Particle Packing Considerations for Pebble Bed Fuel Systems

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This paper provides an insight into modelling the heterogeneity in pebble bed fuel systems and its effect on k-effective.

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1. Introduction

The current development of pebble bed fuel system designs poses many challenges in the computational field. The calculation of k-effective is no exception and many existing methods do not readily lend themselves to accurate modelling of the neutronic behaviour essential for criticality safety. In particular, the fuel geometry is unlike that of most existing power plants and the extent to which the detail of the pebble bed designs can be approximated needs careful consideration. As part of an on-going programme of work, the computer codes WIMS¹ and MONK² have been applied to pebble bed type systems. This paper reports the work performed to date.

2. Background

As part of an international benchmarking programme, the WIMS code is being used to model the fuel management processes in a multi-pass Pebble Bed Modular Reactor (PBMR). WIMS comprises a suite of modules that enable it to model a wide range of reactor types using 2D and 3D deterministic methods, and 3D Monte Carlo methods. These methods can be used in WIMS to model the depletion in the fuel in the PBMR, and enable a detailed fuel management strategy to be developed.

To verify a subset of the data produced by WIMS and with a view towards criticality safety applications, the Monte Carlo criticality code MONK has been used to model explicitly the PBMR geometry. MONK is a well-established criticality tool with a proven track record of application covering the whole of the nuclear fuel cycle, and is ideally suited to modelling geometrically complex systems. The modelling of multi-pass PBMR fuel also requires the code to represent the varying fuel compositions depending on the burn-up of the pebble. A typical system modelled would comprise nearly 500,000 pebbles (with a packing fraction of ~0.6), with each fuel pebble containing 15,000 multi-layered coated particles of fuel in a carbon matrix.

During the process of benchmarking WIMS, several different arrangements for packing

arrangements for the fuel were used. Initially calculations made use of an existing model that employed a very simple pebble packing method to give some indicative values for k-effective. Reference calculations were then attempted by modelling the system as accurately as possible using the full capabilities of MONK. These two results were sufficiently different that they initiated an investigation into the effect of the packing method used on the calculated k-effective.

3. Modelling the Pebble Bed Geometry

For investigating each of the packing methods, use was made of the MONK 'hole geometry' algorithm³). This well-established method is very well suited to modelling complex geometry that is either impractical or prohibitively time-consuming to model by more conventional solid body algorithms. The production version of MONK has two hole algorithms applicable to pebble bed systems. A new development version of the code includes a recently developed third option, written especially for the PBMR.



Fig. 1 A T-Hole showing the spheres cut by the container.

The first algorithm in MONK, the T-Hole (Figure 1), models the pebbles as a regular array of spheres all of the same radius, and has many streaming paths due to the regularity of the array. This is not a problem for many applications such as compacted waste systems

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or fuel dissolution but can lead to an under-estimate of k-effective for systems with no interstitial moderator.



Fig. 2 A Random hole showing some of the spheres cut by the container.

The second algorithm, the Random Hole (Figure 2), avoids much of the regularity of the T-Hole and allows for a distribution of spherical radii. This hole has been used successfully for waste systems, fuel dissolution and low-density moderation effects but still possesses some streaming paths. In addition, both the T-Hole and the RANDOM Hole cut any spheres that intersect the containing body (for example, the cylindrical container of a PBMR core) - this is a clear lack of modelling realism that may be significant in reactor applications.



Fig. 3 PBMR hole packing spheres into a reactor core.

A third algorithm, the new PBMR Hole (Figure 3), seeks to pack spheres randomly into a container body. Four different algorithms are available to provide a choice of internal packing arrangements and avoid the streaming paths that limit the application of the other hole types. In addition, for the PBMR Hole only, complete spheres are modelled throughout (i.e. no cutback by the container), with the additional option to place several different sphere types within a series of radial zones.



Fig. 4 A fuel grain defined using the PEBBLE hole.



Fig. 5 A pebble defined using the PEBBLE hole.

To augment the PBMR hole, a further hole geometry (the PEBBLE hole, Figures 4 and 5) was developed to model explicitly a pebble and the ~15,000 multi-layered fuel grains found within. This hole also provides for modelling the graphite moderator pebbles used within the PBMR.

Unlike many reactor systems where the geometry, moderator and fuel location are well defined, it is not possible to identify the location and type of all the pebbles in a PBMR. However, the new PBMR hole models those data that are available, such as the packing fraction and the relative proportion of pebble types in various radial zones within the core. Changing a random number seed allows the arrangement of a particular method to be varied between runs, and this feature is used during the later analyses to investigate the effect of random fluctuations of the system geometry.

4. Calculations

The new PBMR hole in MONK was used to model a cylinder 3.7m in diameter and of infinite height. Within the cylinder was a mixture of graphite pebbles and fuel pebbles, the latter containing the fuel grains. These were assigned to four radial zones to model a typical mixture of pebble types in a PBMR. The interstitial material was Helium-4 with traces of Helium-3.

The PBMR hole provides access to four packing methods that evolved during the development process, each aimed at achieving both the selected packing fraction and the correct quantity of fuel:

- Mode 0 close packed hexagonal lattice with tetrahedral groups of four replaced by a single pebble (Figure 6)
- Mode 1 regular packed hexagonal with a separation chosen to give the required packing fraction (similar to the T-Hole, but models complete spheres)
- Mode 2 regular hexagonal, close packed axially, radial separation chosen to achieve packing fraction (Figure 7)
- Mode 3 layers of hexagonal arrays in XY, successive layers randomly oriented and dropped into spaces in previous layers (considered the best packing method of the four, Figures 8, 9 and 10)



Fig. 6 Mode 0 packing.



