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Monte Carlo-Deterministic Hybrid Analysis for a Soluble-Boron-Free SMR

Mohd-Syukri Yahya and Yonghee Kim*

Department of Nuclear & Quantum Engineering, KAIST, Daejeon, Republic of Korea
**Corresponding author: yongheekim@kaist.ac.kr*

Abstract – *This paper documents the calculational procedure of a two-step reactor analysis based on Monte Carlo Serpent and Coredax nodal diffusion codes. Specifically, the paper details all major steps required to build a homogenized group constant database necessary for a 3-D nodal diffusion calculation from Serpent assembly branch calculations. It should be noted that the proposed hybrid Monte Carlo-deterministic procedure is especially advantageous for a light water reactor core analysis requiring explicit modeling of a novel reactor concept. As such, the paper compares results of the two-step hybrid calculation against a reference 3-D Monte Carlo analysis of a soluble-boron-free small modular core design loaded with a new unconventional burnable absorber design named the BigT (burnable absorber-integrated guide thimble). The result clearly demonstrates potential of the hybrid calculational procedure.*

I. INTRODUCTION

Removal of soluble-boron reactivity control from PWRs offers many potential advantageous; chief amongst them is constantly negative moderator temperature coefficients (MTC) at all times, which is very desirable for the safety of PWR operation [1]. In fact, preliminary investigation clearly shows that the MTC of a soluble-boron-free (SBF) PWR is strongly negative [2], suggesting the core could be more sensitive to moderator temperature and density fluctuations. As such, a multi-physics calculation that couples the core neutronics and its thermal-hydraulics feedback is essential to accurately assess the performance of any SBF PWR core. It is upon this observation that a hybrid Monte Carlo-deterministic two-step reactor core analysis was pursued in this research. The said calculation procedure calls for: (1) spatial homogenization of fuel assembly branch depletion calculations, and (2) nodal diffusion analysis of the 3-D core using homogenized group constants (HGCs) generated from the aforementioned lattice calculations. In this work, Monte Carlo Serpent [3] code with ENDF/B-7.1 nuclear data library was used during the fuel assembly spatial homogenization and KAIST-developed Coredax [4] nodal diffusion code was chosen for the 3-D core calculation.

II. CALCULATION TOOLS

The use of the continuous-energy Monte Carlo Serpent code for assembly spatial homogenization is very advantageous. This is because Serpent is inherently capable of handling geometry model and interaction physics without major approximations; we can model the heterogeneous lattice full-scale quite accurately, thus obtaining the best available reference solution for the problem. The capability of producing high quality reference results becomes particularly valuable in the modeling of novel reactor concepts and any other system where experimental data is scarce or not available. In addition, we can also eliminate many lattice resonance approximations by opting to use the unresolved resonance probability table sampling available in Serpent. This is particularly advantageous when coupled with Serpent's direct treatment of resonance up-scattering effects. Besides, Serpent is also equipped with an integrated and accurate nuclide depletion module as well as on-the-fly cross-section temperature treatment, which are desirable features for an efficient lattice branch depletion calculation.

Meanwhile, Coredax offers a 3-D rectangular geometry nodal diffusion calculation that can be coupled with thermal-hydraulics feedback. The nodal diffusion solver is based on Analytic Function Expansion Nodal (AFEN) and is accelerated using partial-current-based coarse-mesh finite difference (p-CMFD) method. The AFEN solver expands solutions to the 3-D diffusion equation in subsets of analytic basis functions. The thermal-hydraulics solver in Coredax is meanwhile based on a simple single channel analysis model, in which radial heat conduction is assumed in the fuel pellet, with mass and energy conserved in the coolant region. It should be noted that Coredax has been validated against many nuclear regulator-approved codes (e.g., US NRC's PARC) in a number of benchmark problems [4].

A wrapper script was also recently developed to link the Monte Carlo Serpent branch calculations to the 3-D Coredax nodal diffusion analysis. This FORTRAN-based program extracts results from Serpent output files, process the constants and tabulate them according to Coredax-formatted HGC database. Details of the wrapper program are presented subsequently.

