

## A SAS2H/KENO-V METHODOLOGY FOR 3D DEPLETION ANALYSIS

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### ABSTRACT

A new SAS2H/KENO-V sequence was set up for 3D full core depletion analysis. This sequence combines a 3D Monte Carlo calculation of node power distribution and a 1D Wigner-Seitz equivalent cell transport method for independent depletion calculation of each of the nodes. This paper describes the new procedure and illustrates its capabilities by applying it to burnup analysis of the IRIS core benchmark. It was found that the SAS2H/KENO-V.a procedure can predict with good accuracy not only  $k_{\text{eff}}$ , but also the space dependent nuclide composition, burnup and power distribution. The prediction of accurate burnup and power distribution in large thermal reactor cores like the IRIS core requires use of a predictor-corrector algorithm and a large number of source neutrons and is therefore time consuming – on the order of one to two weeks on a single 2 GHz Pentium IV processor. This is more than an order of magnitude shorter than the time required for getting comparable results using the MOCUP code system.

### 1. INTRODUCTION

The progress in evaluation of point-wise nuclear data cross section libraries and in coupling of Monte Carlo codes with fuel depletion codes, makes it practical to apply Monte Carlo methods for simulation of neutron transport in complex 3D full-core configurations during fuel depletion. Indeed, the MOCUP code developed by INEEL [1] is in use at UC Berkeley (UCB) for fast reactors full core burnup analysis. MOCUP consists of the MCNP-4C Monte Carlo code [2] and of ORIGEN2.1 depletion code [3] managed by the MOCUP driver [1]. This tool, although very accurate, was found not to be adequate enough for depletion analysis of relatively large thermal core designs due to limitations described below. The specific LWR core design we tried to apply MOCUP to is IRIS – a modular, small/medium size (335 MWe) PWR with integral vessel configuration [4,5]. The reference IRIS core is to operate for four-years without fuel shuffling or partial reloading; it makes enhanced use of burnable absorbers of the IFBA (a thin layer of  $\text{ZrB}_2$  coating fuel pellets) and possibly another type of burnable absorber. The initial space-dependent depletion analysis of IRIS using MOCUP was proven to be unsatisfactory due to: (a) too long running time, (b) a limited number of zones for depletion analysis – 50, (c) a limited number of nuclides for which one-group cross sections for depletion analysis could be determined – 150, and (d) a possible problem with the convergence of the spatial distribution of fission neutron sources, unless a large number ( $10^5$ ) of neutron histories is used in each generation, prohibitively extending the running time.

In order to remove the above-mentioned limitations and at the same time to retain accuracy, we developed a new methodology that involves several modules of the SCALE-4.4a code system [6]. The multigroup Monte Carlo code KENO V.a [7] is used to generate the power distribution per node, and

the SAS2H code sequence [8] is used to perform space-independent depletion analysis for each of the nodes the core is divided into.

The new methodology is first verified by comparing its results for an IRIS 15x15 fuel assembly burnup analysis against results of two well-benchmarked code systems. The first is MOCUP, which we previously verified for thermal reactor applications [9]. The second code system is KENO V.a/ORIGEN2 recently developed at UCB [10]; it is similar to MOCUP except that it uses the KENO V.a code instead of MCNP-4C. It enables inclusion in the fuel depletion analysis of all fission products for which cross section data exist in the SCALE multi-group cross section libraries. It has been found that the latter code system is as accurate as MOCUP and is faster than MOCUP by more than an order of magnitude. The newly developed SAS2H/KENO-V methodology was then applied to the 3-D burnup analysis of two configurations of the IRIS-1000 PWR reactor core with IFBA (Benchmark#44 core [11]) that features different burnable poison distributions; one configuration uses axially symmetric and the other uses axially asymmetric IFBA distribution.

A short description of the IRIS 1000 benchmark core is presented in Section 2. The new SAS2H/KENO-V methodology is described in Section 3, together with its verification results for an IRIS 15x15 fuel assembly burnup analysis. The results and the discussion of the 3-D burnup analysis of the IRIS core are presented in Section 4.

