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SPATIAL EFFECTS IN DANCOFF FACTOR CALCULATIONS FOR PEBBLE-BED HTRs

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ABSTRACT

A Monte-Carlo program, named INTRAPEB, is written to calculate the average value and the space-dependency of the Dancoff factor of one single fuel pebble, as well as the angular distribution of neutrons escaping from the pebble. For the Dancoff factor, the analytical results from literature agree very well with ours. However, for a cubic packing of particles, as is usually modeled in MCNP calculations, a larger Dancoff factor is found for the pebble. The angular distribution of neutrons escaping from the moderator zone of a pebble is much more forwardly peaked than the cosine angular distribution assumed in analytical methods.
A second program, named PEBDAN, is written to calculate the average value and the space dependency of the inter-pebble Dancoff factor (the probability that a neutron escaping from the fuel zone of a pebble crosses a fuel particle in another pebble) and the pebble-pebble Dancoff factor (the probability that a neutron escaping from the fuel zone of a pebble crosses the fuel zone of another pebble). In this program, the coordinates of the pebbles in a randomly packed bed are determined, after which the Dancoff factors are calculated by a Monte Carlo ray-tracing method. Compared with experiments, the radial porosity profile of the packed bed shows less pronounced peaks and a slightly larger average value. Due to the larger first-flight escape probability of neutrons, the Dancoff factors drop several tens of percents along the inner and outer reflector of the core.

KEYWORDS: Dancoff factors, Pebble-bed reactors

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1. INTRODUCTION

Dancoff factors are used in resonance shielding calculations to adjust the first-flight escape probability of a fuel lump for the probability that a neutron that escapes will enter a neighboring fuel lump without interaction in between. Many programs and subroutines exist that calculate Dancoff factors for regular or irregular lattices, see for example Refs. 1 and 2. The calculation of Dancoff factors of HTGR fuel types, both pebble-bed and prismatic types, has always been more problematic than that of LWR fuels, because of the three times smaller scattering cross section of the moderator in the resonance region. Consequently, the influence of the double or even triple heterogeneity involved in HTGR fuel types has to be accounted for in the Dancoff factor calculation.

HTGR fuel typically consists of a fuel kernel with diameter of 350 to 500 μm, covered by a porous buffer layer and a combination of pyrolytic Carbon and SiC layers. The buffer layer accommodates the gaseous fission products that escape from the fuel kernel and protects the outer coating layers from recoiling fission products. The total thickness of all the layers covering the fuel kernel is typically about 200 μm. The coated particles are embedded in a graphite matrix with either spherical shape for pebble-bed reactors or cylindrical shape for prismatic graphite block types. In pebble-bed reactors, which is the main focus of this article, the spherical fuel zone of a pebble, containing about 10-20 thousands of these coated particles, has a radius of 2.5 cm and is covered by a graphite layer with thickness of 0.5 cm. Besides these fuel pebbles, the core may contain moderator pebbles containing graphite but no coated particles, which, from a neutronics point of view, increases the effective thickness of the outer graphite shell of a fuel pebble.

The first issue addressed in this paper is the influence of the particle distribution in the fuel pebble on the Dancoff factor. In a recent paper [3], Kim *et al* found that the eigenvalues of the Next Generation Nuclear Plant (NGNP) under study at INL differ significantly for a random distribution of fuel kernels and for a regular lattice, with the latter values always being lower. They found that this discrepancy is due to an overestimation of the neutron capture rate in the main resonance absorbers by about 1%. To investigate the influence of the kernel packing on the Dancoff factor, a Monte-Carlo program was written that calculates the *intra-pebble* Dancoff factor for a random and cubic packing of particles in a fuel pebble. Besides the pebble-average Dancoff factors, this program also calculates the radial dependence of Dancoff factors, and the first-flight escape probability as well as the angular distribution of the outgoing current. Results are given in Chapter 2.

The second topic is about the calculation of space-dependent Dancoff factors for pebble-bed reactors. Because of enhanced neutron leakage, the *inter-pebble* Dancoff factor will be less at the boundary of a reactor core. For water-moderated reactors, this effect is quite small because of the small diffusion length, but for graphite-moderated reactors, the effect might be more significant. A Monte-Carlo program was written that calculates the different contributions to the Dancoff factor as a function of radius and height in a cylindrical reactor core (although the latter is not a limitation of the ray-tracing method and other geometries could be easily programmed as well). Results are given in Chapter 3. The article's conclusions are given in Chapter 4.