III. CONSTRUCTION OF HOMOGENIZED GROUP CONSTANT DATABASE

Construction of HGC database is one of the most important steps in the conventional two-step reactor analysis procedure. Within this database, homogenized macroscopic cross-section (XS) and other important parameters are listed to reflect the different possible operating state conditions that a specific region in the core may experience during normal irradiation cycle. The macroscopic XSs are parametrized as a function of state variables such as moderator density, fuel temperature, moderator temperature, and soluble poison concentration to account for the instantaneous change of state of the system. Xenon and samarium microscopic absorption XSs are treated separately since they are relatively large and their number densities are very dependent on the flux level.

1. Spatial Homogenization Branch Calculations

In standard practice, the process of generating HGCs involves running assembly burnup calculations covering all assembly types and branch variables. Branch variables are accounted for by performing restart calculations for each burnup point, varying local operating conditions independently and separately, even if the state variables are physically coupled such as moderator temperature and density. The result is that the simulations are typically performed hundreds times or even more. Performing these calculations efficiently often requires the use of automated driver and processing scripts.

Fortunately, the Monte Carlo Serpent code version 2.1.25 (and upwards) provides such automated burnup sequence calculation [5]. When its 'branch' card is invoked, Serpent performs nominal burnup calculation from beginning to end. Afterwards, the code then automatically executes the branches. As such, this automated branching capability conveniently removes unnecessary computational overhead and reduces overall computing time typically associated with spatial homogenization branch calculations.

2. Group Constant Tabulations

Table 1 lists Serpent and Coredax equivalent HGC data. Note that all HGCs in the Serpent calculations are inferred from its infinite spectrum calculations [6]. B1 leakage-corrected spectrum calculations can easily be turned on by replacing the prefix 'INF_' to 'B1_' In Table I of the Serpent group constant outputs.

3. Group Constant Coefficient Calculations

Group constant coefficients (i.e., XS temperature derivatives) are necessary for the thermal-hydraulics feedback consideration in the Coredax calculations. These coefficients are generally determined based on a linear least square fitting of the three branch states. Coefficients for the second-order moderator temperature derivatives are on the other hand based on a quadratic function fit. Coefficients for the Doppler branch are meanwhile calculated with respect to the square root of the fuel temperatures.

Table I: Coredax-Serpent Equivalent Group Constants

Coredax	Serpent	Description
Tr	INF_TRANSPXS	Macroscopic transport XS, Σ_{tr}
R-Abs	INF_RABSXS – (INF_XE135_MACRO_ABS + INF_SM149_MACRO_ABS)	Reduced macroscopic absorption XS, Σ_a
NuFi	INF_NSF	Macroscopic nu-fission XS, $\nu\Sigma_f$
Fi	INF_FISS	Macroscopic fission XS, Σ_f
KaFi	INF_FISS * INF_KAPPA * 1.60218E-13	Macroscopic kappa-fission XS, $\kappa\Sigma_f$
Scat	INF_S0	Macroscopic scattering XS matrix, $\Sigma_{s,g\rightarrow g'}$
ADF	INF_DF	Assembly discontinuity factor
Xi	INF_CHIT	Fission spectrum, X
YIELD_I_XE_PM	(1) INF_I135_YIELD (2) INF_XE135_YIELD (3) INF_PM149_YIELD	Fission yield: (1) I-135, (2) Xe-135, and (3) Pm-149
XE_SM_MIC	(1) INF_XE135_MICRO_ABS (2) INF_SM149_MICRO_ABS	Microscopic absorption XS, σ_a: (1) Xe-135, and (2) Sm-149

IV. WRAPPER VERIFICATION

A study was performed to verify the wrapper's output extraction from Serpent branch calculations and its tabulation of Coredax HGC database. The calculation procedure is illustrated in Figure 1, which clearly distinguishes the level of details in the transport theory calculation (Monte Carlo Serpent) to that of the diffusion theory calculation (Coredax). In the transport code, the detailed lattice was modeled explicitly while in the diffusion code, the homogenized equivalent version of the lattice geometry was executed. Exact operating conditions were modeled in both calculations so that a one-to-one comparison can be performed. If the wrapper functions correctly, the Monte Carlo Serpent calculations should be reproduced **exactly** using the diffusion code Coredax.

