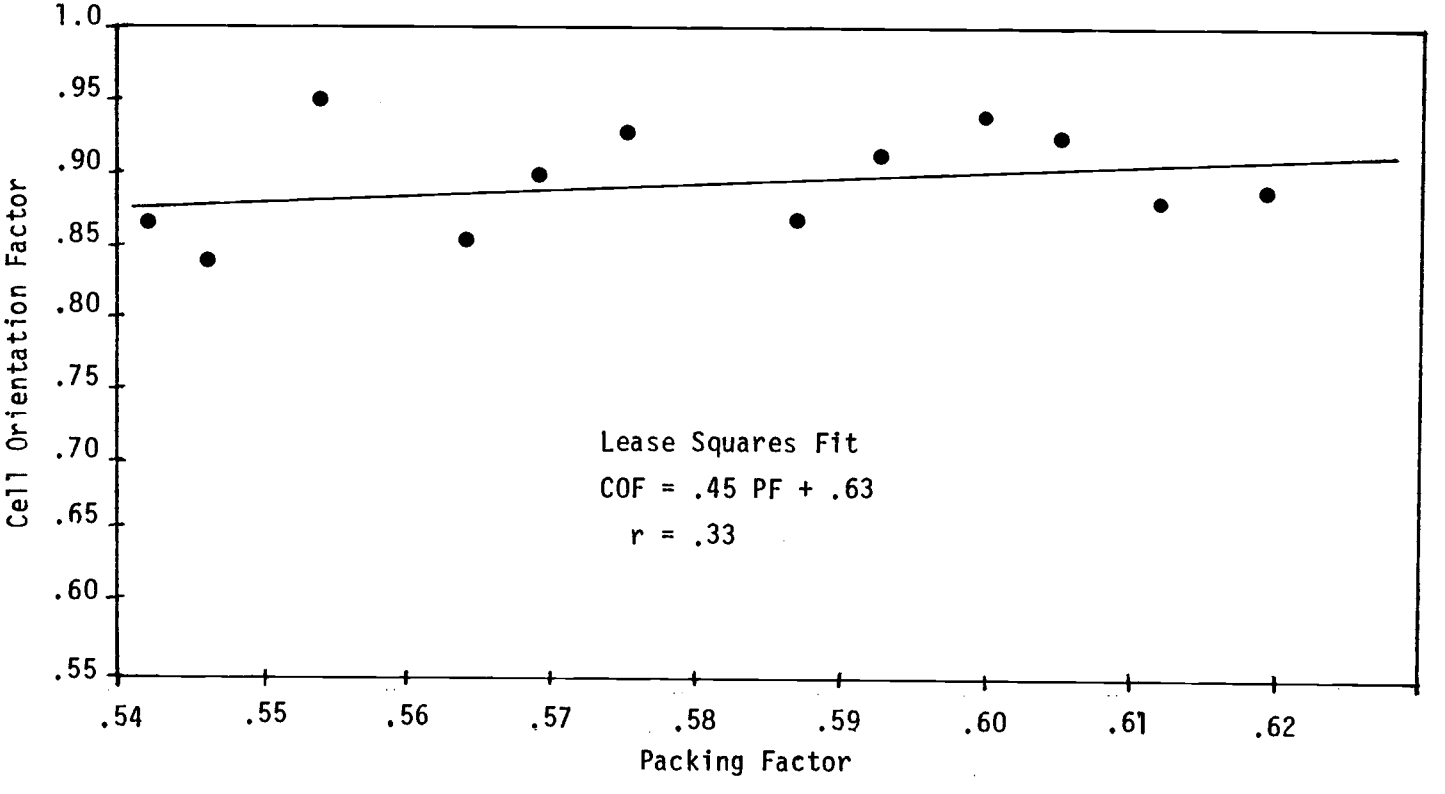
$$R_c = R_s \sqrt{\frac{2}{3PF}},$$

where R_s is the sphere radius, and

PF is the packing factor (4).

The length of the cell is equivalent to one sphere diameter.

The experimental data cited by Ades for comparative purposes (16) involves sphere beds of slightly higher density than have been achieved by RANDPAC (62.53% dense as compared to the RANDPAC maximum of 61.90% dense). For this reason, several beds of successively lower density

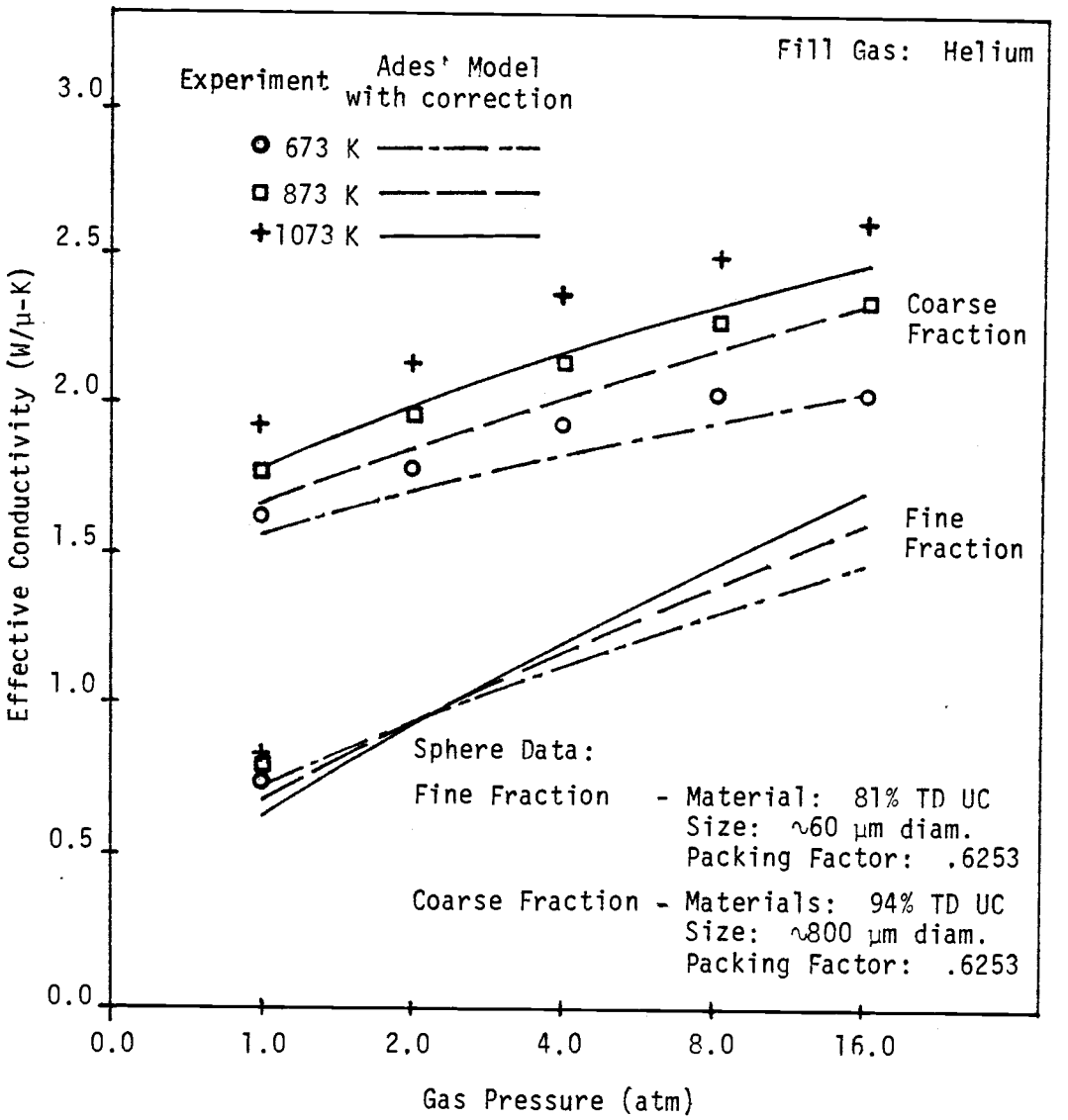


Effect of Packing Factor on
Unit Cell Based Sphere Bed Conductivity Calculation (Ades' Unit Cell (4))

Figure III.4a

were analyzed and the results plotted (Figure III.4a). While there is a great deal of scatter in this data (probably due to the relatively small size of the beds investigated), there appears to be a mild linear correlation corresponding to the second order effect mentioned above. It is interesting to note that the "cell orientation factor" corresponding to this unit cell is almost constant with packing factor. This is due to two competing effects: the overall increase in conductivity that should accompany increasing packing factor in a random bed and the diminished heat flow through the unit cell due to the decreasing cell heat transfer area. These factors are why care must be taken in choosing a unit cell and the boundary conditions applied to it.

A least squares approximation to the data was calculated and the cell orientation factor for the 62.53% dense bed determined by extrapolation to be approximately .91. When Ades' values for effective conductivity are multiplied by the cell orientation factor they fall consistently below the experimental values (Figure III.4b). This is a strong indication of the significance of the cell orientation effect and why it must be considered in sphere bed conductivity calculations involving unit cells.



Ades' Conductivity Calculation Corrected for Cell Orientation Effect

Figure III.4b

IV. Conclusions and Recommendations

Extensive evaluation and application have shown the RANDPAC code to be a useful and accurate tool in the thermal modeling of sphere pac nuclear fuels and cylindrically shaped sphere beds in general. These characteristics should carry over into other areas of investigation, such as mechanical analysis and, possibly, Monte Carlo neutronics. While RANDPAC produced random beds adequate for the analysis presented here, several areas exist which deserve additional study. The code is currently capable of producing what are commonly called "loose random" beds with asymptotic packing factors of approximately 60%. This is some three to four percent below the density of experimentally attainable "dense random" packings. As there are undoubtedly applications which require the densest beds possible, it would be useful for RANDPAC to be capable of simulating denser beds. As mentioned earlier, the inadequacy of the present sphere minimum potential energy algorithm is the predominant reason for not achieving optimum packing. This method does not lend itself to significant improvement, however, and should be discarded in favor of an efficient algorithm for actively seeking the optimum site for each sphere. This could be done by establishing general criteria for the identification of surface spheres and for the geometric stability of a given site. Closely related to optimum packing is the second major shortfall of the code,

the lack of an adequate treatment of infiltration. Once the optimum packing problem has been overcome, infiltration modeling becomes concerned primarily with the location of new holes or potential sphere placement sites within the bed after the new sphere penetrates the surface. This will not be too difficult as the "hole" through which the infiltration occurs greatly reduces the search area. Once infiltration is complete and a potential new site identified, the problem reduces to that of optimum packing.

During the verification of RANDPAC it was noted that a discrepancy exists between the experimental and predicted values of coordination number for a closely packed bed. This should be alleviated in part by improving the packing density. It would be useful, however, to observe the frequency of near contacts (close but not actually touching) as a function of sphere separation distance. These near contacts may contribute significantly to heat transfer within the bed and may, in fact, require an independently formulated unit cell to represent them.

The present version of RANDPAC is still in the developmental stage and little effort has been made to optimize either the FORTRAN or the logic to decrease execution time and central memory requirements. The following items are suggestions for future work in this area which have the most potential for making significant improvements.

1. Central memory storage might be cut by more than fifty percent by keeping track of only the three initial contacts of each sphere. A separate post processor could be written to expand this data into the full contact matrix when necessary.
2. To decrease the time spent searching for neighbor spheres, a method should be devised whereby spheres are flagged and not considered in the search after they become physically inaccessible. If the data for the sphere flagged out is immediately written to mass storage, the central memory space becomes available for treating a new sphere. These two changes will allow essentially infinite packings to be generated without cumulative storage or execution time penalties.

Mention has been made several times of the fact that the simulated beds used in this study were fairly small (less than 500 spheres). An effort needs to be made to benchmark the minimum bed size necessary to avoid large statistical variations in packing factor. Additionally, it would be helpful to repeat some of the calculations reported here to improve upon and examine the validity of the correlations discussed in Chapters Two and Three. This should include some very large radius beds to better determine the asymptotic density achievable by RANDPAC.

Because large, dense packings could not be readily produced, an accurate examination of the effect of the

contact probabilities discussed in Chapter Two was not possible. With the improvement of RANDPAC, the parametric study mentioned in connection with these probabilities would be a valuable exercise because of the potential for gaining valuable insight into the coordination properties of a random bed.

The evaluation of the sphere bed temperature distribution and effective conductivity is performed quickly and accurately by the ORIENT code. Some modifications are necessary, however, before the code can be applied to multiple size fraction beds. First, the generalization discussed in Section III.2 must be incorporated to account for the differences in resistance between the various types of unit cells. Concurrent with this, an algorithm to read in the parameters for the various cells and assign them properly to the links in the resistance network must be developed. These changes are simple and should not significantly affect the execution time although some increase in central memory usage will occur. This can be alleviated by stacking the resistance information in the same memory locations as the contact information.

The analysis presented in Section III.3 indicates that the effect of packing on the effective conductivity of sphere pac nuclear fuels is significant and must be considered in any calculation utilizing the unit cell approach. Observation of the relationship between

orientation factor and packing density for Ades' cell (Figure III.4a) might lead to the additional conclusion that, for packings of interest, bed density is not a significant variable. It is important to note, however, that the magnitude of the orientation factor is highly dependent on unit cell geometry and how it varies with packing factor. That is, different cells may result in orientation factors with markedly different behavior. This enhances the need for care in the selection of unit cells and their boundary conditions.

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APPENDICES

Appendix A

Listing of RANDPAC

This appendix contains a complete listing of RANDPAC and all of its subroutines, with two exceptions. The routines ZRPOLY and VSRTR were accessed through the use of the IMSL Library (21), a commercially available mathematics and statistical package for digital computers. The use of these routines was primarily for reasons of computational speed and could have been avoided by the coding of equivalent FORTRAN routines. The location of the call to each routine and a general description of its purpose is given below.

ZRPOLY - This is called from routine SSCCON and is a root finder capable of determining both real and complex zeros. In SSCCON it is used to determine all the roots of a fourth order polynomial.

