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UNIT-CELL DEPLETION ANALYSIS WITH AXIALLY VARYING COMPOSITION

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ABSTRACT

This paper describes a new procedure for the application of the SCALE-4.3 code system to depletion analysis of unit-cells that are finite and have variable composition in the axial direction. This procedure involves applying KENO-VI for generating the average power density for a pre-selected number of axial zones and for calculating leakage-factors for each of these zones. The SAS2H sequence of SCALE uses this information to perform space-independent depletion analysis for each of the zones. The application of KENO-VI and SAS2H is iterative. The results from this sequence of calculations are benchmarked against those of MOCUP and several other codes. The new methodology is found to be fast while accounting accurately for the axial variation in depletion and effective cross sections.

1. INTRODUCTION

Westinghouse, together with the Massachusetts Institute of Technology, the University of California at Berkeley and the Polytechnic of Milano, has been awarded in 1999 a DOE Nuclear Energy Research Institute (NERI) contract to develop a Generation IV reactor named IRIS. IRIS (International Reactor Innovative and Secure) is an integral primary system configuration, light water cooled modular reactor of small-to-medium power (100-300 MWe per module). More than half-a-dozen non-US organizations currently participate in this development.

A primary design objective of IRIS is long-life core without refueling or fuel shuffling. A desirable feature of this core, in addition to a life of 7 to 15 years, is a small

as practical burnup reactivity swing. This latter feature implies minimum excess reactivity built into the core at beginning of life (BOL) and, consequently, simplified core control system and enhanced reactor safety. More on the overall characteristics of IRIS can be found in (Carelli, 2000) and (Petrovic, 2000).

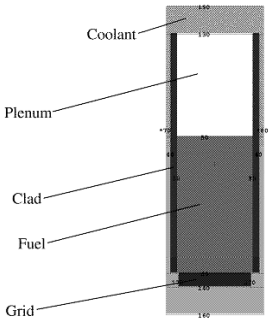
Various approaches are being considered for the design of the long-life core for IRIS. On the one extreme we are considering very tight lattices featuring a conversion ratio close to unity (Lou, 2000). On the other extreme we are considering very well moderated lattices that feature higher BOL k_{eff} for a given fissile fuel content than conventional PWR lattices. The maximum fissile content was set at 20% ^{235}U, according to the DOE specified upper limit to satisfy proliferation resistance considerations. The fuel compositions considered are UO_2 and MOX; their compatibility with water coolant is well established. Some of the benchmarks also considered a metallic alloy with Zr (10 weight %). The metallic fuel was to provide an upper bound on the conversion ratio attainable in water-cooled cores. This is not to imply that metallic fuel is compatible with water coolant.

Generic difficulties with tight lattice cores include high frictional losses of the coolant and positive void coefficient. A remedy for both of these problems may be obtained by designing the core to be of a small height. Indeed, some designs feature core height as low as ~50 cm. Another measure being used to achieve negative void coefficient is to axially segregate the core into fissile layers and fertile (blanket) layers. Short cores, especially when axially of non-uniform composition, cannot be well represented by an infinite lattice approximation, as commonly done in reactor analysis.

For the purpose of the feasibility study of long-life unit cells for IRIS we have adopted a couple of computational tools that can adequately account for axially variable composition. One is the MOCUP code (Moore, 1995). The other is based on the SCALE 4.3 code package (SCALE, 1995). The reason for developing the second methodology was a long running time for depletion analysis with MOCUP. A typical high burnup unit-cell calculation can take more than a week to complete on a single computer. In order to perform a depletion analysis for unit-cells with axially varying composition, a special methodology was developed that employs various SCALE 4.3 sequences. The purpose of this paper is to describe this special methodology developed for SCALE 4.3, and to compare it against MOCUP and several other codes.

2. BENCHMARK DESCRIPTION

Figures 1 and 2 show the geometry of our unit-cell test problem. The scale of X-axis and Y-axis in Figure 1 is 1:115. The plenum height is 75% of the active fuel length. A 20-cm thick stainless steel grid plate, which has a cross-sectional area equal to half of the unit cell, is placed under the fuel rod. The water reflector above and below the core is 40 cm thick.



