In order to properly model the temperature distribution of a nuclear fuel pin, the thermal conductivity of the fuel must be known. For sphere pac fuel, the modeling of the conductivity is complicated due to the fact that the fuel is a collection of spheres in a random packed bed. Current models used to calculate the thermal conductivity of sphere pac fuel treat the fuel pin as having a constant packing factor across the pin diameter, ignoring boundary effects. The models also neglect the effects of neighboring spheres which do not contact each other.

Analysis of previously manufactured sphere pac fuel pins has shown that the packing factor of spheres in cylinders can be treated as consisting of two regions: the boundary region, in which packing is based on local wall curvature, and the infinite bed region, where packing is assumed that of an infinite bed of spheres.

Two sets of "unit cells" were developed to model the heat flow in these two regions. In addition to the
boundary region of large spheres near the clad, the effects of fine spheres bordering on a large sphere was included.

The thermal conductivities obtained from these models was compared to data from previous sphere packing thermal conductivity experiments. The match between experimental data and predictions was good for single size fraction data and matched reasonably well for binary fuel in comparison to current models modified to account for cell orientation effects.
THERMAL CONDUCTIVITY MODELING OF UNRESTRUCTURED SPHERE PAC NUCLEAR FUELS

by

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Typed by J.S. Willison for James Stuart Willison
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Chapter I
Introduction

Since the early days of nuclear power, significant efforts have been devoted to finding new types and configurations of fuel that would allow more efficient utilization of the world's uranium resources. More recently, concern has shifted to include the possible diversion of fissile material from the nuclear fuel cycle for the production of nuclear weapons. A primary goal of these efforts has been to develop a fuel with a longer lifetime while keeping the fuel cycle safe from illicit diversion. One of the concepts which meets these needs is sphere pac nuclear fuel. Since its origin, in the early 1960's, considerable international attention has been focused on the development and production of sphere pac fuel(1).

Sphere pac fuel consists of two or three sizes of fuel spheres which are then loaded into zircaloy or stainless steel cladding tubes, depending on the reactor type. Except for the gaps between the spheres, the spheres completely fill the enclosed volume of the cladding. This is different from current pellet nuclear fuels, which leave a gas gap between the fuel and
cladding to leave room for fuel restructuring.

One group which is involved in sphere pac fuel research is the Swiss Federal Institute for Reactor Research (EIR). Sphere pac fuels made by EIR are produced by forming microspheres of fuel material in a wet chemistry solution-gelation process. The spheres are then sintered and vibrofilled into cladding tubes. A cross-section of a typical sphere pac fuel pin is shown in Figure 1. These procedures are easily adapted to remote handling techniques and are thus resistant to diversion(2).

There is also evidence that fuel clad mechanical interaction is less severe in sphere pac fuel rods than in conventional pellet fuel pins(3). Pellet fuel tends to crack because of high temperature gradients, and the broken pieces can relocate, causing extremely high local stresses in the cladding. The spheres in near the clad of a sphere pac fuel pin are not as susceptible to cracking and can lead to longer pin lifetimes.

An important parameter in adequately modeling a nuclear fuel is the thermal conductivity. This, along with the power distribution in the fuel, determines the temperature profile and the maximum fuel temperature, which must be below certain limits in order to maintain safety margains.

Heat transfer through a packed bed of spheres is less than straightforward because it is not a solid
Figure 1. Cross-Section of Typical 2-size Sphere Pac Fuel Pin (FILOS 4)
material. The spheres have a random orientation within the cladding and the heat flow depends on the number of contacts each sphere has with other spheres. This in turn is dependent upon the packing factor of spheres in the pin.

A two-dimensional unit cell was developed by Ades (4) in an attempt to evaluate the thermal conductivity of a sphere pac bed. However, there are limitations to this model with respect to the orientation of the unit cell relative to the heat flow. Assumptions are also made regarding the accommodation coefficient of mixed carbides and the exclusion of boundary effects in the conductivity calculations.

The present work is divided into three main areas; the determination of boundary effects on the packing density of spheres throughout the pin, the development of a set of unit cells with a more appropriate physical basis than Ades' cell, and the comparison of results from the models with data from experiments performed with sphere pac fuel.
Chapter II
Wall Effects on the Radial Packing Factor Distribution

A basic assumption made in the development of the Ades unit cell (4) was that the packing factor could be treated as a constant across the entire fuel pin. Since the calculated conductivity is a function of the packing factor, the assumption was made that the same unit cell could be used anywhere in the pin. This, however, is not the case. Previous work on the packing of hard spheres into cylindrical containers has shown that the void fraction is in fact similar to a damped sine wave near a boundary (5,6). An example of this is shown in Figure 2.

The reason for this behavior is an imposed order on the packing of the spheres in contact with a boundary. This ordering next to a wall results in a higher void fraction because volumes which would normally be filled by neighboring spheres are blocked as they are too small for whole spheres to fill. This boundary effect is illustrated in Figure 3. As one gets away from the wall, the randomness of the packing causes the sine wave to damp out so that it is negligible at about five sphere diameters.

The exact manner in which the packing factor varies with distance from a wall is dependent on the curvature of the wall with respect to the size of the sphere. It is also essentially independent of whether the wall is
Figure 2. Void Fraction Variation near the Boundary of a Semi-infinite Bed of Spheres
Figure 3. Schematic Representation of Higher Void Fraction Adjacent to Boundaries
concave or convex.

The distance of one sphere radius was selected as the most reasonable transition point between the boundary packing region and the infinite bed region. It is at one radius that the first minimum occurs in the packing factor distribution. The boundary packing region is defined as the region near the clad wall where the packing factor is lower than for an infinite bed and the most significant heat flow is from the spheres to the clad. The infinite bed region constitutes the remainder of the fuel pin where the packing factor is assumed to be that of an infinite bed. Heat transfer in this region is from sphere to sphere and depends upon the number of contacts with neighboring spheres. Because of these differences, two different types of cell are used for these two regions. These cells are described in Chapters 3 and 4.

