NEUTRONIC BENCHMARK ON HOLOS-QUAD MICRO-REACTOR CONCEPT

N. E. Stauff[1]*, C. H. Lee[1], P. Shriwise[1], A. Wells[2], C. Filippone[2]

[1] Argonne National Laboratory
9700 S. Cass Avenue Argonne, IL 60439, USA

[2] HolosGen LLC
Manassas Park, Virginia, USA

* nstauff@anl.gov

ABSTRACT

The Holos-Quad micro-reactor concept is proposed by HolosGen LLC for civilian applications to generate 22 MWt with a lifetime of approximately 8 effective full power years (EFPYs). The design is based on a very innovative high-temperature gas-cooled reactor concept using four Subcritical Power Modules (SPMs) that fit into one commercial 40-foot transport ISO container. Neutronics benchmarks were developed based on a preliminary version of the Holos-Quad design to confirm feasibility of the neutronics design of this non-traditional high temperature gas-cooled (HTGR)-type micro-reactor concept. Calculations were performed using Monte Carlo codes (SERPENT and OpenMC) as well as the PROTEUS high-fidelity deterministic code for two exercises based on a unit cell model and a full core model. The results obtained showed good agreement with all of the evaluated parameters for the unit cell problem and the full core problem. SERPENT and OpenMC display consistently good agreement in eigenvalue within 150 pcm for the unit cell benchmark and less than 270 pcm for the full core benchmark. PROTEUS eigenvalues showed relatively larger differences but still reasonable agreement with the SERPENT solutions. For the depletion benchmark, the observed eigenvalue differences between SERPENT and OpenMC were within 300 pcm throughout the depletion up to 100 GWd/MT, ensuring that the two codes used equivalent input parameters such as the recoverable heat values for fission reactions. This benchmark exercise confirms the neutronic feasibility and core performance of the preliminary Holos-Quad design.

KEYWORDS: micro-reactor, neutronic benchmark, Monte Carlo, HTGR

1. INTRODUCTION

The Holos-Quad micro-reactor concept is proposed by HolosGen LLC for civilian applications to generate 22 MWt with a lifetime of at least 8 effective full power years (EFPYs). The design is based on a very innovative high-temperature gas-cooled reactor concept using four Subcritical Power Modules (SPMs) that fit into one commercial 40-foot transport ISO container. It adopts a non-traditional primary reactivity control mechanism in which the criticality is achieved by moving the four SPMs in close proximity, while the reactor is shut down by moving the SPMs away. The Holos-Quad uses TRISO fuel distributed in graphite hexagonal blocks and cooled with helium gas.

Under the ARPA-E MEITNER program initiated in FY2019, the Argonne National Laboratory (ANL) design team has been contributing to the core design of the Holos-Quad by performing a design optimization of the core [1, 2]. Through this work, ANL has been demonstrating the neutronic feasibility of the Holos-Quad concept. In particular, neutronics benchmarks were developed based on a preliminary version of the Holos-Quad design. The objective of the benchmarks detailed in this paper is to further confirm the feasibility of the neutronics design of this non-traditional high temperature gas-cooled (HTGR)-type micro-reactor concept.

2. DESCRIPTION OF THE HOLOS-QUAD CORE CONCEPT

The Holos-Quad is a HTGR concept generating 22 MWt designed to fully fit into one 40-foot transport ISO container. The core contains 151 fuel assemblies (some of which are axially and/or radially split) 4.0 m-long, which include 3.9 m of fuel and 0.05 m of upper and lower reflectors, as shown in Figure 1 and Table 1. The Holos-Quad is formed by four independent subcritical power modules (SPMs) enabling power generation when a minimum number of SPMs are actively positioned by actuators to satisfy criticality requirements. Each SPM contains its own closed-loop, gas Brayton cycle with a turbine, compressor, inter-cooler and rejection heat exchanger, converting thermal power to 5.5 MW electricity. In the configuration analyzed, each SPM is wrapped inside a shell of zircaloy-4 to prevent outside air from interacting with hot graphite. Two reactivity control systems are being considered in this paper: the capability to manage reactivity by moving SPMs apart and increasing the neutron leakage, and the insertion of hafnium blades in between the SPMs as an emergency shutdown system. Additional and complimentary control systems are being considered in the framework of the project under the ARPA-E MEITNER program.