VSRTR - This is called from routine UBOUND. It is a highly efficient algorithm for sorting a vector by the relative magnitude of its components. In UBOUND it is used to sort the spheres by elevation.

```
      PROGRAM RANDPAC(INPUT,OUTPUT,TAPE6,TAPE7)
      COMMON/COORDS/X(500),Y(500),Z(500)
      COMMON/RADII/R(500)
      COMMON/LOCALN/LOCCN,NLOCN,LOCN(500),DLOCN(500)
      COMMON/INTER/INT(20,500),IB(500),IT(500)
      COMMON/NEW/XN(2),YN(2),ZN(2)
      COMMON RC,PF(6),RF(5),PC(4)
      DIMENSION HMAX(49),ER(48,2),ET(48,2)
      DIMENSION IMARK(4),XP(4),YP(4),ZP(4),DP(4),LOCNP(500)
      DATA(HMAX(I),I=1,49)/49*0./
      REWIND 6
      REWIND 7
      NCNTACT=20
      PI=4.*ATAN(1.)
C$
C$    READ INPUT
C$
      PRINT*,"CLAD RADIUS?"
      READ*,RC
      PRINT*,RC
C$
C$    SET UP THE ENERGY SEARCH BOUNDARY MATRICES
C$
      DO 300 I=1,48
      ER(I,1)=RC/7.
      IF(I.LT.41)ER(I,1)=3.*RC/7.
      IF(I.LT.25)ER(I,1)=5.*RC/7.
  300 ER(I,2)=ER(I,1)+2.*RC/7.
      DO 301 I=1,16
      ET(I+24,1)=FLOAT(I-1)*PI/8.
  301 ET(I+24,2)=FLOAT(I)*PI/8.
      DO 302 I=1,8
      ET(I+40,1)=FLOAT(I-1)*PI/4.
  302 ET(I+40,2)=FLOAT(I)*PI/4.
      DO 303 I=1,24
      ET(I,1)=FLOAT(I-1)*PI/12.
  303 ET(I,2)=FLOAT(I)*PI/12.
      PRINT*,"# OF SPHERES, SIZE FRACTIONS?"
      READ*,NS,NF
      PRINT*,NS,NF
      PRINT*,"PROB., RADIUS OF EACH FRACTION?"
      READ*,((PF(I+1),RF(I)),I=1,NF)
      PF(1)=0.
      NFP=NF+1
      PRINT*,"PROBABILITIES = ",(PF(I),I=1,NFP)
      PRINT*,"RADII = ",(RF(I),I=1,NF)
      PRINT*,"CONTACT PROB. VECTOR?"
      READ*,(PC(I),I=1,4)
      PRINT*,(PC(I),I=1,4)
      PRINT*,"RANDOM # GENERATOR SEED?"
      READ*,ISEED
```

```
      PRINT*,ISEED
      WRITE(6)NS,NF,RC,(PC(I),I=1,4)
      WRITE(6)(PF(I),I=1,NFP)
      WRITE(6)(RF(I),I=1,NF)
      WRITE(6)ISEED
      NFF=NF
C$
C$    INITIALIZE RANDOM # GENERATOR
C$
      CALL RANSET(ISEED)
      DO 998 I=1,100
  998 P=RANF(W)
      ZLAST=0.
C$
C$    BEGIN LOADING LOOP
C$
      NF=1
      DO 997 IS=1,NS
      NL=IS-1
      DO 11 I=1,20
   11 INT(I,IS)=0
      IB(IS)=0
      IT(IS)=0
C$
C$    DETERMINE SIZE FRACTION
C$
      P=RANF(W)
      DO 1 I=1,NFF
    1 IF(P.GE.PF(I).AND.P.LE.PF(I+1))IF=I
      R(IS)=RF(IF)
C$
C$    SEARCH FOR AREA OF LOWEST POTENTIAL ENERGY
C$
      ISITE=0
      HSITE=10000.
      ISTART=IFIX(49.*RANF(W)+1.)
      DO 310 I=1,49
      J=ISTART+I
      IF(J.GT.49)J=J-49
      IF(HMAX(J).GT.HSITE)GO TO 310
      ISITE=J
      HSITE=HMAX(J)
  310 CONTINUE
C$
C$    DETERMINE THE INITIAL DROP COORDINATES
C$
      IF(ISITE.LT.49)GO TO 311
      XT=(2.*RANF(W)-1.)*(RC/7.)
      YMAX=SQRT((RC*RC/49.)-XT*XT)
      YT=(2.*RANF(W)-1.)*YMAX
      GO TO 312
  311 RSUB=0.
```

```
      IF(ISITE.LT.25)RSUB=R(IS)
      R0=RANF(W)*(ER(ISITE,2)-RSUB-ER(ISITE,1))+ER(ISITE,1)
      T0=RANF(W)*(ET(ISITE,2)-ET(ISITE,1))+ET(ISITE,1)
      XT=R0*COS(T0)
      YT=R0*SIN(T0)
  312 CONTINUE
      ZT=ZLAST+10.*R(IS)
C$
C$    RUN FIRST CONTACT SEARCH
C$
      IF(NL.EQ.0)GO TO 8
      ZMAX=100000.
      IC1=0
      CALL SEARCH1(XT,YT,IC1,NF,IS,ZMAX)
      XXX=XT
      YYY=YT
      ZZZ=Z(IS)
      IF(IC1.GT.0)GO TO 2
C$
C$    FIND COORDINATES IF NO FIRST CONTACT
C$
    8 Z(IS)=.001*RANF(W)*RF(1)
      X(IS)=XT
      Y(IS)=YT
      CALL IBSET(RC,IS,IB(IS),RF(1))
      GO TO 999
    2 CONTINUE
C$
C$    SET UP FIRST CONTACT
C$
      IT(IC1)=IT(IC1)+1
      IF(IT(IC1).GT.NCNTACT)GO TO 990
      INT(IT(IC1),IC1)=IS
      IT(IS)=1
      INT(1,IS)=IC1
C$
C$    CHOOSE NUMBER OF CONTACTS TO SEEK
C$
      P=RANF(W)
      DO 3 I=1,3
    3 IF(P.GE.PC(I).AND.P.LE.PC(I+1))NCP=I
      IF(NCP.EQ.1)GO TO 999
      IF(NCP.GT.1)GO TO 20
C$
C$    REVERT TO ORIGINAL FIRST CONTACT POSITION
C$
   12 CONTINUE
CCC   IF(IMAG.EQ.1)PRINT*,"WARNING--IMAG=1 FOR SPHERE ",IS
      X(IS)=XXX
      Y(IS)=YYY
      Z(IS)=ZZZ
      GO TO 999
```

```
   20 CONTINUE
C$
C$    TWO CONTACT SEARCH STARTS HERE
C$    FIND CLOSEST SPHERE IN NEW LOCAL GROUP
C$
      IC2=0
      IFLAG1=0
      IFLAG2=0
      ZT=Z(IS)
      DMAX=R(IS)+3.*RF(1)
      CALL LOCAL(XT,YT,ZT,DMAX,DMAX,DMAX,NF,NL,LOCCN,NLOCN,LOCN,
     &DLOCN)
      IF(NLOCN.GE.2)GO TO 23
      IF(LOCCN.EQ.1)GO TO 24
      GO TO 12
   23 DMIN=1000.
      DO 21 I=1,NLOCN
      IF(LOCN(I).EQ.IC1)GO TO 21
      IF(DLOCN(I).GT.DMIN)GO TO 21
      DMIN=DLOCN(I)
      IC2=LOCN(I)
      IHOLD2=I
   21 CONTINUE
C$
C$    IS CLAD LOCAL? IF SO HOW FAR
C$
      IF(LOCCN.EQ.0)GO TO 22
      DCLAD=RC-PYTHAG(XT,YT,0.)
      IF(DCLAD.GT.DLOCN(IHOLD2))GO TO 22
C$
C$    2ND CONTACT IS WITH CLAD(UNLESS NCP=3),PICK ANGLE
C$
   24 IF(NCP.EQ.3)GO TO 22
   75 CONTINUE
      DO 26 I=1,100
      XI=PI*RANF(W)
      CALL SCCON(IC1,IS,XI,RC,IMAG)
      IF(IMAG.EQ.1)GO TO 22
      II=IFIX(2.*RANF(W))+1
      IF(ZN(II).LT.0.)GO TO 26
      CALL LEGAL(XN(II),YN(II),ZN(II),IS,ILEG)
      IF(ILEG.EQ.1)GO TO 26
      X(IS)=XN(II)
      Y(IS)=YN(II)
      Z(IS)=ZN(II)
      CALL IBSET(RC,IS,IB(IS),RF(1))
      GO TO 999
   26 CONTINUE
CCC   PRINT*,"100 ATTEMPTS AT S-C CONTACT"
   22 CONTINUE
      IF(IFLAG1.EQ.0.AND.IFLAG2.EQ.0)GO TO 71
      IFLAG2=1
```

```
      IF(IFLAG1.EQ.1)GO TO 12
   71 CONTINUE
      IF(IC2.EQ.0)GO TO 12
C$
C$    2ND CONTACT IS WITH SPHERE. PICK ANGLE
C$
      DO 27 I=1,100
      XI=2.*PI*RANF(W)-PI
      CALL SSCON(IC1,IC2,IS,XI,IMAG)
      IF(IMAG.EQ.1)GO TO 12
      IF(IMAG.EQ.2)GO TO 27
      IF(ZN(1).LT.0.)GO TO 27
      CALL LEGAL(XN(1),YN(1),ZN(1),IS,ILEG)
      IF(ILEG.EQ.1)GO TO 27
      X(IS)=XN(1)
      Y(IS)=YN(1)
      Z(IS)=ZN(1)
      IF(NCP.EQ.2)CALL IBSET(RC,IS,IB(IS),RF(1))
C$
C$    SET THE CONTACT MATRICES
C$
      IT(IS)=2
      INT(2,IS)=IC2
      IT(IC2)=IT(IC2)+1
      IF(IT(IC2).GT.NCNTACT)GO TO 990
      INT(IT(IC2),IC2)=IS
      IF(NCP.GT.2)GO TO 30
      GO TO 999
   27 CONTINUE
CCC   PRINT*,"100 ATTEMPTS AT S-S CONTACT"
      IFLAG1=1
      IF(IFLAG2.EQ.1)GO TO 12
      GO TO 75
   30 CONTINUE
C$
C$    THIRD CONTACT SEARCH STARTS HERE
C$    SAVE PRESENT COORDINATES
C$
      XO=X(IS)
      YO=Y(IS)
      ZO=Z(IS)
      DMAX=R(IS)+3.*RF(1)
C$
C$    DEFINE THE LOCAL GROUP
C$
      CALL LOCAL(XO,YO,ZO,DMAX,DMAX,DMAX,NF,NL,LOCCN,NLOCN,LOCNP,
     &DLOCN)
C$
C$    TRY TO FIND A S-S-S CONTACT
C$
      ISSS=0
      DO 55 I=1,4
```

```
      DP(I)=0.
   55 IMARK(I)=0.
      IF(NLOCN.LT.3)GO TO 33
      NNN=NLOCN
      DO 31 I=1,NNN
      DO 32 KJI=1,4
   32 IMARK(KJI)=0
      IF(LOCNP(I).EQ.IC1.OR.LOCNP(I).EQ.IC2)GO TO 31
      CALL SSSCON(IC1,IC2,LOCNP(I),IS,IMAG)
      IF(IMAG.EQ.1)GO TO 31
      CALL LEGAL(XN(1),YN(1),ZN(1),IS,ILEG1)
      CALL LEGAL(XN(2),YN(2),ZN(2),IS,ILEG2)
      IF(ILEG1.EQ.0.OR.ILEG2.EQ.0)ISSS=1
      IF(ILEG1.EQ.0.OR.ILEG2.EQ.0)IC3=LOCNP(I)
      IF(ISSS.EQ.0)GO TO 31
      IF(ILEG1.EQ.0)IMARK(1)=1
      IF(ILEG2.EQ.0)IMARK(2)=1
      IF(ZN(1).LT.0.)IMARK(1)=0
      IF(ZN(2).LT.0.)IMARK(2)=0
      IF(IMARK(1).EQ.0.AND.IMARK(2).EQ.0)ISSS=0
      IF(IMARK(1).EQ.0)GO TO 34
      XP(1)=XN(1)
      YP(1)=YN(1)
      ZP(1)=ZN(1)
   34 IF(IMARK(1).EQ.0.AND.IMARK(2).EQ.0)GO TO 31
      IF(IMARK(2).EQ.0)GO TO 33
      XP(2)=XN(2)
      YP(2)=YN(2)
      ZP(2)=ZN(2)
      GO TO 33
   31 CONTINUE
C$
C$    TRY TO FIND A S-S-C CONTACT
C$
   33 CONTINUE
      ISSC=0
      CALL SSCCON(IC1,IC2,IS,RC,IMAG)
      IF(IMAG.EQ.1)GO TO 37
      CALL LEGAL(XN(1),YN(1),ZN(1),IS,ILEG1)
      CALL LEGAL(XN(2),YN(2),ZN(2),IS,ILEG2)
      IF(ILEG1.EQ.0)IMARK(3)=1
      IF(ILEG2.EQ.0)IMARK(4)=1
      IF(ILEG1.EQ.0.OR.ILEG2.EQ.0)ISSC=1
      IF(ZN(1).LT.0.)IMARK(3)=0
      IF(ZN(2).LT.0.)IMARK(4)=0
      IF(IMARK(3).EQ.0.AND.IMARK(4).EQ.0)ISSC=0
      IF(IMARK(3).EQ.0)GO TO 36
      XP(3)=XN(1)
      YP(3)=YN(1)
      ZP(3)=ZN(1)
   36 IF(IMARK(4).EQ.0)GO TO 37
      XP(4)=XN(2)
```

```
      YP(4)=YN(2)
      ZP(4)=ZN(2)
C$
C$    DETERMINE THE SHORTEST AND MOST PROBABLE MOVE
C$
   37 DO 38 I=1,4
      IF(IMARK(I).EQ.0)GO TO 38
      DP(I)=PYTHAG((XP(I)-X0),(YP(I)-Y0),(ZP(I)-Z0))
   38 CONTINUE
      DO 39 I=1,4
      IF(DP(I).NE.0.)GO TO 40
   39 CONTINUE
CCC   PRINT*,"NO THIRD CONTACT FOUND"
      CALL IBSET(RC,IS,IB(IS),RF(1))
      GO TO 999
   40 DIST=10000.
      ICL=IFIX(10.*RANF(W))
      IF(ICL.GE.1)GO TO 62
      IFF=1
      IF(ISSS.EQ.0.AND.ISSC.EQ.1)IFF=3
      GO TO 63
   62 IFF=3
      IF(ISSC.EQ.0.AND.ISSS.EQ.1)IFF=1
   63 IL=IFF+1
      DO 41 I=IFF,IL
      IF(IMARK(I).EQ.0)GO TO 41
      IF(DP(I).GT.DIST)GO TO 41
      DIST=DP(I)
      NXYZ=I
   41 CONTINUE
      X(IS)=XP(NXYZ)
      Y(IS)=YP(NXYZ)
      Z(IS)=ZP(NXYZ)
      CALL IBSET(RC,IS,IB(IS),RF(1))
      IF(NXYZ.GT.2)GO TO 999
C$
C$    SET THE INTERACTION VECTORS
C$
      IT(IS)=3
      INT(3,IS)=IC3
      IT(IC3)=IT(IC3)+1
      IF(IT(IC3).GT.NCNTACT)GO TO 990
      INT(IT(IC3),IC3)=IS
  999 CONTINUE
      WRITE(7,110)IS,X(IS),Y(IS),Z(IS),R(IS),NCP,IB(IS),IT(IS),
     &(INT(J,IS),J=1,4)
      ENDFILE 7
  110 FORMAT(I4,4(1X,E12.6),1X,I1,1X,I1,1X,I2,4(1X,I4))
C$
C$    UPDATE THE ENERGY SEARCH ARRAY
C$
      R0=PYTHAG(X(IS),Y(IS),0.)
```

```
      TO=ATAN2(Y(IS),X(IS))
      IF(TO.LT.0.)TO=TO+2.*PI
      IF(RO.GT.(RC/7.))GO TO 320
      IF(Z(IS).GT.HMAX(49))HMAX(49)=Z(IS)
      GO TO 997
  320 JF=1
      IF(RO.LT.(5.*RC/7.))JF=25
      IF(RO.LT.(3.*RC/7.))JF=41
      JL=24
      IF(JF.EQ.25)JL=40
      IF(JF.EQ.41)JL=48
      DO 321 I=JF,JL
      IF(TO.LT.ET(I,1).OR.TO.GE.ET(I,2))GO TO 321
      IF(Z(IS).GT.HMAX(I))HMAX(I)=Z(IS)
      GO TO 997
  321 CONTINUE
  997 CONTINUE
      CALL UBOUND(NS,BEDLEN,PACFAC,NBOT,NUP)
      WRITE(6)BEDLEN,PACFAC
      PRINT*,"LENGTH OF BED = ",BEDLEN
      PRINT*,"PACKING FACTOR = ",PACFAC
      PRINT*,"# OF UPPER BOUNDARY SPHERES = ",NUP
      PRINT*,"# OF LOWER BOUNDARY SPHERES = ",NBOT
      WRITE(6)NUP,NBOT
      DO 1000 I=1,NS
 1000 WRITE(6)X(I),Y(I),Z(I),R(I),IB(I),IT(I),(INT(J,I),J=1,20)
      STOP
  990 PRINT*,"TOO MANY CONTACTS FOR SPHERE ",IS
      STOP
      END
      SUBROUTINE SSSCON(I,J,K,L,IMAG)
C$
C$    L       NEW SPHERE
C$    I,J,K   OLD SPHERES
C$    IMAG    COMPLEX SOLUTIONS INDICATOR
C$
      COMMON/COORDS/XP(500),YP(500),ZP(500)
      COMMON/RADII/RAD(500)
      COMMON/NEW/XN(2),YN(2),ZN(2)
      DIMENSION X(3),Y(3),Z(3)
      IMAG=0
C$
C$    SHIFT TO LOCAL COORDINATES
C$
      DO 1 M=1,3
      IF(M.EQ.1)N=I
      IF(M.EQ.2)N=J
      IF(M.EQ.3)N=K
      X(M)=XP(N)-XP(I)
      Y(M)=YP(N)-YP(I)
    1 Z(M)=ZP(N)-ZP(I)
C$
```

```
C$    DETERMINE THE LEG LENGTHS
C$
      S12=PYTHAG(X(2),Y(2),Z(2))
      S13=PYTHAG(X(3),Y(3),Z(3))
      S23=PYTHAG((X(2)-X(3)),(Y(2)-Y(3)),(Z(2)-Z(3)))
      S14=RAD(I)+RAD(L)
      S24=RAD(J)+RAD(L)
      S34=RAD(K)+RAD(L)
C$
C$    DETERMINE COSINES OF ANGLES
C$
      T24=(S12*S12+S14*S14-S24*S24)/(2.*S12*S14)
      T34=(S13*S13+S14*S14-S34*S34)/(2.*S13*S14)
      IF(ABS(T24).LE.1..AND.ABS(T34).LE.1.)GO TO 78
      IMAG=1
      RETURN
   78 CONTINUE
C$
C$    DETERMINE A,B DIRECTION COSINES
C$
      A1=X(2)/S12
      A2=Y(2)/S12
      A3=Z(2)/S12
      B1=X(3)/S13
      B2=Y(3)/S13
      B3=Z(3)/S13
C$
C$    DEFINE CONSTANTS FOR QUADRATIC
C$
      ALFA=A1*B3-A3*B1
      BETA=A2*B3-A3*B2
      IF(BETA.NE.0.)GO TO 77
      PRINT*,"DIRECTION COSINE FLUKE IN SSSCON"
      IMAG=1
      RETURN
   77 CONTINUE
      GAMA=(B3*T24)-(A3*T34)
      SGMA=A1*B2-A2*B1
      ETA=A3*B2-A2*B3
      DLTA=(B2*T24)-(A2*T34)
      Q=1.+((ALFA/BETA)**2.)+((SGMA/ETA)**2.)
      R=(-2.)*((ALFA*GAMA/(BETA**2.))+(SGMA*DLTA/(ETA**2.)))
      S=((GAMA/BETA)**2.)+((DLTA/ETA)**2.)-1.
C$
C$    SOLVE THE QUADRATIC
C$
      DD=R*R-(4.*Q*S)
      IF(DD.GE.0.)GO TO 2
      IMAG=1
      RETURN
    2 DD=SQRT(DD)
      CALL QUAD(Q,R,DD,C11,C12)
```

```
C$
C$    FIND THE REST OF THE DIRECTION COSINES C
C$
      C21=(GAMA-ALFA*C11)/BETA
      C22=(GAMA-ALFA*C12)/BETA
      C31=(DLTA-SGMA*C11)/ETA
      C32=(DLTA-SGMA*C12)/ETA
C$
C$    FIND THE LOCAL COORDINATES
C$
      XN(1)=S14*C11
      XN(2)=S14*C12
      YN(1)=S14*C21
      YN(2)=S14*C22
      ZN(1)=S14*C31
      ZN(2)=S14*C32
C$
C$    CONVERT TO GLOBAL COORDINATES
C$
      DO 3 M=1,2
      XN(M)=XN(M)+XP(I)
      YN(M)=YN(M)+YP(I)
    3 ZN(M)=ZN(M)+ZP(I)
      RETURN
      END
      SUBROUTINE SSCON(I,J,L,XI,IMAG)
C$
C$    L      NEW SPHERE
C$    I,J    OLD SPHERES
C$    XI     ROTATION ANGLE
C$    IMAG   COMPLEX SOLUTIONS INDICATOR
C$
      COMMON/COORDS/XP(500),YP(500),ZP(500)
      COMMON/RADII/RAD(500)
      COMMON/NEW/XN(2),YN(2),ZN(2)
      DIMENSION X(2),Y(2),Z(2),BB(2)
      PI=4.*ATAN(1.)
C$
C$    SHIFT TO LOCAL COORDINATES
C$
      IMAG=0
      DO 1 M=1,2
      IF(M.EQ.1)N=I
      IF(M.EQ.2)N=J
      X(M)=XP(N)-XP(I)
      Y(M)=YP(N)-YP(I)
    1 Z(M)=ZP(N)-ZP(I)
C$
C$    DETERMINE THE LEG LENGTHS
C$
      S12=PYTHAG(X(2),Y(2),Z(2))
      S13=RAD(I)+RAD(L)
```

```
      S23=RAD(J)+RAD(L)
C$
C$    DETERMINE THE INCLUDED ANGLE AND ITS COSINE
C$
      CT23=(S12*S12+S13*S13-S23*S23)/(2.*S12*S13)
      IF(ABS(CT23).LE.1.)GO TO 78
      IMAG=1
      RETURN
   78 CONTINUE
      ST23=SQRT(1.-CT23*CT23)
C$
C$    DEFINE DIRECTION COSINES A
C$
      A1=X(2)/S12
      A2=Y(2)/S12
      A3=Z(2)/S12
C$
C$    DEFINE RANDOM B1
C$
      B1=COS(XI)
      Q=A2*A2+A3*A3
      BSQ=B1*B1
      IF(BSQ.LE.Q)GO TO 76
      IMAG=2
      RETURN
   76 CONTINUE
C$
C$    DEFINE CONSTANTS
C$
      IF(Q.NE.0.)GO TO 77
      PRINT*,"DIRECTION COSINE FLUKE IN SSCON"
      IMAG=1
      RETURN
   77 CONTINUE
      R=2.*A1*A2*B1
      S=((1.-A2*A2)*B1*B1)-A3*A3
      DD=SQRT(R*R-4.*Q*S)
C$
C$    SOLVE THE QUADRATIC
C$
      CALL QUAD(Q,R,DD,BB(1),BB(2))
C$
C$    DETERMINE THE REMAINING DIRECTION COSINES
C$
      II=IFIX(2.*RANF(W))+1
      B2=BB(II)
      B3=(-1.)*(A1*B1+A2*B2)/A3
      C1=B2*A3-A2*B3
      C2=B3*A1-A3*B1
      C3=B1*A2-A1*B2
C$
C$    DETERMINE THE LOCAL COORDINATES
```

```
C$
      XN(1)=S13*(A1*CT23+C1*ST23)
      YN(1)=S13*(A2*CT23+C2*ST23)
      ZN(1)=S13*(A3*CT23+C3*ST23)
C$
C$    CONVERT TO GLOBAL COORDINATES
C$
      XN(1)=XN(1)+XP(I)
      YN(1)=YN(1)+YP(I)
      ZN(1)=ZN(1)+ZP(I)
      RETURN
      END
      SUBROUTINE SCON(I,L,TH,PHI)
C$
C$    L           NEW SPHERE
C$    I           OLD SPHERE
C$    TH, PHI     ROTATION ANGLES
C$
      COMMON/COORDS/XP(500),YP(500),ZP(500)
      COMMON/RADII/RAD(500)
      COMMON/NEW/XN(2),YN(2),ZN(2)
C$
C$    DETERMINE DISTANCE BETWEEN CENTERS
C$
      S12=RAD(I)+RAD(L)
C$
C$    DETERMINE NEW COORDINATES
C$
      XN(1)=XP(I)+S12*COS(TH)*SIN(PHI)
      YN(1)=YP(I)+S12*SIN(TH)*SIN(PHI)
      ZN(1)=ZP(I)+S12*COS(PHI)
      RETURN
      END
      SUBROUTINE FRSTCON(I,L)
C$
C$    L      NEW SPHERE
C$    I      OLD SPHERE
C$
      COMMON/COORDS/XP(500),YP(500),ZP(500)
      COMMON/RADII/RAD(500)
      COMMON/NEW/XN(2),YN(2),ZN(2)
C$
C$    DETERMINE DISTANCE BETWEEN CENTERS
C$
      S12=RAD(I)+RAD(L)
C$
C$    DETERMINE NEW Z-PRIME COORDINATES
C$
      D=SQRT(S12*S12-((XP(I)-XP(L))**2.)-((YP(I)-YP(L))**2.))
      ZN(1)=ZP(I)+D
      ZN(2)=ZP(I)-D
      RETURN
```

```
      END
      SUBROUTINE SCCON(I,L,XI,RC,IMAG)
C$
C$    L      NEW SPHERE
C$    I      OLD SPHERE
C$    XI     ROTATION ANGLE
C$    RC     CLAD RADIUS
C$    IMAG   COMPLEX SOLUTIONS INDICATOR
C$
      COMMON/COORDS/XP(500),YP(500),ZP(500)
      COMMON/RADII/RAD(500)
      COMMON/NEW/XN(2),YN(2),ZN(2)
C$
C$    DETERMINE DISTANCES AND ANGLES
C$
      IMAG=0
      S13=RAD(I)+RAD(L)
      R1=PYTHAG(XP(I),YP(I),0.)
      IF(YP(I).EQ.0.)IMAG=1
      IF(IMAG.EQ.1)RETURN
      THETA=ATAN2(XP(I),YP(I))
      R3=RC-RAD(L)
      CT23=(R1*R1+R3*R3-S13*S13)/(2.*R1*R3)
      IF(ABS(CT23).GT.1.)IMAG=1
      IF(IMAG.EQ.1)RETURN
      ST23=SQRT(1.-CT23*CT23)
C$
C$    CALCULATE XN, YN, AND ZN IN TRANSFORMED COORDINATES
C$
      XM=R3*ST23
      XN(1)=XM*COS(XI)
      XN(2)=(-1.)*XN(1)
      YN(1)=SQRT(R3*R3-XN(1)*XN(1))
      YN(2)=YN(1)
      ZN(1)=(S13*S13-XN(1)*XN(1)-((R1-YN(1))**2.))+1.E-12
      IF(ZN(1).LT.0.)IMAG=1
      IF(IMAG.EQ.1)RETURN
      ZN(1)=SQRT(ZN(1))
      ZN(2)=(-1.)*ZN(1)
C$
C$    TRANSFORM SOLUTION TO GLOBAL COORDINATES
C$
      XT1=XN(1)*COS(THETA)+YN(1)*SIN(THETA)
      XT2=XN(2)*COS(THETA)+YN(2)*SIN(THETA)
      YT1=YN(1)*COS(THETA)-XN(1)*SIN(THETA)
      YT2=YN(2)*COS(THETA)-XN(2)*SIN(THETA)
      XN(1)=XT1
      XN(2)=XT2
      YN(1)=YT1
      YN(2)=YT2
      ZN(1)=ZN(1)+ZP(I)
      ZN(2)=ZN(2)+ZP(I)
```

```
      RETURN
      END
      SUBROUTINE SSCCON(I,J,L,RC,IMAG)
C$
C$    L     NEW SPHERE
C$    I,J   OLD SPHERES
C$    RC    CLAD RADIUS
C$    IMAG  COMPLEX SOLUTIONS INDICATOR
C$
      COMMON/COORDS/XP(500),YP(500),ZP(500)
      COMMON/RADII/RAD(500)
      COMMON/NEW/XN(2),YN(2),ZN(4)
      DIMENSION DD(3,2),AA(5),Z(4)
      COMPLEX Z
C$
C$    FIND LOCAL COORDINATES
C$
      IMAG=0
      X2=XP(J)-XP(I)
      Y2=YP(J)-YP(I)
      Z2=ZP(J)-ZP(I)
C$
C$    FIND DISTANCES
C$
      S13=RAD(I)+RAD(L)
      S23=RAD(J)+RAD(L)
      S12=PYTHAG(X2,Y2,Z2)
C$
C$    DEFINE CONSTANTS
C$
      DLTA=((RC-RAD(L))**2.)-XP(I)*XP(I)-YP(I)*YP(I)-S13*S13
      GAMA=(S12*S12+S13*S13-S23*S23)/2.
      DENOM=X2*YP(I)-XP(I)*Y2
      IF(DENOM.NE.0.)GO TO 77
      PRINT*,"DENOM=0. FLUKE IN SSCCON"
      IMAG=1
      RETURN
   77 CONTINUE
      A=X2/(2.*DENOM)
      B=XP(I)*Z2/DENOM
      C=(DLTA*X2-(2.*GAMA*XP(I)))/(2.*DENOM)
      DENOM=(-1.)*DENOM
      D=Y2/(2.*DENOM)
      E=YP(I)*Z2/DENOM
      F=(Y2*DLTA-(2.*GAMA*YP(I)))/(2.*DENOM)
      AA(1)=A*A+D*D
      AA(2)=2.*(A*B+D*E)
      AA(3)=2.*(A*C+D*F)+B*B+E*E+1.
      AA(4)=2.*(B*C+E*F)
      AA(5)=C*C+F*F-S13*S13
C$
C$    CALL TO IMSL ROUTINE ZRPOLY TO FIND 4 ROOTS
```

```
C$
      NDEG=4
      CALL ZRPOLY(AA,NDEG,Z,IER)
C$
C$    DETERMINE NUMBER OF REAL ROOTS AND DECODE
C$
      K=0
      DO 1 M=1,4
      IF(ABS(AIMAG(Z(M))).GT.1.E-7)GO TO 1
      K=K+1
      ZN(K)=REAL(Z(M))
    1 CONTINUE
      IF(K.EQ.2)GO TO 4
      IMAG=1
      RETURN
    4 CONTINUE
C$
C$    FIND REST OF LOCAL COORDINATES
C$
      XN(1)=D*(ZN(1)**2.)+E*ZN(1)+F
      XN(2)=D*(ZN(2)**2.)+E*ZN(2)+F
      YN(1)=A*(ZN(1)**2.)+B*ZN(1)+C
      YN(2)=A*(ZN(2)**2.)+B*ZN(2)+C
C$
C$    CONVERT ALL TO GLOBAL COORDINATES
C$
      DO 5 M=1,2
      XN(M)=XN(M)+XP(I)
      YN(M)=YN(M)+YP(I)
    5 ZN(M)=ZN(M)+ZP(I)
      RETURN
      END
      FUNCTION PYTHAG(X,Y,Z)
      PYTHAG=SQRT(X*X+Y*Y+Z*Z)
      RETURN
      END
      SUBROUTINE QUAD(Q,R,DD,C11,C12)
      C11=((-1.)*R+DD)/(2.*Q)
      C12=((-1.)*R-DD)/(2.*Q)
      RETURN
      END
      SUBROUTINE LOCAL(X,Y,Z,DX,DY,DZ,NF,NS,LOCC,NLOC,LOC,DLOC)
C$
C$    X,Y,Z     SEARCH CENTER COORDINATES
C$    DX,DY,DZ  SEARCH INCREMENTS
C$    RC        CLAD RADIUS
C$    NF        FIRST SPHERE TO BE EXAMINED
C$    NS        CURRENT NUMBER OF SPHERES
C$    LOCC      CLAD LOCALITY FLAG
C$               0 NOT LOCAL
C$               1 LOCAL
C$    NLOC      NUMBER OF LOCAL SPHERES
```

```
C$    LOC       SPHERE NUMBERS OF LOCAL SPHERES
C$    DLOC      DISTANCES TO LOCAL SPHERES
C$
      COMMON/COORDS/XP(500),YP(500),ZP(500)
      COMMON RC
      DIMENSION RM(4),LOC(1),DLOC(1)
C$
C$    SET UP SEARCH BOUNDS
C$
      XU=X+DX
      XL=X-DX
      YU=Y+DY
      YL=Y-DY
      ZU=Z+DZ
      ZL=Z-DZ
C$
C$    PERFORM LOCAL SEARCH AND CALCULATE DISTANCES TO LOCAL SPHERES
C$
      NLOC=0
      DO 1 I=NF,NS
      IF(XP(I).GT.XU.OR.XP(I).LT.XL)GO TO 1
      IF(YP(I).GT.YU.OR.YP(I).LT.YL)GO TO 1
      IF(ZP(I).GT.ZU.OR.ZP(I).LT.ZL)GO TO 1
      NLOC=NLOC+1
      LOC(NLOC)=I
      DLOC(NLOC)=PYTHAG((XP(I)-X),(YP(I)-Y),(ZP(I)-Z))
    1 CONTINUE
C$
C$    DETERMINE LOCALITY OF CLAD
C$
      RM(1)=PYTHAG(XU,YU,0.)
      RM(2)=PYTHAG(XU,YL,0.)
      RM(3)=PYTHAG(XL,YU,0.)
      RM(4)=PYTHAG(XL,YL,0.)
      LOCC=0
      DO 2 I=1,4
    2 IF(RM(I).GE.RC)LOCC=1
      RETURN
      END
      SUBROUTINE IBSET(RC,IS,IB,RF)
C$
C$    IS    SPHERE #
C$    IB    BOUNDARY TYPE
C$           0 NONE
C$           1 CLAD
C$           2 BOTTOM
C$           3 BOTH
C$    RC    CLAD RADIUS
C$
      COMMON/COORDS/X(500),Y(500),Z(500)
      COMMON/RADII/R(500)
      IB=0
```

```
      RS=PYTHAG(X(IS),Y(IS),0.)+.0000001
      RMAX=RC-R(IS)
      IF(ABS(Z(IS)).LT.R(IS))IB=IB+2
      IF(RS.GE.RMAX)IB=IB+1
      RETURN
      END
      SUBROUTINE SEARCH1(XX,YY,IC1,NF,IS,ZMAX)
C$
C$    XX,YY      X-Y PLANE COORDINATES OF NEW SPHERE
C$    IC1        FIRST CONTACT SPHERE
C$    NF         FIRST SPHERE TO CHECK
C$    IS         NEW SPHERE NUMBER
C$
      COMMON/COORDS/X(500),Y(500),Z(500)
      COMMON/RADII/R(500)
      COMMON/NEW/XN(2),YN(2),ZN(2)
      NL=IS-1
      DO 1 J=NF,NL
      I=NL-J+1
      IF(Z(I).GT.ZMAX)GO TO 2
      D=PYTHAG((XX-X(I)),(YY-Y(I)),0.)
      DMIN=R(IS)+R(I)
      IF(D.GT.DMIN)GO TO 1
      X(IS)=XX
      Y(IS)=YY
      CALL FRSTCON (I,IS)
      Z(IS)=AMAX1(ZN(1),ZN(2))
      IC1=I
      GO TO 2
    1 CONTINUE
    2 RETURN
      END
      SUBROUTINE LEGAL(XX,YY,ZZ,IS,ILEG)
C$
C$    XX,YY,ZZ    CURRENT NEW SPHERE COORDINATES
C$    IS          CURRENT SPHERE NUMBER
C$    ILEG        LEGALITY INDICATOR
C$                 0 YES
C$                 1 NO
C$
      COMMON/COORDS/X(500),Y(500),Z(500)
      COMMON/RADII/R(500)
      COMMON/LOCALN/LOCCN,NLOCN,LOCN(500),DLOCN(500)
      COMMON RC,PF(6),RF(5),PC(4)
      ILEG=0
      NF=1
      NL=IS-1
C$
C$    COMPUTE AND FLAG OUT NEW LOCAL SPHERE DISTANCES
C$
      DMAX=R(IS)+3.*RF(1)
      CALL LOCAL(XX,YY,ZZ,DMAX,DMAX,DMAX,NF,NL,LOCCN,NLOCN,
```

```
     &LOCN,DLOCN)
      DO 1 I=1,NLOCN
      DMIN=R(IS)+R(LOCN(I))
      IF((DMIN-DLOCN(I)).LE..00000001)GO TO 1
      ILEG=1
      RETURN
    1 CONTINUE
C$
C$    CHECK FOR SPHERE OUTSIDE CLAD
C$
      RR=PYTHAG(XX,YY,0.)-.00000001
      RMAX=RC-R(IS)
      IF(RR.LT.RMAX)RETURN
      ILEG=1
      RETURN
      END
      SUBROUTINE UBOUND(NS,BEDLEN,PACFAC,NBOT,NUP)
      COMMON/COORDS/X(500),Y(500),Z(500)
      COMMON/RADII/R(500)
      COMMON/INTER/INT(20,500),IB(500),IT(500)
      COMMON RC
      DIMENSION IUP(100),IBOT(100)
      DIMENSION IORDER(500),ZORDER(500)
      DO 7 I=1,NS
      IORDER(I)=I
    7 ZORDER(I)=Z(I)
      PI=4.*ATAN(1.)
C$
C$    BEGIN UPPER SPHERE SEARCH
C$
      VSTOT=0.
      IMAX=0
      ZMAX=0.
      DO 1 I=1,NS
      VSTOT=VSTOT+4.*PI*(R(I)**3.)/3.
      IF(Z(I).LE.ZMAX)GO TO 1
      ZMAX=Z(I)
      IMAX=I
    1 CONTINUE
      PRINT*,"ALTITUDE OF HIGHEST SPHERE = ",ZMAX
C$
C$    DETERMINE LOWER BOUNDARY SPHERES AND LOWER BOUNDARY HEIGHT
C$
      NBOT=0
      DO 2 I=1,NS
      IF(IB(I).LE.1)GO TO 2
      NBOT=NBOT+1
      IBOT(NBOT)=I
    2 CONTINUE
      RBSUM=0.
      RBZSUM=0.
      DO 9 I=1,NBOT
```

```
      RBSUM=RBSUM+R(IBOT(I))
      RBZSUM=RBZSUM+R(IBOT(I))*Z(IBOT(I))
    9 CONTINUE
      ZBOT=RBZSUM/RBSUM
      PRINT*,"BOTTOM BOUNDARY ALTITUDE = ",ZBOT
C$
C$    DETERMINE (NBOT) TOP SPHERES
C$
      CALL VSRTR(ZORDER,NS,IORDER)
      RSUM=0.
      RZSUM=0.
      NF=NS-NBOT+1
      DO 3 I=NF,NS
      K=IORDER(I)
      IUP(I-NF+1)=K
      RSUM=RSUM+R(K)
      RZSUM=RZSUM+R(K)*Z(K)
    3 CONTINUE
      ZTOP=RZSUM/RSUM
      PRINT*,"TOP BOUNDARY ALTITUDE= ",ZTOP
      NUP=NBOT
      DO 4 I=1,NUP
      IF(IB(IUP(I)).EQ.0.OR.IB(IUP(I)).EQ.1)GO TO 5
      NUP=NUP-1
      NBOT=NBOT-1
      IB(IUP(I))=IB(IUP(I))-2
      GO TO 4
    5 IB(IUP(I))=IB(IUP(I))+4
    4 CONTINUE
      BEDLEN=ZTOP-ZBOT
C$
C$    DETERMINE THE PACKING FRACTION
C$
      VCYL=PI*RC*RC*BEDLEN
      PACFAC=VSTOT/VCYL
      RETURN
      END
```

