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AP1000®† Benchmarking of VERA Neutronics Toolset

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Abstract – *Benchmarking of the VERA tools MPACT and Shift was conducted using simulations of AP1000 2D lattice models with the results from Serpent models serving as a reference. MPACT was found to exhibit closer agreement to Serpent compared to previous benchmarking endeavors due to adoption of consistent kappa heating values in the two codes as well as implementation of a new 51 energy group cross-section library in MPACT. Comparisons between Serpent and Shift indicated excellent agreement with regards to eigenvalue and power distribution, confirming the validity of using the results from either code as a benchmarking reference.*

I. INTRODUCTION

The Consortium for Advanced Simulation of Light Water Reactors (CASL) [1] has made steady strides towards the provision of efficient, high-fidelity simulations of light water reactors (LWRs). Part of this steady progression is the extensive benchmarking activity of the CASL toolset provided through its Virtual Environment for Reactor Applications (VERA) [2] against other established neutronics codes and plant operating data.

Herein presented is a continuation of the benchmarking of VERA neutronics solver MPACT [3–5] as well as the VERA Monte Carlo code Shift [6], focusing on AP1000† pressurized water reactor (PWR) modeling [7]. The AP1000 PWR startup core design is depicted in Figure 1; it is an advanced core design with a very low-leakage 18 month operating cycle which expedites convergence to the equilibrium cycle through the use of several fuel regions mimicking the reactivity distribution of an equilibrium core. This is achieved with a loading pattern of properly arranged fuel assemblies at various enrichments (from close to 5 w/o ^{235}U to natural uranium) in conjunction with intra-assembly enrichment zoning to reduce interface effects and by adopting Integral Fuel Burnable Absorbers (IFBAs) and short and long Wet Annular Burnable Absorbers (WABAs) to provide the desired reactivity hold-down. In addition, banks of "grey" and "black" control rods are adopted as part of the core control strategy MSHIM† [8,9]. The heterogeneity of the AP1000 advanced core provides an excellent benchmarking opportunity for the CASL toolset.

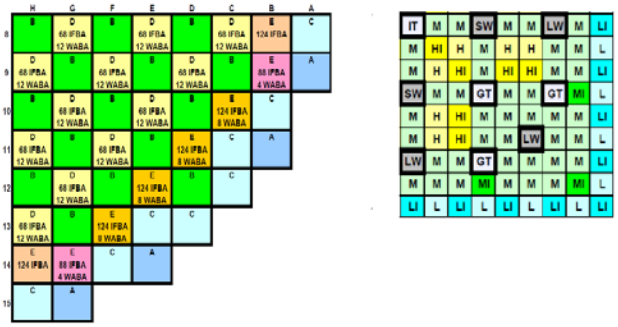

Fig. 1. AP1000 quarter core (left) and sample quarter assembly (right) [1]

II. DESCRIPTION OF THE ACTUAL WORK

Two-dimensional lattice simulations of the various assembly regions characterizing the AP1000 core design were conducted. These included fuel assembly regions A, B, C with uniform radial ^{235}U enrichments of 0.74%, 1.58%, and 3.2%, respectively, regions D and E with heterogeneous fuel, and IFBA loadings and average enrichments of 3.8% and 4.4%, respectively, as well as the 3.2% enriched annular axial blanket region. Additionally, the Region B lattice was modeled with a grey tungsten control rod inserted. A detailed depiction of the assembly layouts along with pin-cell geometries is described in Figure 2, Figure 3, and Table I. All remaining model specifications are summarized in Table II.