Much of the literature currently available on the thermal performance of sphere pac fuel refers to the difference in conductivity in the boundary region near the clad in terminology more appropriate to pellet fuel. Namely, the difference is referred to as a "gap conductance". While the conductivity is different near the cladding as opposed to the center of the pin, it has nothing whatsoever to do with gaps near the clad. Rather, it is due to differing packing factors adjacent to a boundary.
Once a given transition point was chosen, integrated void fraction curves from Benenati and Brosilow (6) could be analyzed to determine a relationship between wall curvature and the boundary region packing factor. This is shown in Figure 4.

This curve was then used to calculate the boundary and infinite bed packing factors for several sphere pac fuel pins which have been previously manufactured (7-11). A summary for these pins is found in Table 1.

It should be noted in Table 1 that the calculated bed packing factor of large spheres for all pins lies around 64-65%, which is near the estimate of 64% for the maximum packing for a random bed (12). It would seem reasonable to assume that for vibrofilled sphere pac fuel that the large fraction packing factor has the maximum bed value in the bed region. The boundary packing factor then can be determined from the relation in Figure 4.

Consistant with the packing of large spheres, it is not possible to assume that the packing of the fine fraction is constant across the pin. In EIR fuel, the fine fraction is loaded only after the large spheres have been loaded and packed down. More void is located in the boundary region, which is then filled by the fine fraction spheres.
Figure 4. Wall Packing Factor as a Function of Wall Curvature

Derived from Benenati and Brosilow (6)
<table>
<thead>
<tr>
<th>Pin ID</th>
<th>Lg. Sphere Pack Fac.</th>
<th>Pin Dia. Sphere Dia</th>
<th>Wall PF</th>
<th>Bed PF</th>
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<td>FILOS 05</td>
<td>61.0</td>
<td>9.975</td>
<td>.478</td>
<td>.641</td>
</tr>
<tr>
<td>Upper Pin 5.1</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>FILOS 05</td>
<td>61.5</td>
<td>9.975</td>
<td>.478</td>
<td>.647</td>
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<td>Lower Pin 5.2</td>
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<td></td>
<td></td>
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<tr>
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<td>10</td>
<td>.478</td>
<td>.637</td>
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<tr>
<td>Lower Zone</td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>FILOS 07</td>
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<td>10</td>
<td>.478</td>
<td>.638</td>
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<tr>
<td>Upper Zone</td>
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<td></td>
</tr>
<tr>
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<td>61.2</td>
<td>9.1</td>
<td>.472</td>
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<tr>
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<td>7.26</td>
<td>.453</td>
<td>.644</td>
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III. Heat Transfer Modes

Calculations involving all gaps between spheres in a packed bed of any significant size would be prohibitive both in terms of cost and computer utilization. In addition, most of the calculations would be redundant.

Because of the regularity of structure of a sphere pac bed, it is assumed that a "unit cell" can adequately model the heat transfer mechanisms between spheres. For packed beds which are not under mechanical load, the contacts between spheres are idealized as points. The heat transfer takes place almost exclusively through the gas gaps. It is also assumed that radiation heat transfer between spheres is negligible. In support of this assumption is a measurement made by Beatty. While performing measurements of sphere pac fuel conductivity, one test was performed with essentially no fill gas. The effective conductivity for vacuum conditions was roughly an order of magnitude less than for one atmosphere of helium. Thus, the accuracy of calculated conductivities should depend upon the gap conductance model used and the proper characterization of the gas gaps throughout the bed.

III.2 Ades Unit Cell

The unit cell which Ades chose to model a packed bed consisted of two hemispheres surrounded by a fill gas
(Figure 5). He assumed that the conductivity calculated from this cell would be representative of the entire pin. For binary fuel, the cell would first be used to calculate a fine fraction conductivity. This value would be inserted into the large cell in place of the fill gas except in the narrow gap between the spheres where the fine fraction could not penetrate. The penetration distance was calculated by using the pin-smear packed packing factors to calculate the large and fine cell void fractions. The remaining gas was assumed to be in the gap. For standard EIR binary fuel (Large Diameter=800um, Fine Diameter=60um), he calculated that fine fraction fuel penetrated to where the separation between the large spheres was 2.79 fine sphere diameters.

A severe shortcoming to this approach is this large gap, which contains no fine fuel. Examination of micrographs of existing fuel show many occurrences of small spheres penetrating such that it actually contacts both large spheres.

Another point raised by Henke(14), is that Ades' cell would only be valid for beds with a "simple cubic" structure and heat flow parallel to its axis. This is shown in Figure 6. As the packed sphere beds have random orientations and are far from ordered, another approach should be utilized which accounts for physical characteristics of the packed bed.
Figure 5. Ades' Unit Cell
Figure 6. Valid Simple Cubic Orientation for Ades' Unit Cell
III.3 The Unit Cell based upon Coordination Numbers of Packed Beds

In his work on packed beds, Henke(14) developed a computer program which mathematically generated a random packing of spheres within a cylindrical container. One of the results of his work was an approximate correlation between the average number of sphere contacts in a packed bed (coordination number) and the bed packing factor. It was found that

\[ n = 2.67P + 3.97 \]  

where \( n \) = average coordination number  
\( P \) = corrected packing factor

The corrected packing factor was defined as the packing factor for the region of the bed away from its edge (infinite bed region). This reduces the wall effects and makes the formula applicable for a wide range of bed sizes. This coordination number is used to calculate the dimensions of the unit cell shown in Figure 7.

For EIR vibrofilled fuel pins, the corrected packing factor is assumed to be the maximum (\( P=0.64 \)) for a packed bed. From this packing factor, an average coordination number is calculated. The inverse of the coordination number(n) should be the fraction of a sphere's volume which is contained in the unit cell. The angle \( \phi \) for the
Figure 7. Basic Unit Cell Based on Coordination Number
unit cell which establishes the right cell volume is expressed as:

$$\phi = \cos^{-1}(1 - \frac{2}{n})$$  \hspace{1cm} (III-2)

The angle $\phi$ can be seen in the basic unit cell shown in Figure 7. The cell shown is a two-dimensional cross-section and is axisymmetric about the left boundary.

Once the angle is determined, the right boundary of the cell is established so that the cell has the proper packing factor. In order to calculate this cell boundary in which there is sphere to sphere contact at the top edge of the cell, the cell is split into a short cylinder of height $X$ and a cone of radius $R$ and height $H$.