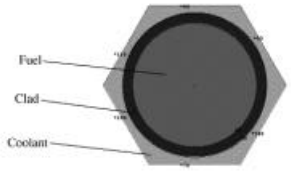


Fig. 1 Unit-cell vertical view

Fig. 2 Unit-cell horizontal view

Table 1a gives a summary of the weight fractions of stainless steel, depleted uranium and plutonium. Unless it is specified in the following sub-sections, most calculations use the material properties given in Table 1b.

Table 1a. Material Composition			Table 1b. Material Specification	
Material	Components	(w/o)	Cladding and Grid Temperature (°C) Nominal density (g/cm^2)	SS3 16L 320(Clad), 290(Grid) 7.8196
SS316L	Fe Cr Ni Mo	69 17 12 2	Coolant Temperature (°C) Pressure (bars) Nominal density (g/cm^2)	H_2O 290 155 0.7465
Depleted Uranium	^{235}U ^{238}U	0.2 99.8	Fuel Temperature (°C) Smear factor for fuel	UO_2, MOX, Metallic 600 0.95 (oxide), 0.85 (metallic)
Plutonium	^{239}Pu ^{240}Pu ^{241}Pu ^{242}Pu	67.2 21.7 6.4 4.7	Nominal density (g/cm^2) UO_2 PuO_2 Metallic fuel	 10.96 11.46 13.61

The fuel density is calculated based on the nominal densities listed in Table 1b with temperature and smear factor taken into account. The metallic fuel considered is an alloy of heavy metal (depleted U with 10 w/o of Pu) and zirconium (Zr content is 10 w/o). No refueling or fuel shuffling is allowed during operation. The average linear heat rate is between 80 to 120 W/cm. The maximum burnup limit is assumed to be 150 GWD/tHM. The maximum neutron fluence on the cladding for neutron energy above 0.1 MeV is assumed to be $4x10^{23}$ n/cm^2.

The geometric specification for the unit-cell used for the benchmarking is: fuel height of 2 m, fuel pellet diameter of 1 cm, clad thickness of 0.08 cm, and pin-cell pitch of 1.276 cm. The resulting pitch-to-diameter (p/d) ratio is 1.1 and the coolant-to-fuel volume ratio is 0.45 (the coolant-to-fuel rod volume ratio is 0.33). The average linear heat rate is 120 W/cm. The burnup proceeds in 14 time steps of full power regardless of whether the infinite multiplication factor is above unity or not.

3. DESCRIPTION OF METHODOLOGY

In this section we will describe two methodologies: (a) using MCNP - Monte Carlo code and ORIGEN2 coupled through the MOCUP code, and (b) a new methodology developed to perform a depletion analysis for unit-cells with axially varying composition that employs various SCALE 4.3 sequences.

The MOCUP Methodology

The initial calculations were done using MCNP (Briesmeister, 1997) and ORIGEN2 (Hermann, 1995) managed by the MOCUP code (Moore, 1995). MCNP calculates k_{eff}, zone-wise fluxes, relative power and effective one group averaged cross sections for use in ORIGEN2, in 3D geometry. ORIGEN2 calculates the change in the isotopic composition as a function of time. When MCNP finishes the neutronics analysis, mcnpPRO, which is part of MOCUP, will generate the effective one-group neutron cross-section data for five types of reactions. Then, these cross sections are stored in a file (Figure 3).

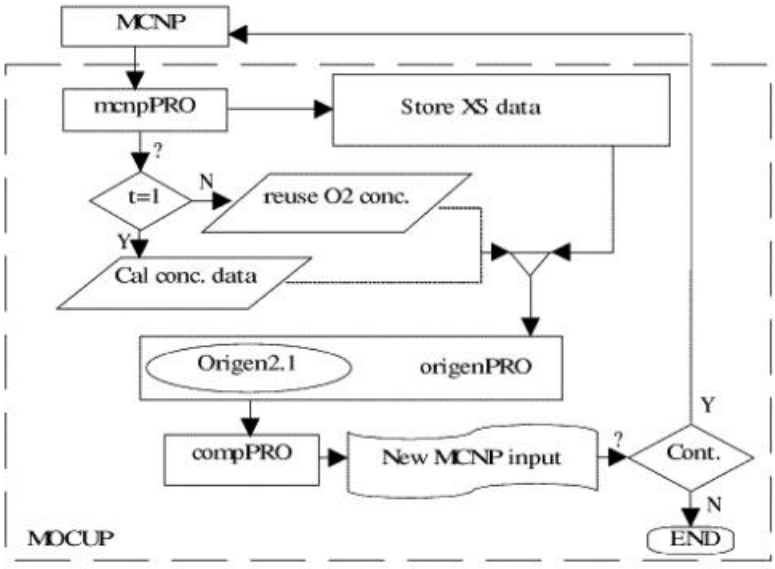


Figure 3. Program Flow for MOCUP

Most MCNP continuous-energy neutron cross-sections used in this study were processed by the NJOY code to account for the Doppler broadened effects. Up to 45