2. INTRAPEBBLE DANCOFF FACTOR

To investigate the effect of the kernel packing on the Dancoff factor, a Monte Carlo program, named INTRAPEB, was written that calculates the intra-pebble Dancoff factor (the probability that a neutron escaping from a fuel kernel in a pebble crosses another fuel particle in the same pebble), the distribution of distances traveled by neutrons until their first intersection with another fuel kernel, the first-flight escape probability, and the angular distribution of the escaping neutrons. In this program, the kernels are positioned either in a cubic lattice, or in a random lattice. The latter is done for each particle by drawing a random position, and checking whether there is no overlap with any other particle (kernel with surrounding coatings). After positioning all particles, a kernel is selected randomly, as well as the position and angular distribution of the emerging neutron. The distances between this escape position and all other particles traversed by the ray are calculated to obtain the first intersection of the ray with a fuel kernel. This process is repeated many times (typically between 100,000 and 1,000,000) to obtain statistically small errors for the Dancoff factor. If there is no fuel kernel intersection, the neutron, corrected for the probability that it might have had a collision with a moderator nucleus, contributes to the first-flight escape probability. In this way, the the intra-pebble Dancoff factors are calculated with a relative standard deviation <<1%. Besides the Monte-Carlo based Dancoff factors, INTRAPEB also calculates the intra-pebble Dancoff factor based on the methods of Bende [4] and Lane [5].

In Fig. 1, we show the intra-pebble Dancoff factor as a function of the kernel density in a standard pebble with fuel zone radius of 2.5 cm for kernel radii of 100 and 250 μm. The difference between the two plots is the number of particles in the cubic lattice geometry. The left plot shows the Dancoff factor as a function of the number of coated particles that fit completely in the fuel zone of the pebble (and for which the calculations have been done), while the right plot shows the Dancoff factor as a function of the total number of particles including the ones that are partly cut by the outer boundary of the fuel zone. Because the latter number is larger then the first, the dotted line in the right plot is a shifted copy of the line in the left plot. Which plot to use depends on where the results need to be compared with. Clearly the cubic lattice gives intra-pebble Dancoff factors significantly higher than the stochastic lattice. However, the total Dancoff factor is composed of the intra-pebble and inter-pebble Dancoff factors, and, as we will see later on, a larger intra-pebble Dancoff factor gives a lower fraction of neutrons that escape from the pebble, and thus a smaller contribution to the inter-pebble Dancoff factor. Whether the total Dancoff factor is larger for the cubic lattice or not cannot be clearly concluded from these results.

Because no definite conclusions can be drawn from Fig. 1 about the total Dancoff factor in a cubic lattice, it is difficult to compare with literature. In Ref. 3, it was found that the eigenvalue of the Next Generation Nuclear Plant is consistently lower for a regular packing of fuel particles due to increased resonance absorption. This would correspond to a lower Dancoff factor for a cubic lattice.

In Ref. 4, Monte Carlo calculations with MCNP for kernels with a radius of 100 μm gave consistently lower Dancoff factors too. This was attributed to channel ray effects that would enhance neutron leakage. Although these channel ray effects might exist for scattered neutrons,

they could not be confirmed for the unscattered neutrons that make up the contribution to the intra-pebble Dancoff factor. Our calculations showed that in a cubic lattice, relatively many neutrons, much more than in a stochastic lattice, intersect the nearest kernels, which results in a relatively high value for the intra-pebble Dancoff factor (see Fig. 2). Furthermore, for kernels with a radius of 250 μm, the first-flight escape probability in a cubic lattice is lower than in a random lattice for all particle densities considered here. The differences increase with particle density, and range from 2% at 5,000 particles per pebble, to 6% at 40,000 particles). In contradiction to previously mentioned literature, Ref. 6 reports a higher eigenvalue for a cubic packing of kernels. Clearly, this issue needs some more research.