If the radius of the sphere is unitized, then the volume of the cell is equal to the volume of a sphere of radius 1.0 divided by the coordination number and also divided by the packing factor of the cell, so that:

$$V = \frac{4\pi}{3nP}$$  \hspace{1cm} (III-3)

where 

- $V = \text{cell volume}$
- $P = \text{cell packing factor}$
- $n = \text{coordination number}$

By splitting the cell into a cylinder and a cone, the cell volume is expressed as:
\[
V = \frac{4\pi}{3nP} = \frac{1}{2}\pi R^2 H + \pi R^2 X \quad (\text{III-4})
\]

However, \(X = 1 - H\). By inserting this into equation (III-4) and reducing, the result is

\[
\frac{4}{nP} = R^2(3 - 2H) \quad (\text{III-5})
\]

Since

\[
\tan \phi = \frac{R}{H} \quad (\text{III-6})
\]

then

\[
R^2 = H^2 \tan^2 \phi \quad (\text{III-7})
\]

and

\[
\frac{4}{nP} = H^2 \tan^2 \phi (3 - 2H) \quad (\text{III-8})
\]

By simplifying equation (III-8), the result is:

\[
H^3 - \frac{3}{2} H^2 + \frac{2}{nP \tan^2 \phi} = 0 \quad (\text{III-9})
\]

This can be solved by using the trigonometric method for cubic equations. Calculations for cell dimensions of close contact cells (cells not in contact at the top
boundary) can be found in Appendix A.

In order to perform the conductivity calculations, the center of the sphere is removed by means of a lumped parameter analysis. When the Biot number of a body is less than 0.1, it can be assumed with little error that it has negligible internal resistance(15).

For a hollow sphere, the heat transmitted is:

\[ Q = \frac{4\pi k\Delta T}{\frac{1}{r_1} - \frac{1}{r_o}} \quad \text{(III-10)} \]

and for convection

\[ Q = hA\Delta T \quad \text{(III-11)} \]

By equating the heat transfer, the convective coefficient becomes:

\[ h = \frac{k}{r_0^2\left(\frac{1}{r_o} - \frac{1}{r_1}\right)} \quad \text{(III-12)} \]

The Biot number is defined as:

\[ Bi = \frac{h(V/A)}{k} \quad \text{(III-13)} \]

By inserting relations for a sphere and normalizing the outer radius to 1.0, equation (III-13) reduces to

\[ Bi = \frac{1}{3}\left(1 - \frac{r_1^3}{r_1^3} - 1\right) \quad \text{(III-14)} \]
For $\text{Bi}=0.1$, equation (III-14) reduces to

$$r_i^4 - 1.3r_i + 0.3 = 0 \quad (\text{III-15})$$

The only two real roots to this equation are at 1.0 and 0.233. For a sphere of 60um diameter, the radius of the removed section would be 6.99um.

The large unit cell differs from the fine fraction unit cell only in the inclusion of a boundary layer around the large sphere. In this model, small spheres may penetrate as far as is physically possible. This boundary layer extends to the leading edge of a sphere at maximum penetration, which is defined by the angle $\beta$, defined as:

$$\beta = \tan^{-1} \left( \sqrt{2u + u^2} - u \right) \quad (\text{III-16})$$

if $u =$ diameter ratio of small to large spheres

This is shown for the spheres in contact unit cell in Figure 8.

For calculations, the unit cell is modeled in finite elements with COYOTE, a two dimensional, non-linear heat conduction program(16). COYOTE treats the cell as axisymmetric around the central axis with adiabatic side boundaries. A constant temperature is fixed across the
Figure 8. Large Unit Cell (Contact)
top of the cell along with a temperature across the bottom. After COYOTE evaluates the steady state heat fluxes across the bottom face, the total heat flow is calculated through the cell.

From this, the conductivity of the cell is calculated as:

$$k_{\text{EFF}} = \frac{LQ}{\Delta T A}$$  \hspace{1cm} (III-17)

where $L$ = the length of the cell (including center of sphere)

- $Q$ = total heat flow across lower face
- $A$ = area of top face of cell
- $\Delta T$ = temperature difference across cell

The gap distances are calculated by dividing the gas element volume by the top element surface area and then doubling the result. This doubling is because the unit cell top surface is a plane of reflection for another unit cell (boundary cell gap distances are not doubled as they are not symmetric about their top surface).

Gap distances are in turn utilized to provide the necessary material conductivity of the gas elements. The gap conductance calculations are based on the Kennard model and are explained in Appendix B(17,18).

III.4 The Cell Orientation Factor

Another result of Henke's work(14) is the "cell
orientation factor". Henke took his packed bed models and treated the heat transport as a network of thermal resistances. He solved the resulting coupled equations in the computer code ORIENT. ORIENT computes a ratio between the input unit cell conductivity and the effective conductivity of a packed bed. This was done for a series of beds with different packing factors. Henke then calculated a relation between the orientation factor and the packing factor. For the range of packing factors of interest in sphere pac fuel, the orientation factor is approximately 0.9.

III.5 The Close Contact Factor

One of the drawbacks of Henke's work was that it only took into account heat transfer between spheres which were in actual contact. An analysis of some of the packed beds he used showed that occasionally neighboring spheres were almost but not quite in contact and thus neglected in his orientation calculations. In order to take this into account, two additional unit cells were developed for the large cell for small separations between neighboring spheres. Additional cells were developed for the fine fraction as well. These cells are shown in Figures 9, 10 and 11. The fine unit cells are identical in configuration to the large cells with the omission of the fine boundary layer next to the large spheres and the clad.

An analysis was made of Henke's packed bed data base
Figure 9. Large Unit Cell (Average Separation)
Figure 10. Large Unit Cell
(Maximum Separation)
Figure 11. Fine Unit Cell (Spheres not in Contact)
using the code CLOSEC to determine the frequency and magnitude of near contacts between spheres. CLOSEC calculated the center to center distance between spheres and compared this to the sphere radius. The separation distances used in the unit cells were the maximum and average separations for spheres in the close contact category. The average distribution for close contact spheres is shown in Figure 12. As can be seen, most close contacts between large spheres are less than 10% of the maximum separation allowed. Beyond 10% of maximum separation, the distribution appears to be constant. This maximum separation is the point at which the leading edge of a fine sphere contacts the axis of symmetry of the cell. It is at this point that no gas gap is defined in the large unit cell, except that which was already defined in the fine cells. At the same time, close contacts between large spheres and the cladding were not found in significant quantity to be deemed important and were thus disregarded.