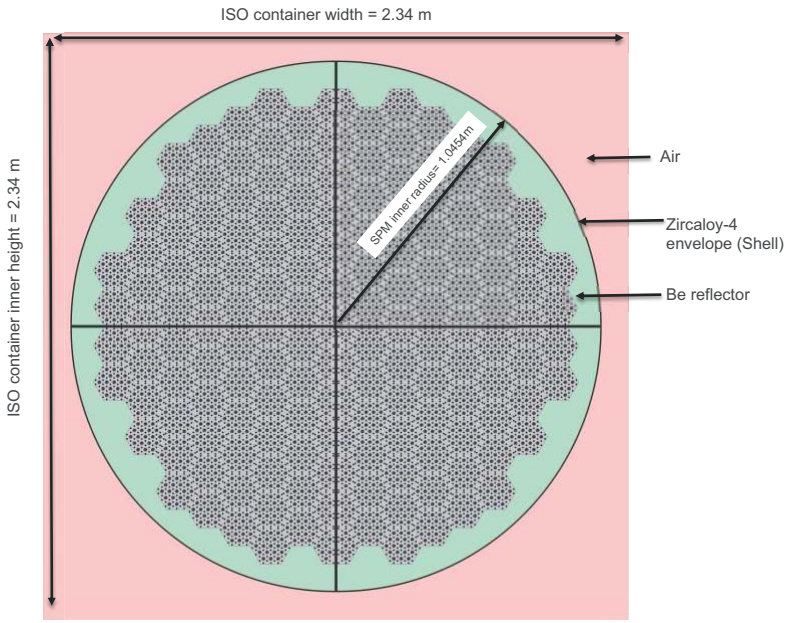

Figure 1. Transversal layout for Holos-Quad core.

To readily access available material technology, the coolant temperature was limited to 650$_{o}$C, but higher temperatures are being considered to enhance thermal efficiency of the Brayton cycle. For improved inherent safety, the Holos-Quad uses TRISO particle fuel distributed in graphite hexagonal blocks as shown with the assembly layout in Figure 2. The assembly "cut" is performed so that pins and coolant channels are not split, as shown in Figure 1. A full assembly contains 19 fuel compacts, each being surrounded by 6 coolant channels. The packing fraction considered is 40% and the fuel uses high-assay low-enriched

uranium with U-235 enrichment of 19.95 at%. Pressurized helium at 70 bars is used as the coolant material circulating through Zirc-4 sleeves located inside the coolant holes. Burnable poisons are used to limit the excess reactivity of the core, considering dilution of B-10 directly within the graphite matrix at this stage of the project.

Table 1. Design parameters used for the Holos-Quad core benchmark (hot conditions).

	Parameters	**Unit**	**Value**
Shell (Zirc-4)	Thickness	cm	0.5
	Inner radius	m	1.045
Core	Power	MWt	22
	Number of full/half/quarter fuel columns		132 / 36 / 4
	Height of the fuel column	m	3.9
	Height of upper/lower reflector	m	0.05
Fuel block	Pitch	cm	14.45
	Number of fuel holes		19
	Number of small coolant holes		54
Fuel cell	Pitch of fuel cell	cm	1.7
	Radius of fuel hole	cm	0.7
	Packing fraction	%	40
	Fuel form		UCO, C/U=0.4, O/U=1.5
	Outside radius of coolant hole	cm	0.3
	Coolant cladding (Zirc-4) thickness	cm	0.057
	Lead buffer thickness (between coolant cladding and graphite)	μm	20
Particle size	Fuel kernel diameter (UCO)	μm	425
	Buffer thickness		100
	Inner pyrolytic carbon thickness		40
	Silicon carbide thickness		35
	Outer pyrolytic carbon thickness		40
Material density	Fuel kernel (UCO)	g/cm^3	10.744
	Buffer		1.04
	Inner pyrolytic carbon		1.882
	Silicon carbide (SiC)		3.171
	Outer pyrolytic carbon		1.882
	Graphite block (matrix)		1.806
	Reflector block (Beryllium)		1.778
	Coolant He		0.00365
	Air (inter-modules – N_2)		0.0012
	Lead		10.253
	Zircaloy-4 (SPM shell)		6.489
B-10 burnable absorbent material (diluted in graphite block)		ppm	20