Appendix B

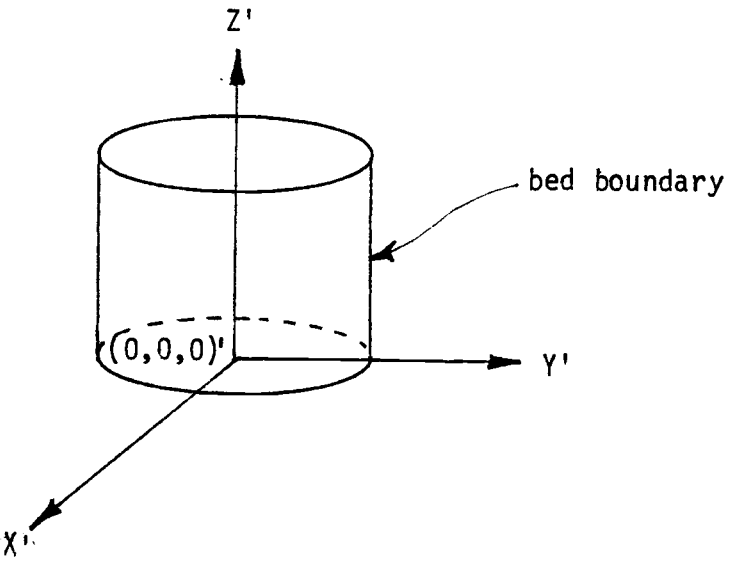
Determination of Solutions to Sphere Interaction Problems Associated with the RANDPAC Code