The conductivities resulting from the three unit cells are weighted with this distribution and the touching contacts to give an effective unit cell conductivity. This, multiplied by the cell orientation factor results in the infinite bed effective conductivity. This number for the fine fraction is then utilized in the large unit cells.
Figure 12. Frequency Distribution of Close Contacts in a Packed Bed of Spheres
Chapter IV

The Boundary Cell

IV.1 General Description

As previously mentioned in Chapter 2, the dominant mode of heat transfer in the boundary packing region is from the spheres to the cladding, instead of to other spheres. Because of this difference, the unit cell developed for the infinite bed region was deemed inappropriate, and a different cell had to be formulated.

As one of its main functions would be to calculate the conductivity of the boundary layer of small spheres on large spheres in EIR two size fuel (Figure 13), a cell which is essentially one-half of Ades unit cell was chosen as the boundary cell. The fine boundary cell is shown in Figure 14.

The packing fractions used in the boundary cells are derived from the relation in Figure 4, being based on local wall curvature. The packing factor for the cell is established by determining the cell radius such that:

\[ a + R = \sqrt{\frac{2R^2}{3P}} \]  (IV-1)

The boundary cells are also axisymmetric about the left boundary.

IV.2 The Large Boundary Cell

The large boundary cell is analogous to the large unit cell as its primary difference with the respective
Figure 13. Relationship of the Fine Boundary Cell to Large Spheres
Figure 14. Fine Boundary Cell
fine cell is the addition of a boundary layer of small spheres next to the large sphere. In addition to this, the large boundary cell has a boundary layer of small spheres adjacent to the cladding (Figure 15).

As the geometry next to a boundary is slightly different than between spheres, the small sphere penetration angle ($\beta$) must be reevaluated. For a small sphere penetrating between two large spheres, the center of the small sphere lies on the top boundary of the large unit cell. This is because the top boundary is a plane of symmetry between two cells. For a large sphere next to a boundary the center of a penetrating small sphere will not be at the top boundary, but one small sphere radius from the top.

The leading edge of this penetrating small sphere defines the angle $\beta$ which is expressed as:

$$
\beta = \cos^{-1}\left(\frac{k - u + 1}{u + 1}\right) - \sin^{-1}\left(\frac{u}{u + 1}\right) \quad (IV-2)
$$

where $u =$ ratio of small to large sphere diameters

$k =$ ratio of large sphere-cladding gap to large sphere radius

(for contact with clad, $k=0$)

Gap distances for material conductivities are calculated in the same was as for the unit cells. The only exception is that the distances are not doubled as
Figure 15. Large Boundary Cell
the cladding boundary is not a plane of symmetry.

IV.3 Packing Factor Differences by Parallel Resistance

An interesting aspect of the fine boundary cell is that the packing factor can be raised by the subtraction of a thin annulus of fill gas. The gas for the calculations done for this work (He) had a much lower conductivity than the fuel. For this reason, lateral heat transfer to and from this annulus was small. To reduce computation expense, an investigation was made to determine if the conductivity of the annulus of gas and the effective conductivity of the fine boundary cell within the annulus could be treated as parallel thermal resistances. This is illustrated in Figure 16. Several COYOTE runs were made with differing pressures and temperatures for He and mixed carbide fuel. In all cases, the difference between the conductivity calculated by parallel resistances from the smaller cell was less than 2%.

A similar investigation was carried out on the large boundary cell. However, in this case the annulus consisted of a narrow length of fine boundary conductivity with the remainder having the conductivity of the fine infinite bed (Figure 17). It was found that the method of parallel resistances gave good agreement for large boundary cells as well as for the fine cells. This method was used for the remainder of the study whenever more than one boundary cell with differing
Figure 16. Normal Boundary Cell with Annulus of Gas to Lower Packing Factor
Figure 17. Large Boundary Cell Showing Annulus for Parallel Resistance Calculation
packing factors was needed.

The total integration of these models is schematically illustrated in Figure 18.
Figure 18. Schematic of Modeling Elements
Chapter V
The Beatty Experiment

V.1 General Experiment Description

In 1977, Dr. R. Beatty performed experiments aimed at determining the thermal conductivity of a packed bed of sphere pac nuclear fuel(13). The fuel parameters which he used are listed in Table 2. These fuel spheres are the same dimensions as EIR two-size fraction fuel. However, due to unavailability of mixed carbide spheres, Beatty used uranium carbide of slightly higher porosity for his experiments.

The Beatty apparatus, shown in Figure 19, consisted of two concentric cylinders with the fuel spheres in the annulus between them. The central cylinder contained an electric resistance heater. The energy from this heater created a temperature difference between the two cylinders which was measured by attached thermocouples. The two cylinders had known thermal conductivities, and as such their effect on the temperature difference was taken into account. The final result was an effective conductivity for an annulus of sphere pac fuel.

Beatty used two different sized apparatus for his experiments. One of these (System II), was only used for measuring the fine fraction. It had an inner diameter of 19mm. The other apparatus (System I), was used for measuring the conductivity of the large fraction, with and without the fine spheres. System I had an inner
Table 2. Fuel Sphere Parameters Used in the Beatty Thermal Conductivity Experiment

Fuel: UC

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Size Fractions</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Large</td>
<td>Fine</td>
</tr>
<tr>
<td>Average Size ($\mu$m)</td>
<td>800</td>
<td>60</td>
</tr>
<tr>
<td>Fuel Porosity (%)</td>
<td>6</td>
<td>19</td>
</tr>
<tr>
<td>Fill Gas</td>
<td>He</td>
<td></td>
</tr>
</tbody>
</table>
Figure 19. Beatty's Experimental Apparatus
diameter of 28mm. The same heater was used in conjunction with both systems. The heater had an outer diameter of 10mm. A calculation of the packing factors for these devices using the method in Chapter II is found in Appendix E.

