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**Applications of Monte Carlo
Methods for the Analysis of MHTGR
Case of the PROTEUS Benchmark**

F. C. Difilippo

**MANAGED BY
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Engineering Physics and Mathematics Division

**APPLICATIONS OF MONTE CARLO METHODS FOR THE ANALYSIS OF MHTGR
CASE OF THE PROTEUS BENCHMARK**

F. C. Difilippo

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APPLICATIONS OF MONTE CARLO METHODS FOR THE ANALYSIS OF MHTGR CASE OF THE PROTEUS BENCHMARK

F. C. Difilippo

1. INTRODUCTION

Monte Carlo methods, as implemented in the MCNP code, have been used to analyze the neutronics characteristics of benchmarks related to Modular High Temperature Gas-Cooled Reactors. The benchmarks are idealized versions of the Japanese¹ (VHTRC) and Swiss² (PROTEUS) facilities and an actual configurations of the PROTEUS Configuration I experiment. The purpose of the unit cell benchmarks is to compare multiplication constants, critical bucklings, migration lengths, reaction rates and spectral indices. The purpose of the full reactors benchmarks is to compare multiplication constants, reaction rates, spectral indices, neutron balances, reaction rates profiles, temperature coefficients of reactivity and effective delayed neutron fractions. All of these parameters can be calculated by MCNP, which can provide a very detailed model of the geometry of the configurations, from fuel particles to entire fuel assemblies, using at the same time a continuous energy model. These characteristics make MCNP a very useful tool to analyze these MHTGR benchmarks.

We have used the MCNP latest version, 4.x, eld = 01/12/93 with an ENDF/B-V cross section library. This library does not yet contain temperature dependent resonance materials, so all calculations correspond to room temperature, $T=300^{\circ}\text{K}$. Two separate reports were made—one for the VHTRC, the other for the PROTEUS benchmark.

2. THE PROTEUS BENCHMARK PROBLEM

The calculations shown here correspond to the specifications of the benchmark described in Ref. 2. The unit cell for the core is a hexagonal compact packing of 6 cm moderator and fuel pebbles in a 1 to 2 ratio (LEUPRO-1 cell of Ref. 2). The fuel pebbles have a 5 cm diameter fuel compact that contains the fuel particles in a graphite matrix and a 0.5 cm thick graphite shell; the moderator pebbles are spheres of graphite. The pebbles, with the fuel regions, were modeled explicitly. The fuel particles were modeled explicitly, referred to as heterogeneous compact calculations, or were homogenized with the particle coatings and matrix, referred to as homogeneous compact calculations. Two types of systems were analyzed: the numerical benchmark related to the LEUPRO-1 cell and the more detailed critical experiments that are in progress at the Paul Scherrer Institute.

2.1 RESULTS FROM THE CALCULATION OF THE UNIT CELL

The unit cell corresponding to the core region of Figs. 1 and 2 consists of a hexagonal compact packing of 6 cm diameter spheres (pebbles). There are two types of pebbles, moderator and fuel pebbles, in a proportion of 1 to 2. The moderator pebbles are spheres of graphite and the fuel pebbles have a 0.5 cm thick graphite shell with a fueled core of fuel particles (diameter 502 μm) in a graphite matrix.

Table 1 describes the five types of calculations that were done in relation to this cell. Case 1 corresponds to a fully explicit calculation for which fuel particles, pebbles and the air in between are modeled. This case would correspond to the double heterogeneous calculations using discrete ordinate codes. Case 2 maintains the description of individual pebbles and the shell of the fuel pebbles, but the fuel compact is homogenized. This case would correspond to the single heterogeneous case. Case 3 corresponds to full homogenization within the core volume of all the core materials. In Case 4, the full description of the fuel particles and the fuel region of the fuel pebble is maintained, but all the rest of the materials, moderator and air, are homogenized. This case was intended to characterize the leakage between pebbles.

Finally, Case 5 corresponds to Case 1, but with 20% (volume) water contamination of the air between pebbles.

Table 1. LEUPRO-1 cell calculations, definitions and CPU times for MCNP runs

Description of fuel			Description of moderator and air	Comments	CPU times ^a (min)
Case	Particle	Homogeneous			
1	Yes	No	Explicit	Fully explicit	470.0
2	No	Yes	Explicit	Single heterogeneous	89.0
3	No	Yes	Homogeneous	Whole homogeneous	51.0
4	Yes	No	Homogeneous	Check leakage between pebbles	448.0
5	Yes	No	Explicit	Fully explicit with 20% water	308.0

^aIBM workstation, 50,000 histories.

Table 2. LEUPRO-1 Cell, critical parameters

Case	$k_{\infty}(0)$	$k_{\infty}(B_c^2)$	M(cm)	$B_c^2(m^{-2})^a$	$R_c(cm)^b$
1	1.72186 ± 0.00305	1.68833 ± 0.00512	29.66 ± 0.19	7.825 ± 0.102	109.48 ± 0.71
2	1.63193 ± 0.00319	1.56760 ± 0.00447	29.24 ± 0.18	6.637 ± 0.081	119.12 ± 0.73
3	1.58775 ± 0.00324	1.53414 ± 0.00607	28.31 ± 0.29	6.667 ± 0.116	118.85 ± 1.04
4	1.71916 ± 0.00250	1.66059 ± 0.00454	29.00 ± 0.20	7.856 ± 0.090	109.27 ± 0.62
5	1.59904 ± 0.00200	1.57985 ± 0.00397	20.65 ± 0.13	13.594 ± 0.149	83.51 ± 0.46

^aExtrapolation lengths used: for Cases 1 to 4, $\delta = 2.82$ cm. For Case 5, $\delta = 1.70$ cm.

^bCritical radius of bare core.

Required CPU times for an IBM workstation are also shown in Table 1 for the case of 50,000 histories (100 generations, 500 neutrons each). In general, CPU times are long because of the nature of the transport of neutrons through the graphite and because of the large number of surfaces to track them. Reasonable precision can be obtained in a reasonable amount of time considering the high degree of details of the models.

Table 2 summarizes critical parameters for each case. Statistical errors are either given by MCNP or are the propagation of the 50,000 histories precision. Case 1, with all the details, gives critical size and $k_{\infty}(0)$ very similar to the values of Case 4, i.e., the higher leakage of Case 1 (relative to Case 4) is compensated with a higher $k_{\infty}(B_c^2)$. Similar conclusions apply to the comparison of Cases 2 and 3. The grouping of the four cases into two appears then for the critical size, one around $R=109$ cm, the other around $R=119$ cm. It suggests that the heterogeneity effects due to the fuel particles is more important than the description of the leakage between the pebbles. Note that the critical dimension here is the radius of a sphere that averages effects in all directions. Had we chosen slab geometry, the results could have been different.

