MCNP Modelling of the PBMR Equilibrium Core

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Abstract

A complete MCNP model of the PBMR equilibrium core is presented, which accounts for the same fuel regions defined in the PBMR core management code, as well as for complete fuel and reflector temperature distributions. This comprehensive 3D model is the means to calculate and characterize the neutron and photon boundary sources of the equilibrium core, and is also used to support some specific core neutronic studies needing detailed geometry modelling.

Due to the geometrical modelling approach followed, an unrealistic partial cutting of fuel kernels and pebbles is introduced in the model. The variations introduced by this partial cutting both on the packing fraction and on the uranium load of the modelled core and its corresponding effect on core reactivity and flux levels, have been investigated and quantified.

A complete set of high-temperature cross-section data was applied to the calculation of the PBMR equilibrium core, and its effect on the calculated core reactivity is also reported.

KEYWORDS: PBMR equilibrium core, pebble-bed modelling with MCNP, high-temperature graphite reactor

1. Introduction

The South African Pebble Bed Modular Reactor (PBMR) is a high-temperature helium-cooled graphite-moderated continuous-fuelled pebble bed reactor, which will become a first-of-a-kind Generation-IV reactor. A multi-pass fuel management is foreseen, in which the fuel pebbles are re-circulated through the core until they reach the target burn-up. The VSOP99 code system is used for the core neutronic design and fuel management. More details on the neutronic design of the equilibrium cycle and the reactor layout can be found in Ref. [1]. Due to the maturity reached in the PBMR 400 MWth reactor design, detailed modelling is needed to support specific core neutronic analyses and to generate core neutron and photon sources to be applied in subsequent radiation transport problems. Consequently, a complete MCNP core model was developed.

There is extensive experience in using MCNP to model HTGR-type fuel. Some of the articles available in the open literature deal with modelling room temperature experiments where the composition and arrangement of the pebbles in the system are well known. [2] Another set of articles is focused on the different approaches followed to model, in a reasonable way, the random distribution of kernels in the pebble, and that of the pebbles in the core. [3-6] Code

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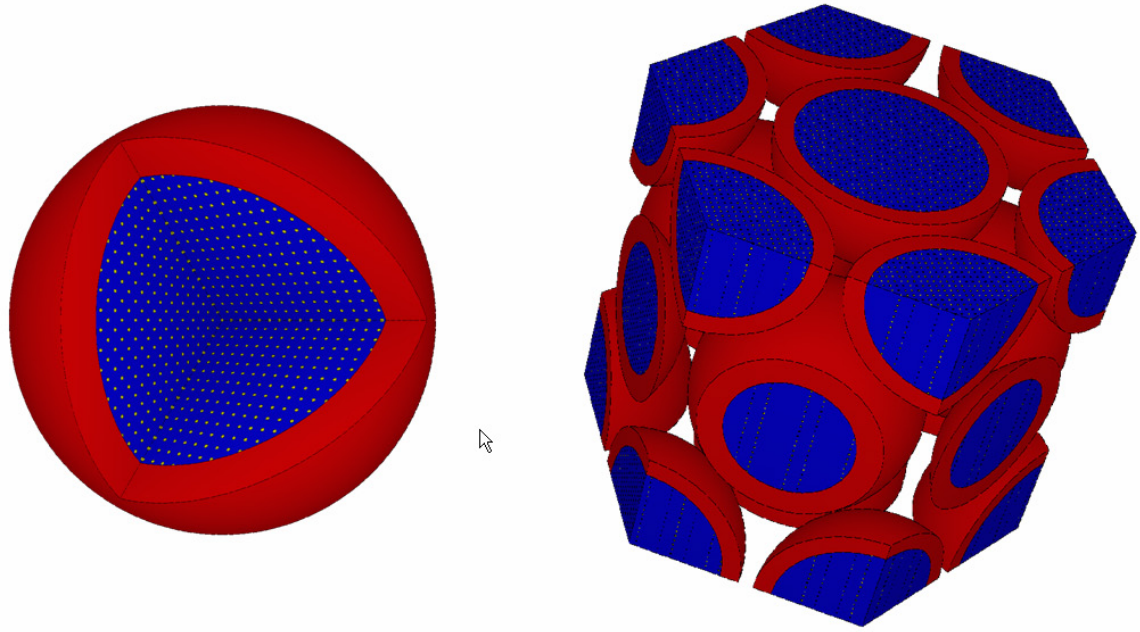
developers are also trying to find efficient and accurate ways of simulating the random distribution of kernels and pebbles. [6-8] However, no information has been found concerning the modelling of a pebble bed equilibrium core with MCNP, with details of the implications of such a modelling as it is presented in this paper.