V.2 Calculational Results

Using the packing factors of Appendix E, a set of unit and boundary cells was developed in an attempt to mathematically reproduce the measurements of Beatty. Calculations were made for a packed bed of fine spheres only, large spheres only and a binary mixture at different temperatures and pressures using the techniques described in previous chapters.

The infinite bed conductivities calculated for all three fuel mixtures is shown graphically in Figure 20 and listed in Table 3. An interesting aspect of the infinite bed results is that both the fine and binary fuel mixtures "cross-over" with increasing pin pressure. At low pressures, the two different fuels have a lower thermal conductivity at higher temperature. However, as pressure increases, the higher temperature conductivity crosses over the lower temperature conductivity. The calculations with only large spheres present does not exhibit this type of response at all. Rather, the conductivity has a higher value at higher temperatures for all pressures.

In large part, this is due to the sizes of the gas
Figure 20. Calculated Infinite Bed Thermal Conductivities of Fuel Used by Beatty
Table 3. Calculated Infinite Bed Thermal Conductivities for Fuel Used by Beatty

<table>
<thead>
<tr>
<th>Pressure (atm)</th>
<th>1</th>
<th>2</th>
<th>4</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fine Spheres (673K)</td>
<td>.834</td>
<td>.971</td>
<td>1.19</td>
<td>1.35</td>
</tr>
<tr>
<td>Fine Spheres (1073K)</td>
<td>.784</td>
<td>.918</td>
<td>1.14</td>
<td>1.36</td>
</tr>
<tr>
<td>Large Spheres (673K)</td>
<td>1.66</td>
<td>1.82</td>
<td>1.87</td>
<td>1.98</td>
</tr>
<tr>
<td>Large Spheres (1073K)</td>
<td>1.79</td>
<td>2.03</td>
<td>2.08</td>
<td>2.14</td>
</tr>
<tr>
<td>Binary Bed (673K)</td>
<td>2.41</td>
<td>2.66</td>
<td>2.85</td>
<td>2.99</td>
</tr>
<tr>
<td>Binary Bed (1073K)</td>
<td>2.36</td>
<td>2.56</td>
<td>2.88</td>
<td>3.05</td>
</tr>
</tbody>
</table>

Conductivity units are W/m°C
gaps involved. The binary and fine fuel beds have small gaps, where the molecular domain has a significant effect. For these small gaps, the conductivity is much more dependent upon pressure than for the large gaps which occur in the bed with large spheres only. For the large gaps, the continuum domain is predominant. Thus, large gaps are less dependent upon gas pressure.

Calculations for the outer boundary layer conductivity (within one sphere radius of the outer wall), are shown in Figure 21 and listed in Table 4. It should be noticed that the boundary cell exhibits cross-over as well as the unit cells. Also of interest is the fact that the boundary cells have higher conductivities than the corresponding unit cells. They also show a much higher pressure dependence than the unit cells.

The infinite bed and boundary conductivities were then used to mathematically reconstruct the results which Beatty's apparatus should have yielded. These effective conductivities were obtained by weighting the calculated values by the volume over which they applied. These effective conductivities are shown in Figure 22 and listed in Table 5. As a result of adding boundary effects, the cross-over point for the fine and binary fuel beds shifted down to lower pressures. The large spheres still showed no cross-over in conductivities.

Finally, the calculation results were compared to
Figure 21. Outer Boundary Thermal Conductivities for the Beatty System I Apparatus
Table 4. Outer Boundary Thermal Conductivities for Fuel Used by Beatty

<table>
<thead>
<tr>
<th>Pressure (atm)</th>
<th>1</th>
<th>2</th>
<th>4</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>673K</td>
<td>2.88</td>
<td>3.39</td>
<td>3.84</td>
<td>4.23</td>
</tr>
<tr>
<td>1073K</td>
<td>2.75</td>
<td>3.15</td>
<td>3.88</td>
<td>4.36</td>
</tr>
</tbody>
</table>

Conductivity units are W/m°C
Figure 22. Calculated Effective Thermal Conductivities of Fuel in Beatty's Apparatus.
Table 5. Calculated Effective Thermal Conductivities for Fuel Used in Beatty's Apparatus

<table>
<thead>
<tr>
<th>Pressure (atm)</th>
<th>1</th>
<th>2</th>
<th>4</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fine Spheres (673K)</td>
<td>.842</td>
<td>.985</td>
<td>1.21</td>
<td>1.39</td>
</tr>
<tr>
<td>Fine Spheres (1073K)</td>
<td>.791</td>
<td>.928</td>
<td>1.26</td>
<td>1.39</td>
</tr>
<tr>
<td>Large Spheres (673K)</td>
<td>1.66</td>
<td>1.82</td>
<td>1.88</td>
<td>1.99</td>
</tr>
<tr>
<td>Large Spheres (1073K)</td>
<td>1.79</td>
<td>2.02</td>
<td>2.10</td>
<td>2.16</td>
</tr>
<tr>
<td>Binary Bed (673K)</td>
<td>2.45</td>
<td>2.72</td>
<td>2.93</td>
<td>3.09</td>
</tr>
<tr>
<td>Binary Bed (1073K)</td>
<td>2.39</td>
<td>2.61</td>
<td>2.96</td>
<td>3.16</td>
</tr>
</tbody>
</table>

Conductivity units are W/m °C
the results Beatty obtained in Figure 23, with some of Ades' results as well (corrected for cell orientation). As can be seen, the fine and large sphere only results tend to agree rather well with Beatty's measurements. On the other hand, the binary mixture, while having approximately the proper magnitude, has much less of a pressure dependence than Beatty's measurements.