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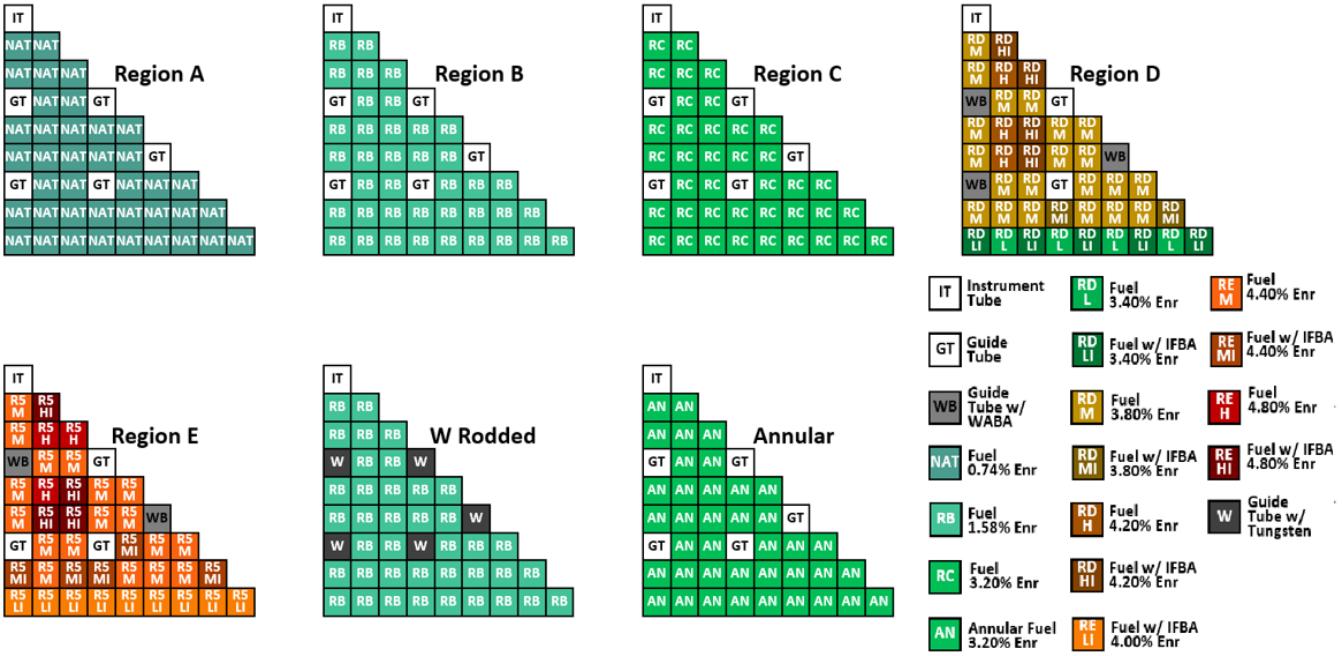

Fig. 2. AP1000 2D Lattice Model Pin Maps. [8]

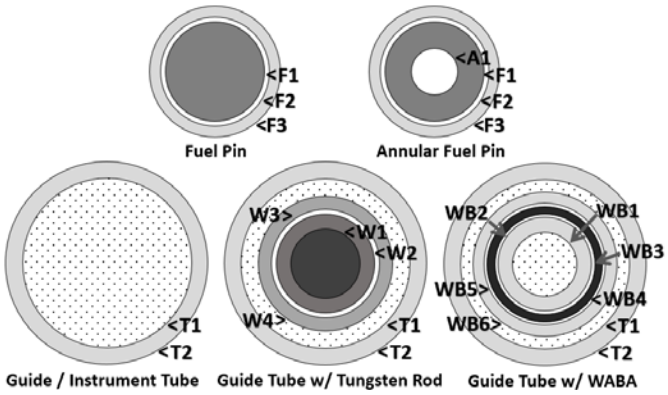

Fig. 3. AP1000 2D Lattice Model Pin-Cell Diagrams. [8,10]

Lattice depletion simulations were conducted in the VERA neutronics solvers MPACT and Shift, as well as in the Monte Carlo code Serpent [11], with Serpent serving as the reference solution because it served as the reference in the previous AP1000 lattice benchmark [4]. Fixed temperatures of 900K for fuel and 600K for the moderator and other non-fuel materials were assumed to facilitate model consistency between codes. The ENDF-VII.0 library was utilized and kappa heating values were made consistent with Serpent in MPACT and Shift. It should be noted that consistent kappa values were not employed in the previous Serpent-MPACT comparisons [4]; as will be shown later, adopting consistent kappa heating provides significant improvements in the results. Seventy-three depletion steps were used to simulate these models for a target burnup of 70 GWD/MTHM (~1 GWD/MTHM per time step). Accurate results could likely be obtained with a coarser time mesh, but the fine mesh was employed to ensure a quality benchmark comparison.