2. Core Geometry and Temperature Distribution Modelling

2.1 Fuel pebble and equilibrium core modelling

The double heterogeneity of the PBMR fuel is treated explicitly in the MCNP core model. The UO_2 kernels in the fuel matrix are arranged in a cubic array. The four coating layers of TRISO particles are homogenized in a single layer surrounding the UO_2 kernel, and the outer graphite fuel-free shell is modelled explicitly. A Hexagonal Close-Packed (HCP) arrangement of pebbles was chosen to distribute pebbles in the core. This approach at kernel and pebble levels is discussed in several works. [2, 4, 5, 9] Fig. 1 shows a fuel pebble and the elementary HCP arrangement, as modelled with MCNP.

Figure 1: (a) 3D view of a fuel sphere, where 1/8 of it was removed to show the internal distribution of coated particles. (b) Elementary unit cell of pebbles in an HCP arrangement.

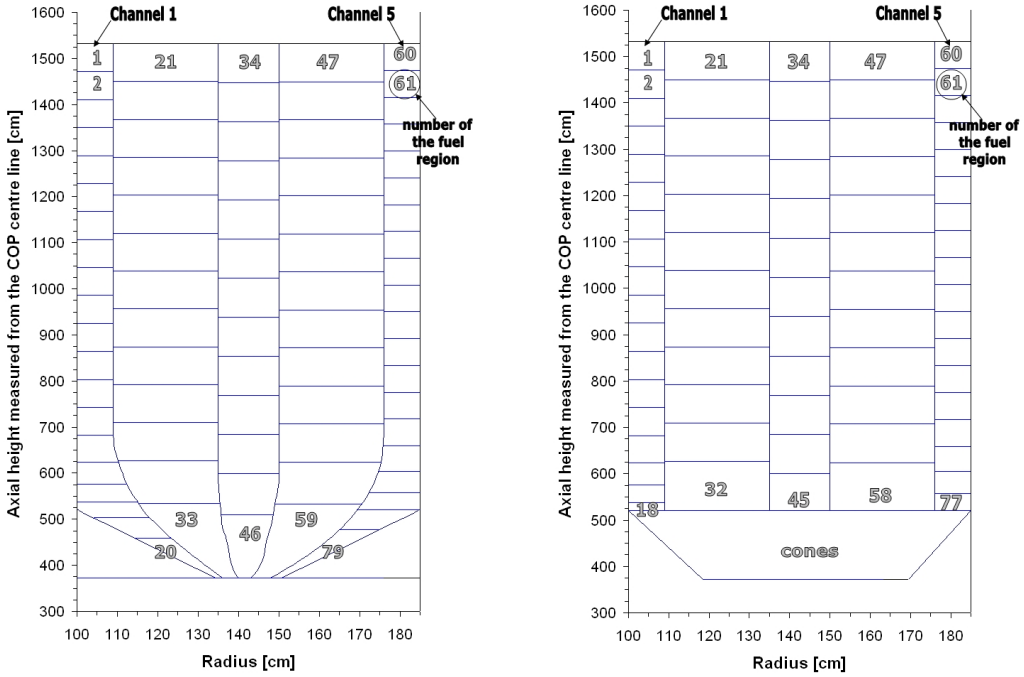


For the first time at PBMR, the same fuel regions defined in VSOP99 for the equilibrium core were incorporated in this MCNP core model. Fig. 2 shows the definition of the fuel regions in the VSOP99 2-D core model. The number densities of the fuel kernels in each one of these fuel regions were derived from the corresponding data calculated with the VSOP99 equilibrium core model. [1] Five flow channels are defined, representing flow paths for pebbles. The different axial discretization of each channel is used to model the different flow rates in the channels. Due to the multi-pass fuel management scheme adopted, every fuel region contains fuel with different burnup levels (batches). In the MCNP equilibrium core model, the number densities from different batches in a given fuel region are averaged to represent the fuel at that position in the

core. It is clear that different fuel regions have a different composition, and a different fuel and moderator temperature, too.