A few simplifications to the core model are considered in this benchmark. First, the graphite and beryllium blocks used in the fuel and reflector assemblies are supposed to be perfectly cut to fit into the cylindrical shell (see Figure 1). Second, no cooling material channel is currently considered in the radial reflector block. However, coolant channels are considered in the axial reflectors. Finally, the channels containing the flow of cold coolant returning to the compressor were not modelled. These channels will be positioned between the radial reflector and the outside shell (whose shape will be extended to accommodate additional volume)

or will be embedded with the radial reflector. For neutronics modeling consideration, three core configurations are considered with following changes in cross-section temperatures.

- Full power: Fuel temp = 900K, Coolant+Structure (including S(α,β)) = 800K
- Hot shutdown: Fuel temp = 800K, Coolant+Structure (including S(α,β)) = 800K
- Cold shutdown: Fuel temp = 300K, Coolant+Structure (including S(α,β)) = 300K

At this stage of our study, changes in density (from thermal expansion) were not considered, and all dimensions provided in Table 1 are at high temperature conditions.

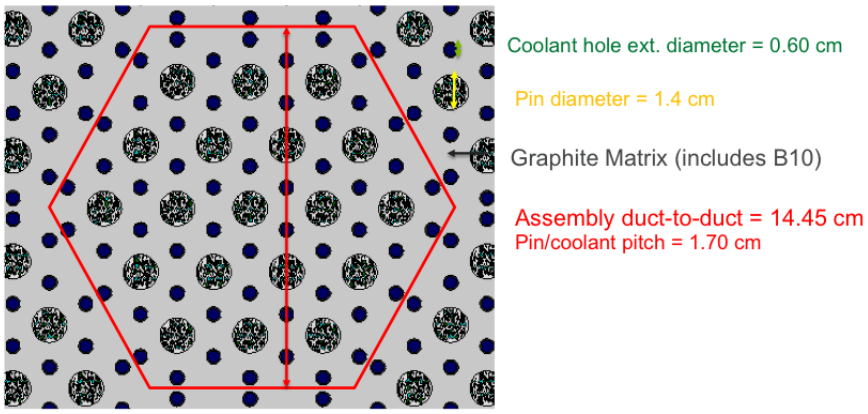

Figure 2. Assembly dimensions for Holos-Quad core.

3. METHODS EMPLOYED

Neutronic calculations were performed using Monte Carlo codes (SERPENT and OpenMC) as well as the PROTEUS high-fidelity deterministic code using consistent geometry, modeling approach, and nuclear data libraries based on the same NJOY-generated ENDF/B-VII.1 library, while each code used their own thermal scattering library. The temperatures for cross-sections of fuel, structure and coolant and for thermal scattering libraries are consistent between different codes. The different neutronics codes used are described in this section.

The Monte Carlo code SERPENT [3] is the main code employed for neutronic simulations for core design and analysis in this project. It is a continuous-energy Monte-Carlo reactor physics burnup calculation code developed at the VTT Technical Research Center of Finland. The fuel region is modeled with an explicit description of the TRISO fuel where particles are distributed with semi-random sampling technique; they are filled in a compact regular lattice, and random TRISO particles are then removed to meet the packing fraction requested.