## 2. THE IRIS 1000 BENCHMARK CORE

The Westinghouse IRIS-1000 PWR core with IFBA (Benchmark#44 core [11]) consists of 89 fuel assemblies arranged as shown in Figure 1. The core is surrounded by a reflector consisting of 50% stainless steel and 50% water. An IRIS core fuel assembly is composed of 15x15 square unit cells 204 of which are fuel cells and the remaining 21 contain guide thimbles (GT) or an instrumentation tube (IT). The GT and IT unit cells are assumed identical for these calculations. The dimensions and other specifications of the fuel assemblies are defined in [5].

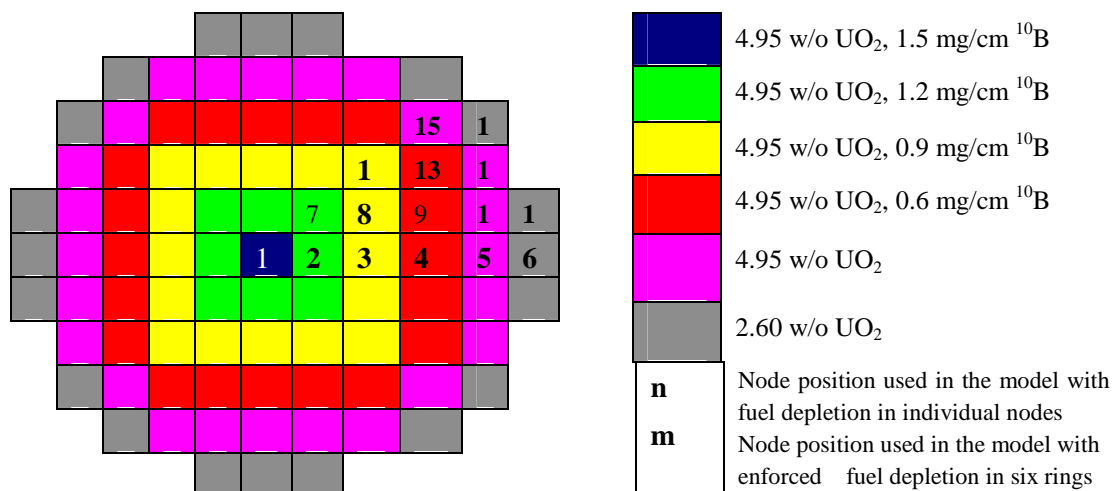


Figure 1. Horizontal cut through the IRIS Benchmark#44 core

The reference fuel assemblies (FAs) contain UO<sub>2</sub> with uranium enrichment of 4.95 w/o <sup>235</sup>U. Peripheral fuel assemblies contain UO<sub>2</sub> with enrichment of 2.6 w/o <sup>235</sup>U. Axial blankets at the top and

bottom are 30.48 cm (1 ft) long and made of  $\text{UO}_2$  with enrichment of 4.95 w/o  $^{235}\text{U}$ . Most FAs have symmetric IFBA coating (IFBA coating is expressed in  $\text{mg } ^{10}\text{B}$  per cm of fuel rod). IFBA coating covers the central 355.76 cm (12 ft) of the fuel, i.e., a fuel rod is axially composed of: 30.48 cm (1 ft) enriched (4.95 w/o  $^{235}\text{U}$ ) uncoated, 355.76 cm (12 ft) enriched (4.95 w/o  $^{235}\text{U}$ ) coated, and 30.48 cm (1 ft) enriched (4.95 w/o  $^{235}\text{U}$ ) uncoated  $\text{UO}_2$ . The fuel assembly is surrounded on each side by a 0.0508 cm (0.020") water gap, hence, the fuel assembly pitch is 22.66442 cm (8.923"). The pin cells are square; their outer fuel radius is 0.46482 cm, the outer gap radius is 0.47371 cm, the outer Zircaloy-4 clad radius is 0.53721 cm and the cell pitch is 1.50419 cm. Grid plates, assumed to occupy 1 volume % of the moderator, are homogenized with the moderator.

