THE DEVELOPMENT OF MODERN DESIGN AND REFERENCE CORE NEUTRONICS METHODS FOR THE PBMR.

T D NEWTON

Serco Assurance
Winfrith Technology Centre
Dorchester
Dorset DT2 8ZE
United Kingdom
Tel +44 (0)1305 202061
Fax +44 (0)1305 202194
Tim.Newton@sercoassurance.com

ABSTRACT

The Pebble Bed Modular Reactor (PBMR) introduces several challenges for core neutronic methods. The particulate fuel is highly heterogeneous with a random distribution within the fuel pebbles and requires unique methods to calculate the effects of fuel resonance self shielding. In addition, the flow of fuel through the core is specific to the PBMR, again requiring specialised methods to model refuelling. This paper describes developments to the ANSWERS core neutronics codes to treat the specific heterogeneity and fuel cycle features of the PBMR. ANSWERS provides both a reference calculational route, provided by the MONK Monte Carlo code (Reference 1), and a fast deterministic route for design calculations, provided by the WIMS9 modular code scheme (Reference 2).

This paper describes some of the main developments implemented in the MONK and WIMS codes to treat PBMRs as well as presenting an inter comparison of the results obtained from the deterministic and Monte Carlo treatments as a first level of validation.

1 PBMR Description

The PBMR is a small modular reactor designed for location at remote sites. Typically it has a total thermal power of about 300 MW with an electrical output of about 120MW. For high thermal efficiency the Brayton cycle is used for energy conversion employing a high temperature helium coolant. The core has an typical inlet temperature of around 530 °C with an outlet temperature of about 900 °C and uses coated particle fuel set in a carbon matrix at the centre of fuel pebbles, see Figure 1.

Each coated particle has an 8.2% ^{235}U enriched UO_2 fuel kernel with surrounding shells of carbon, pyro carbon, silicon dioxide surrounded by a further outer pyro carbon shell. There are around 15,000 coated particles in each two-region fuel pebble which has an inner region consisting of a mixture of coated particles within a carbon support matrix, 5 cm diameter, and an outer moderating carbon shell 0.5 cm thick. The core contains about 450,000 fuel pebbles within a carbon moderating outer reflector. An inner carbon moderator region, at the core centre, acts to limit peak fuel temperatures and further moderate the otherwise under moderated system.

Several different operational fuel management regimes can be employed from the once through then out (OTTO) cycle to the multi-pass cycle. In the multi-pass cycle pebbles pass through the core several times before reaching their discharge burn-up. In representing this burn-up cycle WIMS models a set of fuel batches, each batch being defined by a user specified burn-up range. The burn-up of each pebble is examined after each pass through the core and is either discharged or, if it has not reached its discharge irradiation, its composition is averaged with the other pebbles of the same batch before being reloaded at the top of the core.