OpenMC [4] is an open-source Monte Carlo code originally developed at the Massachusetts Institute of Technology in 2011. Various institutions, laboratories, and organizations contribute to the development of OpenMC. It is capable of continuous energy neutron and photon transport with support for TRISO modeling along with analogous physics models to those found in SERPENT. An identical TRISO fuel particle distribution to the one used in SERPENT is applied in all OpenMC models. All geometry, materials, and depletion zones in SERPENT calculations are matched in the OpenMC model as well.

The PROTEUS code [5] is a high-fidelity capable three-dimensional (3D) deterministic neutron transport code developed by ANL under the Department of Energy (DOE) Nuclear Energy Advanced Modeling and Simulation (NEAMS) program. The Holos-Quad was modeled using the method of characteristics (MOC) transport solver with explicit geometry. The CUBIT mesh generation software was used to generate the geometry model and mesh since the geometry of the Holos core is non-standard. For multigroup cross

sections, the 14-group cross sections were generated using SERPENT. The convergence study in terms of mesh refinement and energy groups were conducted at the assembly calculation, finally determining meshes and energy groups which were optimal in terms of accuracy and computational performance.

4. INFINITE CELL BENCHMARK

A simple unit-cell benchmark was proposed first based on a geometry shown in Figure 3, which is similar (but not equivalent) to the one from the full core. The objective of this exercise is to make sure that satisfactory agreement is reached without error cancellation on the full-core benchmark. For this analysis, various eigenvalue calculations were performed, as listed in Table 2. The results obtained for the infinite cell lattice problem are summarized in Table 2. Very good agreement between OpenMC and SERPENT was obtained for calculations #1, 4, 6, and 8. Larger discrepancy up to 140 pcm is observed on calculations #2, #5 and #7, which appears to come from inconsistencies in the thermal scattering library used. The discrepancies in the estimated MDC and FTC coefficients are within the statistical uncertainty of these evaluations (the uncertainties are quite large when compared with the small value of MDC coefficient). The OpenMC calculation #4 shows that the Doppler broadening rejection correction for U-238 is responsible for ~70 pcm. Relatively larger but still reasonable agreement was obtained with the PROTEUS code.

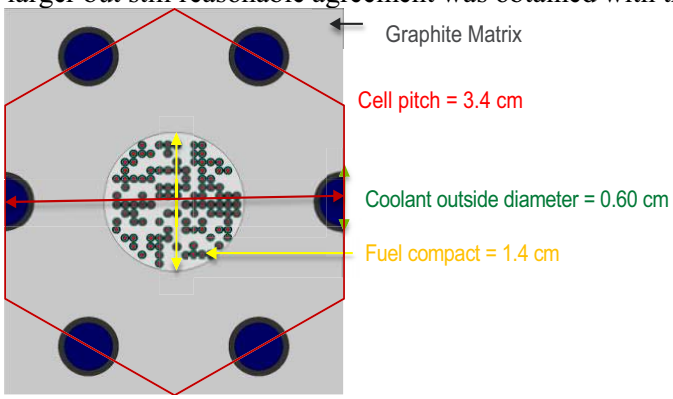

Figure 3. Infinite lattice cell model.

Table 2. Benchmark results comparison for infinite cell problem.

Calculation #	**SERPENT**	**OpenMC (*Δk)**	**PROTEUS (*Δk)**
1: Reference calculation at “Full Power”	1.25442 ± 0.00021	1.25444 ± 0.00046 (2)	1.25389 (-53)
2: Calculation at “Cold shutdown”	1.30220 ± 0.00021	1.30083 ± 0.00042 (-137)	1.30104 (-116)
3: Calculations at “Hot shutdown” with Doppler broadening rejection correction for U-238		1.25821 ± 0.00044	
4: Calculations at “Hot shutdown”	1.25976 ± 0.00021	1.25974 ± 0.00042 (-2)	1.25687 (-289)
5: Reference without thermal scattering for Graphite	1.25516 ± 0.00021	1.25625 ± 0.00043 (+109)	1.25328 (-188)
6: Reference without including B-10 concentration in Graphite matrix	1.53602 ± 0.00019	1.53590 ± 0.00038 (-12)	1.53424 (-178)
7: Calculations at “Cold Shutdown” with He coolant in graphite hole replaced with water (1.0 g/cm3)	1.38246 ± 0.00017	1.38124 ± 0.00041 (-122)	1.38469 (+223)
8: Reference with graphite density reduced by 1% in block and pin	1.25423 ± 0.00021	1.25442 ± 0.00045 (+19)	1.25450 (+27)
MDC[pcm/1%] = 1e5*(1/#1 - 1/#8)	-12 ± 30	-1 ± 64 (+11)	39 (+51)
FTC[pcm/-100K] = -1e5*(1/#1 - 1/#4)	-338 ± 30	-335 ± 62 (+3)	-189 (149)