Reaction rates for the core materials averaged over core volumes are shown in Table 3 for the five cases. Statistical errors depend on the frequency of occurrence which depends on densities and cross sections, and the total number of histories. Precision is high for materials like ^{235}U and low for materials like ^{11}B . Spectral indices appear in Table 4. The energy cutoff is 0.625 eV as specified in Ref. 2.

Table 3. LEUPRO-1 cell, reaction rates^a

Captures — Case ^b					
Isotope	1	2	3	4	5
²³⁵ U	1.4165-1	1.3481-1(0.3)	1.3050-1	1.4120-1	1.1976-1
²³⁸ U	1.3154-1	1.8264-1(0.1)	2.0761-1	1.3326-1	6.5462-2
C	2.6704-2	2.4970-2(1.1)	2.3581-2	2.6586-2	2.5102-2
N	2.4351-3	2.3008-3(4.2)	2.1471-3	2.4271-3	1.8890-3
¹⁰ B	6.9518-3	6.5129-3(20.0)	7.6244-3	8.2470-3	7.5806-3
¹¹ B	1.8452-7	6.9323-8(47.8)	2.9924-9	6.7247-8	1.0355-7
H	5.4114-6	5.9820-6(1.0)	5.9239-6	7.8911-6	1.2961-1
O	6.8785-5	7.5918-5(14.7)	4.2348-5	7.9080-5	5.5910-4
Si	2.6464-3	2.4216-3(4.0)	2.3705-3	2.6426-3	2.5028-3
Fissions — Case ^b					
²³⁵ U	6.8673-1	6.4572-1(0.13)	6.2511-1	6.8433-1	6.4651-1
²³⁸ U	1.2442-3	9.9154-4(13.7)	9.7454-4	1.2248-3	1.0099-3

^aRelative to total absorptions. Estimation of precision between parenthesis (%) for Case 2.

^bSee Table 1 for definition of cases.

Table 4. LEUPRO-1 cell. Spectral indices^a

Case					
Spectral index	1	2	3	4	5
ρ^{28} : Ratio epithermal to thermal captures in ²³⁸ U	7.594(1.6)	11.75	13.88	7.658	3.371
δ^{25} : Ratio epithermal to thermal fission in ²³⁵ U	0.1125(0.84)	0.1156	0.1157	0.1107	0.04789
δ^{28} : Ratio macroscopic ²³⁸ U to ²³⁵ U fissions	0.001845(1.0)	0.001676	0.001554	0.001842	0.001562
C*: Ratio of macroscopic ²³⁸ U captures to ²³⁵ U fissions	0.1906(1.5)	0.2821	0.3290	0.1924	0.1012

^aTypical precisions (in %) are shown for Case 1.

2.2 RESULTS FOR THE WHOLE REACTOR BENCHMARK PROBLEM

2.2.1 LEUPRO-1 Cell

Table 5 describes the parameters of the MCNP runs for 50,000 and 500,000 histories. Note that the pebbles were explicitly modeled. The model of the fuel pebbles includes both the fuel compact and the graphite shell. The fuel compact was modeled as a uniform mix and also explicitly with a model for the UO₂ fuel kernel, buffer, 3 coatings and the graphite matrix. For this last case, a cubic lattice for the fuel

particles was assumed with a distance between particles given by the number of fuel particles per unit volume. Number densities and dimension were taken from Ref. 2. Because of the shape of the cavity containing the pebbles, a cylinder of radius 58 cm, and the explicit modeling of the fuel lattice, the boundaries between the core and reflector cut the pebbles in the way described by Fig. 1 for odd layers, and Fig. 2 for even layers. The pebbles of the first layer sit at the bottom of the cavity as Fig. 3 shows. This figure shows an xz cut across the origin of coordinates in Fig. 1 with details of the air gap (as large as the core), aluminum structure of the upper plug of the cavity, and radial and axial graphite reflectors. Table 6 compares results for k using a homogeneous model for the fuel compact or modeling it with all the details. The fuel particle heterogeneous effects amounts to a $(1.48 \pm 0.61)\%$ difference in reactivity, which is comparable, although larger, than the case of the VH1-HP benchmark. Obviously more histories are needed to have a better precision for this effect.

Table 5. PROTEUS benchmark. Whole reactor with LEUPRO-1 cell. Parameters of MCNP runs

	Homogenized compact	Heterogeneous compact
Number of generations	100	100
Neutron per generation	500	500 and 5,000
Total number of histories	50,000	50,000 and 500,000
CPU time for IBM WS (min) ^a	147.0	43.4 and 3,658

^aFor k calculations only, tallies for reaction rates increase CPU times.

Table 6. PROTEUS benchmark. Whole reactor with LEUPRO-1 cell, 99 cm height core^a

	Homogeneous compact (50,000)	Heterogeneous compact (50,000)	Heterogeneous compact (500,000)
k	0.99726 ± 0.00433	1.01205 ± 0.00429	1.01665 ± 0.00134
Leakage/Absorption ^b	0.20350	0.20604	0.20720
Production/Absorption ^b	1.20021	1.22057	1.22730

^aNumber of histories are shown in parenthesis.

^bReactor average.

Table 7 summarizes the sequence of calculations to obtain the critical height. The fit of these results is shown in Fig. 4, which gives 94.61 cm for the critical height and a reactivity coefficient of 299 pcm per centimeter of layer. This last number is only an indicator because, as Fig. 5 shows, the upper plane cuts the top layer in a nonlinear way.

Table 7. PROTEUS benchmark. Whole reactor with LEUPRO-1 cell.
Approach to critical heterogeneous compact model

Height (cm) ^a	k
92.21	0.99218 ± 0.00387
93.92	0.99438 ± 0.00455
94.49	1.00067 ± 0.00398
95.00	1.00495 ± 0.00415
99.00	1.01205 ± 0.00429

^aMeasured from the plane tangent to the lowest layer.

Fig. 1. PROTEUS benchmark. Whole reactor with LEUPRO-1 cell, odd layers of pebbles. The hexagons mark positions in the lattice only. The two concentric circles indicate the shell of the fuel pebbles.

Fig. 2. PROTEUS benchmark. Whole reactor with LEUPRO-1 cell, even layers of pebbles.

Fig. 3. PROTUS benchmark. Whole reactor with LEUPRO-1 cell. Configuration of core, air gap, axial and radial graphite reactors and the aluminum structure of the upper plug of the cavity.

Fig. 4. PROTEUS benchmark. Whole reactor with LEUPRO-1 cell. MCNP results (with uncertainties) for the reactivity as function of core height.

Fig. 5. PROTEUS benchmark. Whole reactor with LEUPRO-1 cell. Cut at 94.49 cm height (around critical) showing how the pebbles would be cut.