Table I. Pin-Cell Radii and Material Descriptions [8,10]

ID	Material	Radii (cm)
A1	Helium	0.19685
F1	Fuel	0.409575
F2	Helium	0.41783
F3	Zirlo	0.47498
W1	Tungsten	0.25019
W2	Inconel	0.3937
W3	Helium	0.4191
W4	Stainless Steel	0.48387
T1	Coolant	0.56134
T2	Zirlo	0.61214
WB1	Coolant	0.29
WB2	Zircaloy	0.34
WB3	Helium	0.35
WB4	Alumina Boron-Carbide	0.40386
WB5	Helium	0.41783
WB6	Zircaloy	0.48387

Table II. Additional Model Specifications [10]

Parameter	Value
Fuel Temp (K)	900
Non-Fuel Temp (K)	600
Coolant Dens. (g/cc)	0.744
Coolant Boron (ppm)	1321
IFBA Layer Thickness (cm)	0.000508
Assembly Pitch (cm)	21.5
Pin Pitch	1.26
Model Power (MW)	0.05075
Model Height (cm)	1

The Serpent simulations were performed using Serpent version 2.1.24 with a continuous- energy library, over 76,800 cores (4,800 nodes) on the Oak Ridge Leadership Computing Facility (OLCF) Titan supercomputer [12]. In order to reduce the statistical uncertainty on eigenvalue and especially pin power to obtain a benchmark quality power distribution, 100 billion particle histories were simulated with a 1/8 symmetry applied to the model. Some models were simulated using 4.0 million particles per generation with 250 active generations, and others were simulated with 3.5 million particles per generation with 286 active generations due to memory constraints[1]. All models simulated 100 inactive generations prior to the simulation of active generations. Depletion simulations were accomplished using a single individual depletion region for each fuel pin, IFBA coating, and WABA pin. Additionally, a predictor-corrector scheme was employed with constant reaction rate extrapolation with two substeps for the predictor step and linear reaction rate interpolation with one substep for the corrector step. No substep flux renormalization was employed for the Serpent simulations. The computational time was ~ 6 hours per simulation, or ~ 0.5 million core hours.

The Shift simulations were performed with the SCALE [13] continuous-energy library, over 1,032 cores (43 nodes) on the Idaho National Laboratory (INL) Falcon supercomputer [14]. Simulations were performed using 4.0 million particles per generation with 250 active generations like the Serpent models but using full symmetry due to a current lack of 1/4 or 1/8 symmetry modeling capabilities in Shift for depletion calculations. All models simulated 100 inactive generations for the first timestep and then only 10 inactive generations thereafter[2]. Like Serpent, the depletion model utilized single individual depletion regions for each fuel pin, IFBA coating, and WABA pin, as well as employed a predictor-corrector numerical scheme. However, unlike Serpent, Shift was run at recommended settings of linear reaction rate extrapolation with a single substep for the predictor and quadratic reactor rate interpolation with four substeps for the corrector, along with energy integrated substep flux renormalization [15–16]. The computational time for each simulation was ~120 hours, or ~120,000 core hours[3].

The MPACT simulations were performed with transport-corrected P0 scattering, with a 51 energy group cross-section library [17], 0.05 cm ray spacing for models without IFBA, and 0.005 cm ray spacing for models with IFBA. It should be noted that the previous MPACT-Serpent comparison [4] utilized an older 47 energy group library which was superseded by the 51-group library. This 51 group library not only added more energy groups for improved epithermal flux accuracy but also provided more optimized resonance self-shielding factors for important actinide isotopes. As such, some improvement in depletion accuracy was expected. Again, a predictor-corrector depletion scheme was applied; however, three equal-volume depletion regions were applied to each individual fuel pin and single individual depletion regions for the non-fuel depletable materials. Additionally, constant reaction rate extrapolation was used for the predictor, and constant reaction rate interpolation for the corrector, with three substeps for both and no substep flux renormalization for either. These simulations were accomplished on eight cores using ~1.5 hours totaling only 13 core-hours vs. > 100,000 core hours of the Monte Carlo reference simulations.