actinides and 79 fission products (FP) were accounted for. The second module of MOCUP is origenPRO, which combines the MCNP generated one-group neutron cross-section data file and a skeleton ORIGEN2 input file into an ORIGEN2 input file. Next, origenPRO makes a system call to run ORIGEN2. The last module is compPRO which updates the MCNP input file with the calculated isotope concentration from ORIGEN2 for the next time step. The user repeats the process until the desired burnup is reached. A timestep of one year between MCNP simulations is chosen for most of the problems studied with shorter ORIGEN2 depletions steps in between. Shorter time steps (e.g. 5 days, 1 month, etc) had been used at BOL. However, due to the hard neutron spectrum of tight lattices, the results did not indicate any significant changes from larger time step size (Lou, 2000).

Two sets of the MOCUP results are presented in this paper: for 2D and 3D infinite lattices. In the case of the 2D infinite lattices, the axial structure materials were not accounted for and a reflective boundary condition was used on the top and bottom of the fuel. Depletion analysis employed 27 actinides and 54 FPs. The MCNP calculations were performed with 300,000 histories, and a time step of one year was used between the MCNP simulations. The standard deviation for k-inf is ~1.0%.

The geometry for the 3D infinite lattices is described in Figure 1 and 2. In this case we employed 45 actinides and 79 FPs. The length of time steps used at BOL was gradually increased (i.e. 5 days, 1 month, 2 months, 4 months) and a length of 1 year was used for the rest of time steps. The fuel rod is divided into 5 equal-size axial zones to account for the axial dependence of neutron flux and reaction rates. The MCNP calculations were performed with 200,000 histories in the 3-D infinite lattice model.

We initially set up MCNP to run in parallel on a network of workstations (6 Sun UltraSparc 177.8 MHz) using PVM. Due to a non-dedicated computing environment, one depletion calculation with 14 time steps (i.e., about 14 MCNP runs) took about a week to finish. With a cluster of 14 UltraSparc-10 (333 Mhz) the time for a typical MOCUP problem was reduced to about one day. Nevertheless, long running time is still a major drawback of MOCUP, and was one of the reasons to develop an alternative methodology. Another reason for developing the alternative methodology is that memory limitations restricted the number of actinides and FPs we could account for in the MCNP calculations. On the other hand, the ability to accurately account for space dependence in the axial direction makes MOCUP very useful for the 3D depletion analysis.

3.2 Special Depletion Methodology Using SCALE 4.3

Two SCALE 4.3 sequences were used to perform axially dependent unit cell analysis: CSAS26 (Hollenbach, 1995) and SAS2H (Hermann, 1995a). The following procedure was used to model the burnup in 5 axial zones:

(b) 3D calculation was performed using KENO-VI (Hollenbach, 1995a) through the CSAS26 module. SCALE 4.3 limits the number of nuclides per depletion zone to 46. We decided to use 15 actinides, 29 FPs and one pseudo FP (see below). Also, due to limitations for the 3D calculations, it was not possible to use more appropriate 238-group cross section library. We used the 44-group library, which was derived from the 238-group library by using the

characteristic spectrum for LWR. From the 3D calculations we determined the specific power (in MWt/tHM) and axial buckling in each of 5 axial zones.

(c) Using these powers and axial bucklings, we performed the depletion analysis in the 1D-WS geometry with the SAS2H module for each of 5 axial zones independently. The calculation was done using 238-group library with 33 actinides and 165 FPs (see below). The 1D-WS geometry is the standard Wigner-Seitz cylindrical cell, infinite in the axial direction.

(d) The new concentrations obtained after one time step (about 365 days) in each of 5 zones were then used for the 3D calculation, in order to obtain new power (in MWt/tHM) and axial buckling in each zone.