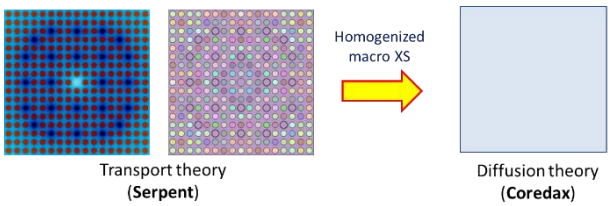

Fig. 1. Verification exercise of the wrapper program.

A BigT- [2] and IFBA-loaded assembly depicted in Figure 2 was arbitrarily chosen as the lattice design in this verification study. The calculation was executed for 30 burnup steps until a burnup of 50 MWd/kgU was

reached, with 100,000 neutrons per batch on 100 inactive and 500 active batches.

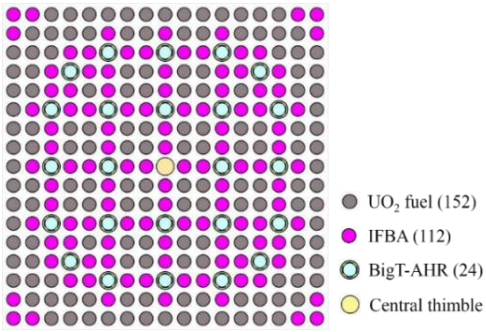

Fig. 2. The representative assembly simulated.

Figure 3 compares the calculations performed by Serpent against Coredax. Secondary y-axis plots differences of the two calculations, which clearly oscillate about zero within ±10 pcm. This oscillatory trend is actually within the statistical Monte Carlo uncertainties (mean value of Serpent collision estimator of k_∞ has an uncertainty of ±10 pcm). Figure 4 meanwhile compares xenon-samarium calculations of the two codes, which match reasonably well when transient option in Coredax was turned on (statistical Monte Carlo uncertainties are ~±70 pcm). One must note that the wrapper program should explicitly exclude xenon and samarium components from Serpent's reduced macroscopic absorption cross-section during the HGC processing and tabulation.

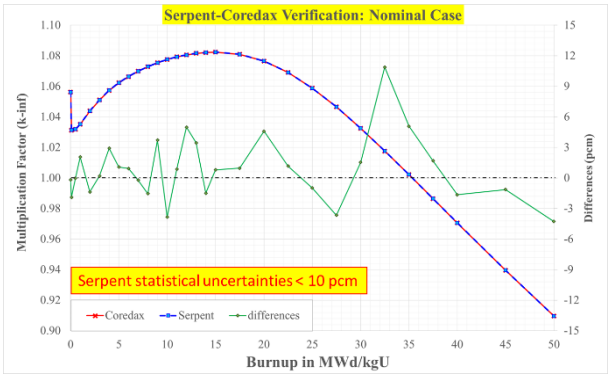

Fig. 3. Serpent-Coredax verification exercise.

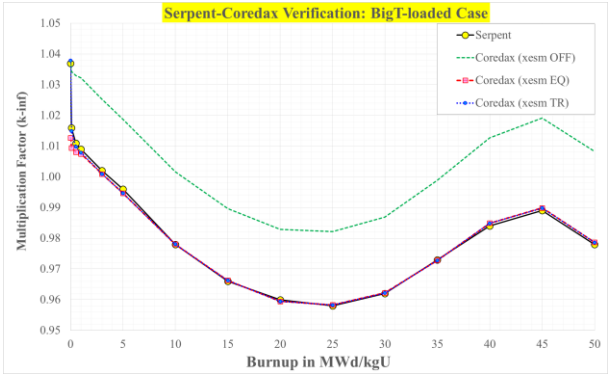

Fig. 4. Comparison of *xesm* calculations.

The study clearly shows good agreement between Serpent and Coredax as their differences are well within the statistical uncertainties of the Monte Carlo calculations. As such, this exercise verifies the extraction of Serpent outputs and its subsequent tabulations into Coredax-formatted HGC database. To get better agreement, a longer transport calculation simulating more neutron histories and batches would be needed. However, current number of neutron histories is sufficient to show the intended comparison.