In this appendix, solutions to the five classes of sphere interactions mentioned in Chapter Two are developed in detail. They are:

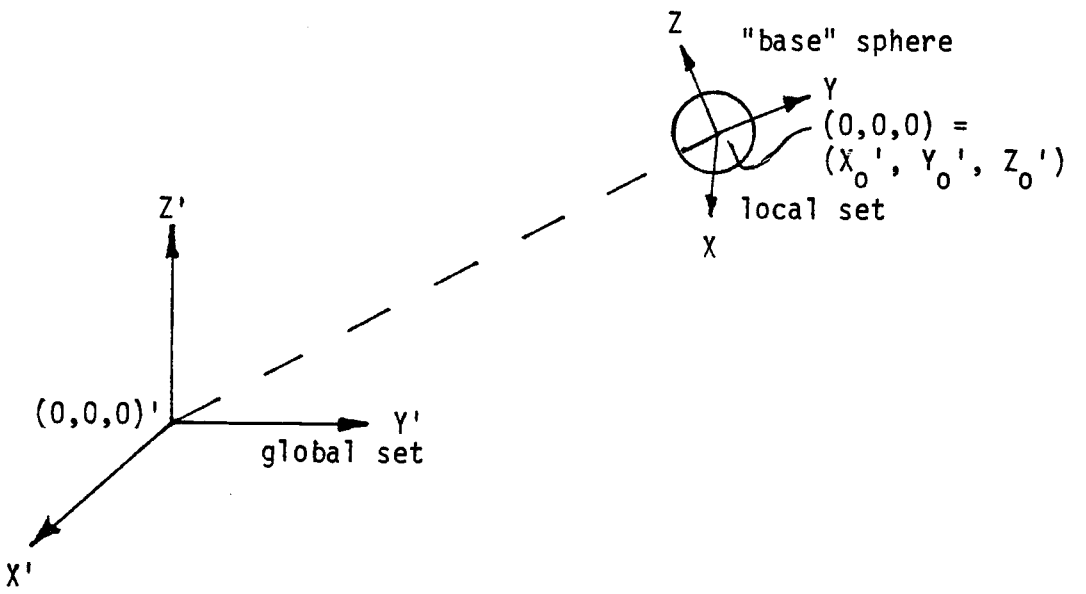
1. one contact with a sphere,
2. two contacts with spheres,
3. one contact with a sphere and one with the boundary,
4. three contacts with spheres, and
5. two contacts with spheres and one with the boundary.

These solutions must be general if they are to be of use in RANDPAC simulations. That is, they must be valid for any boundary radius and any combination of sphere radii.

Two coordinate systems are used throughout this appendix: the "global" and "local" systems. The global system, with the origin at the center of the bottom planar boundary and the z-axis directed along the axis of the cylindrical boundary serves as the overall reference coordinate system (Figure B.1a). A local coordinate set (Figure B.1b) has its origin at the center of a sphere and may be oriented in any direction that will simplify the solution process. Both are right-handed and cartesian.



Global Coordinate Set
Figure B.1a



Local Coordinate Set
Figure B.1b

In most cases, the local coordinate set is a pure translation of the global set such that they are related in the following manner:

$$X = X'-X_o',\ Y = Y'-Y_o',\ Z = Z'-Z_o', \qquad B.1$$

where X, Y, Z are the local coordinates of a point,

X', Y', Z' are the global coordinates of that point, and

X_o', Y_o', Z_o' are the global coordinates of the local origin.

If a rotation is involved, this transformation becomes much more complicated and will be handled on a case by case basis. Special attention should be directed to the above notation as it occurs frequently in the following derivations.

1. One contact with a sphere

Given:	sphere	radius	coordinates of center
	1	R_1	X_1', Y_1', Z_1'
	2	R_2	X_2', Y_2'

Find: All values of Z_2' such that the spheres are in contact.

Solution: This is a simple application of the distance formula. The distance from the center of sphere 1 to any solution to the position of the center of sphere 2, ℓ_{12}, is given by

$$\ell_{12} = R_1 + R_2. \qquad \text{B.1.1}$$

The distance formula can be written down as

$$\ell_{12}^2 = (X_1'-X_2')^2 + (Y_1'-Y_2')^2 + (Z_1'-Z_2')^2. \qquad \text{B.1.2}$$

Solving for Z_2',

$$Z_2' = Z_1' \pm \sqrt{\ell_{12}^2-(X_1'-X_2')^2-(Y_1'-Y_2')^2}. \qquad \text{B.1.3}$$

Observe that zero, one, or two real solutions may exist depending on the relative X' and Y' positions of the spheres.

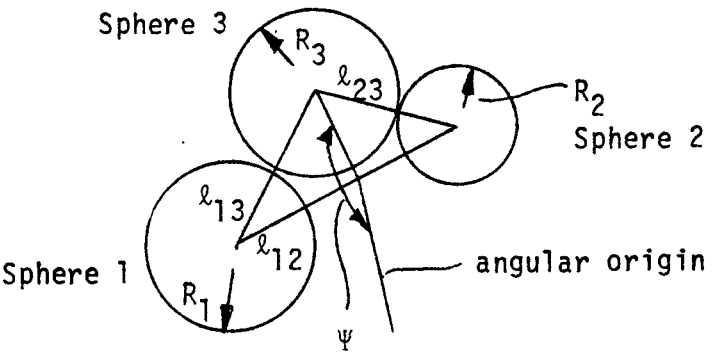
2. Two contacts with spheres

Given: A rotation angle Ψ such that $-\Pi \leq \Psi \leq \Pi$, and

sphere	radius	coordinates of center
1	R_1	X_1', Y_1', Z_1'
2	R_2	X_2', Y_2', Z_2'
3	R_3	

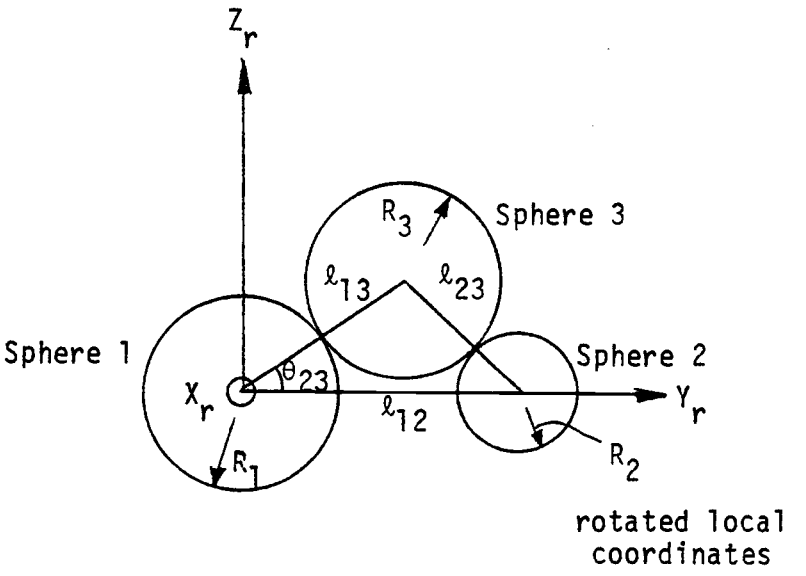
Find: The position of sphere 3 if it is in contact with spheres 1 and 2.

Solution: Obviously an infinite number of solutions exist if only the contact constraint is considered. To remedy this, the angle Ψ may be picked by any method and can be thought of as the rotation of sphere 3 about the line connecting the centers of spheres 1 and 2 relative to some arbitrary angular origin (Figure B.2a).



Two Sphere Contact Geometry
Figure B.2a

This is not precisely the manner in which Ψ is used here, however. Instead, it becomes the means by which a rotated local coordinate set is defined. Suppose we have this rotated coordinate set (X_r, Y_r, Z_r) such that the local origin is at the center of sphere 1, sphere 2 lies on the positive Y_r axis, and sphere 3 lies in the first quadrant of the Y_r-Z_r plane (Figure B.2b). The problem of determining the position of sphere 3 is now much simpler.



Two Sphere Contact Geometry in Rotated Coordinates
Figure B.2b

The indicated lengths may be found as follows:

$$\ell_{13} = R_1 + R_3, \qquad \text{B.2.1}$$

$$\ell_{23} = R_2 + R_3, \qquad \text{B.2.2}$$

$$\ell_{12} = \sqrt{(X_1'-X_2')^2+(Y_1'-Y_2')^2+(Z_1'-Z_2')^2}. \qquad \text{B.2.3.}$$

The cosine of the angle θ_{23} can be obtained by applying the law of cosines,

$$\cos\theta_{23} = \frac{\ell_{12}^2+\ell_{13}^2-\ell_{23}^2}{2\ell_{12}\ell_{13}}, \qquad \text{B.2.4}$$

and can in turn be used to evaluate the sine of θ_{23}:

$$\sin\theta_{23} = \sqrt{1-\cos^2\theta_{23}}. \qquad \text{B.2.5}$$

Now the position of sphere 3 in the rotated local coordinate set can be easily evaluated:

$$\begin{aligned} X_r &= 0 \\ Y_r &= \ell_{13}\cos\theta_{23} \qquad \text{B.2.6} \\ Z_r &= \ell_{13}\sin\theta_{23}. \end{aligned}$$

To complete the solution, a transformation must be found which will shift this solution to the unrotated local coordinate set.

In unrotated local coordinates with the center of sphere 1 as the local origin, the positions of spheres 1 and 2 are given by Equations B.1. They are,

respectively, (0, 0, 0) and (X_2, Y_2, Z_2). The development of the required transformation proceeds as follows:

A) Find the direction cosines a_i of the Y_r axis (Figure B.2c) as given by

$$a_1 = X_2/\ell_{12},\ a_2 = Y_2/\ell_{12},\ a_3 = Z_2/\ell_{12}. \qquad \text{B.2.7}$$

B) Find the direction cosines b_i of the X_r axis as follows:

1) Assume $b_1 = \cos\Psi$ (a restriction will be placed on this later).

2) Construct the inner product of the unit vectors in the X_r and Y_r directions and solve for b_3 (since the coordinate system is orthogonal, this inner product must equal zero).

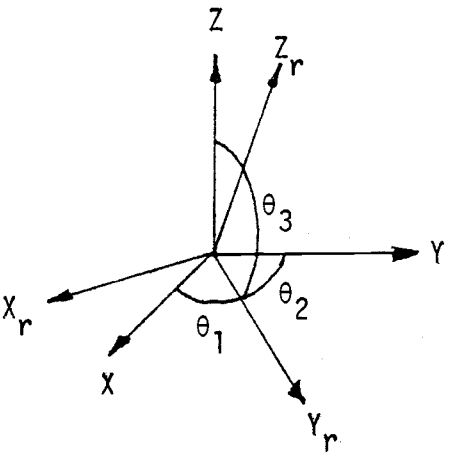
$$\vec{e}_{X_r} \cdot \vec{e}_{Y_r} = a_1b_1+a_2b_2+a_3b_3 = 0$$

$$b_3 = -(a_1b_1+a_2b_2)/a_3. \qquad \text{B.2.8}$$

3) By definition, the direction cosines b_i of the vector $\vec{e}_{Z_r}$ must satisfy the relation

$$b_1^2 + b_2^2 + b_3^2 = 1 \qquad \text{B.2.9}$$

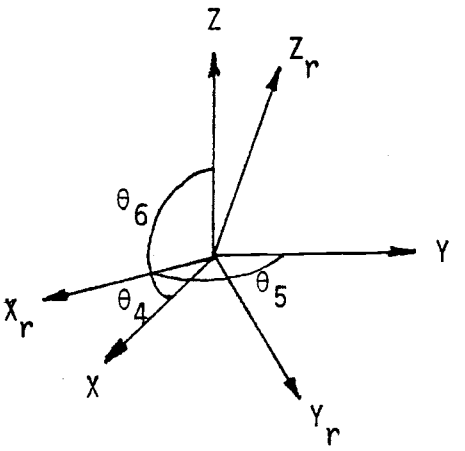
Substituting B.2.8 into B.2.9 and rearranging the terms results in the quadratic equation



$a_1 = \cos\theta_1$

$a_2 = \cos\theta_2$

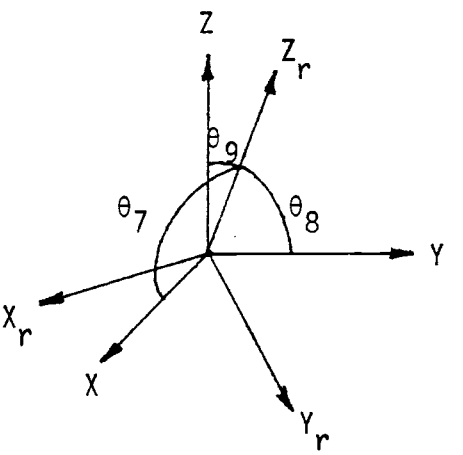
$a_3 = \cos\theta_3$



$b_1 = \cos\theta_4$

$b_2 = \cos\theta_5$

$b_3 = \cos\theta_6$



$c_1 = \cos\theta_7$

$c_2 = \cos\theta_8$

$c_3 = \cos\theta_9$

Definition of Direction Cosines for a Coordinate Rotation

Figure B.2c

$$(a_2^2+a_3^2)b_2^2+(2a_1a_2b_1)b_2+((a_1^2+a_3^2)b_1^2-a_3^2) = 0 \qquad \text{B.2.10}$$

which has the solution

$$b_2 = \frac{-a_1a_2b_1 \pm \sqrt{a_1^2a_2^2b_1^2-(a_2^2+a_3^2)((a_1^2+a_3^2)b_1^2-a_3^2)}}{(a_2^2+a_3^2)} \qquad \text{B.2.11}$$

By reducing the radicand of the above equation, it can be shown that for real solutions to exist,

$$b_1^2 \leq a_2^2+a_3^2 \qquad \text{B.2.12}$$

This is the restriction mentioned in Step B-1. It occurs because the angular separation of the X and X_r axes may be no less than that of the Y and Y_r axes. If this condition is not met, another value of Ψ must be chosen and Step B repeated.

4) Obtain the value of b_3 from Equation B.2.8.

C) Determine the direction cosines c_i by forming the outer product of the unit vectors in the X_r and Y_r directions:

$$\vec{e}_{Z_r} = \vec{e}_{X_r} X \vec{e}_{Y_r} = (b_1\vec{e}_X+b_2\vec{e}_Y+b_3\vec{e}_Z)X(a_1\vec{e}_X+a_2\vec{e}_Y+a_3\vec{e}_Z)$$

$$= (b_2a_3-a_2b_3)\vec{e}_X+(b_3a_1-a_3b_1)\vec{e}_Y+(b_1a_2-a_1b_2)\vec{e}_Z. \qquad \text{B.2.13}$$

This yields

$$c_1 = b_2a_3 - a_2b_3,$$

$$c_2 = b_3a_1 - a_3b_1, \qquad \text{B.2.14}$$

$$c_3 = b_1a_2 - a_1b_2.$$

By performing this operation correctly, an $\vec{e}_{Z_r}$ vector corresponding to a right-handed coordinate set will be found. The final transformation matrix from the rotated to the unrotated local coordinate set is now fully defined as

$$[Q_{r\rightarrow u}] = \begin{bmatrix} b_1 & a_1 & c_1 \\ b_2 & a_2 & c_2 \\ b_3 & a_3 & c_3 \end{bmatrix} \qquad \text{B.2.15}$$

To obtain the solution in unrotated local coordinates, multiply the transformation matrix by the solution in the rotated set:

$$\begin{Bmatrix} X \\ Y \\ Z \end{Bmatrix} = [Q_{r\rightarrow u}] \begin{Bmatrix} X_r \\ Y_r \\ Z_r \end{Bmatrix} . \qquad \text{B.2.16}$$

The final solution in global coordinates is found by the inverse application of Equations B.1. Note that Equation B.2.11 implies that there are either one or two possible solutions for the final sphere position,

as was the case in Problem 1. This is due to the symmetry of the cosine in the evaluation of b_1.

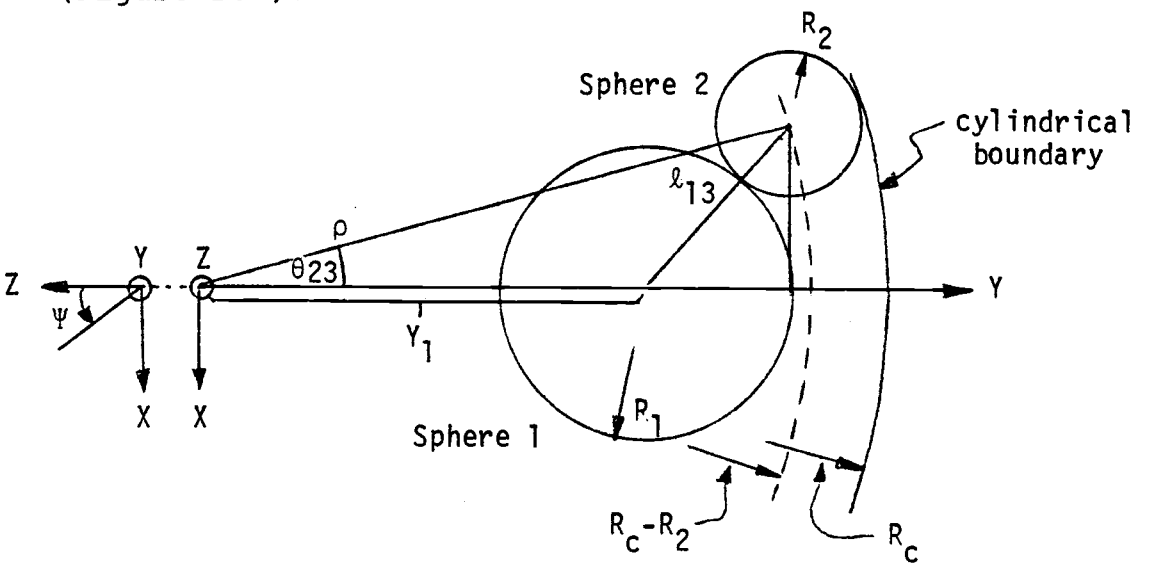
3. One contact with a sphere and one with the boundary

Given: The boundary radius R_c, an orientation angle Ψ, and

sphere	radius	coordinates of center
1	R_1	X_1', Y_1', Z_1'
2	R_2	

Find: A position for sphere 2 such that it touches both sphere 1 and the boundary at an angle Ψ from the vertical.