The primary difference between the binary bed and the fine sphere bed is the large gas gap where no fine spheres may penetrate between two large spheres. Other than this gap, the gap sizes between spheres (and their related pressure dependence) is the same for both fuel mixtures. This, in itself, has brought Beatty's binary measurements into question. Because of the similarities in gap size, the pressure dependence of standard EIR fuel is expected to be roughly the same for binary and fine fuel spheres. This would be in line with the calculational results.
Figure 23. Comparison of Beatty's Results with Calculations from the Unit Cell
Chapter VI
Thermal Conductivity Calculations for AC3 Pins

An experiment is planned in which sphere pac fuel pins, produced by EIR will be placed in a test assembly and irradiated in the Fast Flux Test Facility (FFTF). The test assembly is designated AC3, hence the name. A major effort is under way to try to predict the behavior of the pin prior to its irradiation. This pin was analyzed for packing factor values by the method described in Chapter II. These calculations are detailed in Appendix E. A summary of parameters of the AC3 pin is included in Table 6.

With the packing factor parameters, unit and boundary cells were developed to try to determine the effective thermal conductivity of the AC3 pin. The results of these calculations is shown in Figures 24 and 25, and listed in Tables 7 and 8.

AC3 pin conductivities differ from Beatty's experimental conductivities primarily due to the use of mixed carbide fuel rather than uranium carbide. Also, the porosity of the fine fraction is much lower, resulting in better conductivity in the fine spheres. It should also be noted that while the fine bed exhibits conductivity cross-over similar to calculations for uranium carbide, the binary fuel shows no signs whatsoever of cross-over. This is primarily the result
Table 6. Fuel Sphere Parameters Used in the AC3 Fuel Pin

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Size Fractions</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Large</td>
</tr>
<tr>
<td>Average Size (μm)</td>
<td>800</td>
</tr>
<tr>
<td>Fuel Porosity (%)</td>
<td>6</td>
</tr>
<tr>
<td>Fill Gas</td>
<td>He</td>
</tr>
<tr>
<td>Pin Diameter (mm)</td>
<td>8.38</td>
</tr>
</tbody>
</table>
Figure 24. Infinite Bed Thermal Conductivities for the AC3 Fuel Pin
Figure 25. Boundary Value Thermal Conductivities for the AC3 Fuel Pin
Table 7. Infinite Bed Thermal Conductivities for the AC3 Fuel Pin

<table>
<thead>
<tr>
<th>Pressure (atm)</th>
<th>1</th>
<th>2</th>
<th>4</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fine Spheres (673K)</td>
<td>0.856</td>
<td>0.994</td>
<td>1.21</td>
<td>1.38</td>
</tr>
<tr>
<td>Fine Spheres (1173K)</td>
<td>0.873</td>
<td>1.01</td>
<td>1.25</td>
<td>1.50</td>
</tr>
<tr>
<td>Fine Spheres (1673K)</td>
<td>0.889</td>
<td>0.997</td>
<td>1.16</td>
<td>1.60</td>
</tr>
<tr>
<td>Binary Bed (673K)</td>
<td>2.10</td>
<td>2.29</td>
<td>2.43</td>
<td>2.53</td>
</tr>
<tr>
<td>Binary Bed (1173K)</td>
<td>2.29</td>
<td>2.45</td>
<td>2.72</td>
<td>2.88</td>
</tr>
<tr>
<td>Binary Bed (1673K)</td>
<td>2.43</td>
<td>2.58</td>
<td>2.82</td>
<td>3.14</td>
</tr>
</tbody>
</table>

Conductivity units are W/m °C
Table 8. Boundary Value Thermal Conductivities for the AC3 Fuel Pin

<table>
<thead>
<tr>
<th>Temperature</th>
<th>1</th>
<th>2</th>
<th>4</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>673K</td>
<td>2.69</td>
<td>3.16</td>
<td>3.58</td>
<td>3.93</td>
</tr>
<tr>
<td>1173K</td>
<td>2.80</td>
<td>3.17</td>
<td>3.87</td>
<td>4.40</td>
</tr>
<tr>
<td>1673K</td>
<td>2.87</td>
<td>3.19</td>
<td>3.74</td>
<td>4.66</td>
</tr>
</tbody>
</table>

Conductivity units are W/m°C
of the differing temperature dependence of mixed carbides and pure uranium carbide.
Chapter VII
Model Extensions and Recommendations

As shown earlier, the model presented gives a reasonable estimate for the thermal conductivity of unrestructured, two-size fraction, sphere pac fuel. However, the central portions of a fuel pin reach high temperatures which cause the spheres to sinter together. This restructuring falls outside the applicability of the model. In addition, a form of sphere pac fuel with 3 size fractions of uranium dioxide is being manufactured for light water reactors. The differences in sphere packing with 3 sizes requires a different approach for the same general model to be applicable. These model extensions are discussed below, in turn.

VII.1 Modeling of 3-size Fraction Fuel

The dimensions of the spheres used in 3-size fuel are of the same order of magnitude as 2-size fuel, but differ greatly due to the inclusion of a medium size fraction. The parameters of the fuel are given in Table 9. The medium size fraction also requires a different method of manufacturing.

Two size EIR sphere pac is loaded in two phases. First, the large spheres are poured into the cladding tube. The large spheres are then compacted by vibrating the tube for long periods of time. When the vibrating is complete, the large spheres are in approximately their
Table 9. Fuel Sphere Parameters Used in 3-size Fraction Fuel

Fuel: UO₂

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Large</th>
<th>Medium</th>
<th>Fine</th>
</tr>
</thead>
<tbody>
<tr>
<td>Average Size (µm)</td>
<td>1300</td>
<td>300</td>
<td>35</td>
</tr>
<tr>
<td>Porosity (%)</td>
<td>1.4</td>
<td>0.7</td>
<td>1.4</td>
</tr>
<tr>
<td>Packing Fraction</td>
<td>0.509</td>
<td>0.356</td>
<td>0.394</td>
</tr>
<tr>
<td>Smear Density of Packed Bed</td>
<td></td>
<td></td>
<td>.866</td>
</tr>
<tr>
<td>Fill Gas</td>
<td></td>
<td></td>
<td>Helium</td>
</tr>
</tbody>
</table>


most stable configuration. A perforated clamp is then placed on the top of the packed bed so that the bed will not expand in further manufacturing steps. At this point, a portion of the fine fraction is poured through the clamp and into the bed. The pin is then vibrated to shake the fine fraction down through the voids between the large spheres. This process is repeated until no more fine spheres will penetrate into the bed. The pin is then sealed and is ready for use after inspection.