Fig. 7 Mode 2 packing.



Fig. 8 Mode 3 packing - overview



Fig. 9 Mode 3 packing – sphere relocation



Fig. 10 Mode 3 packing – a VISAGE slice

Each of the calculations was run five times to check the consistency of the results, with the average of the five results being used in the final comparison. The superhistory tracking method was used (ten generations per superhistory) to aid rapid source convergence.

5. Results

The results for each of the calculations, run to a standard deviation of 0.0012, are given in Table 1, and the corresponding leakage (% of total samples tracked) in Table 2.

 Table 1
 MONK k-effective results for each of the
four modes

Mode	0	1	2	3
Run				
1	1.0973	1.1119	1.1097	1.1056
2	1.1007	1.1110	1.1119	1.1060
3	1.0996	1.1109	1.1115	1.1070
4	1.0946	1.1106	1.1123	1.1074
5	1.0941	1.1102	1.1097	1.1041
Mean	1.0973	1.1109	1.1110	1.1060
Stdv	0.0026	0.0006	0.0011	0.0012

Mode	0	1	2	3
Run				
1	26.77	25.78	25.83	26.10
2	26.50	25.69	25.73	26.04
3	26.52	25.74	25.72	26.03
4	26.80	25.76	25.73	26.04
5	26.95	25.86	25.88	26.19
Mean	26.71	25.77	25.78	26.08
Stdv	0.17	0.06	0.06	0.06

Table 2MONK leakage for each of the four modes.Mode0123

The standard deviations (Stdv) given in Tables 1 and 2 are derived using the k-effective and leakage from each set of five runs. A comparison of the standard deviation derived from this small sample with the corresponding MONK values shows consistent behaviour with the possible exception of mode 0.

Inspection of the MONK output files shows a consistent number of pebbles used in each calculation, and no warning messages associated the sampling of the system. The sampling guidance from each case, and the broadly consistent k-effective values for each mode in Table 1 suggest that the calculations converged successfully, and continued to maintain the appropriate source distribution.

We can account for all the material in the problem and, by using other utilities supplied with MONK, demonstrate for all the cases both that the correct packing fraction has been achieved and that the correct distribution of pebbles in each zone has been modelled.

6. Investigation

The MONK calculations show a variation in keffective with packing method of about seven standard deviations between the extremes, well outside the normally accepted limits of two or even three standard deviations. This disparity is intriguing given that these models do not make use of the approximations typical in modelling these systems, such as smearing materials or cutting pebbles. The variation in leakage is consistent with the changes seen in k-effective and perhaps its behaviour gives some indication of the effect the various packing arrangements are having.

One obvious difference between each arrangement is in the number of streaming paths. The T-Hole method (mode 1) is known to have many streaming paths, while mode 3 is expected to have the least. The presence of streaming paths has effects on several processes such as leakage and self-shielding. An early hypothesis was that these streaming paths enabled samples to migrate further within the system, but one consequence of this would be increased leakage whereas the opposite is seen. There was also the problem of how a sample would enter a streaming path and travel along it when there are no pebbles placed to inject such samples: the likelihood of appropriate collisions in the helium or near the edge of a pebble is small.

A further hypothesis is that the more regular an arrangement, the more likely any sample is to interact with pebbles along its path before it can leak from the We can see some evidence of this by system. comparing modes 0 and 1. Mode 1 is similar to the T-Hole where the arrangement of pebbles displays great regularity in all three dimensions and as a consequence has many streaming paths. Mode 0 is like mode 1, but has randomly selected tetrahedral groups of four pebbles replaced by a single centrally placed pebble. This replacement pebble now lies at the point where many streaming paths meet, and its role could be considered as a blockage to many of the streaming paths. Looking at the results, the lowest leakage is seen with mode 1, and the highest with mode 0, possibly suggesting that the new pebble injects samples down the all streaming paths rather than blocks them. In mode 1 there were no pebbles placed which could send a particle directly down a streaming path, in mode 0 such pebbles exist. With this in mind and looking at modes 2 and 3: mode 2 has many streaming paths, but few pebbles in streaming paths; mode 3 is irregular, with few streaming paths and few rows of pebbles. The hypothesis would suggest that mode 2 has a low leakage and high keffective, while mode 3 is the opposite - this is exactly what is observed.

Although this cannot be viewed as definitive proof of a particular hypothesis, it does give an indication of the subtle effects that come into play when modelling such complex systems.

7. Conclusion

The results obtained using the new pebble bed modelling capability in MONK have provided some evidence that the way spheres are packed can affect the final value of k-effective. This suggests that when modelling such systems the modeller needs to represent sensibly the arrangement of the spheres, not simply achieve the correct packing fraction. It is probable that this same effect occurs in other systems where many spheres, or particles, are being modelled. However, the magnitude of the effect is likely to be system dependent: at least a function of both the packing fraction and the materials used. Further studies would be needed to identify under what conditions the effect becomes significant for a variety of packing methods and packing fractions.

The paper has also demonstrated the new sophisticated modelling options available in MONK for pebble bed systems, and the subtle effects they can highlight. It is considered that these methods, as well as having direct applications value, will also be very useful for benchmarking simpler deterministic methods.

Further investigation is now in progress with a

view to finalising this development so that it will form part of the next major release of MONK.

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