* Δk: Eigenvalue difference from SERPENT, pcm

The depletion calculation includes depletion of the graphite matrix region (that includes diluted burnable poison) at all burnup-steps in equivalent full power days (EFPDs): 0.3, 2.0, 36.5, 365, 730, 1095, 1460, 1825, 1737.5, 3650 (representing average burnups of 100 GWd/MT$_{iHN}$) with the cell power of 7.868 kW. The k-eff evolutions obtained from OpenMC and SERPENT are compared in Figure 4, showing agreement within ~300 pcm of each other throughout the depletion. Several verification steps were taken to ensure that SERPENT and OpenMC were using equivalent input parameters for the burnup calculations. Depletion chains, which included all relevant nuclei, were applied in both codes. In OpenMC, adjustments were made to the standard depletion chain, verified in the CASL calculations [6], to include the metastable states of key isotopes, such as Am-241, Ag-109, etc., to match those included in the SERPENT calculation. Additionally, the recoverable heat values for fission reactions were also adjusted in OpenMC to match those in SERPENT.

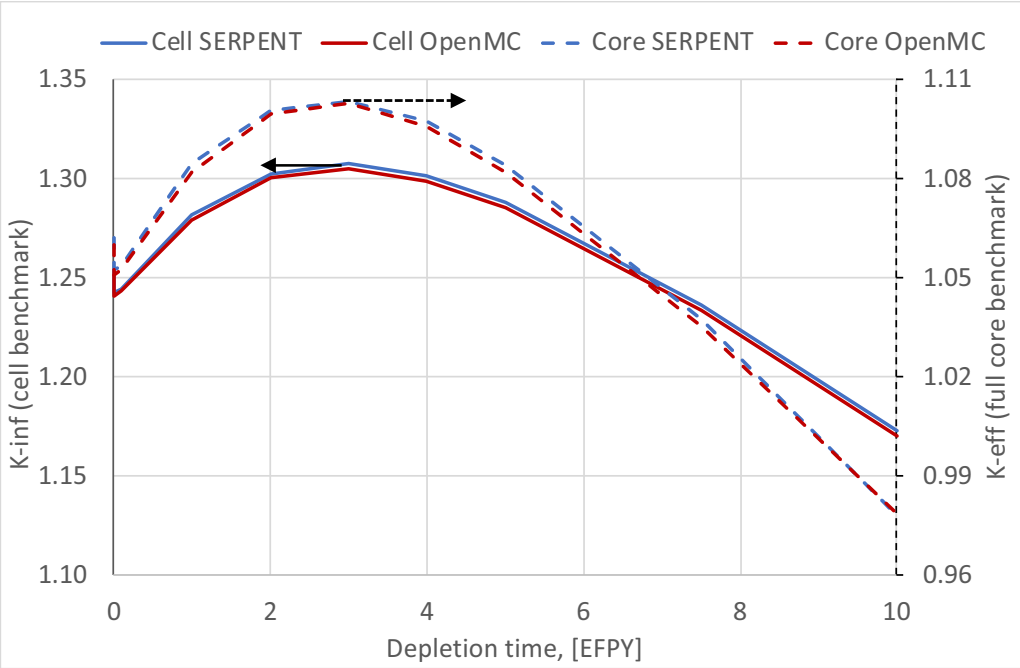

Figure 4. K-eff comparison through infinite cell (plain lines) and full core (dash lines) depletions.