The fine spheres are able to infiltrate between the large spheres because of the ratio of the diameters of the fine and large spheres is small. This infiltration is not possible with the 3-size fuel. As such, all 3 sizes are loaded into a fuel pin at once using a specially designed mixing-loading tool. As a result of the differences in loading the pin with spheres, assumptions made for EIR fuel are not valid for 3-size fuel. The principal assumption which is invalidated is that the fine fraction has no effect on the packing of the large spheres and can thus be homogenized. In 3-size fuel, only the smallest fraction can be homogenized. The large and medium size spheres should require separate unit cells for each contact configuration, namely L-L, L-M, and M-M.

Unfortunately, the dimensions of these cells requires information regarding the coordination number between spheres. All previous work on the coordination
of spheres in random packed beds is in regard to packing of a single size sphere. This information, however, could be derived from the mathematical packed beds which Henke(14) developed. One capability of his RANDPAC computer code is the generation of a packed bed of two-size spheres. However, due to computational expense, the length of the packed beds is necessarily small. Not only could such beds be analyzed to determine the necessary coordination number data, but they could also be used to look for neighboring spheres which are not quite in contact. This information could be used to determine the significance of heat flow across these gaps to the effective thermal conductivity of the bed.

Because of the nature of the packing of the 3-size fuel, it is also not possible to say precisely what effect the clad boundary has on the packing of the spheres. While the boundary lowered the packing factor of large spheres near the wall in EIR fuel, the presence of medium sized spheres loaded simultaneously with the large spheres in 3-size fuel might have just the opposite effect. A definitive answer to this question would have to come from either pin examination or the analysis of Henke's packed beds.

VII.2 Modeling of Restructured Fuel

At the high temperatures experienced in the center of a nuclear fuel pin, the spheres quickly sinter together. The mechanisms for this were explained in
detail by Ades(4). The "necks" which grow between spheres change the mode of heat transfer. While heat in unrestructured fuel must cross a gas gap between spheres, heat in restructured fuel has a bridge of solid fuel material to cross. This greatly increases the conductivity of the bed.

A first approximation for restructured fuel could be obtained by filling in the gas gap with fuel material. While this adds material to the cell and thus increases the packing factor of the cell, the amount of material added is small and should have little effect for this approximation.

VII.3 Using Differing Fill Gas Mixtures

At the outer edges of a sphere pac fuel pin, the temperatures are not high enough to cause significant restructuring. For this reason, the outer regions of the pin retain the physical form of unrestructured fuel over the life of the pin. However, while the structure does not change, the fill gas becomes contaminated with gases resulting from fission, most notably xenon and krypton. These fission gases have not only different thermal conductivities, but should have significantly different accommodation coefficients as well. As the accommodation coefficient reflects the degree to which a gas atom comes into equilibrium with the temperature of a surface it strikes and is highly dependent upon the mass of the gas atoms, the addition of Xe and Kr will undoubtedly alter
the accommodation coefficient and the gap conductance between spheres as well.

In his work, Ades used the model of Brokaw(19) to calculate the conductivity of gases outside the Knudsen domain. The thermal conductivities inside the Knudsen domain were calculated as if each gas acted independently of the other gases. Recent work has shown that Brokaw's model cannot be applied in this manner as it is only valid for the "continuous" domain, while Knudsen's law handles the "molecular" domain (24).

A formulation which was developed for FILOS calculations and could be used is:

\[ k_{\text{gap}} = \frac{1}{k_{\text{mix}}} + \frac{2}{d \cdot n \sum \frac{k_i}{g_i}} \]  \hspace{1cm} (VII-1)

where \( k_{\text{mix}} \) = conductivity of the mixture (e.g. according to Brokaw)

\( k_i \) = conductivity of each gas

\( d \) = gap width

\( g_i \) = temperature jump distance

\( n \) = number of gas components

This model would certainly be applicable to the unit cell for unrestructured fuel developed in Chapter 3. This should also be applicable for gas mixtures (95% He, 5% \( N_2 \)) which EIR has proposed for future use.
Chapter VIII

Summary and Conclusions

Previous efforts at modeling the thermal conductivity of sphere pac fuel have made simplistic assumptions regarding the packing of spheres in a fuel pin. By assuming a constant packing factor across the pin, boundary effects which become more significant for small pins, are neglected. This omission results in an underestimate of the effective thermal conductivity of the pin, and an overestimate of the fuel temperature at power. By splitting off and treating the boundary region separately, more versatility in choosing pin sizes is allowed.

While not precisely matching experimental results, calculations yielded values which were of the proper general magnitude. Calculations basically agreed with experiment, and disagreed significantly only where some doubts exist as to the validity of the experimental results.

Extensions of the model to 3-size fuel in which all sphere sizes are loaded simultaneously should wait for a better understanding of how the spheres actually pack into a fuel pin. However, extensions to model fission gas effects and restructuring should only require minor modifications.
REFERENCES


APPENDICES
Appendix A
Calculation of Cell Dimensions for Spheres Not in Contact

Unit cells for spheres which are not in contact with the top boundary are very similar to normal unit cell with spheres in contact with only slight dimensional differences. As the length of the cell is increased with the separation, the right boundary of the cell must be moved in to maintain the proper packing factor for the cell, as illustrated in Figure A1. The dimensions differ from a contacting cell by noting that $X+H=1+S$ rather than just $X+H=1$. By substituting this into Equation (III-5) and continuing the derivation, Equation (III-9) becomes:

$$H^3 - \frac{3}{2}(1+s)H^2 + \frac{2}{NP\tan\Phi} = 0$$  (A-1)
Figure A1. Dimensional Changes in the Unit Cell for Spheres not in Contact
Appendix B
Gap Conductance Relations used for COYOTE

The relations which were used to calculate the conductivities of gas gaps are taken from Garnier and Begej(18). For each pressure and temperature, the conductance for both the free molecular and continuum regimes was calculated.