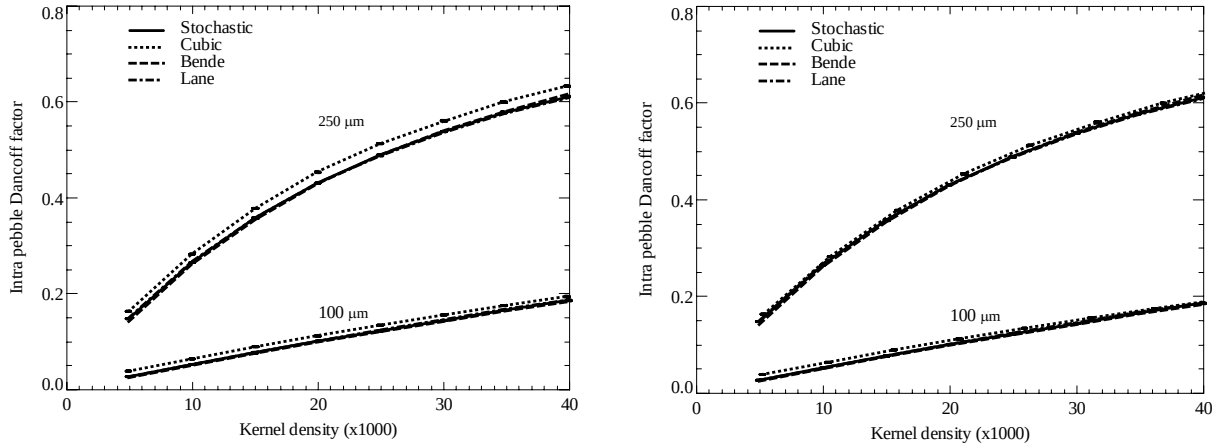

Figure 1: Intra-pebble Dancoff factors as a function of the number of kernels in a standard fuel pebble with radius of 2.5 cm with the kernel radius as a parameter. The left curve shows the Dancoff factor as function of the number of coated particles that fit completely in the fuel zone, while the right plot is the Dancoff factor as a function of the total number of particles including all fractions cut by the outer boundary of the fuel zone. The standard deviations in the results are much less then 1%.

In Fig. 3, the intra-pebble Dancoff factor is shown for a single pebble as a function of the radial position in the fuel zone of the pebble, together with the first-flight escape probability. Clearly both parameters depend strongly on the position in the pebble. For the 15,000 and 30,000 particle cases, the average values of the Dancoff factor reach 0.358 and 0.540, respectively, which agree within 1 percent with the method of Bende *et al* [4]. The neutrons that escape from the pebble contribute partly to the *inter-pebble* Dancoff factor, which means that the total Dancoff factor (the sum of the intra- and inter-pebble contributions) shows a less pronounced dependency on position (see Figs. 10 and 11 in Ref. 4).

In Fig. 4, we show the angular distribution of neutrons escaping from the pebble without any interaction and without crossing another fuel kernel. For the boundary between the fuel zone and the moderator layer, the cosine distribution seems a reasonable assumption, but the angular distribution at the outer boundary of the moderator layer is much more forwardly peaked. This means that the white boundary condition assumed in the calculation of transmission probabilities for the analytical Dancoff factor calculation methods (see Ref. 4) is not fully valid.