The reactivity of the 94.61 cm height core was calculated with a 500,000 histories MCNP run resulting in $k = 0.99765 \pm 0.00130$ which, with the reactivity coefficient of 299 pcm/cm, gives a critical height of (95.39 ± 0.43) cm. Axial and radial reaction rates were computed for the detector regions shown in Figs. 6 and 7 realistically located between the pebbles. The hexagonal cell located immediately above the center in Fig. 6 and at middle core height was chosen to calculate the reaction rates and spectral indices shown respectively in Tables 8 and 9.

Table 8. PROTEUS benchmark. Whole critical reactor with LEUPRO-1 cell. Reaction rates^a for core material in the center of the core. Heterogeneous compact calculation.

Isotope	Fissions/Absorptions	Captures/Absorptions
²³⁵ U	0.67206 (3%)	0.14348
²³⁸ U	0.0011779 (5%)	0.13958 (13%)
C	—	0.025823
¹⁰ B	—	0.012447
Si	—	0.0031127
N	—	0.0025264 (28%)
O	—	2.6831-6
¹¹ B	—	0 ^b
H	—	0 ^b

^aErrors depend on isotopic concentration, cross sections and number of histories, some relative errors in parentheses.

^bFor the 500,000 histories statistics.

Table 9. PROTEUS benchmark. Whole critical reactor with LEUPRO-1 cell. Spectral indices inside fuel particles at the center of the core.

Spectral indices	Value (% error)
ρ^{28}	7.669 (14.3%)
δ^{25}	0.1174 (5%)
δ^{28}	0.001927 (5.6%)
C*	0.1915 (13.3%)

The ratio of infinite diluted Pu isotopes reaction rates to the shielded fission rate of ²³⁵U (per atom) was computed as shown in Table 10.

Table 10. PROTEUS benchmark. Whole critical reactor with LEUPRO-1 cell. Ratio of Pu reaction rates (infinite diluted) to the ²³⁵U fission rate (per atom). Reaction rates inside fuel particles at the center of the core.

Pu isotope	Reaction	Ratio (% error)
²³⁹ Pu	Fission	2.055 (4.3%)
²⁴⁰ Pu	Capture	3.447 (15.0%)
²⁴¹ Pu	Fission	2.349 (4.0%)

Fig. 6. PROTEUS benchmark. Whole reactor with LEUPRO-1 cell. Location of vertical detector regions around the center of the cavity.

Fig. 7. PROTEUS benchmark. Whole reactor with LEUPRO-1 cell. Location of vertical and horizontal detector regions.

Axial and radial fission rates for ^{235}U , ^{239}Pu , ^{238}U , ^{232}Th , and ^{237}Np are shown in Figs. 8-11. They are the sum of the fission rates in the twelve vertical detector regions of Fig. 6 and the two horizontal detector regions of Fig. 7. Note that they correspond to infinitely diluted detector materials located, as in a real experiment, between the interstices of the pebbles. As the detector passes in front of different kinds of pebbles, some structure in the shape of the curve might appear. The statistical precision shown in Figs. 8-11 is not high enough to show this possible behavior, but the models include all the details necessary to explore this possibility. Numerical values are tabulated in Appendix A.

Fig. 8. PROTEUS benchmark. Whole reactor with LEUPRO-1 cell. Axial relative distribution of ^{235}U (continuous line) and ^{239}Pu (+) fission rates.

Fig. 9. PROTEUS benchmark. Whole reactor with LEUPRO-1 cell. Axial relative distribution of ^{238}U (continuous line), ^{232}Th (+), and ^{237}Np (*) fission rates.

Fig. 10. PROTEUS benchmark. Whole reactor with LEUPRO-1 cell. Radial relative distribution of ^{235}U (continuous line) and ^{239}Pu (+) fission rates.

Fig. 11. PROTEUS benchmark. Whole reactor with LEUPRO-1 cell. Radial relative distribution of ^{239}U (continuous line), ^{232}Th (+), and ^{237}Np (*) fission rates.

The reactivity values of control rods located at the center of the core are shown in Table 11. The control rods correspond to the specification of the benchmark (Ref. 2): 1.05 cm radius borated steel inside a 2 mm thick Al cladding both inside a graphite sheath 1 cm thick and with a 2.45 cm external radius.

Table 11. PROTEUS benchmark. Whole reactor with LEUPRO-1 cell.^a
Reactivities of control rods at the center of the core.

Case	k	$\Delta k(\%)$
No CR, core 94.49 cm	0.99901 ± 0.00144	—
CR length 94.49 cm ^b	0.96722 ± 0.00147	-3.18 ± 0.20
CR length 173 cm ^b	0.96422 ± 0.00134	-3.48 ± 0.20

^a500,000 histories, heterogeneous compact.

^bCR totally inserted in core, the longer rod occupies additionally the air above the core.

2.2.2 LEUPRO-1 Cell with 20% Water

The case of the LEUPRO-1 cell contaminated with 20% (volume) water was analyzed with the same model: full explicit representation of pebbles and fuel particles. The air between pebbles was uniformly contaminated with water and the air above the pebbles inside the cavity was assumed to be not contaminated. Table 12 summarizes the reactivity results.

Table 12. PROTEUS benchmark. LEUPRO-1 cell (20% water).
Results for k and critical height.

Core height $H_c = 99$ cm	$k = 1.10864 \pm 0.00111$
Core height $H_c = 71.65$ cm	$k = 1.00209 \pm 0.00117$
Reactivity coefficient	$\frac{\delta k}{\delta H_c} = 399$ pcm/cm
Critical core height	$H_c = (71.11 \pm 0.30)$ cm

Reaction rates, spectral indices and Pu reaction rates at the center of the critical core are shown, respectively, in Tables 13, 14, and 15.

Table 13. PROTEUS benchmark. LEUPRO-1 cell (20% water).
Reaction rates at center of core.

Isotope	Fission/absorption	Capture/absorption
H	—	0.138224
²³⁵ U	0.634172	0.117296
²³⁸ U	0.00143661	0.0739748
C	—	0.0260736
¹⁰ B	—	0.00419218
N	—	0.00238956
Si	—	0.00176353
O	—	0.00004776
¹¹ B	—	0 ^a

^aFor 500,000 histories.

Table 14. PROTEUS benchmark. LEUPRO-1 cell (20% water).
Spectral indices inside fuel kernel at center of core.

Spectral indices	Value (relative error)
ρ^{28}	2.6868 (17%)
δ^{28}	0.04764 (6%)
δ^{28}	0.001663 (4.7%)
C*	0.08438 (12%)

Table 15. PROTEUS benchmark. LEUPRO-1 cell (20% water). Pu reaction rates.

Pu isotope	Reaction	Ratio ^a (relative error)
²³⁹ Pu	Fission	1.6907 (3.7%)
²⁴⁰ Pu	Capture	1.5392 (13%)
²⁴¹ Pu	Fission	2.0932 (3.7%)

^aInfinite diluted cross section divided by shielded ²³⁵U fission cross section.