Solution: This problem is treated in a manner unlike the others in that its local coordinate set has its origin at the center of the circular boundary and at the same axial position as sphere 1. In addition, the X-Y plane remains parallel to the X'-Y' plane and the Y axis passes through the center of sphere 1 (Figure B.3).



Sphere-Clad Contact Geometry

Figure B.3

The following quantities may now be defined:

$$\rho = R_c - R_2 \qquad \text{B.3.1}$$

$$\ell_{12} = R_1 + R_2 \qquad \text{B.3.2}$$

Note that point 3 is a point on the Y axis which is a distance ρ from the local origin. We now consider the triangle defined by the centers of spheres 1 and 2, and point 3. The following definitions are the result of the application of, respectively, the law of cosines and the relationship between sine and cosine:

$$\cos\theta_{23} = \frac{Y_1^2+\rho^2-\ell_{12}^2}{2Y_1\rho}, \qquad \text{B.3.3}$$

$$\sin\theta_{23} = \sqrt{1-\cos^2\theta_{23}}. \qquad \text{B.3.4}$$

The maximum possible X position for sphere 2 can be expressed as

$$Xmax = \rho\sin\theta_{23}. \qquad \text{B.3.5}$$

If $0 \leq \Psi \leq \Pi$, the final X position of the second sphere can now be defined, with no loss of generality, as

$$X_2 = Xmax\ \cos\Psi. \qquad \text{B.3.6}$$

Utilizing this result and the distance formula

$$X_2^2 + Y_2^2 = (R_c-R_2)^2 \qquad \text{B.3.7}$$

Y_2 is found to be

$$Y_2 = +\sqrt{(R_c-R_2)^2-Xmax^2\cos^2\Psi}. \qquad B.3.8$$

Finally, the value of Z is determined from the application of the distance formula between the centers of spheres one and two:

$$(X_1-X_2)^2+(Y_1-Y_2)^2+(Z_1-Z_2)^2 = \ell_{12}^2. \qquad B.3.9$$

The local coordinate set as defined earlier implies that X = 0 and Z = 0. This allows B.3.9 to be reduced to

$$Z_2^2+X_2^2+(Y_1-Y_2)^2-\ell_{12}^2 = 0 \qquad B.3.10$$

which, after the substitution of B.3.6 and B.3.8, yields Z_2:

$$Z_2^2 = \pm\sqrt{\ell_{13}^2-Xmax^2\cos^2\Psi-(Y_1-\sqrt{(R_c-R_2)^2-Xmax^2\cos^2\Psi})^2} \qquad B.3.11$$

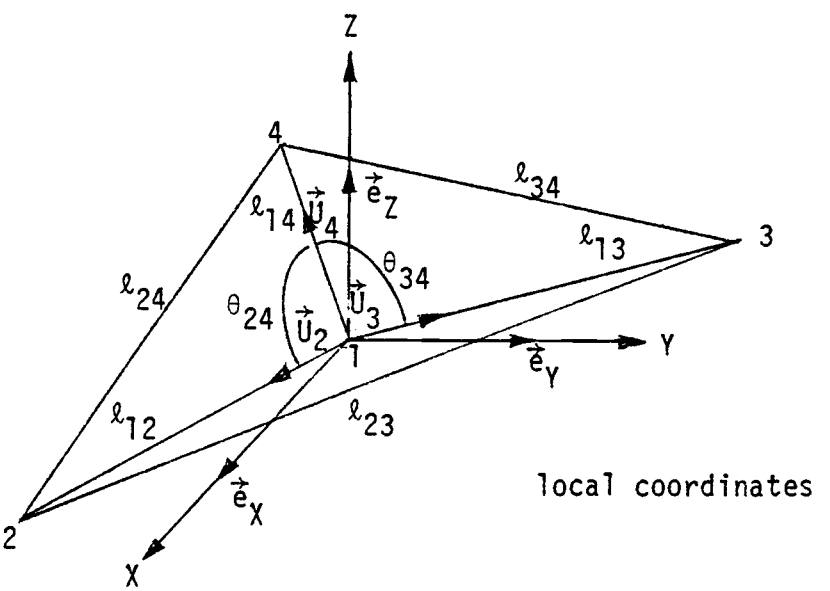
The final solution in global coordinates is found by the inverse application of Equations B.1. Note that B.3.11 implies that there are four unique solutions to the problem. This is due in all cases to the symmetry of the cosine and presents no problem here as one of the four may be picked at random.

4. Three contacts with spheres

Given:	sphere	radius	coordinates of center
	1	R_1	X_1', Y_1', Z_1'
	2	R_2	X_2', Y_2', Z_2'
	3	R_3	X_3', Y_3', Z_3'
	4	R_4	

Find: All positions of sphere 4 such that it is in contact with spheres 1, 2, and 3.

Solution: It is useful to think of the problem as one of finding the fourth vertex of a tetrahedron when three of the vertices and all of the side lengths are known. The first step is to place the origin of the local coordinate set at the center of sphere 1 and orient the local axes in the same direction as the global axes (Figure B.4).



Three Sphere Contact Geometry
Figure B.4

The lengths of the sides are determined in the following manner:

$$\ell_{14} = R_1 + R_4, \qquad \text{B.4.1a}$$

$$\ell_{24} = R_2 + R_4, \qquad \text{B.4.1b}$$

$$\ell_{34} = R_3 + R_4, \qquad \text{B.4.1c}$$

$$\ell_{23} = \sqrt{(X_2-X_3)^2+(Y_2-Y_3)^2+(Z_2-Z_3)^2}, \qquad \text{B.4.1d}$$

$$\ell_{12} = \sqrt{X_2^2+Y_2^2+Z_2^2}, \qquad \text{B.4.1e}$$

$$\ell_{13} = \sqrt{X_3^2+Y_3^2+Z_3^2}. \qquad \text{B.4.1f}$$

The cosines of the angles θ_{24} and θ_{34} can be expressed (from the law of cosines) as

$$\cos\theta_{24} = \frac{\ell_{12}^2+\ell_{14}^2-\ell_{24}^2}{2\ell_{12}\ell_{14}}, \qquad \text{B.4.2a}$$

and

$$\cos\theta_{34} = \frac{\ell_{13}^2+\ell_{14}^2-\ell_{34}^2}{2\ell_{13}\ell_{14}}. \qquad \text{B.4.2b}$$

Three unit vectors, $\vec{U}_2$, $\vec{U}_3$, and $\vec{U}_4$ have been shown. To define the position of sphere 4, the direction of $\vec{U}_4$ must be determined. This proceeds by first defining the three unit vectors in terms of their direction cosines:

$$\vec{U}_2 = a_1\vec{e}_X+a_2\vec{e}_Y+a_3\vec{e}_Z, \qquad \text{B.4.3a}$$

$$\vec{U}_3 = b_1\vec{e}_X+b_2\vec{e}_Y+b_3\vec{e}_Z, \qquad \text{B.4.3b}$$

$$\vec{U}_4 = c_1\vec{e}_X+c_2\vec{e}_Y+c_3\vec{e}_Z. \qquad \text{B.4.3c}$$

where

$$a_1 = X_2/\ell_{12},\ a_2 = Y_2/\ell_{12},\ a_3 = Z_2/\ell_{12},$$

$$b_1 = X_3/\ell_{13},\ b_2 = Y_3/\ell_{13},\ b_3 = Z_3/\ell_{13}, \quad \text{and}$$

$$c_1 = X_4/\ell_{14},\ c_2 = Y_4/\ell_{14},\ c_3 = Z_4/\ell_{14}.$$

Note that a_i and b_i are known. By forming the inner products $\vec{U}_2\cdot\vec{U}_4$ and $\vec{U}_3\cdot\vec{U}_4$, we obtain

$$a_1c_1+a_2c_2+a_3c_3 = \cos\theta_{24}, \qquad \text{B.4.4}$$

and

$$b_1c_1+b_2c_2+b_3c_3 = \cos\theta_{34}. \qquad \text{B.4.5}$$

Eliminating c_3 from B.4.4 and B.4.5, an expression for c_2 in terms of c_1 is found:

$$c_2 = (\gamma-\alpha c_1)/\beta, \qquad \text{B.4.6}$$

where $\alpha = a_1b_3-a_3b_1$,

$\beta = a_2b_3-a_3b_2$, and

$\gamma = b_3\cos\theta_{24}-a_3\cos\theta_{34}$.

Eliminating c_2 in a similar manner, an expression for c_3 in terms of c_1 is developed:

$$c_3 = (\delta-\sigma c_1)/\eta, \qquad \text{B.4.7}$$

where $\sigma = a_1b_2-a_2b_1$,

$\eta = a_3b_2-a_2b_3$, and

$\delta = b_2\cos\theta_{24}-a_2\cos\theta_{34}$.

The definition of the direction cosine requires that

$$c_1^2+c_2^2+c_3^2 = 1. \qquad \text{B.4.8}$$

Substituting B.4.6 and B.4.7 into B.4.8, expanding, and gathering terms results in a quadratic expression for c_1:

$$Qc_1^2+Rc_1+S = 0, \qquad \text{B.4.9}$$

where $Q = 1 + \frac{\alpha^2}{\beta^2} + \frac{\sigma^2}{\eta^2}$,

$R = -2\ (\frac{\gamma\alpha}{\beta^2} + \frac{\sigma\delta}{\eta^2})$, and

$S = \frac{\gamma^2}{\beta^2} + \frac{\delta^2}{\eta^2} - 1$.

This has the solution

$$c_1 = \frac{-R \pm \sqrt{R^2-4QS}}{2Q} \qquad \text{B.4.10}$$

c_2 and c_3 are now determined from B.4.6 and B.4.7 and the values of X_4, Y_4, and Z_4 are determined from

$$X_4 = \ell_{14}c_1;\ Y_4 = \ell_{14}c_2;\ Z_4 = \ell_{14}c_3. \qquad \text{B.4.11}$$

The final solution in global coordinates is found by the inverse application of Equations B.1. Note that two possible solutions are implied. This is entirely physical and corresponds to solutions above and below the plane defined by the centers of spheres 1, 2, and 3.

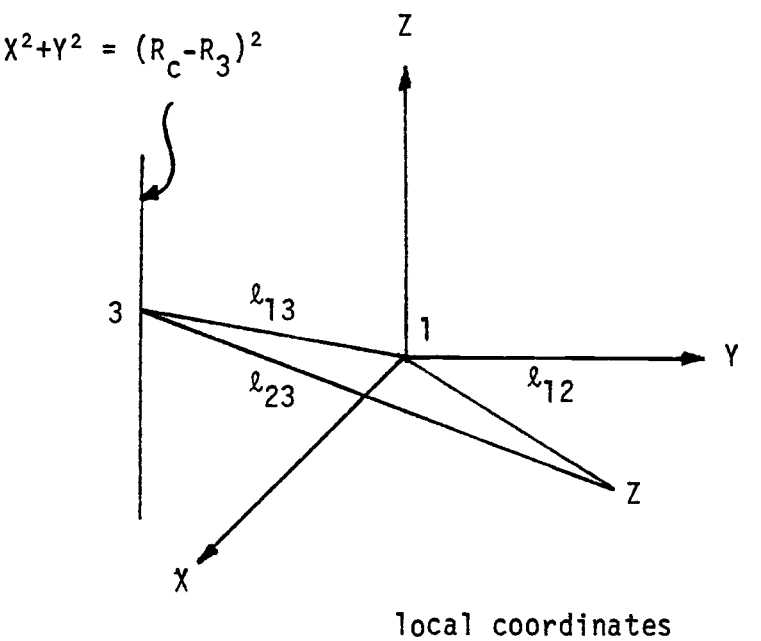
5. Two contacts with spheres and one with the boundary

Given: The boundary radius R_c and

sphere	radius	coordinates of center
1	R_1	X_1', Y_1', Z_1'
2	R_2	X_2', Y_2', Z_2'
3	R_3	

Find: All positions of sphere 3 such that it contacts the boundary and spheres 1 and 2.

Solution: To start the solution, the origin of the local coordinate set is placed at the center of sphere 1 and the local axes aligned with the global axes (Figure B.5).



Clad-Two Sphere Contact Geometry
Figure B.5

The leg lengths of the triangle are given by

$$\ell_{13} = R_1 + R_3, \qquad \text{B.5.1a}$$

$$\ell_{23} = R_2 + R_3, \qquad \text{B.5.1b}$$

$$\ell_{12} = \sqrt{X_2^2+Y_2^2+Z_2^2}. \qquad \text{B.5.1c}$$

Application of the distance formula yields

$$(X_2-X_3)^2+(Y_2-Y_3)^2+(Z_2-Z_3)^2 = \ell_{23}^2, \qquad \text{B.5.2}$$

and

$$X_3^2+Y_3^2+Z_3^2 = \ell_{13}. \qquad \text{B.5.3}$$

Since the third sphere must have a global radial position of R_c-R_3, the distance formula also requires that

$$(X_3+X_1')^2+(Y_3+Y_1')^2 = (R_c-R_3)^2. \qquad \text{B.5.4}$$

Equations B.5.2, B.5.3, and B.5.4 constitute a system of three nonlinear equations in the three unknowns X_3, Y_3, and Z_3. The solution proceeds in the following manner.

Expansion and rearrangement of B.5.4 yields

$$X_3^2+Y_3^2 = -2X_3X_1'-2Y_3Y_1'+(R_c-R_3)^2-X_1'^2-Y_1'^2. \qquad \text{B.5.5}$$

Now combine B.5.3 and B.5.5 to obtain

$$(R_c-R_3)^2-X_1'^2-Y_1'^2-\ell_{13}^2 = \delta, \qquad \text{B.5.6}$$

where $\delta = 2X_3X_1'+2Y_3Y_1'-Z_3$.

The next step is to expand Equation B.5.2 to obtain the linear relationship

$$X_2X_3+Y_2Y_3+Z_2Z_3 = \frac{\ell_{12}^2+\ell_{13}^2-\ell_{23}^2}{2} = \gamma. \qquad \text{B.5.7}$$

By eliminating X_3 from B.5.6 and B.5.7 and rearranging the terms, an expression for Y_3 in terms of Z_3 is found:

$$Y_3 = \underbrace{\frac{X_2}{2(X_2Y_1'-X_1'Y_2)}}_{A}Z_3^2+\underbrace{\frac{X_1'Z_2}{(X_2Y_1'-X_1'Y_2)}}_{B}Z_3+\underbrace{\frac{\delta X_2-2\gamma X_1'}{2(X_2Y_1'-X_1'Y_2)}}_{C}. \qquad \text{B.5.8}$$

In a similar manner, Y_3 is eliminated from B.5.6 and B.5.7 to find X_3 in terms of Z_3:

$$X_3 = \underbrace{\frac{Y_2}{2(X_1'Y_2-X_2Y_1')}}_{D}Z_3^2+\underbrace{\frac{Y_1'Z_2}{(X_1'Y_2-X_2Y_1')}}_{E}Z+\underbrace{\frac{\delta Y_2-2\gamma Y_1'}{2(X_1'Y_2-X_2Y_1')}}_{F}. \qquad \text{B.5.9}$$

Finally, an expression for Z_3 is obtained by inserting B.5.8 and B.5.9 into B.5.3:

$$(A^2+D^2)Z_3^4+2(AB+DE)Z_3^3+(2(AC+DF)+B^2+E^2+1)Z_3^2$$

B.5.10

$$+2(BC+EF)Z_3+(C^2+F^2-\ell_{13}^2) = 0.$$

This solution implies that there are four allowable sphere positions. This is possible if the boundary radius is no more than about three times the sphere radius. If the radius is much larger, two of the Z_3 roots will become a complex conjugate pair, leaving the expected result of zero, one, or two real solutions.