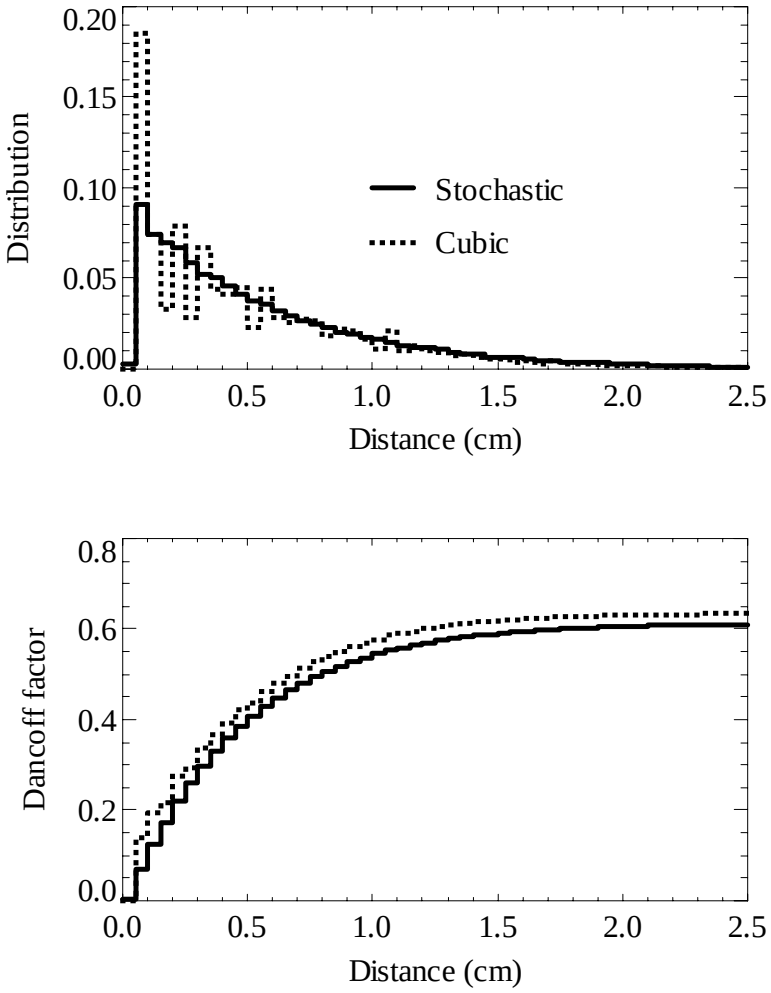

Figure 2: Distribution of the distances traveled by neutrons until their first intersection with another fuel kernel (upper plot), and the cumulative Dancoff factor. In a cubic lattice, neutrons have a large probability to hit one of the nearest neighbors, which results in a relatively large contribution to the Dancoff factor. This is for quite an extreme case, with a particle density of 40,000 per standard fuel pebble, and a fuel kernel radius of 250 μm.

3. SPATIALLY DEPENDENT DANCOFF FACTORS

The results presented in the previous section clearly indicate that the intra-pebble Dancoff factor depends on the radial position in the fuel zone of a pebble. In practice it will be very difficult to account for this effect, as it would require dividing the pebbles in the core in radial zones and performing cross section treatment for each zone. However, a similar effect can be expected for the inter-pebble Dancoff factor, as neutrons originating near the boundary of the reactor core have a larger escape probability than other neutrons. Dividing the core in regions with different cross section sets is common practice, and one could provide each region with its own Dancoff factor. This would especially be useful for those resonance shielding codes that account for the

intra-pebble Dancoff factor (or equivalent treatment) themselves and that only need the inter-pebble Dancoff factors or the pebble-pebble Dancoff factors to be given in the input (the pebble-pebble Dancoff factor is defined as the probability that a neutron escaping from the fuel zone of a pebble enters another fuel zone). This is the case for the MICROX-2 code [7] in use at the INL.