The  $\text{UO}_2$  is assumed to be at a uniform temperature of 810.96 K and have a density of  $10.4164 \text{ g/cm}^3$ . Zircalloy-4 is used for the cladding and structural material. It is assumed to be at a uniform temperature of 616.46 K, have a density of  $6.56 \text{ g/cm}^3$  and composed of (in weight percent): 98.23% Zr, 1.45% Sn, 0.10% Cr; 0.21% Fe and 0.01% Hf. The moderator is made of water (99 volume %;  $0.703 \text{ g/cm}^3$ ) and Zircalloy-4 (1 volume %,  $6.56 \text{ g/cm}^3$ ) at a uniform temperature of 584.16 K. All components outside of the active core are represented by a homogenized reflector having an effective radial and axial thickness of 40 cm. Included in the reflectors are: the fission gap plenum, top and bottom core support plates, core baffle and so on. The homogenized reflector composition consists of 50% (by volume)  $\text{H}_2\text{O}$  and 50% stainless steel SS304. It is assumed that the average linear power is 129.07 W/cm corresponding to an average specific power of 20.7107 MW/tHM and to a total power of 1000 MWt.

### 3. THE NEW SAS2H/KENO-V METHODOLOGY

The proposed methodology for a 3D full core fuel depletion analysis of LWR reactors makes a novel use of several SCALE-4.4a (or SCALE-4.3) modules and sequences. This methodology is based on three approximations/assumptions: First, it is assumed that the calculation of the space-dependent fuel depletion in a full 3D core can be divided into two independent calculations. One calculation determines the power distribution in large volumes called nodes, and the other calculates the burnup-dependent fuel composition. This assumption is commonly done in core depletion analysis. For the first calculation, the Criticality Safety Analysis Sequences (CSASI) [12] is used to provide a Monte Carlo-formatted cross-section library for each of the nodes, and the WAX module [13] is used to combine these libraries into one working library. The KENO-V.a code uses the processed multigroup cross sections and calculates the effective multiplication factor ( $k_{\text{eff}}$ ), neutron flux and fission density of three-dimensional system models. The geometric modeling capabilities available in KENO-V.a coupled with the automated cross-section processing within the control sequences allow complex, 3D systems to be easily analyzed.

The second and third approximations are related to the modeling of fuel depletion. The second approximation assumes that the time-dependent fuel composition in the fuel assembly can be predicted accurately enough by using the SAS2H control sequence for one-dimensional (1D) fuel depletion analysis. In this sequence, 1D neutron transport analyses of the reactor fuel assembly is performed with the XSDRNPM code [14] using a simple lattice-cell model, which is an infinite Wigner-Seitz pin cell having radii that preserve the volumes of each material in the fuel assembly. The fuel neutron flux spectrum obtained from this lattice-cell calculation is used to generate the effective one group cross sections for the fuel isotopes that are needed for burnup analysis. These cross sections are processed by the COUPLE module [15] and used by the ORIGEN-S code [16] to perform point-depletion computation. The outcome is burnup-dependent fuel composition that is to be used in the next KENO-V.a calculation. For reasons of calculation accuracy, SAS2H, CSASI and KENO-V.a use a 44-group library [17] that is based on ENDF/B-V. The third approximation, which is related to the

IRIS 1000 core design, involves smearing the boron layer with the clad (using volume homogenization) for the fuel depletion analysis. This approximation is used only for the SAS2H calculation in order to overcome the inability of the deterministic neutron transport code XDRNPM to adequately account for the effect of a very thin layer of a strong absorber. In the full core modeling using KENO-V.a, each fuel cell is accounted for explicitly and the boron layers are described discretely. The reflector regions are also treated rigorously in the KENO-V.a calculations.

The presence of  $^{10}\text{B}$  and xenon transients in the IRIS Benchmark#44 cores dictate use of small burnup steps between the flux recalculation during the fuel depletion analysis. The following predictor-corrector procedure was found to be effective for reducing the flux calculation frequency and adequately accounting for the coupling between the spatial power distribution and the depletion of fuel and burnable absorber. For each time step, the predictor procedure determines the distribution of fission power in each volumetric node for the initial burnup step B1 (the first KENO-V.a run). In order to reduce the statistical uncertainties and possible problems in the convergence of the spatial distribution of fission neutrons in each neutron generation, we use arithmetic average of this power distribution and power distribution calculated during the corrector step in the previous burnup step. This averaged power distribution is used for burnup calculation (using SAS2H) to burnup level B2. The corrector step is then used to determine the final distribution of fission power for depletion step B2 (the second KENO-V.a run), and this new power distribution is used to do the repeated depletion analysis from the initial (B1) to the final (B2) step (via SAS2H). The final fuel isotope and burnable absorber concentrations in each node at the final (B2) step are determined by averaging the concentrations obtained in the predictor and corrector steps.