Two modifications of the VSOP99 fuel region boundaries were needed in the MCNP model. The first modification is related to the different approach to modelling the defuelling cones in VSOP and MCNP (2D modelling in VSOP vs. a true 3D modelling in MCNP). As a consequence, the fuel regions in VSOP corresponding to the defuelling cones region were modelled as only one fuel region in MCNP. Number densities for this region were calculated by volume-weighting the number densities of the different layers in the defuelling cones. The second modification in the definition of fuel regions between VSOP and MCNP models concerns the radial boundaries of the five different channels, at the core bottom. While in VSOP these radial boundaries change with the axial position, whereas in the MCNP model these boundaries were assumed to be constant and equal to the radial boundaries at the top of the pebble bed. The axial boundaries defining each region were maintained as in VSOP, and a slight difference in the volume of these bottom regions between the VSOP and MCNP core models was introduced.

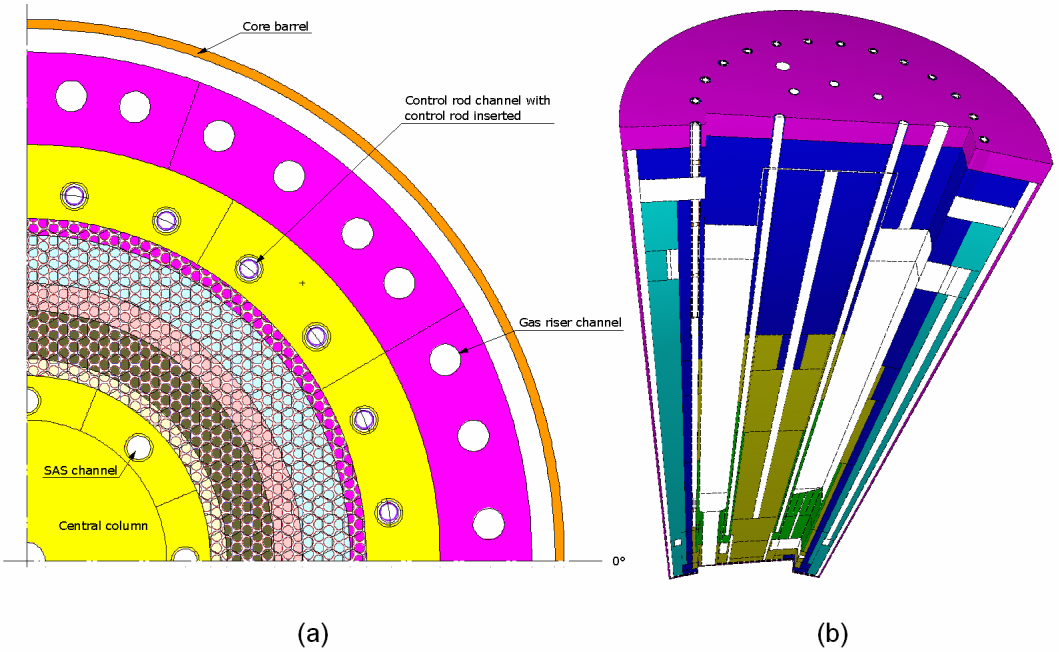
Figure 2: Sketch showing the numbering of flow channels and fuel regions (layers) in the VSOP (left) and MCNP (right) equilibrium core models.



A "coarse mesh" temperature distribution derived from a fine mesh temperature distribution calculated with VSOP99, both within the core and at the graphite reflectors, was also incorporated for the first time in the model. The boundaries of this coarse mesh are determined by the available high-temperature cross-sections (XS) for graphite in the MCNP library.

In addition to modelling of the fuel regions, a great effort was made to represent the core geometry with as much detail as possible. This includes a detailed representation of control rods, small absorber sphere channels, gas riser channels, as well as an explicit modelling of gaps and slits present at the top and bottom reflectors (Fig. 3).

Figure 3: (a) ¼ X-Y section of the MCNP core model, showing the 5 flow channels in the core, the control rods, SAS, and gas riser channels. (b) 3D view of the core model (fuel pebbles not shown) with clipping planes through a control rod channel (left) and a gas riser channel (right). In both plots, the temperature distribution in the reflector is indicated with a different colour.



2.2 Region-wise dependence of modelled packing fraction and uranium loading

If modelled in full detail, a complete PBMR core would require the modelling of ~15 000 kernels per pebble, and ~450 000 pebbles in the core. MCNP5 Release 1.30, currently in use at PBMR, cannot model such a large amount of randomly distributed cells, and then the regular infinite lattice capabilities of MCNP5 are needed. This approach introduces an artificial cutting of pebbles in the core and kernels in the pebble, which is a source of debate concerning the validity of such an MCNP model.