(e) The final burnup calculation in each of 5 axial zones was performed with SAS2H using the algebraic average of the values (the power and leakage parameter) at the beginning and end of the time step. The final calculation of k-eff for the current time step was performed using CSAS 26.

These steps were repeated for each time step. The total number of time steps was 14. It is important to emphasize the following:

(a) The 1D-WS calculations were done using the 238-group cross section library, in order to better account for the effects that characterize the intermediate energy spectrum of IRIS. For each time step and in each axial zone we determined the new microscopic cross sections (by accounting for resonance self-shielding) for all nuclides (actinides and FPs). The accuracy of resonance self-shielding is determined by the accuracy of the SCALE 4.3 modules used: BONAMI (that accounts for resonance self-shielding effects in non-resolved resonances using the Bondarenko methodology), and NITAWL (that uses the Nordheim methodology for resolved resonances). This means that the effects of interference among resonances for various nuclides are not treated in SCALE 4.3 as accurately as in MCNP.

(b) The 3D calculations were performed using KENO-VI through the CSAS26 module. We used the 44-group library, which was derived from the 238-group library by using the characteristic spectrum for LWR. It was not possible to use the 238-group library with SCALE 4.3 for the 3D calculations. Thus, there was a need to check the accuracy of 44-group library, by using the 238-group library in 1D-WS calculations. Both libraries (238groupndf5 and 44groupndf5) were developed based on ENDF/B-V, which means that SCALE 4.3 uses the older libraries than MCNP-4B.

The axial buckling in zone i is defined as

$$B_{z,i}^2 = \frac{\sum_{g=1}^{G} n\Sigma_{f,g,i} f_{g,i} - \sum_{g=1}^{G} \Sigma_{a,g,i} f_{g,i}}{\sum_{g=1}^{G} D_{g,i} f_{g,i}} \quad \text{where} \quad H_{extrapol} = \frac{\pi}{B_z} \quad \text{and} \quad D_{g,i} = \frac{1}{3\Sigma_{tr,g,i}}.$$

Our choice of 15 actinides, 29 FPs and one pseudo fission product is similar to the one used for depletion analysis in WIMS/D-4 (Tabman, 1975). The pseudo fission product (PFP1) has similar characteristics as PFP used in WIMS/D-4, where the absorption cross sections has the form:

$$s_a(E) = \begin{cases} 10\sqrt{\frac{E_0}{E}}, & E < 4\,eV,\ E_0 = 0.0253\,eV; \\ 4.94 - 8.66 \cdot 10^{-6} \cdot E, & 4\,eV \le E \le 9118\,eV, \\ 10\sqrt{\frac{E_0}{E}}, & E > 9118\,eV. \end{cases}$$

Using this formula, we prepared the group data in 238 groups and 44 groups. The 44-group data for PFP1 were added to the existing 44-group SCALE 4.3 library.

The 44-group model with 15 actinides, 29 FPs and one PFP was not used for depletion analysis (it was used for 3D KENO-VI calculations). The 238-group model with 33 actinides and 165 fission products was used for the depletion analysis in the 1D-WS geometry (SAS2H), and the concentrations from these calculations were used for the 3D calculations as follows:

1. For the first 14 actinides (out of 15) in the 44-group 3D calculations we used the same concentrations of the first 14 actinides (out of 33) from 238-group 1D-WS calculations. The concentration of the actinide No. 15 (out of 15), i.e., Pu-238, was corrected in such a way that its total absorption is equal to the total absorption of remaining 19 actinides (out of 33). This correction is performed by using the 238-group total absorption cross sections and the 238-group neutron spectrum from 1D-WS calculations.

2. In the case of fission products, the concentrations for 29 FPs (out of 29) in the 44-group 3D calculations are the same as the concentrations of the first 29 FPs (out of 165) from 238-group 1D-WS calculations. The concentration of the pseudo fission product (PFP1) is determined on such a way that its total absorption is equal to the total absorption of remaining 136 FPs. This calculation was also performed by using the 238-group total absorption cross sections and the 238-group neutron spectrum from 1D-WS calculations (the 238-group cross sections for PFP1 were also used)

3. In addition, we developed an auxiliary module for SCALE 4.3 in order to speed up the calculation of the concentration of Pu-238 and PFP1 for the model with the reduced number of actinides and FPs.