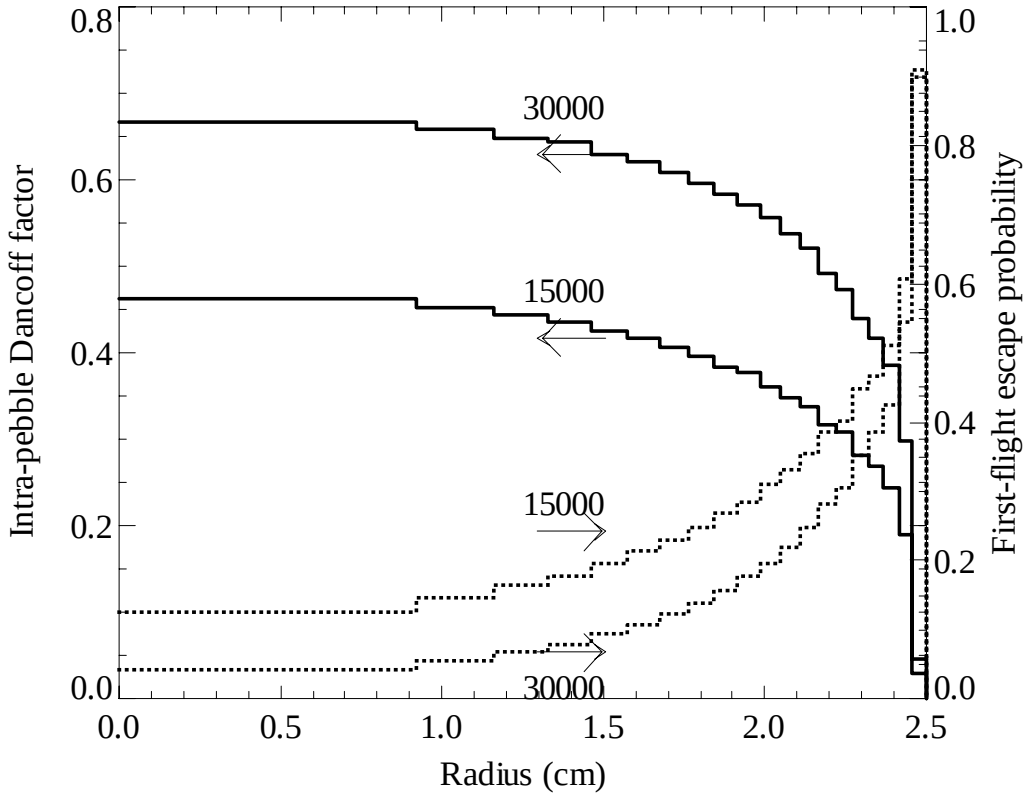

Figure 3: Intra-pebble Dancoff factor and first-flight escape probability as a function of the position in a pebble with the number of kernels as a parameter (15,000 or 30,000 fuel kernels per pebble with fuel zone radius of 2.5 cm).

A program, named PEBDAN, is written that calculates the spatially dependent Dancoff factors in a cylindrical core with outer and inner reflectors. The problem tackled in this code can be subdivided in two parts: 1) Generation of the coordinates of randomly stacked pebbles in the core volume and 2) the calculation of Dancoff factors proper.