Appendix C

RANDPAC Sample Case

This appendix contains an example of a typical RANDPAC run. The data used is described below:

Boundary radius: 8.0

Number of spheres: 300

Number of size fractions: 2

Fraction	Radius	Probability Contribution
1	1	.5
2	.33333	.5
		1.0

Distribution of initial contact:

Contacts	Probability Contribution
1	.05
2	.05
3	.90
	1.00

Random number generator seed: 4565456545654

To avoid loss of precision, most of the output is written to the file TAPE6 in binary form. A short program was written to translate this file and present it in an understandable format.

```
CLAD RADIUS?
8.
# OF SPHERES, SIZE FRACTIONS?
300 2
PROB., RADIUS OF EACH FRACTION?
PROBABILITIES = 0. .5 1.
RADII = 1. .3333333333
CONTACT PROB. VECTOR?
0. .05 .1 1.
RANDOM # GENERATOR SEED?
4565456545654
ALTITUDE OF HIGHEST SPHERE = 8.342511960554
BOTTOM BOUNDARY ALTITUDE = .2605456846817
TOP BOUNDARY ALTITUDE= 5.869467616214
LENGTH OF BED = 5.608921931533
PACKING FACTOR = .6600484975523
# OF UPPER BOUNDARY SPHERES = 63
# OF LOWER BOUNDARY SPHERES = 63
```

NUMBER OF SPHERES = 300
CLAD RADIUS = 8.
NUMBER OF SIZE FRACTIONS = 2
CONTACT VECTOR:
0. .05 .1 1.
FRACTION RADII:
1. .3333333333
FRACTION PROBABILITIES:
0. .5 1.
RANDOM NUMBER GENERATOR SEED = 4565456545654
EFFECTIVE BED LENGTH = 5.608921931533
PACKING FACTOR = .6600484975523
NUMBER OF UPPER, LOWER BOUNDARY SPHERES = 63 63
BED DATA
****
I=SPHERE #, X,Y,Z=COORDINATES, R=RADIUS,
IB=BOUNDARY TYPE, IT=NUMBER OF CONTACTS, INT=VECTOR OF
CONTACTING SPHERES
****

I	X	Y	Z	R	IB	IT	INT												
1	-.641613E+01	.533889E+00	.680710E-04	.100000E+01	2	2	35	59	0	0	0	0	0	0	0	0	0	0	0
2	.639793E+01	-.668473E+00	.475323E-03	.100000E+01	2	4	37	41	83	89	0	0	0	0	0	0	0	0	0
3	-.110688E+01	-.274615E+01	.663898E-03	.333333E+00	2	1	86	0	0	0	0	0	0	0	0	0	0	0	0
4	-.443757E+01	.335231E+01	.405614E-03	.100000E+01	2	5	17	20	44	81	119	0	0	0	0	0	0	0	0
5	-.538715E+01	.209182E+01	.574184E-03	.333333E+00	2	2	17	35	0	0	0	0	0	0	0	0	0	0	0
6	-.815968E+00	.700220E+00	.145991E-03	.100000E+01	2	5	24	71	72	73	109	0	0	0	0	0	0	0	0
7	.382672E+01	.245128E+01	.149766E-03	.333333E+00	2	2	27	30	0	0	0	0	0	0	0	0	0	0	0
8	-.290159E+01	.448656E+01	.998256E-03	.333333E+00	2	3	20	25	50	0	0	0	0	0	0	0	0	0	0
9	.322615E+01	-.110292E+01	.894960E-03	.333333E+00	2	2	90	91	0	0	0	0	0	0	0	0	0	0	0
10	.150206E+01	-.352758E+01	.232557E-03	.333333E+00	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11	.978419E+00	.187858E+01	.213018E-03	.100000E+01	2	4	27	72	73	74	0	0	0	0	0	0	0	0	0
12	-.338657E+01	-.648750E+01	.933883E-04	.333333E+00	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
13	.385531E+01	-.510055E+01	.224426E-03	.333333E+00	2	1	40	0	0	0	0	0	0	0	0	0	0	0	0
14	-.247659E+01	-.888973E+00	.566882E-03	.333333E+00	2	3	24	58	71	0	0	0	0	0	0	0	0	0	0

15	-.603682E+01	-.248726E+01	.957217E-03	.100000E+01	2	3	33	56	78	0	0	0	0	0	0	0	0	0	0	0
16	-.854254E+00	-.572573E+01	.117435E-03	.100000E+01	2	4	45	48	64	105	0	0	0	0	0	0	0	0	0	0
17	-.635758E+01	.292937E+01	.367404E+00	.100000E+01	3	4	4	5	44	110	0	0	0	0	0	0	0	0	0	0
18	.102453E+01	-.297404E+01	.379745E-03	.333333E+00	2	2	82	132	0	0	0	0	0	0	0	0	0	0	0	0
19	-.156194E+01	.397617E+01	.607596E-03	.333333E+00	2	3	20	25	53	0	0	0	0	0	0	0	0	0	0	0
20	-.255327E+01	.338700E+01	.669887E+00	.100000E+01	2	6	8	4	19	25	81	123	0	0	0	0	0	0	0	0
21	.379635E+00	.732461E+01	.994198E-03	.333333E+00	2	1	100	0	0	0	0	0	0	0	0	0	0	0	0	0
22	.177550E-01	.527826E+01	.691913E-03	.333333E+00	2	2	53	108	0	0	0	0	0	0	0	0	0	0	0	0
23	-.411929E+01	-.414784E+01	.314330E-03	.333333E+00	2	2	36	78	0	0	0	0	0	0	0	0	0	0	0	0
24	-.275693E+01	.367123E+00	.349003E+00	.100000E+01	2	6	6	14	35	58	71	109	0	0	0	0	0	0	0	0
25	-.185071E+01	.523127E+01	.345737E+00	.100000E+01	2	11	20	19	8	50	51	53	55	57	108	120	167	0	0	0
26	-.127274E+01	.297201E+01	.721905E-03	.333333E+00	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
27	.286722E+01	.179419E+01	.652357E+00	.100000E+01	2	5	11	7	30	38	113	0	0	0	0	0	0	0	0	0
28	.519966E+01	.304556E+01	.884361E-03	.100000E+01	2	3	30	37	38	0	0	0	0	0	0	0	0	0	0	0
29	.846105E+00	-.414049E+01	.555916E-03	.333333E+00	2	1	45	0	0	0	0	0	0	0	0	0	0	0	0	0
30	.330407E+01	.367200E+01	.120400E+00	.100000E+01	2	4	28	7	27	38	0	0	0	0	0	0	0	0	0	0
31	.434329E+01	.170015E+01	.669225E-03	.333333E+00	2	1	37	0	0	0	0	0	0	0	0	0	0	0	0	0
32	.497464E+01	-.109304E+01	.882105E-03	.333333E+00	2	1	94	0	0	0	0	0	0	0	0	0	0	0	0	0
33	-.641940E+01	-.152757E+01	.843806E+00	.333333E+00	0	2	15	56	0	0	0	0	0	0	0	0	0	0	0	0
34	.178193E+01	.663397E+01	.133111E-03	.100000E+01	2	1	70	0	0	0	0	0	0	0	0	0	0	0	0	0
35	-.458672E+01	.115740E+01	.514337E+00	.100000E+01	2	5	24	5	1	59	81	0	0	0	0	0	0	0	0	0
36	-.477505E+01	-.426015E+01	.427605E-01	.333333E+00	0	3	23	78	79	0	0	0	0	0	0	0	0	0	0	0
37	.549075E+01	.108912E+01	.296929E+00	.100000E+01	2	7	28	31	2	41	83	98	99	0	0	0	0	0	0	0
38	.418911E+01	.285306E+01	.171603E+01	.100000E+01	0	5	30	28	27	95	102	0	0	0	0	0	0	0	0	0
39	.580339E+01	-.329780E+01	.825312E-03	.100000E+01	2	4	40	89	93	129	0	0	0	0	0	0	0	0	0	0
40	.495161E+01	-.494788E+01	.743594E+00	.100000E+01	3	4	39	13	93	129	0	0	0	0	0	0	0	0	0	0
41	.698088E+01	.517067E+00	.150203E+01	.100000E+01	1	7	37	2	83	98	99	122	222	0	0	0	0	0	0	0
42	.366817E+01	-.251313E+01	.832658E-03	.100000E+01	2	3	90	92	93	0	0	0	0	0	0	0	0	0	0	0
43	.388407E+01	.652567E+01	.590498E-03	.333333E+00	2	1	88	0	0	0	0	0	0	0	0	0	0	0	0	0
44	-.544659E+01	.439712E+01	.137527E+01	.100000E+01	1	4	17	4	50	119	0	0	0	0	0	0	0	0	0	0
45	.738206E+00	-.502866E+01	.989139E+00	.100000E+01	2	7	29	16	48	63	67	76	132	0	0	0	0	0	0	0
46	.242528E+01	-.651089E+01	.793837E-03	.100000E+01	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47	.668003E+01	.251833E+01	.986760E-03	.333333E+00	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48	.180106E+00	-.620283E+01	.693122E+00	.333333E+00	0	3	16	45	63	0	0	0	0	0	0	0	0	0	0	0
49	-.167952E+01	-.376888E+01	.581367E-03	.333333E+00	2	2	52	87	0	0	0	0	0	0	0	0	0	0	0	0

50	-.383992E+01	.525741E+01	.551551E+00	.100000E+01	2	9	25	8	44	51	55	119	120	121	166	0	0	0	0	0
51	-.270231E+01	.645736E+01	.167670E+01	.100000E+01	1	11	25	50	55	57	120	121	134	167	168	170	171	0	0	0
52	-.136035E+01	-.339607E+01	.451793E+00	.333333E+00	0	3	49	86	105	0	0	0	0	0	0	0	0	0	0	0
53	-.265399E+00	.401247E+01	.309523E+00	.100000E+01	2	6	25	22	19	73	74	108	0	0	0	0	0	0	0	0
54	-.280845E+01	-.239528E+01	.309094E-03	.333333E+00	2	1	106	0	0	0	0	0	0	0	0	0	0	0	0	0
55	-.283951E+01	.612447E+01	.392905E+00	.333333E+00	0	5	25	51	50	167	168	0	0	0	0	0	0	0	0	0
56	-.582946E+01	-.132064E+01	.612315E+00	.333333E+00	0	3	15	33	59	0	0	0	0	0	0	0	0	0	0	0
57	-.940768E+00	.693649E+01	.859761E+00	.100000E+01	3	4	51	25	100	134	0	0	0	0	0	0	0	0	0	0
58	-.311078E+01	-.910309E+00	.204994E+00	.333333E+00	2	2	24	14	0	0	0	0	0	0	0	0	0	0	0	0
59	-.542315E+01	-.386209E+00	.147228E+01	.100000E+01	0	8	35	56	1	60	61	96	117	118	0	0	0	0	0	0
60	-.686406E+01	-.137285E+01	.244711E+01	.100000E+01	1	7	59	61	96	97	117	197	271	0	0	0	0	0	0	0
61	-.697302E+01	.613951E+00	.224530E+01	.100000E+01	1	5	60	59	110	190	202	0	0	0	0	0	0	0	0	0
62	-.204092E+01	-.649722E+01	.773475E-03	.333333E+00	2	1	64	0	0	0	0	0	0	0	0	0	0	0	0	0
63	.887426E+00	-.694352E+01	.154685E+01	.100000E+01	1	5	48	45	65	66	147	0	0	0	0	0	0	0	0	0
64	-.212639E+01	-.593122E+01	.342505E+00	.333333E+00	0	3	16	62	68	0	0	0	0	0	0	0	0	0	0	0
65	.389591E+00	-.698915E+01	.348336E+01	.100000E+01	1	6	63	66	67	69	147	154	0	0	0	0	0	0	0	0
66	.227981E+01	-.661834E+01	.294525E+01	.100000E+01	1	6	65	63	67	76	77	229	0	0	0	0	0	0	0	0
67	.939415E+00	-.513430E+01	.297619E+01	.100000E+01	0	7	65	66	45	76	147	148	179	0	0	0	0	0	0	0
68	-.235331E+01	-.659257E+01	.147781E+01	.100000E+01	1	2	64	69	0	0	0	0	0	0	0	0	0	0	0	0
69	-.159577E+01	-.681568E+01	.331529E+01	.100000E+01	1	6	68	65	154	155	173	204	0	0	0	0	0	0	0	0
70	.269694E+01	.683910E+01	.947997E+00	.333333E+00	0	2	34	88	0	0	0	0	0	0	0	0	0	0	0	0
71	-.140674E+01	-.104364E+01	.781137E+00	.100000E+01	2	5	6	14	24	109	131	0	0	0	0	0	0	0	0	0
72	.966997E+00	-.594588E-01	.494034E+00	.100000E+01	2	6	11	6	113	114	140	162	0	0	0	0	0	0	0	0
73	-.555362E+00	.225871E+01	.122619E+01	.100000E+01	0	5	53	11	6	74	123	0	0	0	0	0	0	0	0	0
74	.117533E+01	.323397E+01	.145767E+01	.100000E+01	0	4	73	11	53	75	0	0	0	0	0	0	0	0	0	0
75	.137485E+01	.218653E+01	.314973E+01	.100000E+01	0	5	74	103	159	160	177	0	0	0	0	0	0	0	0	0
76	.256030E+01	-.499373E+01	.181301E+01	.100000E+01	0	4	66	67	45	77	0	0	0	0	0	0	0	0	0	0
77	.405828E+01	-.570354E+01	.293203E+01	.100000E+01	1	3	76	66	228	0	0	0	0	0	0	0	0	0	0	0
78	-.453003E+01	-.335422E+01	.989877E+00	.100000E+01	2	8	15	23	36	79	96	101	106	198	0	0	0	0	0	0
79	-.452242E+01	-.534301E+01	.778542E+00	.100000E+01	3	4	78	36	101	133	0	0	0	0	0	0	0	0	0	0
80	.187168E+01	-.196243E+01	.449421E-03	.333333E+00	2	3	82	90	92	0	0	0	0	0	0	0	0	0	0	0
81	-.399846E+01	.257927E+01	.179194E+01	.100000E+01	0	10	20	4	35	110	118	123	124	125	126	128	0	0	0	0
82	.148711E+01	-.250091E+01	.816514E-01	.333333E+00	2	3	18	80	130	0	0	0	0	0	0	0	0	0	0	0
83	.673011E+01	.607983E+00	.195649E+00	.333333E+00	2	4	41	2	37	84	0	0	0	0	0	0	0	0	0	0
84	.579723E+01	-.220183E+00	.666442E+00	.100000E+01	0	4	83	94	98	156	0	0	0	0	0	0	0	0	0	0

85	-.249071E+01	-.459661E+01	.404233E-03	.333333E+00	2	1	87	0	0	0	0	0	0	0	0	0	0	0	0	0
86	-.171008E+01	-.286193E+01	.259879E+00	.333333E+00	2	2	52	3	0	0	0	0	0	0	0	0	0	0	0	0
87	-.226685E+01	-.400468E+01	.210066E+00	.333333E+00	2	3	85	49	105	0	0	0	0	0	0	0	0	0	0	0
88	.363673E+01	.591760E+01	.116113E+01	.100000E+01	0	2	43	70	0	0	0	0	0	0	0	0	0	0	0	0
89	.667363E+01	-.211252E+01	.135647E+01	.100000E+01	1	6	39	2	122	151	156	158	0	0	0	0	0	0	0	0
90	.242638E+01	-.134012E+01	.104103E+01	.100000E+01	0	11	42	9	80	91	92	113	130	140	162	163	235	0	0	0
91	.378910E+01	.939539E-02	.473768E+00	.100000E+01	2	3	90	9	112	0	0	0	0	0	0	0	0	0	0	0
92	.235736E+01	-.237292E+01	.200596E+00	.333333E+00	2	4	42	90	80	104	0	0	0	0	0	0	0	0	0	0
93	.463557E+01	-.317815E+01	.162005E+01	.100000E+01	0	7	42	40	39	129	152	164	219	0	0	0	0	0	0	0
94	.534354E+01	-.145063E+01	.425721E+00	.333333E+00	0	2	84	32	0	0	0	0	0	0	0	0	0	0	0	0
95	.436215E+01	.401045E+01	.235500E+01	.333333E+00	0	2	38	102	0	0	0	0	0	0	0	0	0	0	0	0
96	-.499080E+01	-.207346E+01	.245526E+01	.100000E+01	0	6	78	60	59	97	117	197	0	0	0	0	0	0	0	0
97	-.637198E+01	-.289791E+01	.364380E+01	.100000E+01	1	9	96	60	197	259	260	261	271	272	276	0	0	0	0	0
98	.515007E+01	.817599E+00	.224891E+01	.100000E+01	0	7	84	37	41	99	122	157	176	0	0	0	0	0	0	0
99	.624604E+01	.237264E+01	.163189E+01	.100000E+01	0	4	98	41	37	165	0	0	0	0	0	0	0	0	0	0
100	.119724E+00	.766573E+01	.511410E+00	.333333E+00	1	2	57	21	0	0	0	0	0	0	0	0	0	0	0	0
101	-.535125E+01	-.451266E+01	.239828E+01	.100000E+01	1	7	79	78	133	174	195	198	240	0	0	0	0	0	0	0
102	.387131E+01	.370736E+01	.268915E+01	.333333E+00	0	3	38	95	194	0	0	0	0	0	0	0	0	0	0	0
103	.172766E+01	.299053E+01	.415317E+01	.333333E+00	0	2	75	153	0	0	0	0	0	0	0	0	0	0	0	0
104	.205988E+01	-.218081E+01	.765432E+00	.333333E+00	0	2	92	130	0	0	0	0	0	0	0	0	0	0	0	0
105	-.160203E+01	-.439899E+01	.129649E+01	.100000E+01	0	6	87	52	16	106	149	208	0	0	0	0	0	0	0	0
106	-.266273E+01	-.270344E+01	.128933E+01	.100000E+01	0	6	105	78	54	107	145	146	0	0	0	0	0	0	0	0
107	-.107655E+01	-.308976E+01	.244467E+01	.100000E+01	0	6	106	131	145	146	148	209	0	0	0	0	0	0	0	0
108	-.521011E+00	.531851E+01	.391275E+00	.333333E+00	0	4	22	25	53	111	0	0	0	0	0	0	0	0	0	0
109	-.159287E+01	.259970E+00	.990289E+00	.333333E+00	0	3	24	6	71	0	0	0	0	0	0	0	0	0	0	0
110	-.593397E+01	.232275E+01	.222551E+01	.100000E+01	0	5	61	81	17	181	190	0	0	0	0	0	0	0	0	0
111	-.109081E+01	.529239E+01	.159644E+01	.100000E+01	0	5	108	134	161	171	225	0	0	0	0	0	0	0	0	0
112	.399570E+01	-.882620E+00	.144300E+01	.333333E+00	0	2	91	152	0	0	0	0	0	0	0	0	0	0	0	0
113	.223405E+01	.423658E+00	.196413E+01	.100000E+01	0	9	90	72	27	140	163	176	184	188	235	0	0	0	0	0
114	-.663038E-02	.159692E+00	.222725E+01	.100000E+01	0	4	72	131	139	184	0	0	0	0	0	0	0	0	0	0
115	.445873E+00	.632363E+01	.576617E-03	.333333E+00	2	1	116	0	0	0	0	0	0	0	0	0	0	0	0	0
116	.985806E+00	.607553E+01	.119418E+01	.100000E+01	0	2	115	141	0	0	0	0	0	0	0	0	0	0	0	0
117	-.544116E+01	-.411134E+00	.347204E+01	.100000E+01	0	9	59	96	60	118	190	201	202	203	206	0	0	0	0	0
118	-.410244E+01	.710923E+00	.249797E+01	.100000E+01	0	5	81	117	59	124	262	0	0	0	0	0	0	0	0	0
119	-.418325E+01	.408473E+01	.108515E+01	.333333E+00	0	3	50	44	4	0	0	0	0	0	0	0	0	0	0	0