The above procedure was verified for a 2D X-Y model of the IRIS 15x15 fuel assembly (infinitely long in the Z-direction with reflective boundary condition) against two well benchmarked code systems: MOCUP [3] and the KENO-V.a/ORIGEN2.1 code system recently developed at UCB [10]. Figures 2 and 3 show that the newly developed SAS2H/KENO-V.a procedure is in good agreement with the reference computational tools in predicting the burnup evolution of  $k_{\text{eff}}$  and  $^{10}\text{B}$  concentration.

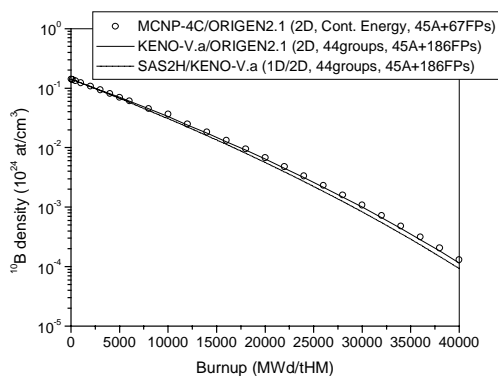


Fig. 2 Comparison of results for the change of  $^{10}\text{B}$  atomic density during the fuel depletion obtained by proposed (SAS2H/KENO-V.a) and reference (MOCUP and KENO-V.a/ORIGEN2.1) procedures

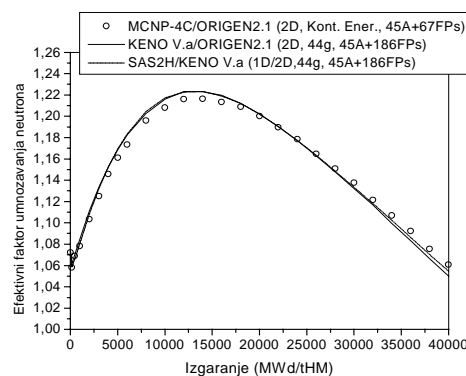


Fig. 3 Comparison of results for the change of  $k_{\text{eff}}$  during the fuel depletion obtained by proposed (SAS2H/KENO-V.a) and reference (KENO-V.a/ORIGEN2.1) procedure.

Also tested is the adequacy of the SAS2H/KENO-V.a methodology to predict the neutron spectrum in specific nodes. Figures 4 and 5 show that the flux spectrum obtained with the simplified SAS2H 1D model of equivalent cell for the fuel assembly (neglecting the neutron flux interdependence of different nodes) is in good agreement with the energy spectra obtained for the detailed 3D core

calculation (with SAS2H/KENO-V.a).

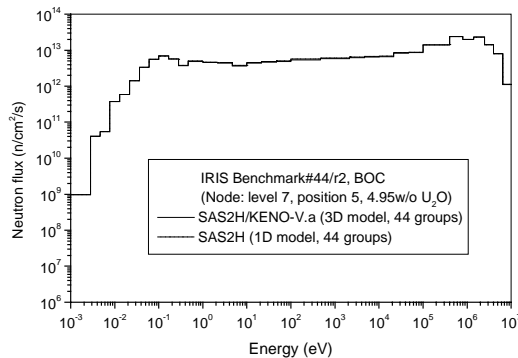


Figure 4. Comparison of energy spectrum of neutron flux in node 7x5 (level 7, pos. 5) of IRIS Bench#44 core with uniform boron distribution obtained at 0 GWd/tHM, obtained by two methodologies

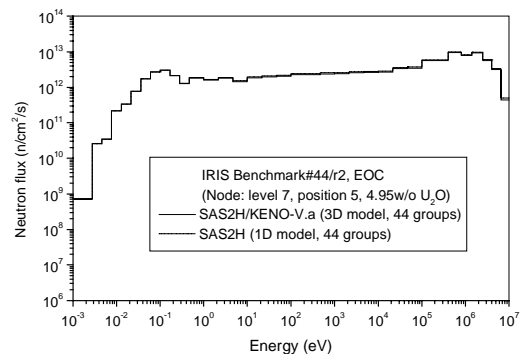


Figure 5. Energy spectrum of neutron flux in node 7x5 of IRIS Bench#44 core with uniform boron distribution at 38 GWd/tHM, obtained by two methodologies