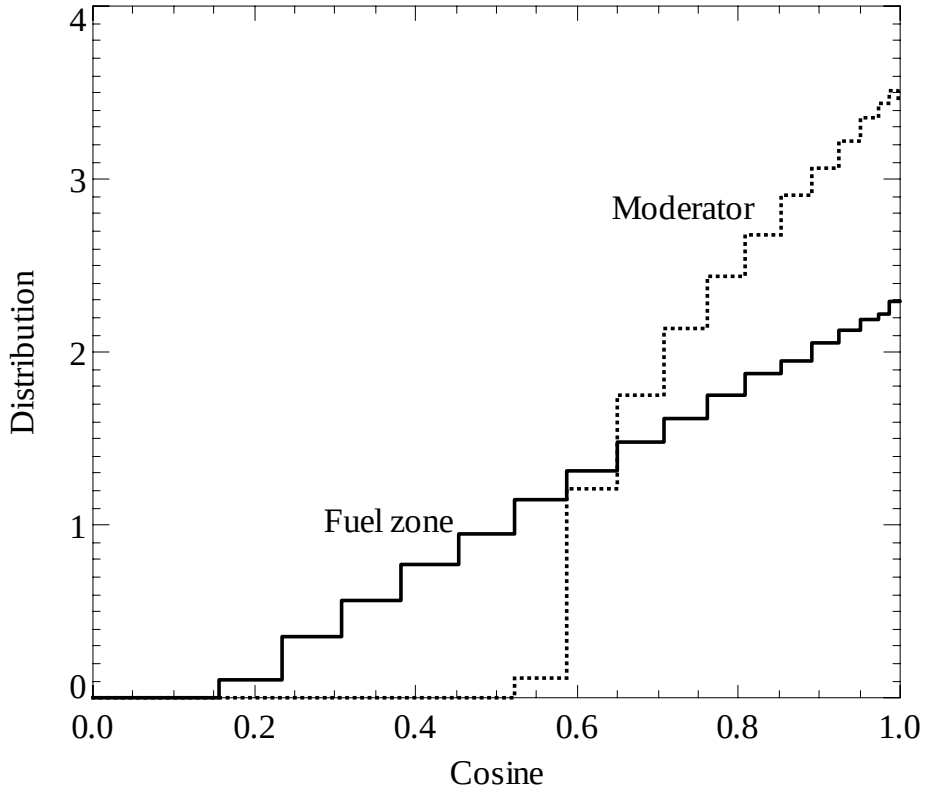

Figure 4: The angular distribution (neutrons per unit cosine) escaping from the pebble without interaction with a moderator nuclide and without crossing another fuel kernel. This figure is for a standard pebble (radii 2.5 and 3.0 cm for the fuel zone and moderator) containing 15,000 kernels with a radius of 250 μm, but the results for 30,000 kernels are very similar.

3.1. Generation of Randomly Packed Pebble Coordinates

The literature on the first problem can be subdivided in two approaches. One is to use rigorous algorithms that simulate pebble flow as accurate as possible based on physics laws [8-10]. The other approach is based on synthetic techniques [10-12], such as a rain model in which a pebble is randomly dropped in the vessel until it reaches another pebble, after which a Monte Carlo shaking routine is used to increase the packing fraction of the bed. The first method is expected to give realistic packing fractions and porosity profiles, while the second class of methods may not.

This paper presents a new method, developed and employed at the INL that belongs to the second class. First a large collection of random points is generated, about 100,000 times the number of pebbles that fit into the vessel. Then, starting at the bottom of the vessel, each random point is checked as to whether it is suitable as a pebble center coordinate. If a pebble at that

coordinate would overlap with any other pebble or structure in the core, it is rejected; otherwise it is accepted, and a pebble is located at that position. Besides some problems that need to be avoided, such as integer overflows, this algorithm is extremely simple to program. Furthermore, overlap of pebbles is easily avoided, whereas for the rigorous methods this is much more difficult. For example, in a packed bed of 5-cm pebbles within a nuclear reactor, it is reported [9] that the average overlap for the rigorous method is 1% with a maximum of 20%. However, as may be expected from the discussion above, no physics are simulated in our model and the resultant pebble-bed packing does not necessarily reflect all characteristics of a real packed bed. Nevertheless, this method was incorporated into the PEBDAN code.

Some results are shown in Fig. 5, which displays a comparison with experiments performed by Benenati and Brosilow [13] in the early sixties. Although the calculations reflect the main trends in radial porosity, there are a few remarkable differences. First of all, the peaks in the calculated porosity profile are not as pronounced as in the measurements. Second, in the calculations, the porosity profile reaches its average value already after two oscillations, while in the measurements; at least four oscillations are clearly visible. Thirdly, the average porosity in the calculations (0.40) seems to be larger than the experimental value (0.38). In the algorithm, the density of the packed bed can be increased by generating more random points or by allowing a small overlap between pebbles (as is usual the case in algorithms of the first kind [9]). The first option is not very practical, as more random points deteriorate the simplicity and performance of the algorithm, while the second option is unrealistic. Since completion of the PEBDAN code, co-workers at INL have developed an enhanced version of the rigorous method that produces the correct packing fraction and boundary density fluctuations while suffering very little overlap (of the order of microns at pebble surfaces). This latter method is being verified and corrected for an overly simple treatment of friction between pebbles before incorporation into PEBDAN [14]. Despite some shortcomings in our current model, the results were used to calculate Dancoff factors for the 600 MW Next Generation Nuclear Plant in development at INL.

3.2. Calculation of Dancoff factors

Once the pebble coordinates are known, Dancoff factors are calculated by PEBDAN using a ray-tracing method. First a starting coordinate is uniformly sampled in an arbitrary fuel pebble in the core (the core can also contain moderator pebbles, but these are discarded as starting points for the ray-tracing method). Subsequently, a direction is uniformly sampled, and the contribution to the *intra-pebble* Dancoff factor is determined by calculating the probability that the neutron will interact with a fuel kernel in the same pebble. This is done using Lane's method [5]. Subsequently, all pebbles that the ray intersects are stored and ordered with ascending distances to the starting pebble. During the ray tracing, each trajectory through a pebble (either through the moderator zone or through the fuel zone) reduces the weight of the neutron, while each trajectory through the fuel zone of a pebble contributes to the *inter-pebble* Dancoff factor (again using Lane's method [5]). The intra-pebble Dancoff factor should not depend on the starting position in the core, and should virtually be equal to that calculated with Bende's method [4], while the inter-pebble Dancoff factor will depend on position, as neutrons originating in pebbles in the outer regions of the core experience a large escape probability.