V. SBF SMR CORE DESIGN

The hybrid Serpent-Coredax two-step analysis was used to assess neutronic potential of KEPCO E&C's SMR design. Rated power of the reactor is 200 MWth with active core height is 2 m. The core is consisted of 37 fuel assemblies, each loaded with 4.9 w/o UO_2 fuel rods. Stainless steel reflector assemblies are used to reduce the radial neutron leakage and, thus, enhance the core neutron economy. For a successful SBF operation, the core reactivity swing should be < 1,000 pcm [1].

1. BigT Burnable Absorber

The core uses "Burnable absorber-Integrated Guide Thimble" (BigT) absorber [2] as depicted in Figures 5 and 6, which is essentially a standard guide thimble but coated with azimuthally heterogeneous burnable absorber (BA) materials on its annulus surface. Thickness and span of the BA can be adjusted per design requirement. In this study, the BA material of choice is 90 w/o ^{10}B boron carbide (B_4C).

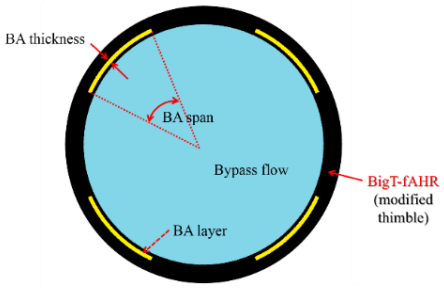

Fig. 5. Design concept of the BigT absorber.

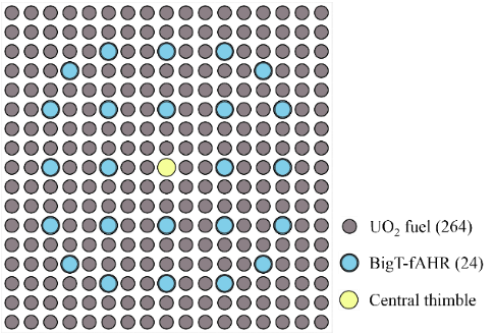

Fig. 6. A BigT-loaded fuel assembly.

2. Core Loading Pattern

Figure 7 shows fuel loading pattern of the core, which is consisted of three different BigT designs as tabulated in Table II and whose unique assembly depletion patterns are shown in Figure 8.

Table II. Three BigT designs in the SMR core.

FA (#)	B_4C thick (mm)	B_4C span (°)
FA-01 (9)	0.090	70
FA-02 (12)	0.089	55
FA-03 (16)	0.019	60

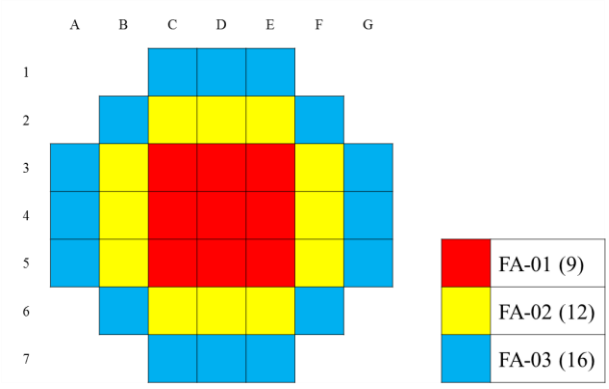

Fig. 7. Core loading pattern.

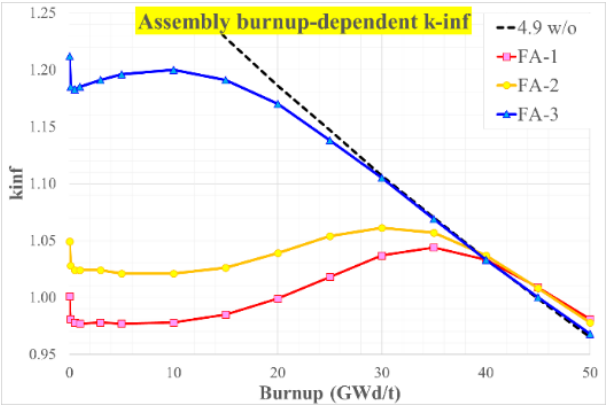

Fig. 8. Assembly neutronic characteristics.