#### 4. FULL CORE ANALYSIS

Criticality calculations using MCNP-4C and KENO-V.a can suffer from two potential problems. The first is the failure to converge the spatial distribution of the fission source from its initial guess to a distribution fluctuating around the fundamental eigenfunction solution. The second potential problem arises from the fact that the criticality algorithm produces a very small negative bias in the estimated eigenvalue. The bias depends upon  $1/N$ , where  $N$  is the number of source neutrons per generation. Thus, it is desirable to make  $N$  as large as possible. In the current 3D calculation of Benchmark#44 the following strategy for KENO-V.a calculations was chosen: (a) at least 50000-100000 histories per generation are used, (b) at least 150 of the initial generations are discarded (since the problem is loosely-coupled), (c) at least 600 active generations are run, and (d) 95% confidence intervals (2-sigma), not 1-sigma, are used. After all, it is expected that the true answer lies outside of  $\pm 1$ -sigma 33% of the time, but only 5% of the time for 2-sigma confidence intervals.

The fuel depletion analysis for Benchmark#44 cores is performed assuming a core average linear power of 129.07 W/cm (20.7107 MW/tHM); it corresponds to a total power of 1000 MWt. The initial core composition is shown in Figure 1. KENO calculations were done using the following burnup increments: 150 MWd/tHM, 350 MWd/tHM, 500 MWd/tHM, 1000 MWd/tHM from 1000 MWd/tHM to 12000 MWd/tHM, and 2000 MWd/tHM from 12000 MWd/tHM to 40000 MWd/tHM (EOC). Typical CPU time for chosen parameters and for Benchmark#44 core with 16(radial)x14(axial) nodes on a 2 GHz Pentium IV PC with Windows 2000P is 12 days for 60,000 source neutrons per generation and 16 days for 100,000 source neutrons per generation.

Figures 6 through 14 give illustrative results from full core simulation of IRIS-1000 Benchmark#44 having 89 fuel assemblies and uniform axial distribution of  $^{10}\text{B}$  obtained by SCALE-4.4a code system using 16(radial)x14(axial) burnup nodes. The initial composition of this core is defined in Figure 1. Figure 6 shows the evolution of  $k_{\text{eff}}$  whereas Figure 7 shows the evolution of the ratio of peak to average core power. Illustration of the variation in the core average radial and axial power distribution in nodes are given in Figures 8 to 14. It is observed that the power density distribution varies widely both radially and axially.