III. RESULTS

The outcomes of the comparisons between the MPACT and Shift against SEPRENT are summarized in Figure 4, Figure 5, Figure 6, Figure 7, and Table III[4]. As can be seen in Figure 4, Figure 5, and Table III, the agreement between MPACT and Serpent, both in terms of eigenvalue and power distribution, is good. Eigenvalue agreement remains within

[1] Fewer particles per generation require a smaller memory footprint.

[2] This was recommended by the Shift development team, being that Shift can utilize the fission sources of the previous timestep as an initial guess for the current step source distribution and thus converge the source distribution in much fewer inactive generations.

[3] It may be noted by the reader that the difference in core hours between Serpent and Shift is substantial; however, it must be kept in mind that neither code was run for the sake of optimality but rather to produce results in low amount of wall-time. Serpent could be parallelized to a much larger number of cores before enormous inefficiencies were encountered, whereas with Shift this barrier was considerably lower. This led to Serpent runs with shorter wall-times but much less efficient runs overall and Shift simulations with considerably longer runtimes but with more efficient core utilization. This is simply stated so that the reader might not draw erroneous conclusions regarding the scaling efficiency of the two Monte Carlo codes.

[4] It should be noted by the reader that some data sets for the Shift results are not entirely complete (i.e., did not simulate all 73 depletion steps) due to runtime errors caused by unphysical upscattering from Shift not performing a fix-up of the ENDF-VII.0 data. However, a sufficient number of time steps was completed so that meaningful assessments of performance could be ascertained.

115 pcm of the Serpent reference for all models. Generally, the difference begins fairly small, within 50 pcm, increases with an MPACT under-prediction within ~50 pcm to ~100 pcm and gradually decreases with burnup to a 0 pcm to ~75 pcm MPACT over-prediction. In the previous AP1000 lattice comparisons [4], maximum eigenvalue differences approached 200 pcm for the early Δk peak but now can be seen to only approach about ~100 pcm, which indicates an improvement from the previous benchmark.

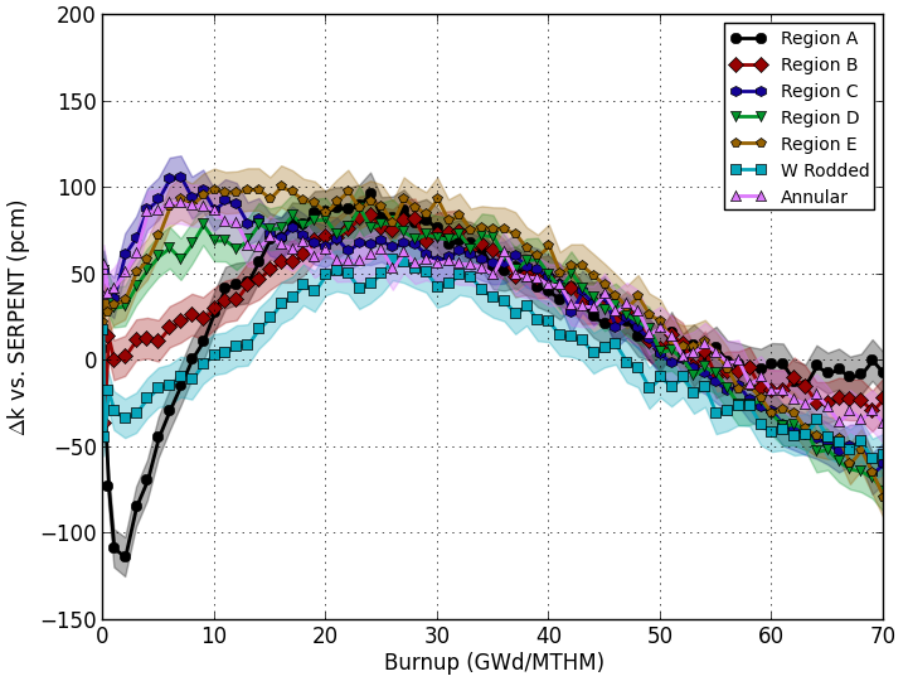

Fig. 4. Serpent-MPACT k_{eff} comparison with 3σ uncertainty bands.