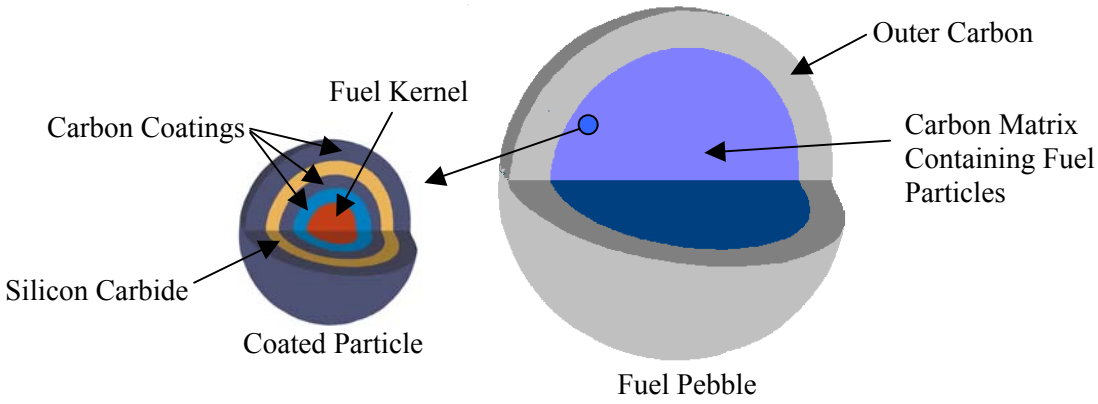

Figure 1 : Fuel Pebble and Coated Particle

2 MONK Monte Carlo Treatment

2.1 Woodcock tracking

The Monte Carlo code MONK uses Woodcock tracking in selected areas where complex geometry is required. This avoids the need to identify surface crossings during the random walk of sampled particles. Instead, it is only necessary to identify the material present at a collision site. This form of tracking is extremely suitable for modelling a PBMR which contains thousands of randomly distributed pebbles each with thousands of randomly distributed fuel grains. Explicit tracking through such a system would not be viable.

The special geometries in which Woodcock tracking is applied are referred to in MONK as 'hole geometries' Two new hole geometries have been devised for PBMR modelling: the *pebble* hole for modelling individual pebbles; the *pbmr* hole for modelling distributions of pebbles within a reactor. The principles of these new geometries are outlined below.

2.2 Modelling a fuel pebble : the PEBBLE hole.

Typical data for a PBMR pebble are as follows.

- 15,000 fuel grains
- Coated particle radius 0.46 mm
- Inner radius of matrix support material (material containing coated particles) = 25mm
- Packing fraction of coated particles = 0.093

With a packing fraction this low it is possible to choose sufficient sites for the grain centres by random sampling. The process rejects sites that would lead to mutual intersection of grains or intersection of grains by the bounding radius of the support matrix.

To reduce the amount of data stored, coated particle sites are sampled and recorded in one octant of the bounding sphere. The remaining octants are filled by flipped/rotated replications of the sampled octant. For efficiency during a Monte Carlo calculation, the sampled octant is overlaid by a regular grid of 10x10x10 cubes. For each cell of the grid a list is created of the grains that lie wholly or partially in that cell. When a collision occurs in the Monte Carlo calculation it is a simple process to identify the cell it occurs in. A relatively short list of coated particle positions can then be processed to identify whether the collision is within a coated particle or in the support matrix.

A coated particle has a central fuel kernel and may have several surrounding shells of different materials. A buffer radius may be specified to achieve a minimum separation of coated particles in the random sampling of their centres to more accurately model the fuel manufacturing process. Typically,

all fuel pebbles in a reactor would be represented by a relatively small set of pebble holes – sufficient, say, to represent the variations in burn-up of pebbles that have passed through different numbers of cycles.

2.3 Modelling pebbles within a reactor.

A PBMR reactor contains hundreds of thousands of pebbles with a typical packing fraction of 0.61. This is too high to be achieved by random sampling of pebble sites. Pebbles arranged in an infinite, close-packed hexagonal array have a packing fraction of 0.744 – slightly less in a finite array if no truncation of pebbles is allowed. In principle, the desired packing fraction of 0.61 could be achieved by a slight increase in the centre spacing of a close packed array: an increase of about 5% in the spacing gives a packing fraction of 0.61 in an infinite array.

However, the regularity of such an array can introduce bias into a Monte Carlo criticality calculation: some particle tracks might stream along paths that do not intersect any fuel; others may penetrate lines of pebbles leading to unrealistic self shielding. Figure 2 illustrates these effects.

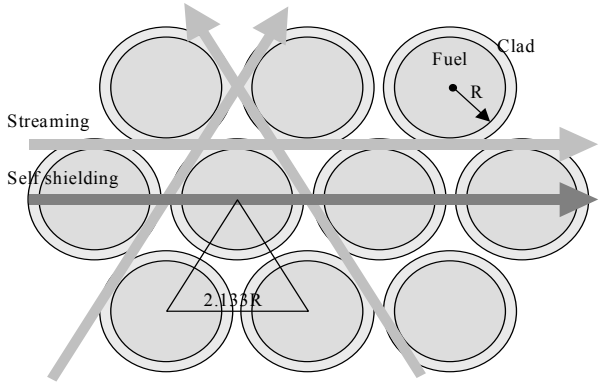

Figure 2 : Two dimensional slice through a regular array

One solution is to reduce the packing fraction of a close packed array by replacing tetrahedral groups of four spheres by a single sphere at their centre. Applied to an appropriate number of sites (chosen at random) this technique can reduce the packing fraction from 0.744 to 0.61 and disturb the regularity of the initial array. This principle is illustrated, in two dimensions, in Figure 3. Although more realistic than a totally regular array, this model still includes unrealistic clumps of regularly spaced spheres with localised areas having lower than average packing fraction.