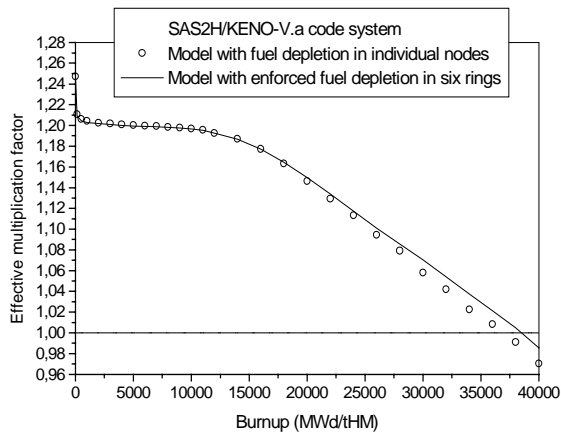


Figure 6.  $k_{eff}$  evolution with burnup

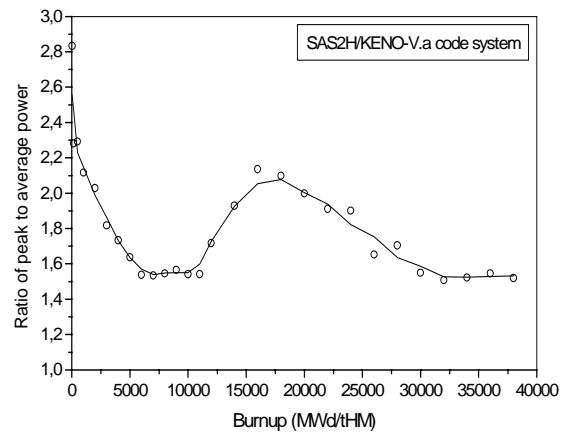


Figure 7. Evolution, with burnup, of core peak to average power density ratio

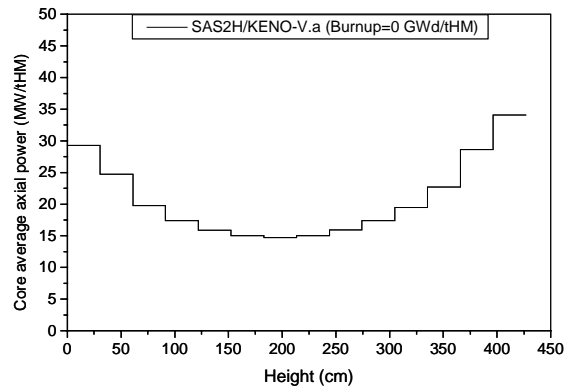
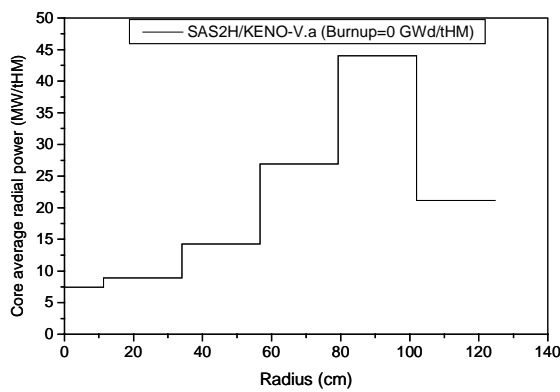


Figure 8. Radial and axial power distribution at 0 GWd/tHM

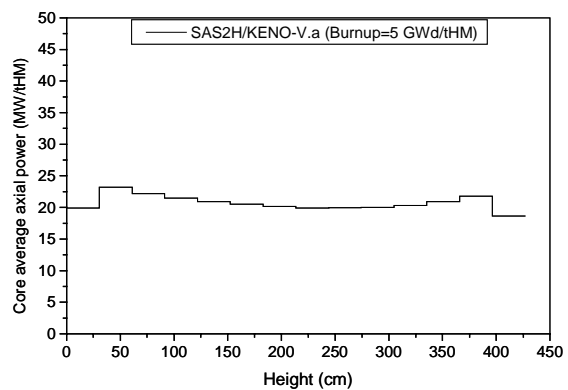
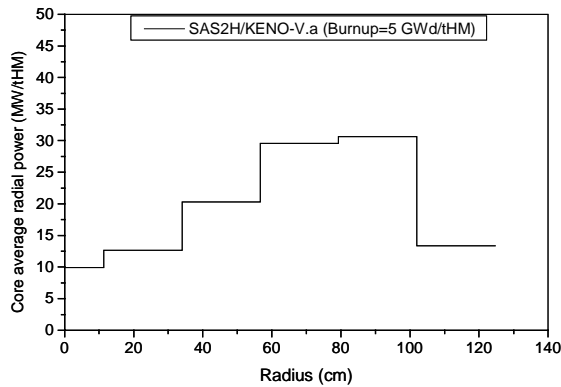