The free molecular conductance is given by:

\[ H_{FM} = \frac{P}{4} \left( \frac{2R \gamma}{\gamma - 1} \right)^{1/2} \left( \frac{\gamma + 1}{\gamma - 1} \right) \frac{1}{T} \left( \frac{a}{2-a} \right) \]  

(B-1)

where \( P \) = gas pressure (Pa)
\( R \) = gas constant (8.31 J/mole-K)
\( \gamma \) = ratio of specific heats \( C_p/C_v \)
\( T \) = temperature (K)
\( a \) = accommodation coefficient (see Appendix C)

The Kennard relation is used for the continuum regime where

\[ H_g = \frac{K_{GAS}}{d + g_1 + g_2} \]  

(B-2)

\( K_{GAS} \) = thermal conductivity of the gas (W/m-K)
\( d \) = gap distance (m)
$q_i$ is the temperature jump distance and is defined by:

$$q_i = \frac{0.2174 \text{ KGAS} \sqrt{T}}{P} (\frac{2 - a}{a}) \sqrt{M}$$  \hspace{1cm} (B-3)

$M =$ molecular weight of the gas (kg/mole)

The free molecular conductance is valid for Knudsen Numbers (KN) of greater than 100, while the continuum value is valid for KN less than 0.01. For the transition region, the conductance is defined by:

$$H_{tr} = H_{fM} e^{-1/KN} + H_{g}(1 - e^{-1/KN})$$  \hspace{1cm} (B-4)

The resulting conductance is then multiplied by the gap distance to give the needed material conductivity to be used by COYOTE.
Appendix C

Estimation of the Thermal Accommodation Coefficient of Uranium Carbide and Mixed Carbide Fuel

Calculations of the gap conductance require a value for the accommodation coefficient of the gas on the fuel. Due to a lack of available experimental data, Ades(4) assumed that values for He on UC and (U,Pu)C would be similar to values for helium on UO$_2$, namely

$$\alpha = 26.5 \times 10^{-12}T^3 - 0.0834 \times 10^{-6}T^2 - 28 \times 10^{-6}T + 0.31 \quad (C-1)$$

However, the thermal accommodation coefficient is the measure of the degree to which a gas atom comes into thermal equilibrium with a wall after a collision. If the wall is composed of atoms which are quite massive in comparison to the gas atoms, then the coefficient will approach zero.

For the case of UO$_2$, there are two light atoms for every heavy uranium atom so that the coefficient is much higher than for pure uranium when using He as a fill gas. A much better approximation could be obtained by choosing a coefficient somewhere between UO$_2$ and pure uranium. As oxygen and carbon are approximately the same mass and UO$_2$ has double the light atoms of UC and (U,Pu)C, the monocarbide coefficient should be midway between values for UO$_2$ and U.
Unfortunately, no data exists for pure uranium. The heaviest element for which data exists is tungsten, with He the incident gas. The values for tungsten range from 0.015 to 0.069 with a median value of approximately 0.030 at a temperature of 250K. Some work has shown that the accommodation coefficient of monatomic gases should be inversely proportional to the mass of the wall atoms (20). The accommodation coefficient of uranium should therefore be about 77% of that of tungsten yielding a value of about 0.023 at 250K. The UO$_2$ accommodation coefficient at this temperature is 0.298. Averaging the two values and assuming the same temperature dependence for monocarbide fuel as for uranium dioxide gives an estimate that the UC and (U,Pu)C accommodation coefficient is 54% of the UO$_2$ value when helium is the incident gas. This value was used in all gap conductance calculations.
Appendix D

Material Properties Used to Calculate Gap Conductances

The following thermal conductivities were used to calculate gap conductances

UC, Reference 21

\[ K_{100} = 21.7 - 3.04 \times 10^{-3} T + 3.61 \times 10^{-6} T^2 \text{ W/m°C} \]  \hspace{1cm} (D-1)

for \( T < 700 \text{ °C} \)

and

\[ K_{100} = 20.2 + 1.48 \times 10^{-3} T \text{ W/m°C} \]  \hspace{1cm} (D-2)

for \( T > 700 \text{ °C} \)

where \( k_{100} \) = thermal conductivity of 100% theoretical density fuel

\((U_{0.85}Pu_{0.15})C\), Reference 22

\[ K_{100} = 17.5 - 5.65 \times 10^{-3} T + 8.14 \times 10^{-6} T^2 \text{ W/m°C} \]  \hspace{1cm} (D-3)

for \( T < 500 \text{ °C} \)

and

\[ K_{100} = 12.76 + 8.71 \times 10^{-3} T - 1.88 \times 10^{-6} T^2 \text{ W/m°C} \]  \hspace{1cm} (D-4)

for \( T > 500 \text{ °C} \)
He, Reference 22

\[ K = 3.366 \times 10^{-3} (T(°C) + 273.15)^{0.668} \text{ W/m°C} \]  \hspace{1cm} (D-5)

The thermal conductivity correction factor for porosity within the spheres is expressed as (23):

\[ K_p = K_{100}^{e^{-2.14P}} \]  \hspace{1cm} (D-6)

where \( P \) = porosity
Appendix E

Packing Factor Calculations for the Beatty Apparatus and the AC3 Fuel Pin

Beatty Apparatus:

Fine Sphere Diameter = 0.06 mm
Large Sphere Diameter = 0.8 mm

Fine Sphere Boundary on Large Sphere:
D/d = 800/60 = 13.33 Wall PF = .496

Fine Sphere Boundary on Heater Wall:
D/d = 10/.06 = 166.7 Wall PF = .565

Fine Sphere Boundary on Outer Cylinders:
System I: D/d = 466.7 Wall PF = .572
System II: D/d = 316.7 Wall PF = .572

Large Spheres at System I Outer Cylinder (ID=28mm):
D/d = 28/0.8 = 35 Wall PF = .540

Large Spheres at Inner Heater (OD=10mm):
D/d = 10/0.8 = 23.75 Wall PF = .492

AC3 Pin:

As the sphere sizes for the AC3 pin are the same as for the Beatty experiment, the packing factor of fine spheres next to large spheres is the same (PF=.496).

Pin Diameter = 8.38mm
Large Spheres Bordering on Clad:

\[ \frac{D}{d} = \frac{8.38}{0.8} = 10.48 \text{ Wall PF = .479} \]

Fine Spheres Bordering on Clad:

\[ \frac{D}{d} = \frac{8.38}{.06} = 139.7 \text{ Wall PF = .564} \]