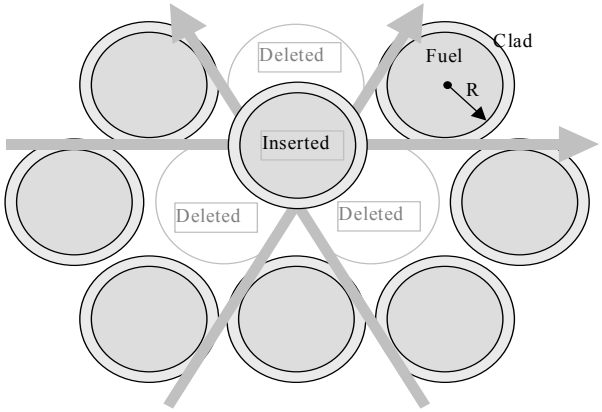

Figure 3 : Two dimensional illustration achieving a given packing fraction by disturbing a regular lattice.

The best algorithm so far obtained is based on the following mechanism.

- A layer of pebbles is created with their centres on a hexagonal lattice within a plane. Pebbles intersecting a cylindrical reactor boundary are rejected. In isolation, this arrangement has a packing fraction slightly less than 0.61.
- A similar layer is placed over the first with the lattice orientation at a random angle.
- Pebbles in the second layer are individually dropped onto the first until they touch one of the first layer pebbles.
- The position of the second layer relative to the first is adjusted to minimise the combined height of the two layers.
- The second layer is now slightly uneven and the packing fraction of the combination is higher than that of the first layer alone.
- The process is repeated.
- After (typically) ten layers the required packing fraction is achieved and the top layer is desirably uneven. The situation in two dimensions is illustrated in Figure 4.

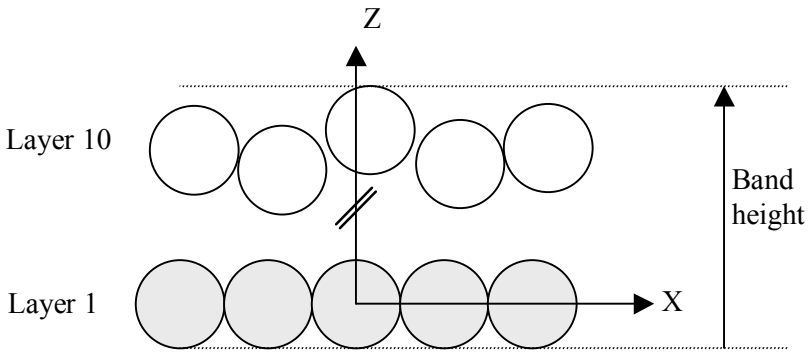

Figure 4 : Two dimensional representation of packing in disturbed layers of hexagons

The 'band' of ten layers has a flat base and irregular upper surface. Suppose now that a sequence of such bands are placed one above the other up the height of a reactor. The axial position of the pebbles at the bottom of each band may be dropped onto the irregular top of the band below to remove their regularity. This allows the axial positions of the pebbles in layer 2 to be further adjusted – and so on up to layer 10. This enhances the irregularity of the layers. The entire process may be repeated several times over the height of the band.