The above described procedure was used in order to increase the accuracy in the calculation of k-eff, the axial distribution of fission power and axial bucklings in the 3D model with reduced number of groups, and reduced number of actinides and FPs.

4. RESULTS AND DISCUSSION

4.1 Sensitivity Analysis

(a) Number of Histories in MCNP. In the MOCUP depletion analysis, MCNP needs to be run at least once per time step. The cross sections needed for the OREGIN2 depletion calculations are generated by MCNP. There is always a question with how many neutron histories the MCNP should be run in order to assure converged solution? Both the accuracy of the result and the time needed to perform this calculation may be very dependent on the number of histories in MCNP.

We ran MCNP for the IRIS hexagonal unit-cell (MOX fuel, 10 w/o Pu) with: (a) 3 x 10^5 and (b) 3 x 10^6 source neutrons. Figure 4 shows the spatial (axial) dependence of the U-238 average capture cross section obtained with MCNP-4B, while Figure 5 shows the same for the Pu-239 average fission cross section. The error bars shown represent the statistical error of one standard deviation.

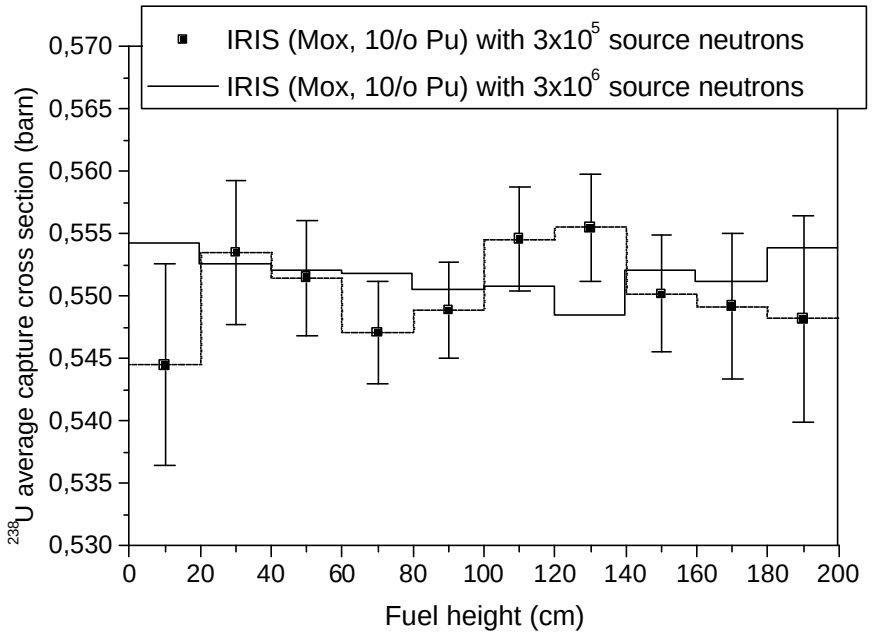


Figure 4. Spatial dependence of ^{238}U average capture cross section in IRIS unit cell (MOX, 10 w/o Pu) obtained with MCNP-4B code for different number of source neutrons

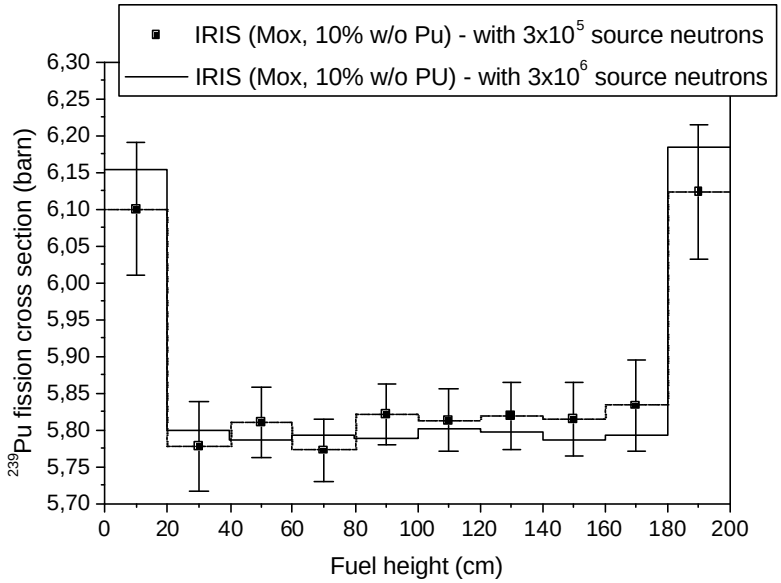


Figure 5. Spatial dependence of ^{239}Pu average fission cross section in IRIS unit cell (MOX, 10%w/o PU) obtained with MCNP-4B code for different number of source neutrons