The effect of the partial cutting on both the packing fraction and the uranium load of the modelled core was analyzed and quantified. The stochastic volume calculation capability in MCNP was used at every fuel region to calculate, the volume occupied by kernels, graphite in the fuel matrix, graphite shells and helium in between pebbles. Several runs were made, each one with a different random number seed, and the results were collected by using the *mcnp_pstudy* script. [10] Fig. 4 shows the kernel volume ratio (MCNP model/theoretical), calculated at every fuel region with the MCNP model. Thus, Fig. 4 gives an indication of the region-wise discrepancy in the uranium loading, introduced by the partial cutting of kernels in the MCNP model. A weak underestimation of uranium loading is seen (< 1%) on average, with fluctuations above and below the expected value of 1. Maximum and minimum deviations occur in fuel regions at the bottom of the core, which make a small contribution to total core reactivity. Concerning the flow channels, higher fluctuations are observed in channel 1 (next to the central column). The volume of fuel regions in this channel are the smallest ones, compared to the volume of fuel regions in the other four channels. Consequently, channel 1 is where the effect of partial cutting on the different volume fractions is more noticeable.

Figure 4: Kernel volume fraction (MCNP/theoretical) per fuel region in the MCNP core model. Values for each one of the 5 fuel channels in the model are shown in different colours.

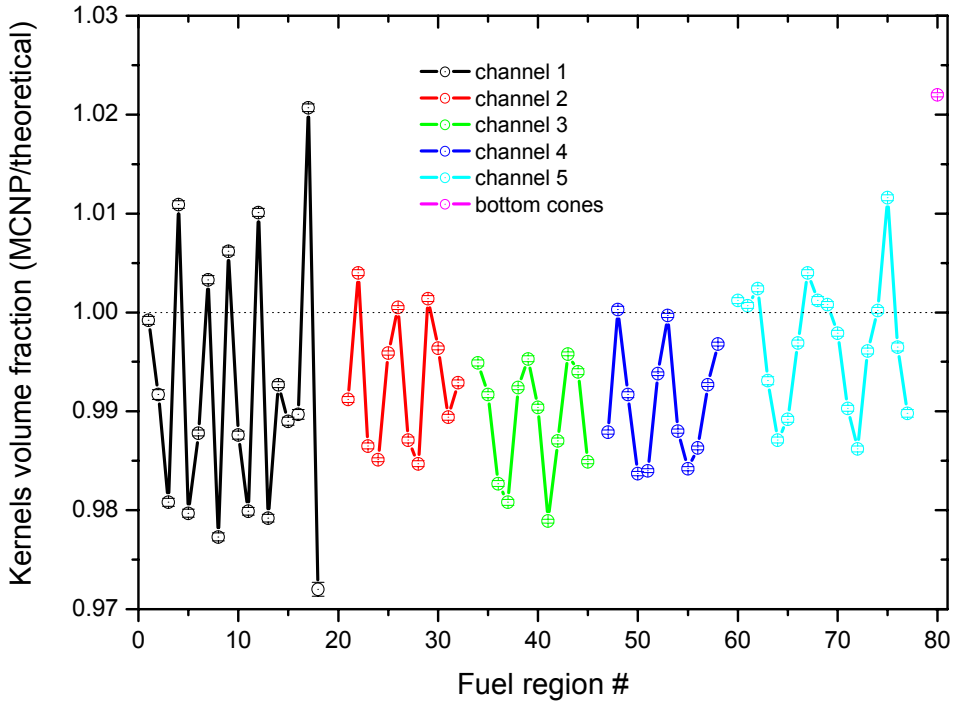


Figure 5: Volume fraction (MCNP/theoretical) calculated for kernels, fuel matrix, graphite shell and helium in between pebbles, for all fuel regions in flow channel 4. The corresponding ratio of packing fraction (MCNP/theoretical) is also shown.