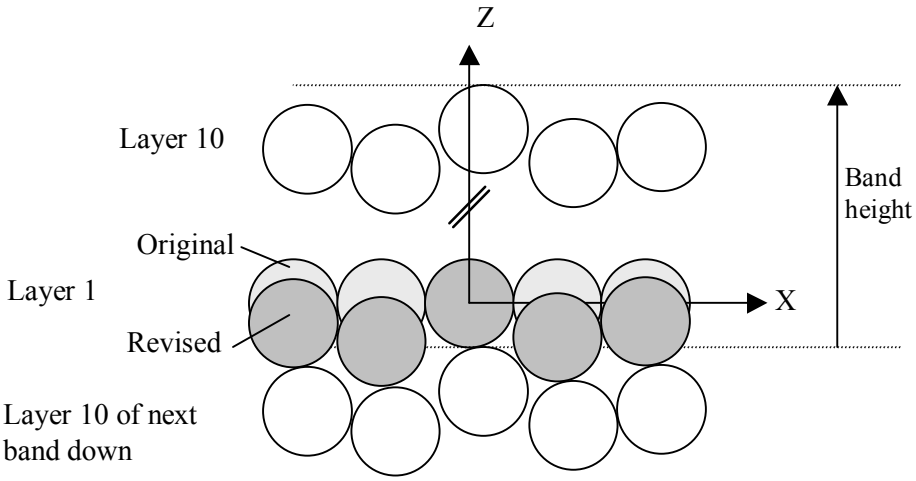

Figure 5 : Two dimensional representation of the final distribution achieved by packing in disturbed layers of hexagons

The net result is an irregular band of pebbles that can be repeated up the axis of the reactor without the pebbles in one band intersecting those of its neighbours, see Figure 5.

Once a distribution has been obtained and recorded, a regular mesh may be overlaid to assist the process of pebble location during Monte Carlo tracking. A type identifier can be allocated to each pebble to give a distribution of moderator and fuel according to an input specification. In this way a distribution of fuel pebbles with different loading or burn history may be included.

For flexibility and to allow the effects of regularity to be investigated, the PBMR hole supports four alternative packing algorithms:

- A regular, close packed, hexagonal array with pebble spacing adjusted to give a specified packing fraction.
- A regular array in which the pitch is increased only within horizontal layers to give a specified packing fraction.
- A regular, close packed, hexagonal array with clusters of four pebbles replaced by a single, central pebble at sufficient sites to give a specified packing fraction.
- Tessellating bands of irregularly positioned pebbles created by the process described above.

3 WIMS Deterministic Treatment

3.1 Resonance Self Shielding

The resonance shielding environment of the fuel in a PBMR contains three levels of heterogeneity:

- Each pebble is surrounded by other pebbles of different burn-up.
- The fuel pebble consists of an outer carbon moderator region surrounding a central carbon matrix material containing the coated particle fuel.
- The coated particle fuel consists of a central fuel kernel surrounded by shells of carbon, pyro carbon, silicon carbide and a further outer pyro carbon shell.

WIMS treats this system by a method termed sub-group theory. The starting point is a data library which contains tabulated resonance integrals for each broad energy group and resonance nuclide as a function of temperature and the potential scattering cross section. The resonance integrals are defined as:

$$I(\sigma_p) = \int \sigma_a(u)\phi(u)du = \frac{1}{\delta u}\int \frac{\sigma_p \sigma_a(u)}{\sigma_p + \sigma_a(u)}du$$

where u denotes lethargy, a denotes absorption and p denotes potential scattering. These integrals are calculated by the NJOY code, Reference 3, which performs a detailed solution of the neutron slowing down equations. NJOY is run at different temperatures and for different homogeneous mixtures of each resonance nuclide with a hydrogen like scattering nuclide to provide the full parameterisation of the data library. Figure 6 shows the typical form of the resonance integral as a function of potential scattering at room temperature for the 6.7eV U238 absorption resonance.

To interpret which value of potential scattering is appropriate to a specific problem many code schemes use equivalence theory in which the heterogeneous problem is reduced to a homogeneous, or to the sum of a series of homogeneous problems, through the use of an appropriate Bell and Dancoff factors. In WIMS a sub-group theory treatment is used instead to allow the effect of the problem geometry to be more exactly represented. The scattering potential dependence of the resonance integrals in any given broad energy group is represented by expressing the resonance integrals as a weighted summation over several sub-groups (as a Lebesgue-Stieltjes integral). Omitting the broad energy group index for clarity, allows the absorption resonance integral to be written as:

$$I(\sigma_p) = \frac{1}{\delta u}\int \frac{\sigma_p \sigma_a(u)}{\sigma_p + \sigma_a(u)} du = \sum_j \frac{w_j \sigma_p \sigma_a^j}{\sigma_p + \sigma_a^j}$$

where the w_j and the σ_a^j are the sub-group weights and absorption cross-sections respectively. As long as the number of sub-groups employed is at maximum one half the number of points at which the resonance integrals are tabulated then it is possible to derive the sub-group weights and absorption cross-sections by a fitting process to the resonance integrals.