As can be seen from Figs. 4 and 5, the difference is within the statistical error. It was recently shown (Takeda, 1999) that the error propagation in number densities in Monte Carlo burnup calculation due to the statistical error is much smaller (below 1.0%) than the cross section errors. Thus, we decided to run MCNP within MOCUP with 2-3 x 10^5 source neutrons. However, in the case of SCALE 4.3, we used 10^6 source neutrons for the 3D KENO-VI calculations.

(b) Time Step Length for Depletion Analysis. The 1D-WS cell with MOX fuel (10% Pu) was analyzed by SAS2H/SCALE-4.3 once with 14 time steps – each 350 day long, and the second time with 56 time steps – each 87.5 days long. We observed no difference between the results. Thus, we decided to use 14 time steps, each one year long.

(c) Number of Fission Products Accounted For. The 1D-WS cell with MOX fuel (10% Pu) was analyzed by SAS2H/SCALE-4.3, once with 165 FPs, and the second time with 70 FPs. In both cases, the 238-group cross section library was used. Again, we did not see a considerable difference between these two models.

4.2 Axial Variation of Cross Sections

The microscopic cross sections do not change very much axially, with the exclusion of the top and bottom zones, where the neutron spectrum is different (see Figs. 4 and 5). Based on this analysis, we decided to follow the depletion independently in each of the 5 axial zones using SAS2H module with 1D-WS cell model. Using the methodology described in Section 3.2 we obtained the axial dependence of Pu-239 fission cross section for one time step, and compared it with the MCNP-4B results. Figure 6 shows a good

agreement with MCNP, and the capability of this methodology to include axial dependence of cross sections in the SAS2H 1D-WS cell model.

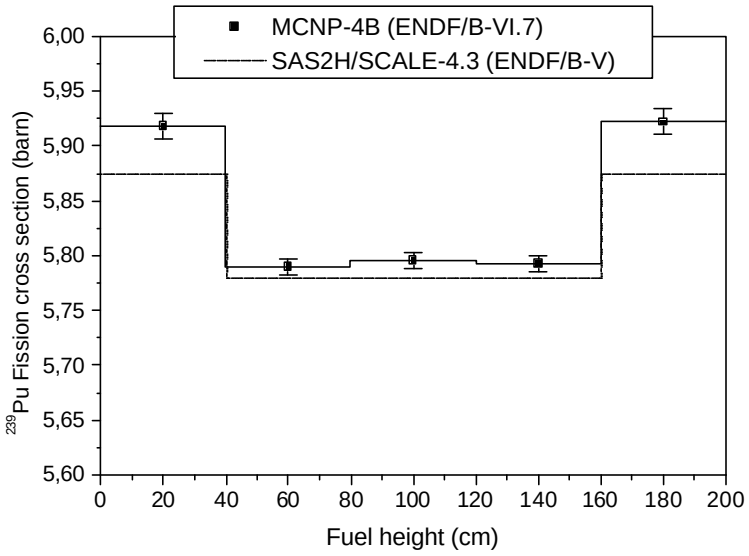


Figure 6. Comparison of spatial dependence of ^{239}Pu average fission cross section in IRIS unit-cell (MOX, 10 w/o PU) obtained with MCNP-4B and SAS2H (SCALE-4.3) codes

4.3 Unit-Cell Depletion Analysis

Various methodologies and codes in 1D, 2D and 3D were used to perform the depletion analysis for four IRIS hexagonal unit-cell test cases: (a) MOX fuel with 10w/o Pu, (b) metallic fuel with 10w/o Pu, (c) MOX fuel with 19.5 w/o, and (d) metallic fuel with 19.5 w/o Pu.

(1) SCALE 4.3 was run using the SAS2H sequence with 1D-WS cylindricized representation of the IRIS unit-cell, with (a) 238-group cross section library, including 33 actinides and 165 FPs, and (b) 44-group cross section library, including 15 actinides and 29 FPs, and one pseudo FP.