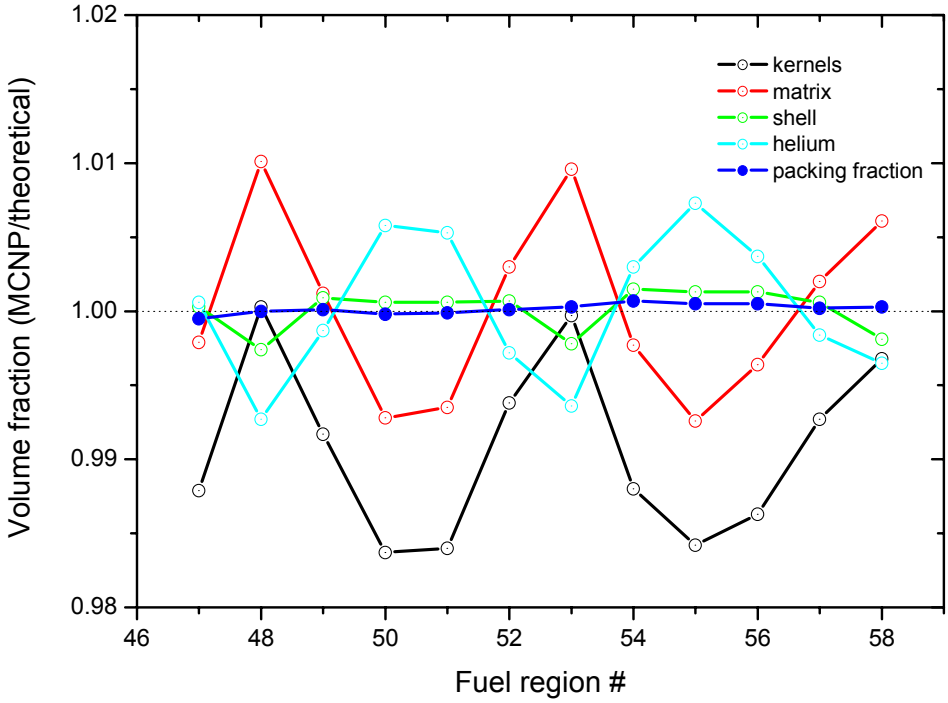


Fig. 5 allows a closer look at the fluctuations of volume fractions in channel 4. Even though the fluctuation in a kernel's volume could be as high as 2%, this fluctuation is compensated by the change in graphite volume (matrix and shell). As a result, the packing fraction and the fuel-to-moderator ratio (not plotted in Fig. 5) show a much smoother behaviour, suggesting that the overall effect on core reactivity should be limited.

To confirm this, the effect that the fluctuations in packing fraction and uranium loading have on core reactivity was investigated with VSOP99, by means of a specific VSOP99 model having the same packing fraction and uranium loading, region per region, as in the MCNP core model. [11] The results obtained show that the region-wise perturbations in packing fraction and uranium loading introduced in the MCNP equilibrium core model do not affect the core characteristics (k_{eff}, flux and power distribution) significantly. In terms of core reactivity, the difference observed was less than 100 pcm.

2.4 Effect of different packing arrangements (regular and random)

Different regular arrangements of pebbles were chosen to quantify their effect on core reactivity. A small, cubic, 1 m^3 core was selected for this purpose. This volume was chosen for two main reasons:

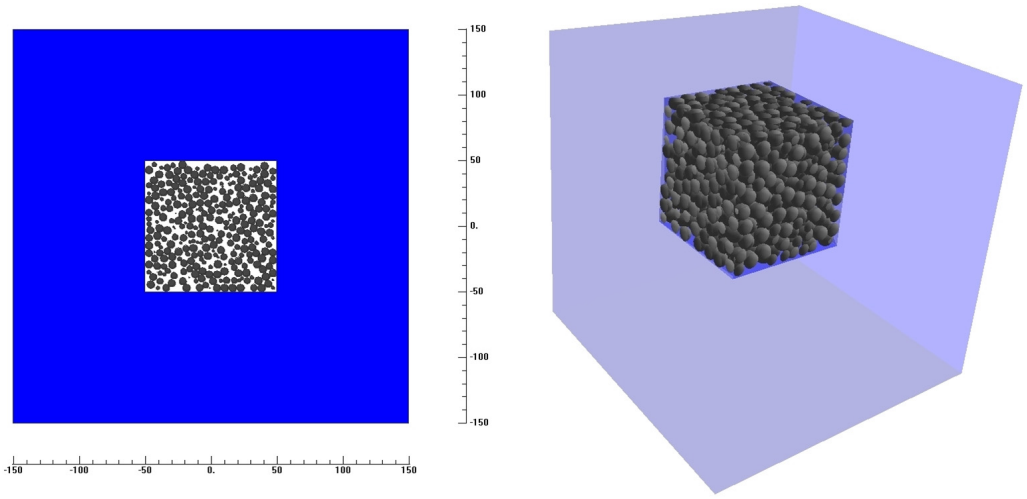
1. When reflected with graphite, 1 m^3 of pebbles (about 5 000 spheres) containing 9 grams of fresh fuel (9.6 wt% enriched) at room temperature is close to critical;
2. Due to the simplicity of this proposed system, it becomes possible with MCNP to model a true random distribution of pebbles in a core of such a size. A random distribution of 4 790 pebbles filling a 1 m^3 cube was calculated with PFC^{3D}. [12] This distribution was then used to model each pebble in the core with MCNP. This case was used as a reference case to compare k_{eff}.