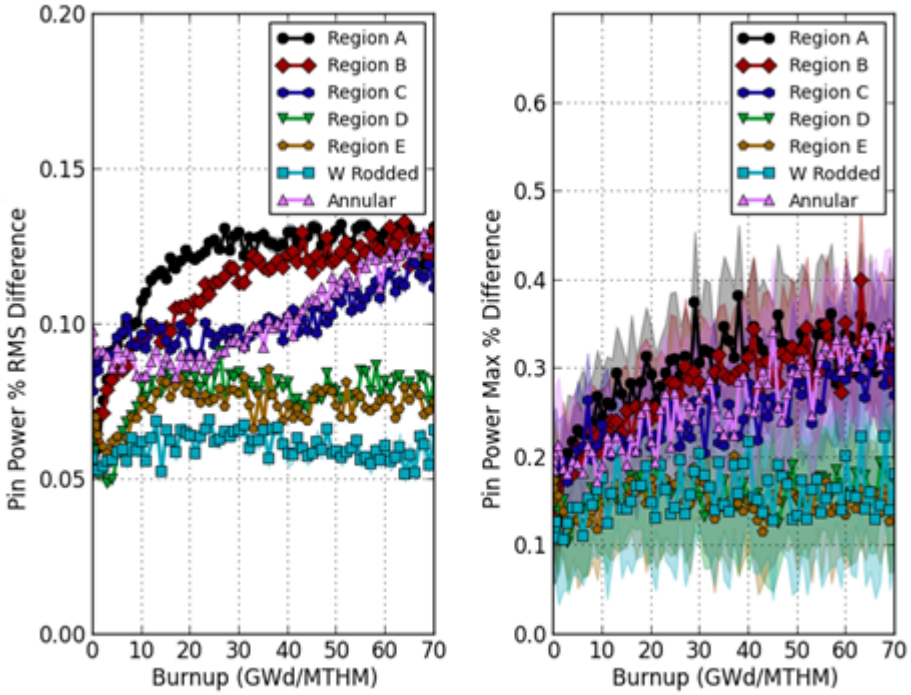

Fig. 5. Serpent-MPACT power distribution comparison with 3σ uncertainty bands.

Table III. Summary of Eigenvalue and Pin Power Differences

Model ID	Serpent - Shift		Serpent – MPACT 51g	
	Δk_{eff} (pcm)	**ΔPin Power (%)**	**Δk_{eff} (pcm)**	**ΔPin Power (%)**
	Max Abs Avg Diff Std Dev Max Unc (1σ)	**Max ABS Max RMS Max RMS Unc (1σ) Max Unc (1σ)**	**Max Abs Avg Diff Std Dev (1σ) Max Unc (1σ)**	**Max ABS Max RMS Max RMS Unc (1σ) Max Unc (1σ)**
Reg A	68 48 10 5	0.17 0.05 0.003 0.05	114 24 47 4.	0.38 0.13 0.001 0.03
Reg B	70 51 14 5	0.21 0.05 0.004 0.05	84 29 34 4	0.40 0.13 0.001 0.03
Reg C	82 50 23 5	0.17 0.05 0.003 0.05	106 36 47 4	0.33 0.12 0.001 0.03
Reg D	83 39 35 5	0.18 0.05 0.004 0.05	89 34 47 4	0.20 0.09 0.001 0.03
Reg E	103 42 37 5	0.20 0.05 0.004 0.05	101 45 51 4	0.20 0.09 0.001 0.03
W Rod	78 52 20 5	0.20 0.05 0.004 0.06	58 3 34 4	0.22 0.07 0.002 0.03
Ann	89 55 27 5	0.18 0.05 0.003 0.05	91 37 36 4	0.35 0.13 0.001 0.03

This improvement in eigenvalue compared to the previous study is fostered by using both the Serpent kappa heating values, which improves consistency, as well as the new 51 energy group cross-section library, which improves accuracy.