5. FULL CORE BENCHMARK

The full-core analysis is based on the geometry described in Section 2. A wide range of eigenvalue calculations described in Table 4 are computed, and the different core configurations are displayed in Table 3. The results obtained for the full core benchmark problem are summarized in Table 4. The agreement obtained between OpenMC and SERPENT is relatively good, within 300 pcm of discrepancy. The PROTEUS simulation displays relatively good agreement as well, with ~200 pcm off on k-eff, showing consistent results for the MDC and FTC calculations. However, PROTEUS for calculation #4 (water flooding) resulted in a relatively large underestimation of k-eff which is under investigation in terms of multigroup cross section and mesh refinement. Figure 5 illustrates fast and thermal flux distributions for calculation #2 (3 SPM separation) results from PROTEUS, in which neutron leakages can be seen through the separation gaps. Under the configuration analyzed, the core is under-moderated as shown with large reactivity excursion due to flooding in the event of water ingress scenarios (external events). The flooding-induced reactivity excursion is being mitigated in this project with alternative reactivity shutdown and control systems, however, these are not considered in this benchmark exercise.

Table 3. Holos-Quad core geometry with different SPM configurations.

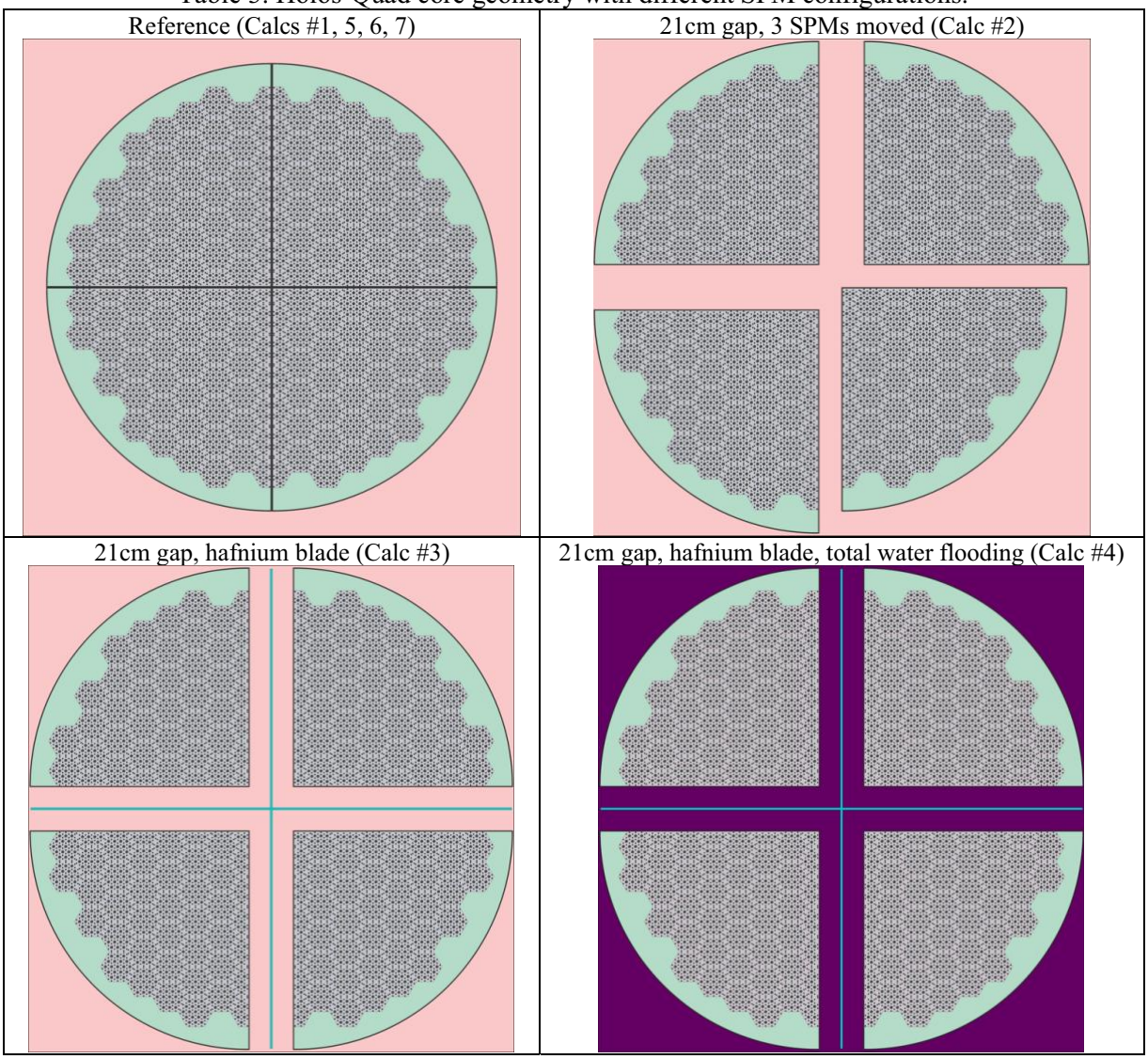

Table 4. Benchmark results comparison for full core problem.

Calculation #	**SERPENT**	**OpenMC (Δk*)**	**PROTEUS (Δk*)**
1: Reference k-eff calculation at "Full Power"	1.06165 ± 0.00016	1.06255 ± 0.00021 (+90)	1.05956 (-218)