The core-averaged packing fraction of the randomly-packed core is 0.542 instead of 0.61 as used in the PBMR case, due to the different core geometry and size. To compare results against this reference case, a second core was modelled with MCNP by choosing an HCP arrangement with the same packing fraction as the random core. The uranium load in both cores (random- and HCP-packed) was almost the same (< 1% difference). Table 1 shows the results obtained. Even though the difference in k_{eff} is about seven standard deviations (which indicates that the systems modelled do not behave neutronically in the same way), the difference in reactivity is ~350 pcm, which is considered as an acceptable difference for the calculation of an equilibrium core.

Table 1: k_{eff} calculated for the cubic core for different arrangements of pebbles (regular and random)

Packing arrangement	Packing fraction	$k_{eff} \pm \sigma$
Random	0.542	0.9891 ± 0.0005
HCP	0.542	0.9926 ± 0.0003
Random + URAN option	0.542	0.9884 ± 0.0006
BCC	0.61	1.0266 ± 0.0004
HCP	0.61	1.0232 ± 0.0004
FCC	0.61	1.0238 ± 0.0004

Figure 6: (a) X-Z section of the cubic core with randomly distributed pebbles. (b) 3D view of 1/8 of the cubic core and reflector.



(a) (b)

The cubic core was also filled with three different regular packing arrangements: BCC (body-centered cubic), FCC (face-centered cubic), and HCP. This time a packing fraction equal to 0.61 was used, as in the PBMR equilibrium core model. The results obtained are also listed in Table 1. The FCC and HCP results are statistically the same, while the core filled with a BCC arrangement of pebbles is more reactive. Given the reasonable agreement obtained when using the HCP and random packing, and since the HCP lattice is simpler to model than the FCC lattice, the HCP lattice was selected to model the PBMR equilibrium core. The HCP lattice also gives enough flexibility to model different fuel-to-moderator ratios as needed to evaluate different options for the PBMR start-up core.

The latest version of the MCNP5 code (release 1.40) provides a limited capability to simulate the stochastic arrangement of fuel kernels in HTGR fuel (URAN card). [8] If this new option is used, each time a neutron enters a lattice element containing a universe defined as stochastic, the position of this universe will be uniformly sampled within limits given by user input. When this is applied to the cubic lattice containing the fuel kernels, the kernel's position is not fixed within the lattice element, but it is stochastically determined within it. This new option in MCNP5 was applied to the randomly packed core described above. The difference in reactivity is < 100 pcm, as shown in Table 1.

2.5 High temperature cross-section libraries

The XS libraries included in the RSICC distribution of MCNP5 contain a limited number of isotopes with high temperature XS data. Therefore, only high temperature data for U^{235}, U^{238} and Pu^{239}, and thermal scattering S(α,β) data for graphite at high temperature were used in the first attempts of calculating the equilibrium core with the MCNP model. Besides this, not all the fission products included in the fuel regions provided by VSOP were available in the RSICC libraries, so these isotopes were not included in the MCNP description of the fuel materials.

At the same time and at the request of PBMR, a comprehensive library including

high-temperature XS data for all isotopes contained in the ENDF/B-VI Release 8 evaluation was developed by NRG. [13] This new XS library was also applied to the calculation of the PBMR equilibrium core.

Several cases were calculated, in order to make a separate evaluation of the effect of different combinations of XS sets on k_{eff}. Table 2 summarizes the results obtained. In Table 2, XS data taken from the new NRG library is referred to as "NRG", while XS data from the MCNP libraries included in the RSICC distribution is indicated as "RSICC". Similarly, when high-temperature XS are indicated, it means that sets at 800 K, 900 K and 1200 K (U^{235}, U^{238} and Pu^{239}, RSICC XS), or at 800 K, 1000 K, 1200 K (all isotopes and graphite thermal-scattering data, NRG XS; and graphite thermal-scattering data, RSICC XS) were used.

As shown in Table 2, the maximum difference in reactivity observed after using one or other set of XS is about -800 pcm. The two main contributors to this difference are the high temperature data used for U^{235}, U^{238} and Pu^{239} (case NRG-1), and the inclusion of all the isotopes in the fuel, as provided by VSOP (compare cases NRG-4 and NRG-5). In the first case, the difference could be at least partially due to, a different temperature discretization in the fuel as determined by the available high temperature XS in both sets. On the other hand, the S(α,β) thermal data in both libraries seems to be of similar quality.