VI. CALCULATION PROCEDURE

Since the core employs three unique BigT-loaded fuel assembly designs, three different assembly branch calculations (Figure 9) were then needed; one for each design. Furthermore, the core also contains top and bottom fuel blanket and BigT cutback regions, necessitating two additional branch calculations for non-poisonous assemblies of 2.0 and 4.9 w/o UO_2 respectively. In addition, three different radial reflector assembly (Figure 10) branch calculations were required; one for FA-03 assembly as it is the only BigT-loaded design located on the core periphery, and two for the two non-poisonous lattices. Moreover, three spatial homogenization of top and bottom axial reflectors (Figure 11) were also performed for the three unique BigT-loaded assembly configurations. As soon as the branch calculations were completed, Serpent-Coredax wrapper program was invoked to automate the processing and tabulation of Coredax HGC database. Once all necessary HGC database were ready, Coredax was called to finally assess the neutronics-thermal-hydraulics performance of the SBF SMR core design.

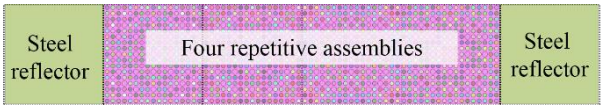

Fig. 10. Representative radial reflector calculations with all reflective boundary conditions.

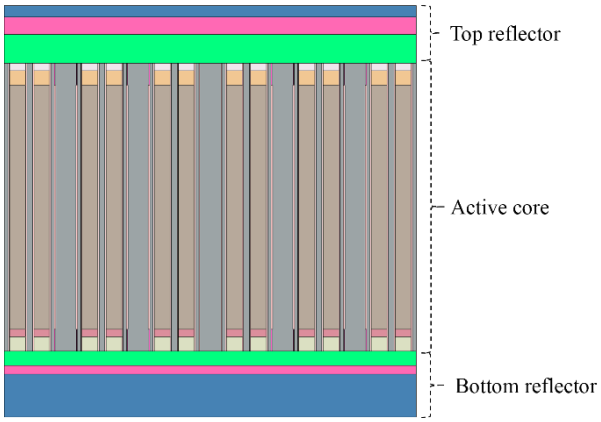

Fig. 10. Representative axial reflector calculation.

VII. SBF SMR CORE CHARACTERISTICS

Figure 12 depicts burnup-dependent k-eff trends of the BigT-loaded SBF SMR core calculated by Serpent-Coredax procedure against reference 3-D Monte Carlo Serpent calculations. In the thermal-hydraulic-coupled Serpent-Coredax analysis, the core was modeled octant-symmetry, with 4 by 5 radial assemblies and 14 axial nodes that include 4 layers of fuel blanket and BigT cutback stacks. Depletion steps were maintained reasonably small, < 1 GWd/t. It should be noted that during spatial homogenization of the assemblies, the Monte Carlo calculations were performed on 1,000 active and 500 inactive cycles, with each cycle is consisted of 120,000 histories. The resulting standard deviations of the k-inf estimations are < 8 pcm.

Meanwhile, the 3-D Monte Carlo Serpent core was modeled explicitly, with depleted materials defined assembly-wise and in octant-symmetry. 14 axial depletion meshes were also used as in the hybrid procedure. However, due to the current limitation in our computing platform capability and Serpent code, multi-physics Monte Carlo calculation was not performed in this study. Instead, the core was modeled with the average core conditions obtained from the previous