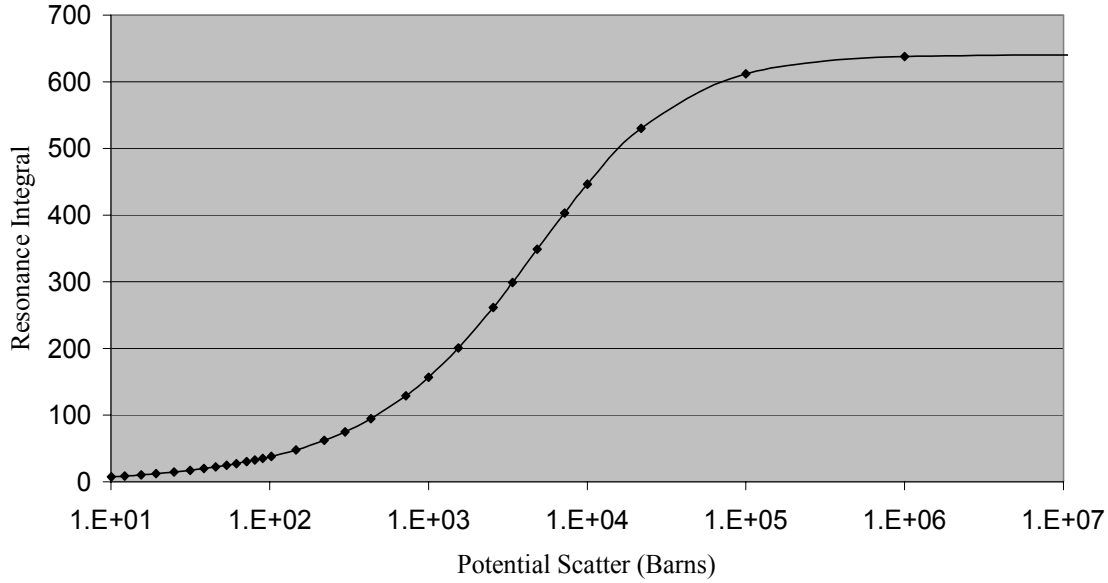

Figure 6 : Resonance Integral for U238 Absorption at 293 Degrees K

Once the sub-group absorption cross-sections have been found, a mono-energetic flux calculation can be performed for each sub-group to derive sub-group fluxes. This is achieved by calculating the collision probabilities, for each sub-group j, $P_{x,r,j}$ than a neutron born in region x will have its next collision in region r. The sub-group fluxes are then given by:

$$\Sigma_t^{r,j}\phi_{r,j} = \sum_x P_{x,r,j}[\Sigma_s^{x,j} - \Sigma_p^x]\phi_{x,j} + \Sigma_p^r$$

where:

$\phi_{r,j}$ = the flux in region r sub-group j.

$\Sigma_t^{r,j}$ = the macroscopic total cross-section in region r, sub-group j.

$P_{x,r,j}$ = the probability, in sub-group j, that a neutron born in region x will have its next collision in region r.

$\Sigma_s^{x,j}$ = the total scatter cross-section in region x, sub-group j.

Σ_p^r = the macroscopic potential scatter cross-section in region r given in the form:

$$\Sigma_p^r = \sum_n N_{n,r}\lambda_n \Sigma_{pot}^n$$

where:

$N_{n,r}$ = atomic number density on nuclide n in region r.

λ_n = the Goldstein/Cohen intermediate resonance parameter giving the probability that nuclide n will scatter a neutron out of the resonance, relative to hydrogen.

Σ^n_{pot} = the background scatter cross-section of nuclide n assumed constant over the resonance energy range.

The problem of calculating the collision probabilities for the imprecise form of the PBMR geometry is returned to following the completion of the sub-group method.