Axial and radial fission rates for ²³⁵U, ²³⁹Pu, ²³⁸U, ²³²Th, and ²³⁷Np are shown in Figs. 12—15. They are the sum of the fission rates in the twelve vertical detector regions of Fig. 6 and the two horizontal detection regions of Fig. 7. Note that they correspond to infinitely diluted detector materials located, as in a real experiment, between the interstices of the pebbles. As the detector passes in front of different kinds of pebbles, some structure in the shape of the curve might appear. The statistical precision of Figs. 12—15, shown in the figures, is not high enough to show this possible behavior, but the models include all the details necessary to explore this possibility. Numerical values are tabulated in Appendix A.

Fig. 12. PROTEUS benchmark. Whole reactor with LEUPRO-1 cell (20% water). Axial relative distribution of ^{235}U (continuous line) and $^{239}\text{Pu}(+)$ fission rates.

Fig. 13. PROTEUS benchmark. Whole reactor with LEUPRO-1 cell (20% water). Axial relative distribution of ^{238}U (continuous line), $^{232}\text{Th}(+)$, and $^{237}\text{Np}(*)$ fission rates.

Fig. 14. PROTEUS benchmark. Whole reactor with LEUPRO-1 cell (20% water). Radial relative distribution of ^{235}U (continuous line) and $^{239}\text{Pu}(+)$ fission rates.

Fig. 15. PROTEUS benchmark whole reactor with LEUPRO-1 cell (20% water). Radial relative distribution of ^{238}U (continuous line), $^{232}\text{Th}(+)$, and $^{237}\text{Np}(*)$ fission rates.

3. RESULTS FOR THE PROTEUS CRITICAL CONFIGURATIONS

A more realistic model of the cavity that contains the pebbles was developed. This 12-sided polygon was designed for the real experiments, and modeled with MCNP to contain 361 pebbles at odd layers and 345 at even ones with layer number 1 at the bottom of the cavity. Figures 16, 17, and 18 are MCNP plots of odd and even layers; odd layers fit the cavity, even layers need spacers (also modeled). Vertical cross section views of the pebble bed and the whole reactor are shown in Figs. 19, 20, and 21. Figure 21 shows the model beyond the pebble bed, air above the bed, aluminum structure of the upper plug, axial and radial reflectors. Dimensions and number densities are from Ref. 2, and the portion of the model beyond the pebble bed is still schematic, especially with the description of the upper plug. Note also that the model does not describe any control device. Both simplifications can be eliminated easily in future models.

Table 16 summarizes typical parameters of MCNP runs. Considering the degree of details, 7421 pebbles in a 21-layers configuration with 9394 fuel particles per fuel pebble, the CPU times are quite reasonable.

Table 16. PROTEUS critical configuration, LEUPRO-1 cell. Parameters of MCNP runs.

	Homogenized compact	Heterogeneous compact
Number of generations	100	100
Neutrons per generations	500	500 and 5,000
Total number of histories	50,000	50,000 and 500,000
CPU ^a time for IBM WS (min)	155	386 and 5,846

^aCalculations of k only.

Results for configurations with 19 and 21 layers are in Table 17. Note that at the time of this calculation the spacers were not included in the model.

Table 17. PROTEUS critical configurations, LEUPRO-1 cell.
Heterogeneous compact. Spacers at even layer not included.

Case	k^a
21 layers	1.01929 ± 0.00369
19 layers	0.99284 ± 0.00426

^a50,000 histories.

The reactivity effects of the spacers were calculated for the 19-layers configuration. Table 18 summarizes the results.

Table 18. PROTEUS critical configurations, LEUPRO-1 cell.
Heterogeneous compact. Spacers included.

19 layers	$k = 0.99711 \pm 0.00367$
Reactivity effects of spacers ^a	$\Delta k = 0.43\%$

^aFrom Tables 17 and 18.

Note that the error in Δk is as large as Δk itself and more histories in the Monte Carlo calculations are necessary for higher precision in the calculation of this parameter.

Fig. 16. Critical configurations of PROTEUS, LEUPRO-1 cell, odd layers of 361 pebbles.

Fig. 17. Critical configurations of PROTEUS, LEUPRO-1 cell, even layers of 345 pebbles with graphite spacers to fit them within the 12-sided polygon.

Fig. 18. Critical configuration of PROTEUS, LEUPRO-1 cell, details of even layers.

Fig. 19. yz view of the pebble bed at $x = -5.2$ cm (Fig. 16 coordinate axis).

Fig. 20. yz view of the pebble bed at $y = 3$ cm (Fig. 16 coordinate axis). Note spacers at even layers.

Fig. 21. yz view of the whole reactor at $x = -5.2$ cm (Fig. 16 coordinate axis).

Higher statistical precisions were obtained for the model that includes the spacers, the results are shown in Table 19.

Table 19. PROTEUS critical configuration, k as function of number of layers for 500,000 histories.

Number of layers	k
19	0.99466 ± 0.00132
21	1.02635 ± 0.00120
22	1.04318 ± 0.00128

Figure 22 shows that the results of Table 19 fit very well to a linear behavior with a reactivity coefficient ($\Delta \rho / \Delta$ layer) of 1558 pcm/layer or 318 pcm/cm (2 layers in one hexagonal cell with 9.8 cm high). This number is very consistent with the result of the benchmark (299 pcm/cm, see Section 2.2.1). Note that we are showing results for a whole number of layers and not for a fraction (like in Section 2.2.1). From Table 19 a 22-layer configuration would have $k = 1.04318$, 1.2% larger than the experimental value of 1.0311 quoted in Ref. 3.

A word of caution about this result: (1) the model is based exclusively on data from Ref. 2; more data are being collected related to effective diameter of the fuel region of the pebbles, effective absorption of the graphite, etc., (2) more details about the upper plug and its aluminum structure can be included in the model, and (3) new experimental data, this time without the perturbations of the rest worth of the Zebra rod (taking into account anyway in the experimental k) are being measured.

4. NOTE ABOUT ^{10}B EQUIVALENT CONTAMINATION

MCNP calculations of the reaction rates of nuclides present in the benchmark show that 3.51% of the absorptions in the reactor occur in the ^{10}B . This number is 0.98% for the core volume; 80.36% of the absorptions in the ^{10}B occur in the reflector. For the VH1-HP benchmark, these numbers are, respectively 0.284%, 0.04%, and 84.84%. There is an order of magnitude difference in the effects of the impurities between both benchmarks; therefore, interpretations of the PROTEUS benchmark are going to rely on accurate measurements of the impurities of the reflector graphite (measurements are in progress).