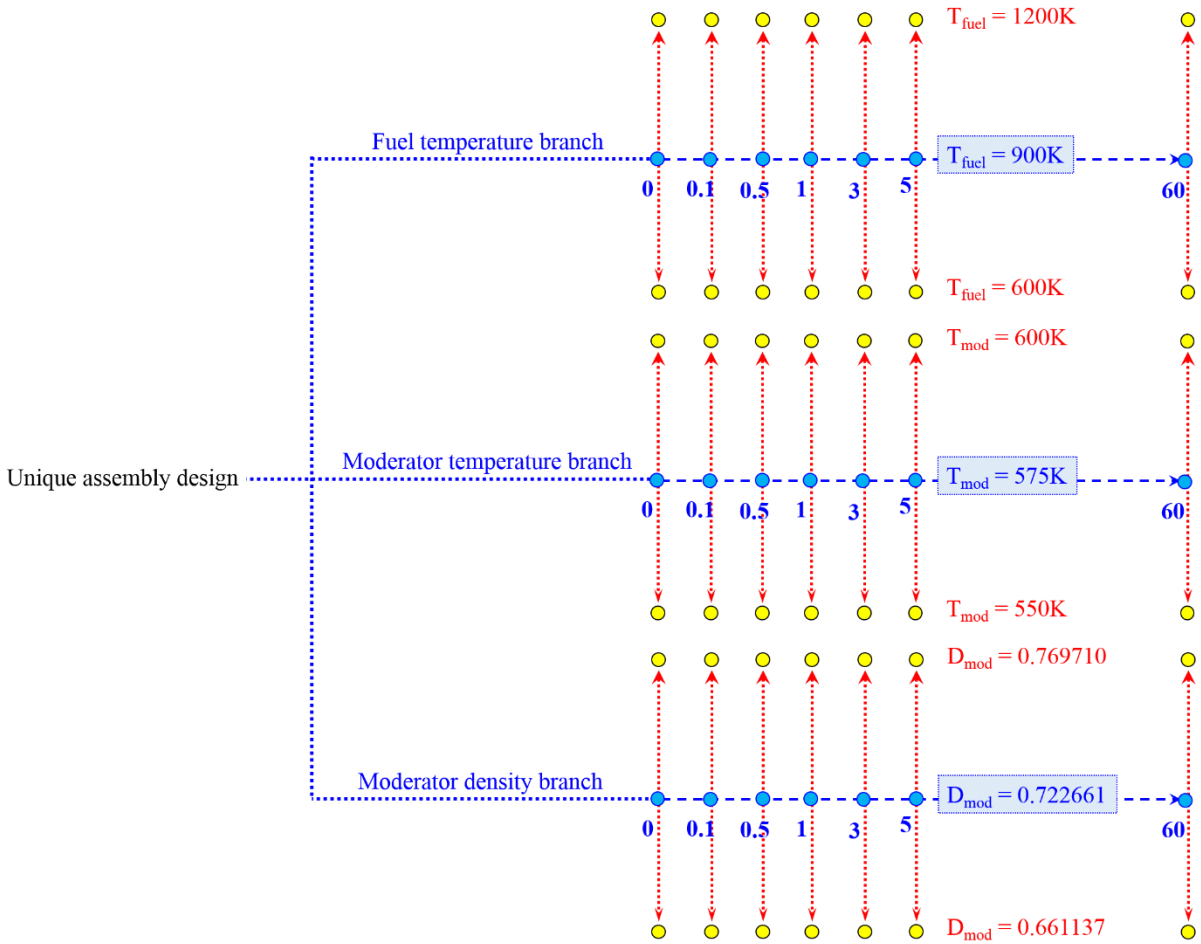

Fig. 9. Serpent branch calculations for the unique assemblies in the SBF SMR design.

Coredax calculation throughout the reactor lifetime: average fuel temperature 697K, average moderator temperature 575K, and average moderator density 0.7231 g/cm^3. The 3-D Serpent calculation was simulated on 1000 active and 500 inactive cycles, with each cycle is consisted of 500,000 particles. Resulting stochastic uncertainties of the core k-eff are < 4 pcm.

It is clear from Figure 12 that despite the differences in the basic methodologies (diffusion versus transport) and in the absence of thermal-hydraulic feedback in reference 3-D Serpent estimation, the two calculations produce reasonably similar k-eff trends of the SMR cores. Secondary axis of the plot depicts discrepancies between the two estimations (Serpent-Coredax minus reference 3-D Serpent), which fluctuate from -558 pcm at BOC to 242 pcm at MOC and to -320 pcm at EOC. While these differences are relatively big to be reasonably practical (as we hope to minimize the core burnup reactivity swing < 1,000 pcm), this study still demonstrates potential of the hybrid Serpent-Coredax procedure. It is quite possible that with multi-physics feedback considerations in reference 3-D Serpent calculation, the discrepancies can actually be reduced.