As in the definition of the resonance integral the flux is assumed to be of the form:

$$\phi(u) = \frac{\sigma_p}{\sigma_p + \sigma_a(u)}$$

The broad energy group average absorption cross-section in region r is then simply given by:

$$\overline{\sigma}_a^r = \frac{\sum_j w_j \phi_{r,j} \sigma_a^j}{\sum_j w_j \phi_{r,j}}$$

In practice, sub-group cross-sections are also derived for fission, scatter and broad energy group removal and the broad energy group average for these reactions are formed by a similar weighting to the absorption cross-section.

The problem that remains is the derivation of the sub-group collision probabilities from the cross-sections for the individual sub-groups for a system consisting of the heterogeneous coated particles within the fuel pebbles which are surrounded by pebbles of different fuel batches.

In the first instance the coated particle is considered surrounded by an additional shell containing the particles associated matrix material. The collision probabilities for this simple spherical system are derived using standard techniques, see for example Reference 4. The total cross-section of an artificial material is then searched for that gives the same boundary to boundary transmission probability as the coated particle with associated matrix material. This artificial material is then used in place of the matrix material and coated particles in the region at the centre of the fuel pebble. The collision probabilities for a spherical system consisting of the fuel pebble surrounded by its associated amount of coolant can then be solved. The two sets of collision probabilities, those for the coated particle and those for the pebble, can then be combined to give collision probabilities for the complete fuel pebble.

The above method can be used to produce collision probabilities for each individual fuel batch. However, these collision probabilities can in turn be combined to form those for the system of fuel batches in interaction by a simple consideration of the system of probabilities giving the probability of a neutron leaving one fuel batch to have its next interaction in each of the other batches.

The current favoured PBMR design has a solid carbon reflector at its centre. However, some designs use a reflector consisting of carbon spheres which flow through the reactor in a similar manor to the fuel pebbles. In these designs there is a mixing zone of fuel pebbles and carbon pebbles next to the central reflector. The above method of creating a system of collision probabilities for the interacting fuel batches can equally be used to create a system containing both fuel batches and prescribed ratios of fuel to carbon pebbles.

In the above description the sub-group collision probabilities were used to calculate sub-group fluxes which allowed the detailed geometry effects to be included in the calculation of the self shielded broad energy group cross-sections. Having obtained the broad energy group cross-sections the system collision probability calculations can be repeated, this time using the broad energy group cross-

sections, to obtain the standard neutron fluxes relating the ratings and power production between the interacting fuel batches.

3.2 Whole Core Flux Solution

To perform a whole core flux solution the reactor is first divided into a coarse R, Z, θ mesh on which the fuel burn-up will be followed. Each region will contain a set of unique materials representing the different fuel batches in the region. A resonance self shielding calculation is then performed, as described in the last section, for each of these coarse regions and the neutron fluxes relating the ratings and power production between the interacting fuel batches are calculated.

For the whole core flux solution the detail of the fuel batches within each coarse model region are of no interest, they are only needed to follow the detail of the fuel burn-up. A flux volume weighting is therefore used to reduce all the materials in a coarse to a single material. Before solving the whole core flux the coarse regions are overlaid with a finer mesh to better follow the spatial dependence of the flux.

3.3 Fuel Management and Burn-up

To perform a fuel burn-up calculation the detailed coarse region neutron fluxes, relating the ratings and power production between the interacting fuel batches, are rebalanced using the coarse mesh averaged fluxes of the whole core solution. These rebalanced fluxes are then used to solve the fuel burn-up equations in each coarse region of the reactor.

The next stage is to follow the downward movement of the fuel through the reactor. Effectively, the coarse mesh is moved downward, relative to its start of time step position, using a velocity profile dependent on the radial location of the fuel. The intersection of the mesh describing the new fuel location with that of the mesh at the start of the time step is calculated and new batch compositions are calculated by smearing together fuel within the same batch (defined range of burn-up). Fuel that is discharged from the reactor during the time step is either discarded, if it has reached the maximum burn-up limit, or is smeared to into batches and reloaded at the top of the reactor. Fuel which has been discarded is replaced by new unirradiated fuel which again is loaded into the top of the reactor.

WIMS also allows the modelling of the inward (toward the reactor centre) flow of fuel through the discharge cone at the bottom of the core, however, this is effectively just additional detail in the overall modelling.