5. SIMULATION OF PULSED NEUTRON EXPERIMENTS

One technique to check the equivalent boron concentration of the impurities in the graphite is to measure the decay constant of the neutron population (α) after the injection of pulses of neutrons in the system to be checked.⁵ The measured decay constant is then compared with calculated values in order to fit the α 's by changing the amount of boron in the model. It is then crucial to have a realistic model in order to avoid biases related to approximations. This requirement is very difficult to meet with discrete ordinates and multigroup codes because of the complicated geometry of the materials surrounding the core (a hollow piece of graphite with structural materials) and the lack of fissile materials (reactor physics codes compute α only for multiplicative-systems).

Fig. 22. PROTUS configurations within the 12-sided polygon, k vs. number of layers.

For these reasons MCNP is an ideal tool to compute α because of the flexibility of the geometrical specifications, the continuous energy model, and the mimic of the events suffered by a neutron after its injection into the system.

A typical result for the counting rate of $1/v$ neutron detectors after the injection of 14 MeV pulses of neutrons is shown in Fig. 23. The point source was located 10 cm below the floor of the cavity shown in Fig. 21, and the calculations correspond to the system without fuel and moderator pebbles, i.e., radial and axial graphite reflectors around the 12-sided empty cavity and the aluminum structure of the upper plug.

Exponential fits of the asymptotic part of the temporal responses give the α 's to be compared with the experiment. We report the results of 6 calculations: (1) the one described, (2) the same, but with 4 times the boron concentration, (3) one that corresponds to the system described, but without the upper axial reflector and its associated structural part, (4) cylindrical like 1, but 58 cm cylindrical cavity, and (5-6) like 3, but 58 cm and 60.78 cm cylindrical cavities.

Case 5 was computed in Ref. 5 using the discrete ordinate transport code TWODANT and a 13 energy group (4 thermal) cross section library as the asymptotic value (zero fuel) of a series of calculations with diluted fuel in the cavity. This laborious method, necessary because of the way discrete ordinate codes compute α 's, gives $\alpha = 167 \text{ sec}^{-1}$.

The sensitivity of α with respect to the boron concentration is, from Cases 1 and 2 of Table 20, $(3.86 \pm 0.54) \text{ sec}^{-1}/\text{nominal boron concentration (nbc)}$. This value was also computed in Ref. 5 as $\sim 6 \text{ sec}^{-1}/\text{nbc}$. A pure absorbing effect of the boron (i.e., no implication in leakage) would give a sensitivity of $7.6 \text{ sec}^{-1}/\text{nbc}$.

The effects of the cylindrical idealization of the cavity on calculated α 's are also shown in Table 20. The 12-sided cavity has an equivalent radius of 60.78 cm that conserves the transverse areas, volumes, and amount of materials. When Case 6 ($\alpha = 165 \text{ sec}^{-1}$) is compared to Case 3 ($\alpha = 167 \text{ sec}^{-1}$) it became apparent that the idealization does not conserve the internal axial surface of the cavity and

Table 20. Neutron decay constant^a for the graphite around the cavity of PROTEUS

Case	System	$\alpha(\text{sec}^{-1})$
1	12-sided cavity nominal boron concentration ^b	129.81 ± 0.14
2	12-sided cavity, 4 times nominal boron concentration	145.24 ± 0.52
3	12-sided cavity, without the upper plug, nominal boron concentration	167.30 ± 0.31
4	58 cm cylindrical cavity nominal boron concentration	128.65 ± 0.12
5	Without the upper plug, nominal boron, 58 cm cylindrical cavity	161.89 ± 0.20
6	Without the upper plug, nominal boron, 60.78 cm cylindrical cavity	164.98 ± 0.21

^a100,000 histories.

^b0.1 ppm.

Fig. 23. MCNP simulation of PNS experiment in the system of Fig. 21 without the fuel and moderator pebbles.

consequently the leakage through it. The radius 58 cm for Cases 4 and 5 was taken from Ref. 2 and corresponds to an arrangement with the same lattice, but rotated with respect to axis z. Comparing Cases 1 and 4 for the whole cavity (i.e., with the aluminum structure) the α 's show less sensitivity to the value of the radius, probably due to the presence of the Al absorber. By contrast, for Cases 3 and 5, for the cavity without the upper plug reflector, the difference between the α 's, 167 sec vs 162 sec⁻¹, shows more sensitivity to the equivalent radius.

6. CYLINDRICAL IDEALIZATION OF THE PROTEUS CONFIGURATION

Section 3 shows how MCNP allows the creation of models with details that are not possible to simulate with other types of codes. Boundary conditions like the 12-sided polygon of the PROTEUS cavity are simulated in discrete ordinate codes as cylinders. Furthermore, the core is simulated as uniform mixtures after cell calculations despite the fact that the symmetry of the lattice disappears at the boundaries (including those at the top and bottom of the core).

This section addresses how to define an equivalent radius ($\bar{R}$) and height ($\bar{H}$) of a LEUPRO-1 cell core inside the 12-sided PROTEUS cavity and what are the biases related to the cylindrical idealization.

The whole reactor benchmarks and the PROTEUS critical configurations were calculated with the c axis of the hexagonal compact cell along the axial axis. This is the case of the present series of experiments at PSI. However, the original definition² of the benchmark corresponds to a rotated cell; for a model which homogenizes the cell the rotation does not matter, but MCNP models might be sensitive to the rotation. Table 21 shows different criterias for the definitions of $\bar{R}$ and $\bar{H}$.

Table 21. Different criterias for the cylindrical idealization of the PROTEUS configurations

Criteria	$\bar{R}(cm)$	$\bar{H}(cm)$	Comment
1	58.0	9.7979 cm each 2 layers	$\bar{R} = 58$ cm from Ref. 2
2	Core: 60.12 Gap: 60.78	Conserve volume of pebbles $\bar{H} = 104.46$ cm for 22 layers	Conserve areas and volumes

Case 1 corresponds to the acceptance of the $\bar{R}$ value from Ref. 2 which corresponds to the rotated lattice. The value $c = 9.7979$ cm per 2 layers corresponds to the symmetry of the hexagonal compact lattice with the c axis vertical. Figure 24 checks this criteria by the comparison of the reactivities from Table 7, which corresponds to the 58 cm cylindrical cavity to the reactivities in Table 19, which corresponds to the 12-sided cavity with a whole number of layers. The "translation" of layers to height is 9.7979 cm per 2 layers. Figure 24 shows also the linear fits of ρ vs H for each set of data; they agree very well. We conclude then that criteria #1 for the cavity gives the right critical height (or number of layers) but not the critical mass because the equivalent radius of the cavity to conserve area is 60.12 cm (see later) rather than 58 cm. The bias for the critical mass is then $(60.12/58)^2 = 1.074$.