Figure 13 depicts normalized radial power distributions in the BigT-loaded SMR core, estimated using Serpent-Coredax procedure. Radial power distribution in the core is quite uniform (0.71~1.36). Meanwhile, Figure 14 shows evolution of the core normalized axial power profiles, also generated using Serpent-Coredax procedure. As expected in a typical PWR design, the core is bottom-skewed at BOC but gradually becomes slightly top-skewed at EOC.

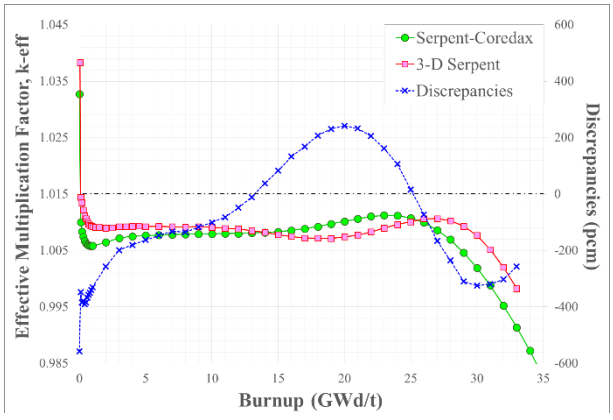

Fig. 12. Comparison of the SMR k-eff trends estimated by Serpent-Coredax against 3-D Serpent calculations.

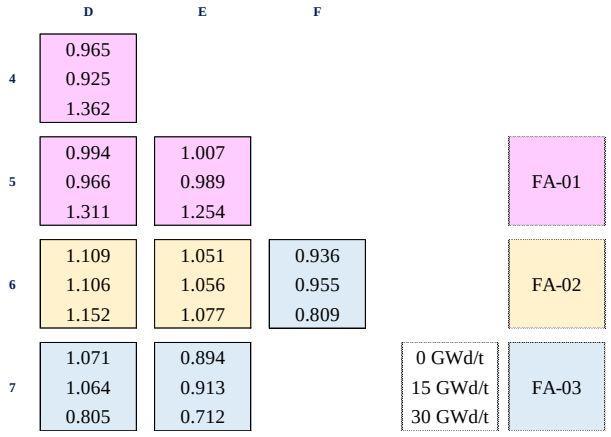

Fig. 13. Burnup-dependent normalized radial power distribution as estimated by Serpent-Coredax procedure.

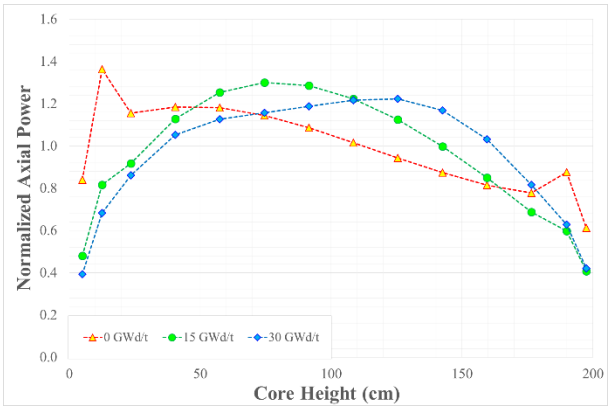

Fig. 14. Burnup-dependent normalized axial power distribution as estimated by Serpent-Coredax procedure.

VIII. CONCLUSIONS

Feasibility of a hybrid Monte Carlo-deterministic reactor analysis procedure was fairly demonstrated in this paper. The hybrid calculation procedure enables explicit full-scale heterogeneous modeling of the novel BigT-loaded assembly designs, while at the same time offers efficient design turn-around as the computing time required for each 3-D core simulation was considerably shorter; as such, trial-and-error design iterations to optimize the BigT-loaded SBF SMR core in order to attain the desired reactivity swing and discharge burnup is now possible. Verification of the hybrid Monte Carlo-deterministic two-step core calculation against a 3-D high fidelity multi-physics Monte Carlo simulation shall be performed next so as to gain more confidence in the proposed methodology.

ACKNOWLEDGMENT

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