2: Reactivity worth of controlling SPM separation at "Hot Shutdown" moving 3 SPMs, with gap of 21 cm	0.92772 ± 0.00018	0.92503 ± 0.00021(-269)	0.92986 (+187)
3: Shutdown margins at "Cold Shutdown" with gap of 21cm between SPMs, and hafnium blade (1cm thick, 13.2 g/cm3)	0.80582 ± 0.00023	0.80543 ± 0.0002 (-39)	0.80526 (-63)
4: Water flooding during "Cold Shutdown" (#3) with water in coolant holes and outside SPMs	1.04607 ± 0.00018	1.04603 ± 0.00022 (-4)	
5: Reduction of graphite density of the fuel pin matrix and the graphite block by 1% at "Full Power"	1.05974 ± 0.00016	1.06114 ± 0.0002 (+140)	1.05781 (-227)
6: Doppler coefficient calculated at "Full Power" by increasing the temperature of the UCO fuel by 300K	1.05083 ± 0.00015	1.05155 ± 0.00019(+72)	1.04971 (-85)
MDC[pcm/1%] = 1e5*(1/#1 - 1/#5)	-170 ± 22	-125 ± 30	-156
FTC[pcm/+300K] = 1e5*(1/#1 - 1/#6)	-970 ± 23	-984 ± 30	-886

* Δk : eigenvalue difference from SERPENT, pcm

The k-eff evolutions through burnup are obtained from OpenMC and SERPENT using the same burnup-steps as used for the cell benchmark with 22 MWt power. To simplify the burnup benchmark, only one depletion zone is considered throughout the core for both the fuel and the graphite regions. The results shown in Figure 4 display relatively good agreement, with discrepancy of consistently less than 300 pcm. The densities from the main isotopes (U-235, U-238, Pu-238 to 242, Am-241, B-10, B-11, Xe-135, Sm-149, Sr-90, and Cs-137) at the end of the depletion simulations were compared, displaying small discrepancy (less than 2.5%) between SERPENT and OpenMC, with variations relatively consistent between the cell and core benchmarks.