The radius of the circles with the same areas of the odd and even layers of Figs. 16 and 17 are, respectively, 60.78 cm and 59.47 cm which give an average $\bar{R} = 60.12$ cm. Using this radius, conserving the volume of the pebbles and considering the packing fraction of 0.7405 for an infinite hexagonal compact lattice, results $H = 104.46$ cm for 22 layers. Note that this number is smaller than $22 \cdot 9.7979/2 = 107.78$ cm which corresponds to criteria #1. Then we have that the dimensions of Table 21 for criteria #2 conserve masses, areas, and volumes.

Fig. 24. Reactivity vs. H for the cylindrical and 12-sided cavity.

The 22 layers case of Table 19 was idealized with criteria #2 for an MCNP run resulting in $k = 1.04663 \pm 0.00118$ rather than $k = 1.04318 \pm 0.00128$ that corresponds to the more realistic calculation. Indeed, like in the case of the α calculations, the cylindrization conserves the volumes, but not the axial surfaces resulting in the calculation of a system with less leakage and consequently larger k 's. The biases for criteria #2 are then (345 ± 167) pcm for k , (-1.15 ± 0.56) cm or (-0.23 ± 0.11) layers for the critical height and $(-1.22 \pm 0.60)\%$ for the critical mass.

7. COMPARISON WITH OTHER CALCULATIONS

The PROTEUS benchmark is presently the object of study of an international group of laboratories. Tables 22 to 28 summarize the comparison of the results of this work with the results of a group of 5 laboratories in the form of averages and their dispersions. The only Monte Carlo and continuous energy analysis is ours; the rest used discrete ordinates codes and multigroup cross sections. The other five laboratories are: Paul Scherrer Institute (PSI) (Switzerland), Institute of Nuclear Energy Technology (China), KFA Research Center Julich (Germany), Japan Atomic Energy Research Institute and the Kurchatov Institute (Russia).

The results for the unit cells agree, in general, quite well within our statistical errors and their dispersion. However, for the whole reactor cases, our critical heights are about 3 cm (0.61 layer) higher than their results. Our evaluation of the reactivity worth of a central borated-steel rod agrees better with the PSI results.

Table 22. LEUPRO-1 cell. Comparison of results.

Parameter	This work ^a	Other labs ^b
$k_{\infty}(0)$	1.722 ± 0.003	1.716 ± 0.006
$k_{\infty}(B_c^2)$	1.688 ± 0.005	1.669 ± 0.008
$B_c^2(m^{-2})$	7.82 ± 0.10	7.75 ± 0.16
$M^2(cm^2)$	880.0 ± 11.0	871.0 ± 23.0
ρ^{28}	7.59 ± 0.12	7.77 ± 0.24
δ^{25}	0.112 ± 0.001	0.114 ± 0.012
δ^{28}	0.00184 ± 0.00002	0.00154 ± 0.00015
C^*	0.191 ± 0.003	0.194 ± 0.005

^aFrom Tables 2 and 4.

^bFrom Ref. 4, averages and dispersions are from the results of 5 laboratories.

Table 23. LEUPRO-1 cell with 20% vol. water. Comparison of results.

Parameter	This work ^a	Other labs ^b
$k_{\infty}(0)$	1.599 ± 0.002	1.596 ± 0.011
$k_{\infty}(B_c^2)$	1.580 ± 0.004	1.578 ± 0.012
$B_c^2(m^{-2})$	13.6 ± 0.1	13.2 ± 0.7
$M^2(cm^2)$	426.0 ± 5.0	439.0 ± 20.0
ρ^{28}	3.37 ± 0.005	3.32 ± 0.11
δ^{25}	0.0479 ± 0.0004	0.0468 ± 0.0021
δ^{28}	0.00156 ± 0.00002	0.00126 ± 0.00013
C^*	0.101 ± 0.002	0.100 ± 0.003

^aFrom Tables 2 and 4.^bFrom Ref. 4, averages and dispersions are from the results of 3 laboratories.

Table 24. LEUPRO-1 cell. Singly heterogeneous model (no grain structure).

Parameter	This work ^a	Other labs ^b
$k_{\infty}(0)$	1.6319 ± 0.0032	1.6313 ± 0.0040
$k_{\infty}(B_c^2)$	1.5676 ± 0.0045	1.5742 ± 0.0025
$B_c^2(m^{-2})$	6.64 ± 0.08	6.95 ± 0.20
$M^2(cm^2)$	855.0 ± 10.0	826.0 ± 28.0

^aFrom Tables 2 and 4.^bFrom Ref. 4, averages and dispersions are from the results of 2 laboratories.

Table 25. LEUPRO-1 cell. Critical radius (cm).

Case	This work ^a	Other labs ^b
Double heterogeneous (DH)	109.48 ± 0.71	110.03 ± 1.13
Single heterogeneous	119.12 ± 0.73	116.35 ± 1.67
DH and 20% water	83.51 ± 0.46	84.77 ± 2.25

^aFrom Table 2.^bFrom Ref. 4 using $\delta = 2.82$ cm for the normal cell and $\delta = 1.70$ cm for the 20% water case.

Table 26. Whole reactor results for LEUPRO-1 cell.

Parameter	This work ^a	Other labs ^b
k_{eff} 99 cm core height	1.0166 ± 0.0013	1.0248 ± 0.0038
Critical height, $H_c(\text{cm})$	95.39 ± 0.43	92.29 ± 0.62
Spectral indices core center:		
ρ^{28}	7.67 ± 1.10	7.67 ± 0.15
δ^{25}	0.117 ± 0.006	0.114 ± 0.015
δ^{28}	0.00193 ± 0.00011	0.00162 ± 0.000015
C^*	0.191 ± 0.025	0.193 ± 0.005

^aFrom Tables 6 and 9, and text section 2.2.1.

^bFrom Ref. 4, averages and dispersions are from the results of 5 laboratories.

Table 27. Whole reactor results for LEUPRO-1 cell with 20% v water.

Parameter	This work ^a	Other labs ^b
k of 99 cm core height	1.1086 ± 0.0011	1.1162 ± 0.0005
Critical height, $H_c(\text{cm})$	71.11 ± 0.30	68.60 ± 0.13
Spectral indices core center:		
ρ^{28}	2.69 ± 0.46	3.31 ± 0.12
δ^{25}	0.0476 ± 0.0028	0.0442 ± 0.0024
δ^{28}	0.00166 ± 0.00008	0.00134
C^*	0.0844 ± 0.0101	0.101 ± 0.001

^aFrom Tables 1, 2, and 14.

^bFrom Ref. 4, averages and dispersions are from the results of 3 laboratories (only one contribution for δ^{28}).

Table 28. Reactivity worth^a of a central borated-steel rod in LEUPRO-1.

	This work ^b	Other labs ^c
Core height rod	$- 3.18 \pm 0.20$	$- 2.67 \pm 0.33$
173 cm high rod	$- 3.48 \pm 0.20$	$- 2.96 \pm 0.45$

^a δk in %.

^bFrom Table 11.