120	-.275578E+01	.517289E+01	.132309E+01	.333333E+00	0	5	50	51	25	121	166	0	0	0	0	0	0	0	0	0
121	-.326026E+01	.524874E+01	.175226E+01	.333333E+00	0	4	51	120	50	166	0	0	0	0	0	0	0	0	0	0
122	.619681E+01	-.799247E+00	.278755E+01	.100000E+01	0	9	98	89	41	150	152	156	157	222	250	0	0	0	0	0
123	-.210810E+01	.258035E+01	.244503E+01	.100000E+01	0	9	81	20	73	124	125	128	137	138	139	0	0	0	0	0
124	-.360601E+01	.221516E+01	.371896E+01	.100000E+01	0	11	123	81	118	125	126	137	138	203	262	263	269	0	0	0
125	-.328369E+01	.310998E+01	.278452E+01	.333333E+00	0	6	123	124	81	126	128	137	0	0	0	0	0	0	0	0
126	-.416296E+01	.404692E+01	.314061E+01	.100000E+01	0	5	125	124	81	127	181	0	0	0	0	0	0	0	0	0
127	-.466967E+01	.521481E+01	.468311E+01	.100000E+01	1	3	126	268	297	0	0	0	0	0	0	0	0	0	0	0
128	-.309694E+01	.345173E+01	.224343E+01	.333333E+00	0	3	123	125	81	0	0	0	0	0	0	0	0	0	0	0
129	.566149E+01	-.390644E+01	.117862E+01	.333333E+00	0	4	39	93	40	143	0	0	0	0	0	0	0	0	0	0
130	.141777E+01	-.209658E+01	.607156E+00	.333333E+00	0	4	104	90	82	132	0	0	0	0	0	0	0	0	0	0
131	-.141655E+01	-.114734E+01	.277842E+01	.100000E+01	0	6	114	107	71	139	145	205	0	0	0	0	0	0	0	0
132	.824343E+00	-.305742E+01	.131596E+01	.100000E+01	0	4	130	18	45	148	0	0	0	0	0	0	0	0	0	0
133	-.509352E+01	-.573008E+01	.191951E+01	.333333E+00	1	3	79	101	174	0	0	0	0	0	0	0	0	0	0	0
134	-.113042E+01	.685115E+01	.284892E+01	.100000E+01	0	4	111	51	57	225	0	0	0	0	0	0	0	0	0	0
135	.223997E+01	.535260E+01	.904857E-03	.333333E+00	2	1	136	0	0	0	0	0	0	0	0	0	0	0	0	0
136	.254446E+01	.611862E+01	.104889E+01	.100000E+01	0	3	135	141	142	0	0	0	0	0	0	0	0	0	0	0
137	-.288230E+01	.325260E+01	.329735E+01	.333333E+00	0	4	124	125	123	138	0	0	0	0	0	0	0	0	0	0
138	-.202276E+01	.328126E+01	.431624E+01	.100000E+01	0	8	124	137	123	159	161	185	277	280	0	0	0	0	0	0
139	-.163017E+01	.794327E+00	.320774E+01	.100000E+01	0	5	131	114	123	185	186	0	0	0	0	0	0	0	0	0
140	.146647E+01	-.605142E+00	.160333E+01	.333333E+00	0	5	113	90	72	162	163	0	0	0	0	0	0	0	0	0
141	.190786E+01	.673499E+01	.284189E+01	.100000E+01	1	6	136	116	144	224	248	288	0	0	0	0	0	0	0	0
142	.350368E+01	.498650E+01	.238986E+01	.100000E+01	0	3	136	194	196	0	0	0	0	0	0	0	0	0	0	0
143	.498808E+01	-.407201E+01	.231743E+01	.100000E+01	0	3	129	192	193	0	0	0	0	0	0	0	0	0	0	0
144	.144210E+01	.564497E+01	.445277E+01	.100000E+01	0	5	141	196	224	242	248	0	0	0	0	0	0	0	0	0
145	-.279943E+01	-.250431E+01	.327469E+01	.100000E+01	0	7	131	107	106	146	195	205	206	0	0	0	0	0	0	0
146	-.237145E+01	-.340228E+01	.238686E+01	.333333E+00	0	5	107	145	106	195	200	0	0	0	0	0	0	0	0	0
147	.281035E+00	-.616343E+01	.244213E+01	.333333E+00	0	3	67	65	63	0	0	0	0	0	0	0	0	0	0	0
148	.724556E+00	-.317411E+01	.331006E+01	.100000E+01	0	8	132	107	67	172	179	207	218	220	0	0	0	0	0	0
149	-.935894E+00	-.536135E+01	.193517E+01	.333333E+00	0	2	105	175	0	0	0	0	0	0	0	0	0	0	0	0
150	.694083E+01	.908256E+00	.351616E+01	.100000E+01	1	3	122	222	252	0	0	0	0	0	0	0	0	0	0	0
151	.685824E+01	-.342670E+01	.148533E+01	.333333E+00	1	1	89	0	0	0	0	0	0	0	0	0	0	0	0	0
152	.431960E+01	-.146293E+01	.259890E+01	.100000E+01	0	7	122	112	93	157	164	192	219	0	0	0	0	0	0	0
153	.118707E+01	.340642E+01	.529885E+01	.100000E+01	4	11	103	159	160	177	178	212	214	215	216	274	287	0	0	0
154	-.707755E+00	-.763393E+01	.388069E+01	.333333E+00	1	2	69	65	0	0	0	0	0	0	0	0	0	0	0	0

155	-.319434E+01	-.622866E+01	.436409E+01	.100000E+01	1	5	69	173	204	275	284	0	0	0	0	0	0	0	0	0
156	.663823E+01	-.790921E+00	.152943E+01	.333333E+00	0	3	89	122	84	0	0	0	0	0	0	0	0	0	0	0
157	.476094E+01	-.922924E-01	.398691E+01	.100000E+01	0	6	152	122	98	176	237	238	0	0	0	0	0	0	0	0
158	.654211E+01	-.277405E+01	.250663E+01	.333333E+00	0	2	89	192	0	0	0	0	0	0	0	0	0	0	0	0
159	-.101696E+00	.338469E+01	.376960E+01	.100000E+01	0	5	138	153	75	160	161	0	0	0	0	0	0	0	0	0
160	.299638E+00	.169600E+01	.476320E+01	.100000E+01	0	10	159	153	75	177	185	186	212	231	232	274	0	0	0	0
161	-.128775E+01	.498166E+01	.356231E+01	.100000E+01	0	6	159	138	111	225	242	258	0	0	0	0	0	0	0	0
162	.114078E+01	-.110405E+01	.130423E+01	.333333E+00	0	3	140	90	72	0	0	0	0	0	0	0	0	0	0	0
163	.182289E+01	-.835388E+00	.211752E+01	.333333E+00	0	5	113	140	90	180	235	0	0	0	0	0	0	0	0	0
164	.399288E+01	-.275105E+01	.270739E+01	.333333E+00	0	3	152	93	219	0	0	0	0	0	0	0	0	0	0	0
165	.631498E+01	.302011E+01	.352293E+01	.100000E+01	1	5	99	194	213	238	255	0	0	0	0	0	0	0	0	0
166	-.312636E+01	.464710E+01	.149820E+01	.333333E+00	0	3	121	120	50	0	0	0	0	0	0	0	0	0	0	0
167	-.228289E+01	.649090E+01	.411500E+00	.333333E+00	0	4	55	51	25	168	0	0	0	0	0	0	0	0	0	0
168	-.287854E+01	.678998E+01	.397609E+00	.333333E+00	0	4	167	55	51	169	0	0	0	0	0	0	0	0	0	0
169	-.304025E+01	.597264E+01	.143856E+01	.100000E+01	0	3	168	170	171	0	0	0	0	0	0	0	0	0	0	0
170	-.390266E+01	.659901E+01	.223961E+01	.333333E+00	1	2	169	51	0	0	0	0	0	0	0	0	0	0	0	0
171	-.221458E+01	.538874E+01	.230753E+01	.333333E+00	0	4	169	51	111	191	0	0	0	0	0	0	0	0	0	0
172	.226893E+01	-.341321E+01	.455815E+01	.100000E+01	0	7	148	179	218	220	227	234	244	0	0	0	0	0	0	0
173	-.153996E+01	-.682851E+01	.531447E+01	.100000E+01	5	4	155	69	245	247	0	0	0	0	0	0	0	0	0	0
174	-.502283E+01	-.579214E+01	.257950E+01	.333333E+00	1	2	133	101	0	0	0	0	0	0	0	0	0	0	0	0
175	-.985158E+00	-.517668E+01	.257386E+01	.333333E+00	0	1	149	0	0	0	0	0	0	0	0	0	0	0	0	0
176	.349040E+01	.127434E+01	.326717E+01	.100000E+01	0	5	157	113	98	178	238	0	0	0	0	0	0	0	0	0
177	.140158E+01	.238608E+01	.446777E+01	.333333E+00	0	4	160	75	153	178	0	0	0	0	0	0	0	0	0	0
178	.263524E+01	.209227E+01	.487953E+01	.100000E+01	4	8	176	177	153	212	214	215	217	237	0	0	0	0	0	0
179	.591364E+00	-.446781E+01	.482947E+01	.100000E+01	4	7	172	148	67	207	218	244	245	0	0	0	0	0	0	0
180	.113474E+01	-.984932E+00	.324972E+01	.100000E+01	0	4	163	184	187	230	0	0	0	0	0	0	0	0	0	0
181	-.600712E+01	.359368E+01	.376803E+01	.100000E+01	1	5	110	126	182	183	281	0	0	0	0	0	0	0	0	0
182	-.592576E+01	.486448E+01	.337279E+01	.333333E+00	1	1	181	0	0	0	0	0	0	0	0	0	0	0	0	0
183	-.508718E+01	.287464E+01	.441184E+01	.333333E+00	0	4	181	263	269	281	0	0	0	0	0	0	0	0	0	0
184	.119827E+01	.264478E+00	.278851E+01	.333333E+00	0	5	180	114	113	187	188	0	0	0	0	0	0	0	0	0
185	-.166094E+01	.147243E+01	.508902E+01	.100000E+01	4	4	160	139	138	186	0	0	0	0	0	0	0	0	0	0
186	-.795077E+00	.135703E+01	.408168E+01	.333333E+00	0	3	160	185	139	0	0	0	0	0	0	0	0	0	0	0
187	.151428E+01	.287080E+00	.337508E+01	.333333E+00	0	3	180	184	188	0	0	0	0	0	0	0	0	0	0	0
188	.148640E+01	.830784E+00	.299031E+01	.333333E+00	0	4	187	184	113	189	0	0	0	0	0	0	0	0	0	0
189	.288030E+00	.843591E+00	.357471E+01	.100000E+01	0	2	188	230	0	0	0	0	0	0	0	0	0	0	0	0

190	-.624039E+01	.135862E+01	.395079E+01	.100000E+01	0	7	117	110	61	201	202	203	270	0	0	0	0	0	0	0
191	-.283730E+01	.592641E+01	.335677E+01	.100000E+01	0	1	171	0	0	0	0	0	0	0	0	0	0	0	0	0
192	.567516E+01	-.261902E+01	.350770E+01	.100000E+01	0	6	158	143	152	193	250	251	0	0	0	0	0	0	0	0
193	.539503E+01	-.446023E+01	.423672E+01	.100000E+01	1	5	192	143	227	228	249	0	0	0	0	0	0	0	0	0
194	.460249E+01	.402626E+01	.375755E+01	.100000E+01	0	5	142	102	165	196	213	0	0	0	0	0	0	0	0	0
195	-.337043E+01	-.427277E+01	.253543E+01	.100000E+01	0	7	146	145	101	198	204	208	211	0	0	0	0	0	0	0
196	.343467E+01	.555435E+01	.430631E+01	.100000E+01	0	7	194	144	142	224	248	278	288	0	0	0	0	0	0	0
197	-.591665E+01	-.168410E+01	.333217E+01	.333333E+00	0	4	96	97	60	260	0	0	0	0	0	0	0	0	0	0
198	-.445442E+01	-.353003E+01	.230940E+01	.333333E+00	0	4	101	195	78	199	0	0	0	0	0	0	0	0	0	0
199	-.521300E+01	-.301529E+01	.327759E+01	.100000E+01	0	4	198	240	259	261	0	0	0	0	0	0	0	0	0	0
200	-.157422E+01	-.252806E+01	.300161E+01	.100000E+01	0	3	146	205	209	0	0	0	0	0	0	0	0	0	0	0
201	-.699258E+01	-.322249E+00	.473109E+01	.100000E+01	1	3	190	117	270	0	0	0	0	0	0	0	0	0	0	0
202	-.579800E+01	.721720E+00	.286616E+01	.333333E+00	0	3	190	117	61	0	0	0	0	0	0	0	0	0	0	0
203	-.451382E+01	.783774E+00	.478056E+01	.100000E+01	0	6	190	124	117	262	270	282	0	0	0	0	0	0	0	0
204	-.187215E+01	-.487564E+01	.371513E+01	.100000E+01	0	7	195	155	69	208	209	245	284	0	0	0	0	0	0	0
205	-.181821E+01	-.150757E+01	.470428E+01	.100000E+01	0	6	200	145	131	206	207	239	0	0	0	0	0	0	0	0
206	-.370552E+01	-.101776E+01	.425916E+01	.100000E+01	0	5	205	145	117	239	259	0	0	0	0	0	0	0	0	0
207	-.194945E+00	-.263707E+01	.500302E+01	.100000E+01	4	5	205	179	148	233	253	0	0	0	0	0	0	0	0	0
208	-.217202E+01	-.484496E+01	.241631E+01	.333333E+00	0	3	195	204	105	0	0	0	0	0	0	0	0	0	0	0
209	-.129829E+01	-.367576E+01	.362163E+01	.333333E+00	0	4	204	200	107	210	0	0	0	0	0	0	0	0	0	0
210	-.226540E+01	-.341936E+01	.450296E+01	.100000E+01	0	3	209	239	295	0	0	0	0	0	0	0	0	0	0	0
211	-.440285E+01	-.488360E+01	.413574E+01	.100000E+01	0	4	195	240	275	284	0	0	0	0	0	0	0	0	0	0
212	.140872E+01	.176916E+01	.642590E+01	.100000E+01	4	6	178	153	160	214	231	232	0	0	0	0	0	0	0	0
213	.586282E+01	.382456E+01	.529731E+01	.100000E+01	5	3	194	165	255	0	0	0	0	0	0	0	0	0	0	0
214	.276552E+01	.323584E+01	.651516E+01	.100000E+01	4	6	212	178	153	215	216	217	0	0	0	0	0	0	0	0
215	.251732E+01	.337787E+01	.521285E+01	.333333E+00	4	4	214	178	153	216	0	0	0	0	0	0	0	0	0	0
216	.238003E+01	.397534E+01	.547481E+01	.333333E+00	4	3	214	215	153	0	0	0	0	0	0	0	0	0	0	0
217	.350678E+01	.292332E+01	.545184E+01	.333333E+00	4	2	178	214	0	0	0	0	0	0	0	0	0	0	0	0
218	.143577E+01	-.416862E+01	.384192E+01	.333333E+00	0	4	172	179	148	220	0	0	0	0	0	0	0	0	0	0
219	.362503E+01	-.252813E+01	.219803E+01	.333333E+00	0	4	164	152	93	221	0	0	0	0	0	0	0	0	0	0
220	.184304E+01	-.389545E+01	.339031E+01	.333333E+00	0	3	172	218	148	0	0	0	0	0	0	0	0	0	0	0
221	.422020E+01	-.304954E+01	.327120E+01	.100000E+01	0	3	219	227	234	0	0	0	0	0	0	0	0	0	0	0
222	.729589E+01	-.544486E-01	.266475E+01	.333333E+00	0	4	122	150	41	223	0	0	0	0	0	0	0	0	0	0
223	.667237E+01	-.487992E+00	.376067E+01	.100000E+01	0	2	222	250	0	0	0	0	0	0	0	0	0	0	0	0
224	.237747E+01	.567667E+01	.350310E+01	.333333E+00	0	3	141	144	196	0	0	0	0	0	0	0	0	0	0	0

225	-.509183E+00	.567710E+01	.273287E+01	.333333E+00	0	4	134	161	111	226	0	0	0	0	0	0	0	0	0	0
226	-.152364E+01	.599197E+01	.353880E+01	.100000E+01	0	4	225	242	243	256	0	0	0	0	0	0	0	0	0	0
227	.413886E+01	-.328395E+01	.525574E+01	.100000E+01	4	8	221	193	172	234	249	251	264	266	0	0	0	0	0	0
228	.401716E+01	-.573258E+01	.493140E+01	.100000E+01	5	4	77	193	229	246	0	0	0	0	0	0	0	0	0	0
229	.223215E+01	-.663457E+01	.494462E+01	.100000E+01	5	5	228	66	244	246	247	0	0	0	0	0	0	0	0	0
230	.885237E+00	-.291768E+00	.510909E+01	.100000E+01	4	6	189	180	231	232	233	300	0	0	0	0	0	0	0	0
231	-.280695E+00	.699097E+00	.639703E+01	.100000E+01	4	5	230	212	160	233	300	0	0	0	0	0	0	0	0	0
232	.123381E+01	.967427E+00	.537500E+01	.333333E+00	4	3	230	212	160	0	0	0	0	0	0	0	0	0	0	0
233	-.162210E+00	-.129541E+01	.648588E+01	.100000E+01	4	5	231	230	207	253	300	0	0	0	0	0	0	0	0	0
234	.327844E+01	-.169390E+01	.440051E+01	.100000E+01	0	4	227	172	221	237	0	0	0	0	0	0	0	0	0	0
235	.246921E+01	-.850115E+00	.228032E+01	.333333E+00	0	4	113	163	90	236	0	0	0	0	0	0	0	0	0	0
236	.222651E+01	-.127427E+01	.352087E+01	.100000E+01	0	2	235	241	0	0	0	0	0	0	0	0	0	0	0	0
237	.312950E+01	.168543E+00	.511402E+01	.100000E+01	4	4	234	157	178	265	0	0	0	0	0	0	0	0	0	0
238	.499801E+01	.183779E+01	.445445E+01	.100000E+01	0	4	176	157	165	252	0	0	0	0	0	0	0	0	0	0
239	-.332859E+01	-.228429E+01	.576043E+01	.100000E+01	4	4	210	205	206	295	0	0	0	0	0	0	0	0	0	0
240	-.549109E+01	-.424970E+01	.369793E+01	.333333E+00	0	4	211	199	101	261	0	0	0	0	0	0	0	0	0	0
241	.960914E+00	-.126229E+01	.506946E+01	.100000E+01	4	3	236	253	254	0	0	0	0	0	0	0	0	0	0	0
242	-.415058E+00	.575620E+01	.518666E+01	.100000E+01	4	8	226	161	144	256	257	277	279	287	0	0	0	0	0	0
243	-.233141E+01	.660034E+01	.526431E+01	.100000E+01	5	4	226	256	279	297	0	0	0	0	0	0	0	0	0	0
244	.222050E+01	-.488428E+01	.591227E+01	.100000E+01	4	4	229	179	172	246	0	0	0	0	0	0	0	0	0	0
245	-.120760E+01	-.487731E+01	.560149E+01	.100000E+01	4	4	179	173	204	283	0	0	0	0	0	0	0	0	0	0
246	.301232E+01	-.594893E+01	.578068E+01	.333333E+00	4	3	229	244	228	0	0	0	0	0	0	0	0	0	0	0
247	.415485E+00	-.698766E+01	.570293E+01	.100000E+01	5	2	229	173	0	0	0	0	0	0	0	0	0	0	0	0
248	.244808E+01	.640250E+01	.401466E+01	.333333E+00	0	5	144	196	141	273	288	0	0	0	0	0	0	0	0	0
249	.596097E+01	-.366972E+01	.598452E+01	.100000E+01	5	4	227	193	251	264	0	0	0	0	0	0	0	0	0	0
250	.672325E+01	-.179486E+01	.350127E+01	.333333E+00	0	3	192	223	122	0	0	0	0	0	0	0	0	0	0	0
251	.551092E+01	-.183116E+01	.533863E+01	.100000E+01	4	7	249	227	192	264	265	266	267	0	0	0	0	0	0	0
252	.678691E+01	.171402E+01	.534018E+01	.100000E+01	5	4	238	150	255	290	0	0	0	0	0	0	0	0	0	0
253	.123057E+01	-.272834E+01	.640287E+01	.100000E+01	4	3	241	233	207	0	0	0	0	0	0	0	0	0	0	0
254	.227482E+01	-.921386E-01	.602047E+01	.100000E+01	4	1	241	0	0	0	0	0	0	0	0	0	0	0	0	0
255	.671047E+01	.292744E+01	.479288E+01	.333333E+00	0	3	252	213	165	0	0	0	0	0	0	0	0	0	0	0
256	-.166953E+01	.554597E+01	.478682E+01	.333333E+00	0	3	242	243	226	0	0	0	0	0	0	0	0	0	0	0
257	-.940740E+00	.693650E+01	.671328E+01	.100000E+01	5	1	242	0	0	0	0	0	0	0	0	0	0	0	0	0
258	-.655745E-01	.357614E+01	.429089E+01	.100000E+01	0	2	161	274	0	0	0	0	0	0	0	0	0	0	0	0
259	-.520271E+01	-.208402E+01	.504751E+01	.100000E+01	4	4	199	97	206	260	0	0	0	0	0	0	0	0	0	0