With regards to power distribution, it can be seen that maximum pin power differences are within 0.5% and RMS differences are within 0.15%. The general trend is that errors increase with burnup, with most lattice models reaching plateau at some point over the course of the burnup, with the exception of the Annular fuel pellet model. Also, the lower enriched assemblies tend to exhibit the greatest disagreement with Serpent.

Figure 6, Figure 7, and Table III illustrate the differences observed between Serpent and Shift, showing excellent agreement in the results. Generally, eigenvalue disagreement begins within ~50 pcm and gradually increases with burnup to within a ~100 pcm Shift under-prediction for all cases. The pin power agreement is also remarkable, with a maximum difference of 0.3% (vs. 0.5% for MPACT) and RMS differences within ~0.05% (vs. 0,15% for MPACT); notably, the agreement remains consistent during the depletion and for the various lattice types simulated.

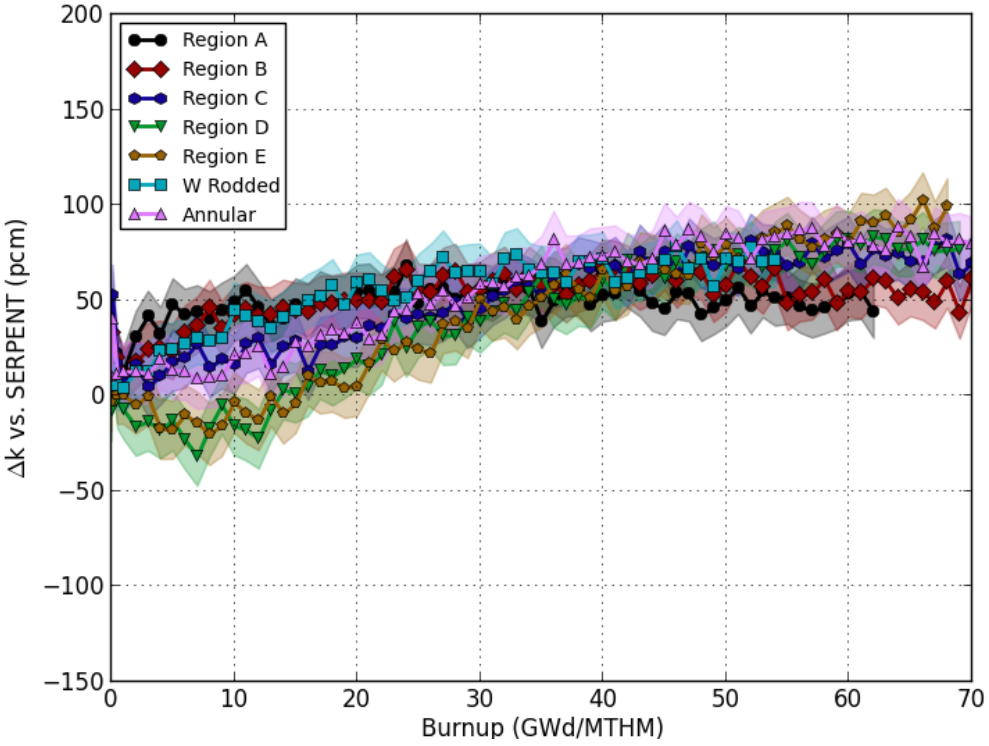

Fig. 6. Serpent-Shift k_{eff} comparison with 3σ uncertainty bands.