Table 2: Effect on k_{eff} due to using NRG XS libraries. Δk_{eff} is the difference in reactivity of the NRG-cases compared to the reference case (NRG – Reference).

Case	Δk_{eff} [pcm]	Description
Reference		• U^{235}, U^{238} and Pu^{239}: RSICC XS, high temperature • Graphite (moderator, reflector): RSICC S(α,β), high temperature • Remaining isotopes in fuel: RSICC XS, room temperature
NRG-1	-349	• U^{235}, U^{238} and Pu^{239}: NRG XS at high temperature • Graphite (moderator, reflector): RSICC S(α,β), high temperature • Remaining isotopes in fuel: RSICC XS, room temperature.
NRG-2	-17	• U^{235}, U^{238} and Pu^{239}: RSICC XS at high temperature • Graphite (moderator, reflector): NRG S(α,β), high temperature • Remaining isotopes in fuel: RSICC XS, room temperature.
NRG-3	-334	• U^{235}, U^{238} and Pu^{239}: NRG XS at high temperature • Graphite (moderator, reflector): NRG S(α,β), high temperature • Remaining isotopes in fuel: RSICC XS, room temperature.
NRG-4	-381	• U^{235}, U^{238} and Pu^{239}: NRG XS at high temperature • Graphite (moderator, reflector): NRG S(α,β), high temperature • Remaining isotopes in fuel (only those isotopes provided by VSOP which are available in RSICC libraries): NRG XS, high temperature.
NRG-5	-774	• U^{235}, U^{238} and Pu^{239}: NRG XS at high temperature • Graphite (moderator, reflector): NRG S(α,β), high temperature • Remaining isotopes in fuel (all isotopes provided by VSOP): NRG XS at high temperature.

3. VSOP99–MCNP Comparison of the k_{eff} of the PBMR Equilibrium Core

The purpose of this paper is to describe the approach and assumptions adopted to develop the MCNP equilibrium core model in detail. However, it is worthwhile giving an initial indication of the differences in results obtained with the VSOP99 and MCNP core models. During the first stages of development of this MCNP equilibrium core model, the multiplication factor obtained was systematically higher than the value obtained by VSOP (about 2400 pcm in some cases). This disagreement was important and the need to explain and reduce the difference was identified. The MCNP model was under scrutiny until we completed the analysis of the effect of the assumptions embedded in the model. Since none of these assumptions could justify the difference with VSOP, the focus was moved to finding reasons in VSOP which could help to understand the difference. Thus, a newer version of VSOP was developed with a different treatment for leakage [14], which is applied at every one of the several spectrum regions in the VSOP model. This new version of VSOP was used to calculate an updated set of number densities and temperature distribution for the equilibrium core. When these sets are incorporated in MCNP, the difference in reactivity between VSOP and MCNP is reduced from ~2400 pcm to ~200 pcm, when RSICC XS data are used. Taking into account the effect of using the NRG library, the agreement between VSOP and MCNP is now in the range of ~600 pcm. A complete comparison effort (including flux profiles and control-rod worth) is already underway and some results will be presented at the next HTR-2006 Conference. [15]

4. Conclusions

A full 3D model of the PBMR equilibrium core has been developed. For the first time, this 3D modelling accounts for the same 79 fuel spectrum regions defined in the VSOP99 equilibrium core model, as well as a complete fuel and reflector temperature distribution. Two different sets of high temperature XS data were used and its results were compared. The use of a complete set of high-temperature XS allowed for quantifying the effect on reactivity of fission-products that were missing in the standard distribution of MCNP, and for properly accounting for temperature in the whole system. The overall effect of using a complete high-temperature XS library, as compared to the limited one available from RSICC, is ~800 pcm.

The calculation of an equilibrium core implies the need to model a large number of fuel spheres containing fuel kernels at different burnup levels. It therefore becomes very difficult to avoid making some modelling simplifications such as the artificial cutting of kernels and pebbles. However, we showed that the effect of this artificial cutting is very limited, as long as the fluctuation in packing fraction and heavy-metal mass are kept below 1% of the target values. In the same way, we showed that the effect on k_{eff} of different packing arrangements is also within reasonable margins for calculation of an equilibrium core.