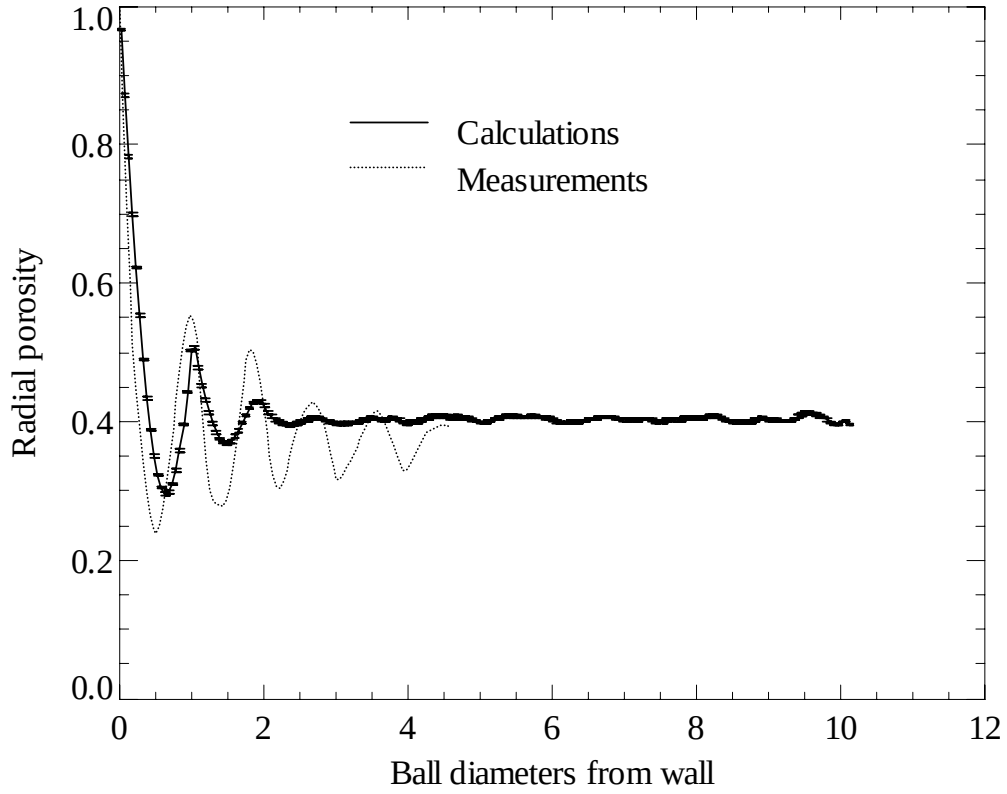

Figure 5: Measured and calculated radial porosity profiles in a cylinder with radius 10.15 times the pebble diameter (0.080 inch). The measurements were read from a plot in literature [12, case 2] and interpolated with a spline fit to get a smooth curve.

Besides the intra- and inter-pebble Dancoff factor, the pebble-pebble Dancoff factor is also calculated. The pebble-pebble Dancoff factor is defined as the probability for a neutron that leaves the fuel zone of a pebble to enter another fuel zone without any interaction in between. Actually, it is this Dancoff factor that is used at INL.

In Fig. 6, we show the pebble-pebble Dancoff factor as a function of height and radial position in the packed bed of the Next Generation Nuclear Reactor under development at INL. Clearly the Dancoff factor to be input to the MICROX-2 code decreases several tens of percents along the boundaries of the reactor core. The center values (≈0.46) are slightly larger than the average value according to Bende's model (0.4436), which could be due to the more forwardly peaked (non-cosine) angular distribution of the neutron current at the outer boundary of the moderator shell of the fuel pebbles (see Fig. 4). In total, the volume fraction along the boundaries having a significantly lower Dancoff factor equals about 15%. The influence of this effect on the eigenvalue of the system is something to be investigated in the future.