260	-.592681E+01	-.169224E+01	.399871E+01	.333333E+00	0	4	97	259	197	271	0	0	0	0	0	0	0	0	0	0
261	-.564538E+01	-.385871E+01	.421539E+01	.333333E+00	0	4	199	240	97	276	0	0	0	0	0	0	0	0	0	0
262	-.367498E+01	.883954E+00	.374901E+01	.333333E+00	0	4	124	203	118	298	0	0	0	0	0	0	0	0	0	0
263	-.484043E+01	.270994E+01	.381482E+01	.333333E+00	0	3	124	183	269	0	0	0	0	0	0	0	0	0	0	0
264	.468941E+01	-.252811E+01	.702368E+01	.100000E+01	4	6	251	249	227	265	266	267	0	0	0	0	0	0	0	0
265	.436808E+01	-.635404E+00	.646294E+01	.100000E+01	4	8	251	264	237	267	290	291	292	293	0	0	0	0	0	0
266	.429749E+01	-.208969E+01	.582703E+01	.333333E+00	4	3	251	264	227	0	0	0	0	0	0	0	0	0	0	0
267	.617536E+01	-.119249E+01	.711363E+01	.100000E+01	4	6	264	265	251	290	291	292	0	0	0	0	0	0	0	0
268	-.431146E+01	.399248E+01	.507728E+01	.333333E+00	4	1	127	0	0	0	0	0	0	0	0	0	0	0	0	0
269	-.479178E+01	.228336E+01	.432483E+01	.333333E+00	0	3	263	183	124	0	0	0	0	0	0	0	0	0	0	0
270	-.613637E+01	.103734E+01	.592207E+01	.100000E+01	4	4	203	201	190	281	0	0	0	0	0	0	0	0	0	0
271	-.652075E+01	-.157507E+01	.371953E+01	.333333E+00	0	3	97	260	60	0	0	0	0	0	0	0	0	0	0	0
272	-.655896E+01	-.343924E+01	.484787E+01	.333333E+00	4	2	97	276	0	0	0	0	0	0	0	0	0	0	0	0
273	.183805E+01	.589355E+01	.508546E+01	.100000E+01	4	2	248	287	0	0	0	0	0	0	0	0	0	0	0	0
274	-.572190E+00	.289807E+01	.610295E+01	.100000E+01	4	4	258	153	160	277	0	0	0	0	0	0	0	0	0	0
275	-.452687E+01	-.618751E+01	.438520E+01	.333333E+00	1	2	211	155	0	0	0	0	0	0	0	0	0	0	0	0
276	-.624638E+01	-.391338E+01	.449868E+01	.333333E+00	0	3	261	272	97	0	0	0	0	0	0	0	0	0	0	0
277	-.177965E+01	.447936E+01	.589910E+01	.100000E+01	4	4	274	242	138	279	0	0	0	0	0	0	0	0	0	0
278	.351500E+01	.459735E+01	.523123E+01	.333333E+00	4	1	196	0	0	0	0	0	0	0	0	0	0	0	0	0
279	-.151719E+01	.578607E+01	.593646E+01	.333333E+00	4	3	277	243	242	0	0	0	0	0	0	0	0	0	0	0
280	-.313556E+01	.320259E+01	.504649E+01	.333333E+00	4	2	138	282	0	0	0	0	0	0	0	0	0	0	0	0
281	-.563523E+01	.295060E+01	.562495E+01	.100000E+01	4	5	270	183	181	282	296	0	0	0	0	0	0	0	0	0
282	-.375084E+01	.231045E+01	.582321E+01	.100000E+01	4	3	281	280	203	0	0	0	0	0	0	0	0	0	0	0
283	-.222068E+01	-.570586E+01	.711384E+01	.100000E+01	4	2	245	295	0	0	0	0	0	0	0	0	0	0	0	0
284	-.318349E+01	-.510625E+01	.364447E+01	.333333E+00	0	4	211	155	204	285	0	0	0	0	0	0	0	0	0	0
285	-.424905E+01	-.466294E+01	.431216E+01	.100000E+01	0	3	284	286	294	0	0	0	0	0	0	0	0	0	0	0
286	-.452927E+01	-.568321E+01	.512352E+01	.333333E+00	4	1	285	0	0	0	0	0	0	0	0	0	0	0	0	0
287	.827670E+00	.494374E+01	.652664E+01	.100000E+01	4	4	273	242	153	289	0	0	0	0	0	0	0	0	0	0
288	.296315E+01	.661346E+01	.364772E+01	.333333E+00	0	3	141	248	196	0	0	0	0	0	0	0	0	0	0	0
289	.315850E+00	.600976E+01	.714261E+01	.333333E+00	4	1	287	0	0	0	0	0	0	0	0	0	0	0	0	0
290	.578717E+01	.739551E+00	.677229E+01	.100000E+01	4	4	265	267	252	291	0	0	0	0	0	0	0	0	0	0
291	.523819E+01	-.292673E+00	.741332E+01	.333333E+00	4	5	290	265	267	292	293	0	0	0	0	0	0	0	0	0
292	.498447E+01	-.873097E+00	.762111E+01	.333333E+00	4	4	265	291	267	293	0	0	0	0	0	0	0	0	0	0
293	.434460E+01	.477308E-01	.834251E+01	.100000E+01	4	3	292	291	265	0	0	0	0	0	0	0	0	0	0	0
294	-.505705E+01	-.484006E+01	.613309E+01	.100000E+01	5	1	285	0	0	0	0	0	0	0	0	0	0	0	0	0

295	-.313876E+01	-.424590E+01	.610111E+01	.100000E+01	4	3	239	283	210	0	0	0	0	0	0	0	0	0	0	0
296	-.614158E+01	.335872E+01	.751626E+01	.100000E+01	5	1	281	0	0	0	0	0	0	0	0	0	0	0	0	0
297	-.382291E+01	.586391E+01	.637475E+01	.100000E+01	5	2	243	127	0	0	0	0	0	0	0	0	0	0	0	0
298	-.323558E+01	-.294688E+00	.419118E+01	.100000E+01	0	2	262	299	0	0	0	0	0	0	0	0	0	0	0	0
299	-.218651E+01	-.193330E+01	.465421E+01	.100000E+01	0	1	298	0	0	0	0	0	0	0	0	0	0	0	0	0
300	.658755E+00	-.246723E+00	.642228E+01	.333333E+00	4	3	231	233	230	0	0	0	0	0	0	0	0	0	0	0

Appendix D

Listing of ORIENT

```
      PROGRAM ORIENT(INPUT,OUTPUT,TAPE6)
      DIMENSION IB(500),IT(500),INT(12,500),T(500),TN(500),Z(500)
      PI=4.*ATAN(1.)
      READ(6)NS,D,RC
      READ(6)
      READ(6)
      READ(6)
      READ(6)BEDLEN,PACFAC
      READ(6)
      DO 1 I=1,NS
    1 READ(6)D1,D2,Z(I),D4,IB(I),IT(I),(INT(J,I),J=1,12)
      PRINT*,"INPUT:"
      PRINT*," "
      PRINT*,"WHAT IS THE PACKING DISTANCE MULTIPLIER",
      READ*,DM
      PRINT*,"THE UNIT CELL K, L, AND A (TRUE DIMENSIONS)",
      READ*,CCOND,CL,CA
      CK=2.*CL/(CCOND*CA)
C
C     CK IS A LINKAGE RESISTANCE (2 SPHERES)
C
      PRINT*,"THE UPPER AND LOWER BOUNDARY TEMPERATURES ",
      READ*,TU,TL
      PRINT*,"MAXIMUM FRACTIONAL ERROR IN TEMPERATURE",
      READ*,ERR
      PRINT*,"MAXIMIUM NUMBER OF ITERATIONS, SOR CONSTANT",
      READ*,ITMAX,ALPHA
      PRINT*,"PRINT ALL TEMPERATURE FIELDS (1=YES,0=NO)",
      READ*,IPRT
      BEDLEN=BEDLEN*DM
      DO 40 I=1,NS
   40 Z(I)=Z(I)*DM
      RC=RC*DM
      PRINT*," "
      PRINT*,"DATA FROM TAPE6 (MODIFIED)"
      PRINT*," "
      PRINT*,"PACKING FACTOR (UNCORRECTED) =",PACFAC
      PRINT*,"EFFECTIVE BED LENGTH =",BEDLEN
C
C     ASSUMES R-SPHERE = 1., ONE SIZE FRACTION
C
      RM=RC-(1.*DM)
      AT=PI*RM*RM
      PRINT*,"EFFECTIVE BED AREA =",AT
      PRINT*," "
      PRINT*,"INITIAL CONDITIONS ASSUME A LINEAR TEMPERATURE VARIATION",
      PRINT*," WITH Z."
      PRINT*," "
      SLOPE=(TU-TL)/BEDLEN
      DO 2 I=1,NS
      T(I)=SLOPE*Z(I)+TL
```

```
      IF(IB(I).EQ.2.OR.IB(I).EQ.3)T(I)=TL
      IF(IB(I).EQ.4.OR.IB(I).EQ.5)T(I)=TU
      TN(I)=T(I)
    2 CONTINUE
      PRINT*,"*** INITIAL TEMPERATURE FIELD ***"
      CALL TEMOUT(T,NS)
C
C     BEGIN THE SOLUTION ITERATION
C
      DO 98 L=1,ITMAX
      EMAX=0.
      DO 10 I=1,NS
      IF(IB(I).EQ.2.OR.IB(I).EQ.3)TN(I)=TL
      IF(IB(I).EQ.4.OR.IB(I).EQ.5)TN(I)=TU
      IF(IB(I).GT.1)GO TO 10
      NN=IT(I)
      IF(NN.EQ.0)GO TO 10
      TSUM=0.
      DO 20 J=1,NN
   20 TSUM=TSUM+TN(INT(J,I))
      TN(I)=TN(I)*(1.-ALPHA)+(ALPHA*TSUM/FLOAT(NN))
      E=ABS((TN(I)-T(I))/TN(I))
      EMAX=AMAX1(EMAX,E)
   10 CONTINUE
      IF(L.EQ.ITMAX)GO TO 12
      IF(EMAX.LT.ERR)GO TO 12
      IF(IPRT.EQ.0)GO TO 11
   12 CONTINUE
      PRINT*,"*** ITERATION ",L," ***"
      PRINT*,"MAXIMUM ERROR = ",EMAX
      IF(EMAX.LT.ERR)PRINT*,"CONVERGENCE REACHED"
      PRINT*,"-----------------------------------------"
      PRINT*," "
      PRINT*,"*** TEMPERATURE FIELD ***"
      CALL TEMOUT(TN,NS)
   11 IF(EMAX.LT.ERR)GO TO 99
      DO 21 K=1,NS
   21 T(K)=TN(K)
   98 CONTINUE
      PRINT*,"***************************************"
      PRINT*,"MAXIMUM NUMBER OF ITERATIONS PERFORMED - CHECK",
      PRINT*,"ERROR  RANGE"
      PRINT*,"***************************************"
      PRINT*," "
      PRINT*," "
   99 CONTINUE
C
C     THE TEMPERATURES HAVE BEEN CALCULATED - EVALUATE THE TOTAL HEAT
C     IN AND THE EFFECTIVE BED CONDUCTIVITY
C
      QSUM=0.
      DO 88 I=1,NS
```

```
      IF(IB(I).NE.2.AND.IB(I).NE.3)GO TO 88
      NN=IT(I)
      IF(NN.EQ.0)GO TO 88
      DO 87 J=1,NN
      I1=I
      I2=INT(J,I)
      IF(Z(I2).LT.Z(I1))GO TO 86
      I1=I2
      I2=I
   86 CONTINUE
   87 QSUM=QSUM+(TN(I1)-TN(I2))/CK
   88 CONTINUE
      QFLUX=QSUM/AT
      PRINT*,"AVERAGE HEAT FLUX = ",QFLUX
      BCOND=QFLUX*BEDLEN/(TU-TL)
      PRINT*,"EFFECTIVE BED CONDUCTIVITY = ",BCOND
      STOP
      END
      SUBROUTINE TEMOUT(T,NS)
      DIMENSION T(1)
      PRINT 101
      NLOOP=NS/10+1
      DO 1 I=1,NLOOP
      NF=10*(I-1)+1
      IF(NF.GT.NS)GO TO 2
      NL=NF+9
      IF(NL.GT.NS)NL=NS
    1 PRINT 102,NF,(T(J),J=NF,NL)
    2 CONTINUE
      PRINT 103
  101 FORMAT(1X,"SPHERE #",7X,"+0",10X,"+1",10X,"+2",10X,"+3",10X,"+4",
     &10X,"+5",10X,"+6",10X,"+7",10X,"+8",10X,"+9"/)
  102 FORMAT(3X,I3,3X,10(3X,F9.4))
  103 FORMAT(///)
      RETURN
      END
```

Appendix E

ORIENT Sample Case

This appendix contains an example of a typical ORIENT run. In addition to a binary file TAPE6 generated by RANDPAC, the following sample data was used:

Packing distance multiplier	1.0
(This is a constant that can be used to scale the dimensions in the RANDPAC datafile TAPE6)	
Unit cell parameters:	
Effective conductivity	1.0
Effective length of cell	1.0
Effective heat transfer area of cell	2.331977
Fractional temperature convergence	0.0000001
Iteration limit	100
SOR constant	1.48

Print initial and final temperatures only

The ORIENT calculation shows that the bed conductivity is only 43.1% of the unit cell conductivity. The low magnitude of this value is due primarily to the use of a bed containing only 100 spheres.

INPUT:

```
WHAT IS THE PACKING DISTANCE MULTIPLIER? 1
THE UNIT CELL K, L, AND A (TRUE DIMENSIONS)? 1 1 2.331977
THE UPPER AND LOWER BOUNDARY TEMPERATURES ? 800 300
MAXIMUM FRACTIONAL ERROR IN TEMPERATURE? 1.E-7
MAXIMIUM NUMBER OF ITERATIONS, SOR CONSTANT? 100 1.48
PRINT ALL TEMPERATURE FIELDS (1=YES,0=NO)? 0

DATA FROM TAPE6 (MODIFIED)

PACKING FACTOR (UNCORRECTED) =.4155646742564
EFFECTIVE BED LENGTH =12.83394297861
EFFECTIVE BED AREA =50.26548245744

INITIAL CONDITIONS ASSUME A LINEAR TEMPERATURE VARIATION
 WITH Z.
```

*** INITIAL TEMPERATURE FIELD ***

SPHERE #	+0	+1	+2	+3	+4	+5	+6	+7	+8
1	300.0000	300.0000	300.0000	300.0000	300.0000	300.0000	300.0000	300.0000	300.0000
11	300.0000	300.0000	300.0000	300.0000	300.0000	300.0000	300.0000	300.0000	300.0000
21	363.6370	364.1251	372.8858	363.6309	364.6199	363.6543	369.2081	376.9170	410.2361
31	386.3292	373.8395	439.3841	375.6533	442.7686	508.3131	424.4908	410.0104	437.9776
41	501.1061	464.1761	466.2352	506.7470	438.0008	572.0329	436.7738	484.3261	468.7785
51	627.6284	625.5759	545.6387	483.8529	500.7906	432.3203	693.8774	570.2958	518.0153
61	557.2139	571.1124	609.8736	469.3017	691.8249	497.8778	553.7002	615.2477	555.0697
71	800.0000	800.0000	642.7956	800.0000	510.8433	800.0000	599.3710	800.0000	530.3573
81	597.3880	800.0000	646.4997	591.3567	800.0000	800.0000	800.0000	800.0000	567.8488
91	800.0000	800.0000	666.0550	800.0000	800.0000	800.0000	800.0000	800.0000	671.4166

*** ITERATION 59 ***
MAXIMUM ERROR = 8.929131640508E-8
CONVERGENCE REACHED

*** TEMPERATURE FIELD ***

SPHERE #	+0	+1	+2	+3	+4	+5	+6	+7	+8
1	300.0000	300.0000	300.0000	300.0000	300.0000	300.0000	300.0000	300.0000	300.0000
11	300.0000	300.0000	300.0000	300.0000	300.0000	300.0000	300.0000	300.0000	300.0000
21	344.8182	342.8878	323.5221	332.0477	333.6876	349.7871	347.0442	370.1286	381.1280
31	383.1457	411.1847	466.0770	376.0120	486.2413	509.7809	401.9992	398.1804	390.1098
41	501.7822	438.5708	454.2387	531.8148	405.2174	559.9544	503.5383	542.5460	462.0372
51	638.2675	683.6755	527.5446	454.3345	466.6529	375.8932	746.5847	511.4084	490.9807
61	500.8299	545.1420	504.8985	443.9529	757.5650	463.7526	565.1205	608.8379	508.9261
71	800.0000	800.0000	704.4189	800.0000	437.6409	800.0000	517.1825	800.0000	511.6921
81	586.3674	800.0000	640.6692	503.2711	800.0000	800.0000	800.0000	800.0000	487.7223
91	800.0000	800.0000	504.0848	800.0000	800.0000	800.0000	800.0000	800.0000	800.0000

AVERAGE HEAT FLUX = 16.78985839224
EFFECTIVE BED CONDUCTIVITY = .4309601704501