^cFrom Ref. 4, averages and dispersions are from the results of 2 laboratories.

8. CONCLUSIONS AND RECOMMENDATIONS

MCNP calculations of the PROTEUS benchmark allow unprecedented degree of details in the models not available with other methods (see Appendix B for a geometry tour). The reactor was modeled in all of its details from the fuel particles (502 microns diameter) to the radial reflector (3.26 m outside diameter) and with continuous energy representation of the cross sections. Details like each one of the thousands of pebbles or the spacers can be modeled exactly with the flexibility of MCNP.

All the requested parameters from the specifications of the benchmarks can be calculated (e.g., see the report about VH1-HP benchmark). In addition, pulsed neutron experiments (usual technique at PROTEUS and VHTRC facilities) can be modeled explicitly with MCNP, providing an important role in the interpretation of experiments to determine the impurities of the graphite and reactivities.

Our results for the critical heights are different with respect to the calculations of five independent groups, although very promising in relation to the experimental finding at PROTEUS.

The model can be easily improved by the introduction of more geometric details of the reflectors and upper plug and more updated values for the number densities. Required CPU times are large; in a good proportion this is due to the long lifetime of the neutrons in the graphite system. The problem is particularly severe when PNS experiments near critical are simulated. It is strongly recommended to use the high performance computer resources at ORNL to take advantage of the flexibility of MCNP to work on parallel architectures.

9. REFERENCES

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APPENDIX A. TABULATION OF FISSION RATES

Table A.1. Benchmark LEUPRO-1 whole reactor axial values of reaction rates

z(cm)	Region	Fissions U235	Rel. error	Fissions U238	Rel. error
4.0	Bottom Reflector	6.65966E-03	0.0622	7.48273E-11	0.1325
13.0		1.91121E-02	0.0420	1.99487E-10	0.0916
23.0		3.13378E-02	0.0334	6.97744E-09	0.6271
33.0		4.72664E-02	0.0286	6.09306E-08	0.4425
43.0		6.09515E-02	0.0240	1.03562E-07	0.3620
53.0		7.78520E-02	0.0218	3.06650E-07	0.2143
63.0		8.25399E-02	0.0208	1.38388E-06	0.1140
70.5		7.59483E-02	0.0255	2.47162E-06	0.1161
75.5		6.67324E-02	0.0264	4.87431E-06	0.0785
80.5	Core	5.81615E-02	0.0250	8.01495E-06	0.0590
85.5		5.06156E-02	0.0268	1.09269E-05	0.0537
90.5		4.74258E-02	0.0268	1.12136E-05	0.0513
95.5		4.36186E-02	0.0267	1.19602E-05	0.0510
100.5		4.09877E-02	0.0268	1.15661E-05	0.0523
105.5		4.01023E-02	0.0272	1.16059E-05	0.0535
110.5		3.96903E-02	0.0289	1.17034E-05	0.0518
115.5		4.06339E-02	0.0271	1.13040E-05	0.0517
120.5		4.00060E-02	0.0285	9.83012E-06	0.0542
125.5		3.83970E-02	0.0296	1.09998E-05	0.0541
130.5		3.68246E-02	0.0279	1.1032 e-05	0.0531
135.5		3.25712E-02	0.0302	9.98499E-06	0.0572
140.5		3.12028E-02	0.0302	9.96479E-06	0.0553
145.5		3.01266E-02	0.0307	8.93325E-06	0.0594
150.5		2.89655E-02	0.0312	7.54016E-06	0.0644
155.5		2.62107E-02	0.0356	7.35182E-06	0.0640
160.5		2.68024E-02	0.0331	6.71965E-06	0.0681
165.5		2.46510E-02	0.0375	5.854 e-06	0.0699
170.245		2.49159E-02	0.0357	4.72434E-06	0.0853
175.245	Air	2.90072E-02	0.0298	3.04307E-06	0.0943
183.0		2.86319E-02	0.0224	2.49470E-06	0.0832
193.0		3.00409E-02	0.0225	2.24401E-06	0.0907
203.0		2.82073E-02	0.0225	1.86661E-06	0.1005
213.0		2.88309E-02	0.0222	1.68152E-06	0.1047
223.0		2.88533E-02	0.0224	1.18143E-06	0.1290
233.0		2.96676E-02	0.0219	1.08908E-06	0.1678
244.5		2.71118E-02	0.0200	9.04600E-07	0.1445
259.15	Al	2.70816E-02	0.0185	1.05868E-06	0.1352
272.3	Top Reflector	2.91329E-02	0.0306	5.12213E-07	0.1932
282.3		2.63982E-02	0.0337	1.39893E-07	0.4293
292.3		2.36900E-02	0.0366	6.34177E-08	0.5374
302.3		1.95351E-02	0.0416	2.82272E-08	0.6308
312.3		1.33614E-02	0.0470	1.12684E-08	0.9801
322.3		1.02396E-02	0.0558	2.21318E-08	0.7042
333.3		6.30964E-03	0.0690	6.60665E-11	0.1289
341.3		1.90763E-03	0.1138	1.78623E-11	0.1112

Table A.2. Benchmark LEUPRO-1 whole reactor radial values of reaction rates

r(cm)	Region	Fissions U235	Rel. error	Fissions U238	Rel. error
3.46	Core	3.68045E-02	0.0413	9.89698E-06	0.0775
9.16		3.63767E-02	0.0397	1.04336E-05	0.0741
15.10		3.86522E-02	0.0387	1.09158E-05	0.0765
21.07		3.66548E-02	0.0375	1.11837E-05	0.0728
27.05		3.53010E-02	0.0409	9.41290E-06	0.0806
33.04		3.68983E-02	0.0406	1.13792E-05	0.0720
39.04		3.81345E-02	0.0383	1.23480E-05	0.0694
45.03		4.16866E-02	0.0387	1.03827E-05	0.0721
51.03		4.29161E-02	0.0422	9.10472E-06	0.0798
57.03		4.84161E-02	0.0364	6.10027E-06	0.0979
63.02	Radial Reflector	6.10529E-02	0.0366	2.43017E-06	0.1531
69.02		6.70505E-02	0.0367	8.82025E-07	0.2367
75.02		6.26684E-02	0.0386	6.06400E-07	0.2868
81.02		5.96339E-02	0.0385	3.32444E-07	0.3661
91.02		4.63044E-02	0.0417	1.94367E-07	0.5278
101.01		3.93147E-02	0.0463	4.36679E-10	0.0800
111.01		2.88899E-02	0.0503	8.60520E-10	0.5803
121.01		1.95521E-02	0.0646	1.84082E-10	0.0625
131.01		1.41513E-02	0.0720	1.31488E-10	0.0702
141.01		7.86084E-03	0.0932	7.27482E-11	0.0912