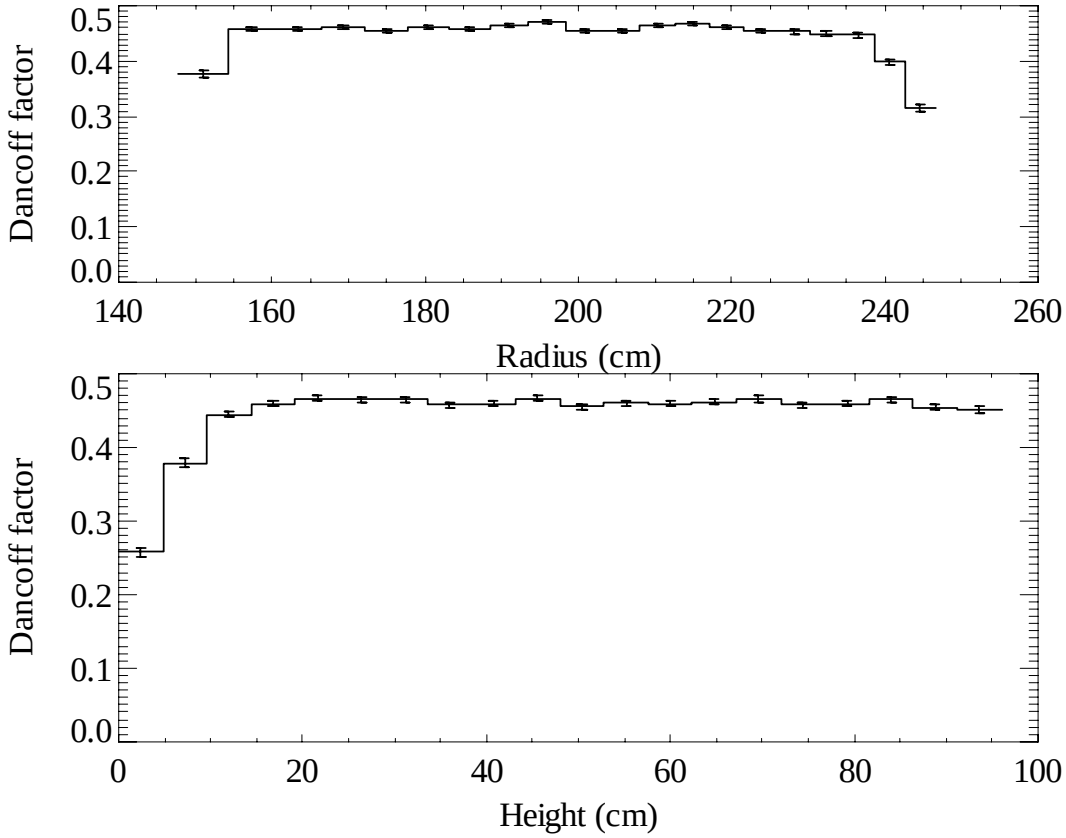

Figure 6: Pebble-Pebble Dancoff factor for the NGNP as a function of radial position (top figure) and height (with a reflective boundary at 96 cm from the bottom). The radial inner reflector has a radius of 147.8 cm, while the outer reflector starts at 246.6 cm.

4. CONCLUSIONS

The intra-pebble Dancoff factor for a single pebble is calculated by a Monte Carlo program named INTRAPEB. The resultant Dancoff factor depends strongly on the radial position in the pebble; it decreases sharply towards the edge of the pebble, while the first-flight escape probability shows the opposite tendency. The Dancoff factor for an isolated pebble with a cubic kernel packing arrangement is several percents larger than for the same pebble with a stochastic packing of kernels. The angular distribution at the boundary between the fuel zone and the moderator zone is very similar to a cosine distribution, while at the outer boundary of the moderator shell, the angular distribution is much more forwardly peaked. This means that the assumption of a cosine angular distribution that is usually applied in analytical methods is not valid at the outer boundary of the pebble.

A program named PEBDAN is written that calculates the pebble coordinates in a stochastically packed bed and the pebble-pebble Dancoff factor as a function of the radial and axial positions in

the reactor core. Along the radial and axial boundaries, this Dancoff factor decreases several tens of percents due to enhanced neutron leakage.

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