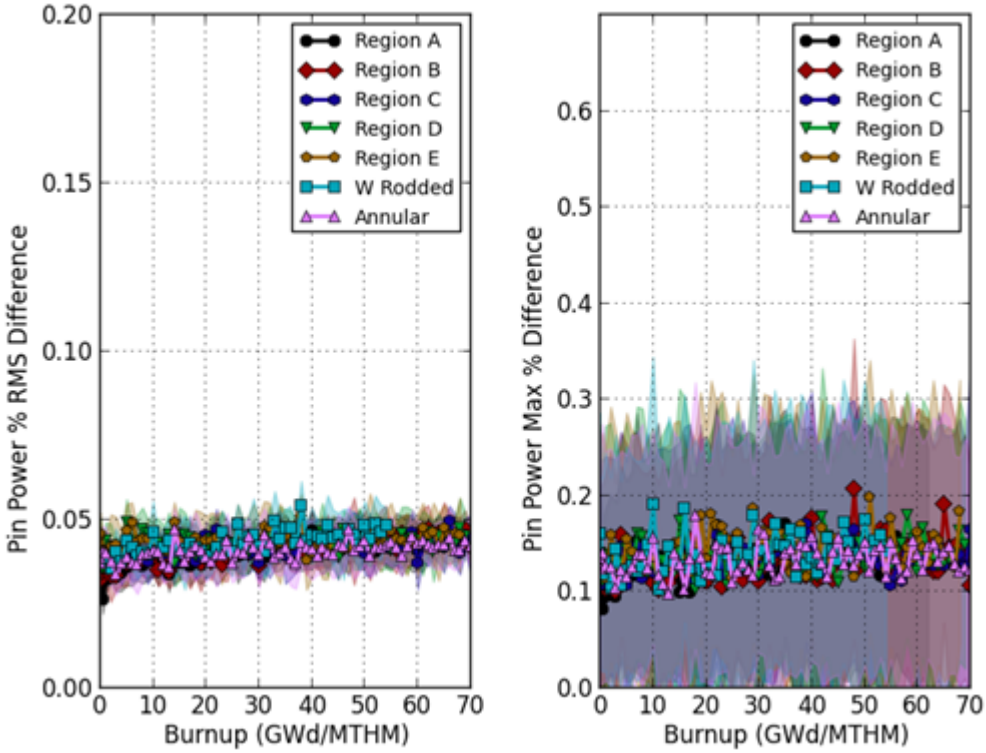

Fig. 7. Serpent-Shift power distribution comparison with 3σ uncertainty bands.

This excellent level of agreement between Shift and Serpent helps to assuage concerns regarding the differences in predictor-corrector models and substep flux renormalization between models. This indicates that the time mesh is so fine as to prevent substantial accumulation of errors brought about by differences in predictor-corrector / substepping treatments. The remaining differences might possibly be attributed to differences in modeled depletion chains or differing levels of source convergence.

IV. CONCLUSIONS

Benchmarking and improvement of the CASL toolset continues through extensive validation against plants measurement as well as comparison to continuous-energy Monte Carlo tools. This work builds on prior comparison of MPACT, VERA deterministic neutron transport solver to Serpent for 2D lattice simulations representative of the AP1000 advanced first core. It is shown that thanks to the adoption of consistent kappa heating values in Serpent and MPACT, as well as a new 51 energy group cross-section library in MPACT, significantly improved agreement between Serpent and MPACT is observed compared to what was reported in previous literature. A comparison of the results from the Shift, the VERA Monte Carlo code, to Serpent is also given, showing an excellent level of agreement between these codes and strengthening confidence in their use to generate numerical benchmarks reference solutions. Further benchmarking of the VERA toolset will continue, particularly with any introduction of improved cross-section libraries for MPACT or enhanced kappa heating approximations to account for gamma heating contributions.

The accuracy of VERA in predicting the eigenvalue and power distribution for these AP1000 lattices supports the reliability of VERA to obtain cycle-depletion predictions relative to the AP1000 advanced first core operation. This is an ongoing endeavor at Westinghouse of high industrial relevance, where the VERA predictions eventually will be confirmed against plants measurements for the first AP1000 units to come on line.

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