Table A.3. Benchmark LEUPRO-1 (20% water) whole reactor axial values of reaction rates

z(cm)	Region	Fissions U235	Rel. error	Fissions U238	Rel. error
4.0	Bottom Reflector	6.77131E-03	0.0672	1.49218E-10	0.5364
13.0		1.84363E-02	0.0421	2.64100E-08	0.9930
23.0		2.98396E-02	0.0328	7.72169E-08	0.6501
33.0		4.36849E-02	0.0275	9.60170E-08	0.4090
43.0		6.07907E-02	0.0242	2.20833E-07	0.2973
53.0		7.62243E-02	0.0223	4.60445E-07	0.1942
63.0		8.26810E-02	0.0203	1.73585E-06	0.0995
70.5		8.51670E-02	0.0246	3.74695E-06	0.0952
75.5		8.61243E-02	0.0241	6.65386E-06	0.0722
79.9	Core	8.21325E-02	0.0276	1.00902E-05	0.0641
83.7		8.22485E-02	0.0272	1.16399E-05	0.0570
87.5		7.33177E-02	0.0268	1.36474E-05	0.0544
91.3		7.63945E-02	0.0276	1.55349E-05	0.0501
95.1		7.47003E-02	0.0274	1.43495E-05	0.0522
98.9		7.11173E-02	0.0273	1.50442E-05	0.0529
102.7		6.97211E-02	0.0279	1.45905E-05	0.0524
106.5		7.00036E-02	0.0264	1.45432E-05	0.0540
110.3		7.17670E-02	0.0283	1.53405E-05	0.0534
114.1		7.32923E-02	0.0280	1.67047E-05	0.0493
117.9		6.70728E-02	0.0291	1.25933E-05	0.0558
121.7		6.44815E-02	0.0294	1.43396E-05	0.0529
125.5		6.24358E-02	0.0307	1.14158E-05	0.0575
129.3		5.18137E-02	0.0315	1.22857E-05	0.0584
133.1		5.03718E-02	0.0337	1.10326E-05	0.0596
136.9		4.23107E-02	0.0335	9.41791E-06	0.0661
140.7		3.81222E-02	0.0362	7.79873E-06	0.0708
144.5		3.55247E-02	0.0378	7.12943E-06	0.0760
148.02		3.07879E-02	0.0412	4.54232E-06	0.0973
154.82	Air	2.98631E-02	0.0232	3.70983E-06	0.0771
166.5		2.94857E-02	0.0199	2.60366E-06	0.0744
179.5		2.91011E-02	0.0198	2.37358E-06	0.0912
192.5		2.94789E-02	0.0213	1.89767E-06	0.0934
205.5		2.88133E-02	0.0217	1.45021E-06	0.1158
218.5		2.69157E-02	0.0207	1.04326E-06	0.1303
231.5		2.73418E-02	0.0218	1.01617E-06	0.1470
244.5		2.60234E-02	0.0211	5.42118E-07	0.1727
259.15	Al	2.60604E-02	0.0197	7.42051E-07	0.1543
272.3	Top Reflector	2.66597E-02	0.0307	4.63648E-07	0.2226
282.3		2.57007E-02	0.0352	7.34952E-08	0.3729
292.3		2.11892E-02	0.0385	8.58119E-08	0.5072
302.3		1.63972E-02	0.0438	2.07540E-08	0.9839
312.3		1.23224E-02	0.0487	2.46230E-08	0.9950
322.3		7.78785E-03	0.0582	7.28316E-11	0.0573
333.3		4.34766E-03	0.0766	4.06286E-11	0.0749
341.3		1.36820E-03	0.1212	1.87058E-11	0.3296

Table A.4. Benchmark LEUPRO-1 (20% water) whole reactor radial values of reaction rates

r(cm)	Region	Fissions U235	Rel. error	Fissions U238	Rel. error
3.46	Core	6.77722E-02	0.0419	1.42529E-05	0.0782
9.16		6.86403E-02	0.0397	1.52886E-05	0.0712
15.10		6.31082E-02	0.0347	1.47553E-05	0.0674
21.07		6.65116E-02	0.0359	1.29770E-05	0.0645
27.05		6.37232E-02	0.0343	1.23876E-05	0.0646
33.04		5.87181E-02	0.0341	1.26012E-05	0.0650
39.04		5.60050E-02	0.0368	1.27211E-05	0.0672
45.03		5.44465E-02	0.0367	1.08280E-05	0.0708
51.03		5.37987E-02	0.0379	9.02773E-06	0.0763
57.03		5.57595E-02	0.0399	6.83578E-06	0.0930
63.02	Radial Reflector	6.01479E-02	0.0383	3.32173E-06	0.1269
69.02		5.58195E-02	0.0383	1.63246E-06	0.1797
75.02		5.29684E-02	0.0399	1.09608E-06	0.2195
81.02		4.95501E-02	0.0418	5.01649E-07	0.3470
91.02		4.32925E-02	0.0535	4.52985E-08	0.6102
101.01		3.05618E-02	0.0501	1.45144E-08	0.9726
111.01		2.31391E-02	0.0555	2.32473E-10	0.0724
121.01		1.65078E-02	0.0731	2.09651E-10	0.2710
131.01		1.12326E-02	0.0752	1.04681E-10	0.0736
141.01		6.77295E-03	0.1017	6.34485E-11	0.0993

APPENDIX B. MCNP GEOMETRY TOUR TO PROTEUS BENCHMARKS

MCNP has the capability to generate plots of 2-dimensional cuts of the assembly being calculated. These plots are extremely useful to edit the input to the program. In our case, the degree of details includes the explicit description of the fuel compact: (1) 502 μm UO_2 kernel, its coatings, (2) buffer (3) pyrolytic graphite, (4) SiC, (5) pyrolytic graphite, and (6) the graphite matrix.

The degree of details can be appreciated in the next series of figures. Figure B1 is an xy cut of the LEUPRO-1 cell whole reactor benchmark. The double circles indicate fuel pebbles (fuel and graphite shell) and the single circles indicate moderating graphite pebbles. The black fuel pebble at the center is magnified and shown in Fig. B2 to emphasize the fuel particles inside the fuel region. Note that the squares indicate only the limits of the cubic cells with the fuel particles at the centers. Further magnification allows one to see the structure of the fuel in Fig. B3, that is the fuel kernels, their 4 coatings and the graphite matrix. Figure B4 shows the boundary between the fuel and shell regions of the fuel pebbles.

Fig. B.1. Core region of the LEUPRO-1 cell whole reactor benchmark. The black fuel pebble is magnified in Figs. B2 to B4. MCNP output.

Fig. B.2. Fuel pebble at the center of the core with explicit fuel particles. MCNP output.

Fig. B.3. Fuel particles at the center of the core with their 4 coatings and graphite matrix. MCNP output.

Fig. B.4. Fuel pebble, interface between fuel region and graphite shell. MCNP output.

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