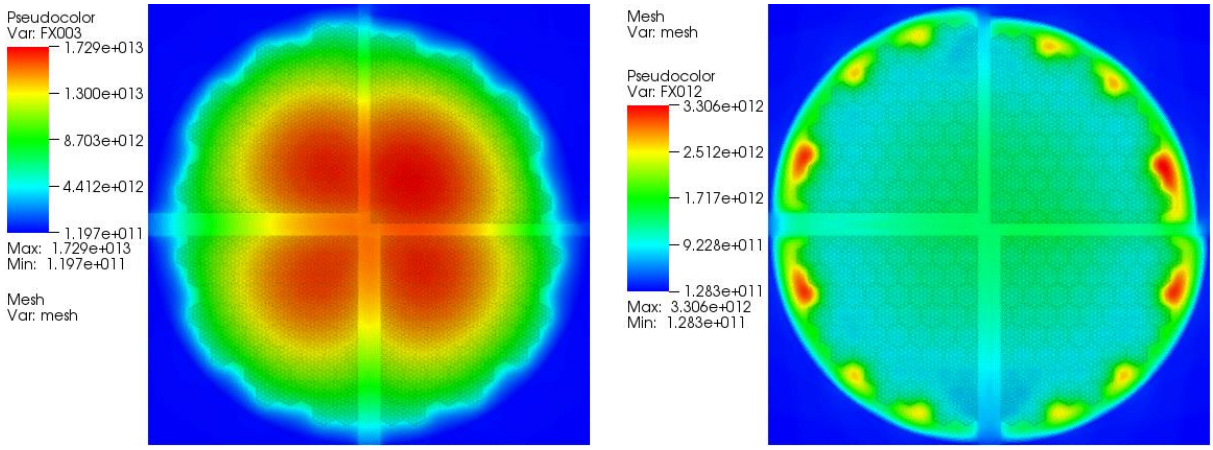

Figure 5. Fast (left) and thermal (right) neutron flux distributions for calculation #2 (3 SPM separation) generated from PROTEUS.

6. CONCLUSIONS

Neutronic benchmark exercises were conducted to confirm the methods used for the design analysis of the non-traditional Holos-Quad micro-reactor concept. Calculations were performed using Monte Carlo codes (SERPENT and OpenMC), and the PROTEUS high-fidelity deterministic code. Two separate exercises were proposed based on a unit cell model and a full core model for the rigorous verification of solutions, and the results obtained showed good agreement in all the evaluated parameters. SERPENT and OpenMC display consistently good agreement in eigenvalue within 150 pcm for the unit cell benchmark and 270 pcm for the full core benchmark. PROTEUS eigenvalues showed relatively large differences but still reasonable agreement with the SERPENT solutions. For the depletion benchmark, the observed eigenvalue differences between SERPENT and OpenMC were within 300 pcm throughout the depletion up to 100 GWd/MT. This benchmark exercise confirms the neutronic feasibility and core performance of the preliminary Holos-Quad design.

ACKNOWLEDGMENTS

Argonne National Laboratory's work was supported by U.S. Department of Energy (DOE) under Contract number DE-AC02-06CH11357. The direction and support of the U.S. DOE Office of Nuclear Energy and the ARPA-E MEITNER Program is greatly appreciated.

REFERENCES

1. N. Stauff *et al.,* "Neutronic Design and Analysis of the Holos-Quad Concept," ANL/NSE-19/8, Argonne National Laboratory (2019). (https://www.osti.gov/biblio/1524786-neutronic-design-analysis-holos-quad-concept)
2. Nicolas E. Stauff *et al.,* "Design Optimization of the Holos-Quad Micro-Reactor Concept," PHYSOR 2020, Cambridge, United Kingdom, March 29-April 2 (2020).
3. J. Leppanen, "Serpent – a Continuous-energy Monte Carlo Reactor Physics Burnup Calculation Code," User's Manual, June 18 (2015).
4. P. K. Romano *et al.,* "OpenMC: A State-of-the-Art Monte Carlo Code for Research and Development," Ann. Nucl. Energy, 82, 90–97 (2015).
5. Y. S. Jung *et al.*, "PROTEUS-MOC User Manual (Rev.0)," ANL/NSE-18/10, Argonne National Laboratory (2018).
6. K. S. Kim, Specification for the VERA Depletion Benchmark Suite. doi:10.2172/1256820.