4 Inter Comparison of Results from MONK and WIMS

4.1 Infinite Array of Fuel Pebbles

In the development of the methods described in the previous sections inter comparisons were made between the MONK Monte Carlo results and those from the WIMS deterministic treatment for an infinite array of fuel pebbles.

The first case considered was for an infinite array of two region fuel pebbles consisting of a central region of smeared fuel and matrix material surrounded by an outer layer of carbon moderator. This case omits the heterogeneity of the coated particles, to define a base case against which the heterogeneity effect can be calculated, and omits the presence of the coolant. The coolant is omitted so that the outer boundary condition for the WIMS collision probability calculation, a white boundary condition, is approximately the same as that for the MONK Monte Carlo calculation, which, for a sphere, returns neutrons with a cosine distribution about the outward normal. These two boundary

conditions are equivalent only in the case of an isotropic flux at the outer boundary, a condition more precisely met with heavy scattering carbon rather than helium gas at the outer problem boundary.

WIMS gave a reactivity 460 ± 100 pcm higher than the MONK point energy Monte Carlo reactivity indicating a cross-section bias in the WIMS calculation for this case.

When the coated particles were represented explicitly rather than smeared with their support matrix, to treat the full fuel heterogeneity effect, WIMS gave only a slight difference in reactivity relative to MONK of 50 ± 30 pcm.

The reactivity increase due to the coated particle heterogeneity effect is large, of the order of 11,000 pcm for an infinite array.

4.2 Whole Core Calculation

For the whole core calculation WIMS was run using two mesh structures, a standard mesh 1 structure which had a mesh of approximately 5 cm in the fuelled regions and 2 cm in the carbon reflector regions and a mesh 2 structure in which all mesh dimensions were halved. An infinitely fine mesh k-effective (k_∞) was then extrapolated using the relation:

$$k_\infty = \frac{4k_2 - k_1}{3}$$

Where the suffixes 1 and 2 refer to mesh structure 1 and 2 respectively.

The accuracy of this extrapolation was tested by using the broad energy group of WIMS in the MONK code. In this mode of operation MONK performs a Monte Carlo calculation using the broad group cross-sections in place of the continuous energy representation of the cross-sections and verifies that there are no mesh structure effects which have been omitted in the deterministic solution. The agreement between MONK and WIMS was excellent, WIMS had a higher k-effective by 19 ± 100 pcm.

The MONK calculation was then repeated using the continuous energy representation of the cross-sections. MONK gave a k-effective 245 ± 100 pcm higher than WIMS. This indicates a potential small bias in the WIMS cross-section set. However, the bias is sufficiently small for design calculations and may in part be due to the detail of the algorithm used in MONK to pack the pebbles in the reactor. No allowance has been included in the assigned uncertainty for this effect. More work is planned to validate the algorithms in MONK including comparison with experiment.

5 Conclusion

Methods have been developed within the ANSWERS Monte Carlo code MONK and the deterministic treatment WIMS modular code scheme to provide both reference and design routes for PBMR core neutronic calculations.

An inter comparison of results between MONK and WIMS for an infinite array of heterogeneous fuel pebbles indicates a minor over estimate of k-infinity by WIMS of 50 ± 30 pcm.

For a whole core calculation MONK gives a k-effective 245 ± 100 pcm higher than WIMS.

These results are encouraging and provide an initial validation of the methods in WIMS. Full validation awaits comparison with experiment.

6 Acknowledgement

The author gratefully acknowledges the work of several colleagues at Serco Assurance for their assistance in performing the work described in this paper. Particular thanks are due to Ted Shuttleworth for the design and implementation of the methods employed in the MONK Monte Carlo code.

7 References

1. N R Smith, N T Gulliford and D Hansin, "Achieving Industry Acceptance of a JEF2.2 Nuclear Data Library for MONK", *International Conference on Nuclear Criticality Safety*, ICNC '99, Versailles, September 1999.

2. T D Newton and J L Hutton, The next Generation WIMS Lattice Code : WIMS9, Physor 2002, Seoul, Korean, October 2002.

3. R E MacFarlane, D W Muir, The NJOY Nuclear Data Processing System Version 91, LA-12740-M Manual, October 1994.

4. R J J Stamm'ler and M J Abbate, Methods of Steady State Reactor Physics in Nuclear design. Academic Press 1983.