The model developed provides an alternative way to calculate core physics parameters such as the multiplication factor, control-rod worth, distribution of flux, and energy deposition in the core and reflectors. Since it is a completely independent tool (in the sense of software, resolution method and XS data) when compared to VSOP, this model will play an important role in the inter-code comparison effort scheduled for the next stages of PBMR design. The first contribution to this effort has been the identification of the need of a better leakage treatment in VSOP, which resulted in a closer agreement between both codes. In addition to this, some

particular problems that are difficult or even impossible to represent with a VSOP 2D model, can now be calculated with this MCNP model. Examples of such particular problems include a complete heating distribution produced by neutrons and gammas (if the contribution from fission-product gammas is included), the inadvertent insertion of SAS spheres in only one SAS channel, or a detailed 3D distribution of fast neutron flux in one reflector block.

References

1) F. Reitsma, "The Pebble Bed Modular Reactor Layout and Neutronics Design of the Equilibrium Cycle," PHYSOR 2004, Chicago, Illinois, April 25-29, 2004, on CD-ROM, ANS, LaGrange Park, IL (2004).
2) F. C. Difilippo,. "Monte Carlo Calculations of Pebble Bed Benchmark Configurations of the PROTEUS Facility," Nuc. Sci. Eng., 143, 240 (2003).
3) "Evaluation of High Temperature Gas Cooled Reactor Performance: Benchmark Analysis Related to Initial Testing of the HTTR and HTR-10," IAEA TECDOC 1382 (2003).
4) Z. Karriem, C. Stoker and F. Reitsma, "MCNP Modelling of HTGR Pebble-Type Fuel," Proc. of the Monte Carlo 2000 Conference, Lisbon, Portugal, Oct. 23-26, 2000, 841 (2000).
5) H. Chang et al., "Monte Carlo Method Treatment of Stochastic Geometry in a Pebble Bed Reactor", The Monte Carlo Method: Versatility Unbounded in a Dynamic Computing World, Chattanooga, Tennessee, April 17-21, 2005, on CD-ROM, ANS, LaGrange Park, IL (2005).
6) M. Armishaw, N. Smith and E. Shuttleworth, "Particle Packing Considerations for Pebble Bed Fuel Systems," Proc. Int. Conf. on Nuclear Criticality Safety, ICNC2003, Tokai-Mura, Japan, Oct. 20-24, 2003, 401 (2003).
7) I. Murata et al., "New Sampling Method in Continuous Energy Monte Carlo Calculation for Pebble Bed Reactors," J. Nuc. Sci. Technol., 34, 734 (1997).
8) F. B. Brown, W. R. Martin, "Stochastic Geometry Capability in MCNP5 for the Analysis of Particle Fuel," Ann. Nucl. Energy, 31, 2039 (2003).
9) U. Colak and V. Seker, "Monte Carlo Criticality Calculations for a Pebble Bed Reactor with MCNP," Nuclear Mathematical and Computational Sciences: A Century in Review, A Century Anew," Gatlinburg, Tennessee, April 6-11, 2003, on CD-ROM, ANS, LaGrange Park, IL (2003).
10) F. Brown, J. Sweezy and R. Hayes, "Monte Carlo Parameter Studies and Uncertainty Analyses with MCNP5," PHYSOR 2004, Chicago, Illinois, April 25-29, 2004, on CD-ROM, ANS, LaGrange Park, IL (2004).
11) S. Sen, "The Effect of the Fluctuations in the Modelled Packing Fraction and HM Loading in the MCNP Core," DIT000740, PBMR (Pty) Ltd. (2005)
12) A. Polson, "Non-overlapping Sphere Positions in a 1 Cubic Metre Volume Using PFC^{3D}," Memorandum 024917 Rev. A, PBMR (Pty) Ltd. (2004)
13) M. C. Duijvestijn, A. Hogenbirk and S. C. van der Marck, "ENDF/B-VI.8-PBMR Contents of the ENDF/B-VI.8 Based MCNP Neutron Transport Cross Section Libraries for PBMR," NRG 21526/05.64901/C, Petten, The Netherlands (2005).
14) H. Brockmann et al., "Review of the Neutron Spectrum Calculation Methods in the Computer Code System VSOP-99," FZJ-ISR-RC-5084/2004, Jülich, Germany (2004).
15) S. Sen, F. Albornoz and F. Reitsma, "Comparison of VSOP and MCNP Results of PBMR Equilibrium Core Models," accepted for presentation at the 3rd International Topical Meeting on HTR Technology - HTR 2006, Sandton, South Africa, Oct. 1-4 (2006).