Figure 9. Radial and axial power distribution at 5 GWd/tHM

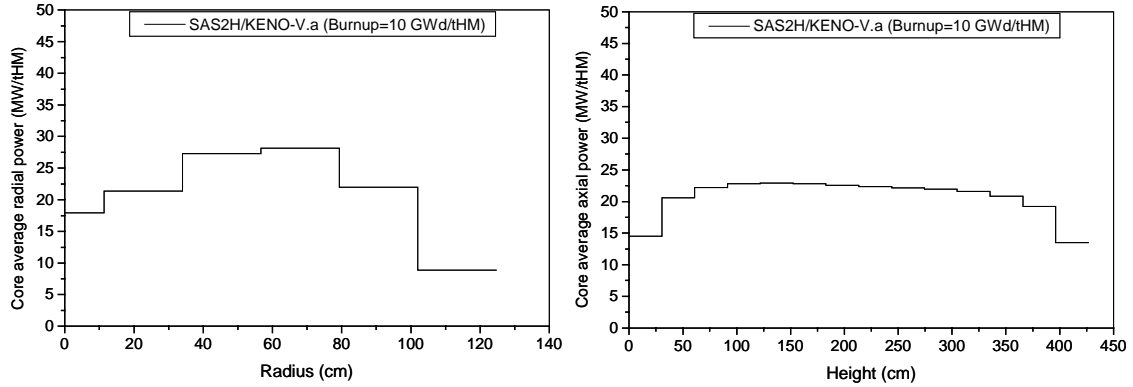


Figure 10. Radial and axial power distribution at 10 GWd/tHM

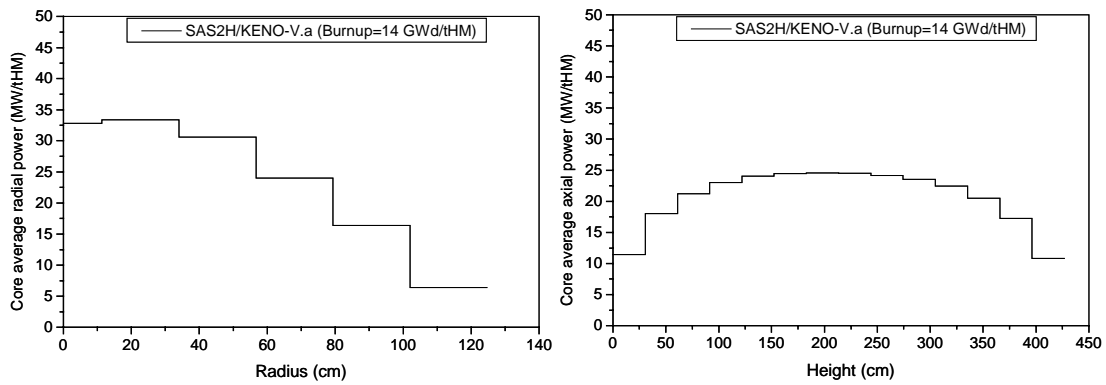


Figure 11. Radial and axial power distribution at 14 GWd/tHM

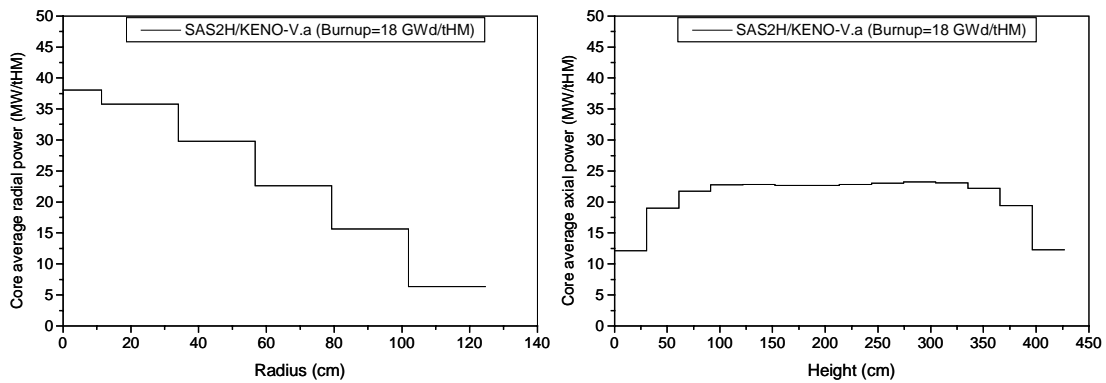


Figure 12. Radial and axial power distribution at 20 GWd/tHM

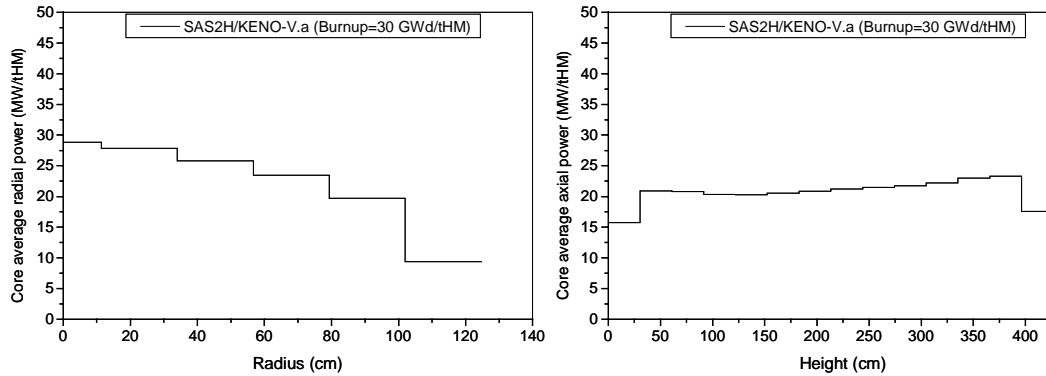


Figure 13. Radial and axial power distribution at 30 GWd/tHM

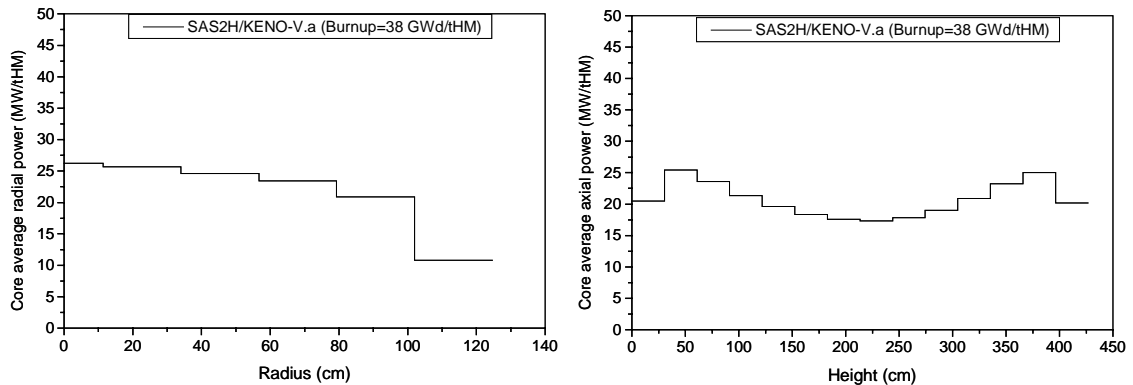


Figure 14. Radial and axial power distribution at 38 GWd/tHM

The pronounced power deep at the core center at BOC (Figure 8) is due to the relatively high loading of boron. For this reason the power peaking factor at BOC is so high (Figure 7). As the boron depletes the power shape is flattening (Figure 9); it reaches a minimum at  $\sim 7.5$  GWd/tHM (Figure 7). Thereafter the power density keeps increasing at the core center (Figure 11) reaching a peak at  $\sim 17$  GWd/tHM (Figure 7). As burnup proceeds, the fuel depletion at the core center exceeds that in the core periphery causing the power shape to flatten once again (Figure 13). Towards EOC the axial power shape deeps at the core center (Figure 14) and the power peaking factor is declining (Figure 7). The oscillatory behavior of the power distribution described above pertains to a benchmark core and not to a realistic core. A realistic core will be designed to have a much more stable power shape.

The benchmark problem was defined to be axially symmetric. Indeed, the axial power shape predicted by the new SAS2H/KENO-V methodology is nearly symmetric. This symmetry is a sensitive test for the ability of the Monte Carlo method to predict power shape distribution. The power shape evolution predicted by SAS2H/KENO-V was found to be in good agreement with the corresponding power shape calculated using CASMO/SIMULATE.



## CONCLUSIONS

The newly developed SAS2H/KENO-V.a methodology was found adequate for 3D burnup analysis of full LWR cores. The new methodology can predict with good accuracy not only  $k_{\text{eff}}$ , but also the space dependent nuclide composition, burnup and power distribution. The prediction of accurate burnup and power distribution in large thermal reactor cores like the IRIS core requires use of a predictor-corrector algorithm and a large number of source neutrons and is therefore time consuming – on the order of one to two weeks on a single 2 GHz Pentium IV processor. This is more than an order of magnitude shorter than the time required for getting comparable results using the MOCUP code system.

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