(2) Westinghouse calculations were done in a modified 2D geometry (equivalent square lattice), employing a 70-group cross section library based on ENDF/B-VI data. For this study, axial leakage was approximated by a constant axial buckling. Depletion analysis employed 15 actinides and 29 FPs including one pseudo FP.

(3) SCALE 4.3 was also run using our new CSAS26/SAS2H methodology with 3D hexagonal representation of IRIS unit-cell and a 44-group cross section library (KENO-VI). Depletion analysis was done using SAS2H in 1D-WS geometry for 5 axial zones independently, including 15 actinides, 29 FPs, and one pseudo FP in 238 groups. Both cross section libraries are based on ENDF/B-V.

(4) MOCUP was run with a 3D hexagonal geometry, with continuous energy spectrum, employing 45 actinides and 79 FPs.

(5) Two sets of the 2D MOCUP results for 10 w/o Pu MOX fuel and 10 w/o Pu metallic fuel are also presented. In this case, 27 actinides and 54 FPs were used for depletion analysis.

Figure 7 and 8 show the results for MOX and metallic fuel with 10 w/o Pu, while Figure 9 and 10 show the results for MOX and metallic fuel with 19.5 w/o Pu. The 2D results of MOCUP are in good agreement with the Westinghouse 2D calculation (Figures 7 and 8). The deviation of these two results from the other results shown on Figures 7 and 8 is probably due to the smaller number of nuclides traced in the MOCUP 2D and the Westinghouse calculation. The small number of nuclides is adequate for a thermal system design, and may not be adequate for a harder spectrum in IRIS. Good agreement between two SAS2H/SCALE 4.3 results with 1D-WS representation of the IRIS unit-cell as described in (1), shows the importance of using the proper spectrum when collapsing cross sections from 238 groups to 44 groups, and reducing number of actinides and FPs. A very good agreement between the results of the CSAS26/SAS2H 3D methodology and MOCUP 3D for all four test cases prove that our new SCALE 4.3 based 3D methodology is accurate for this unconventional design.

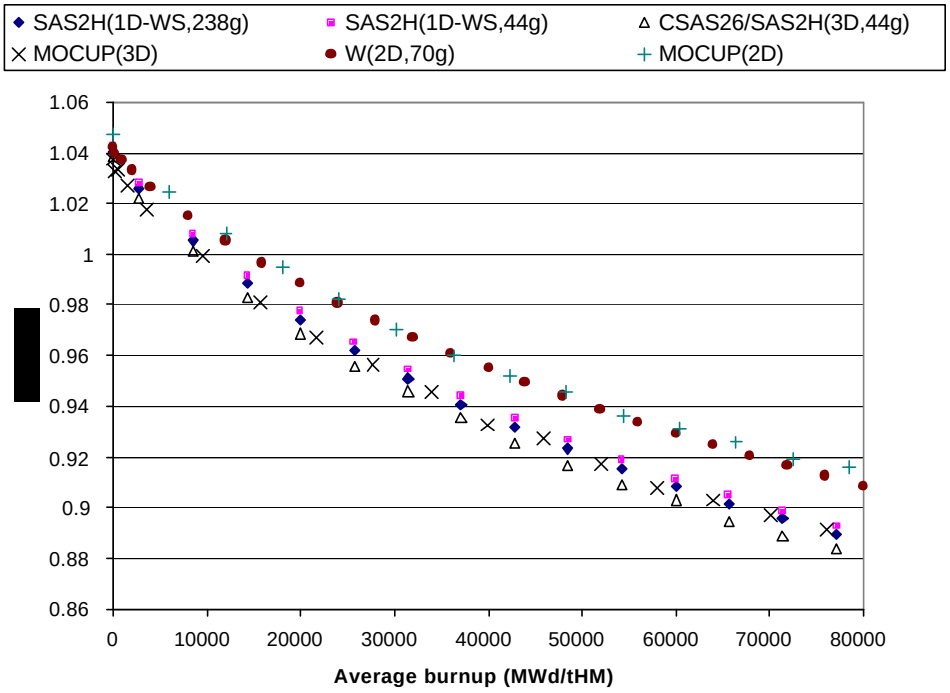


Figure 7. Comparison of *k* calculation results for unit cell of IRIS long-life core with MOX fuel (10%w/o Pu) and H_2O coolant

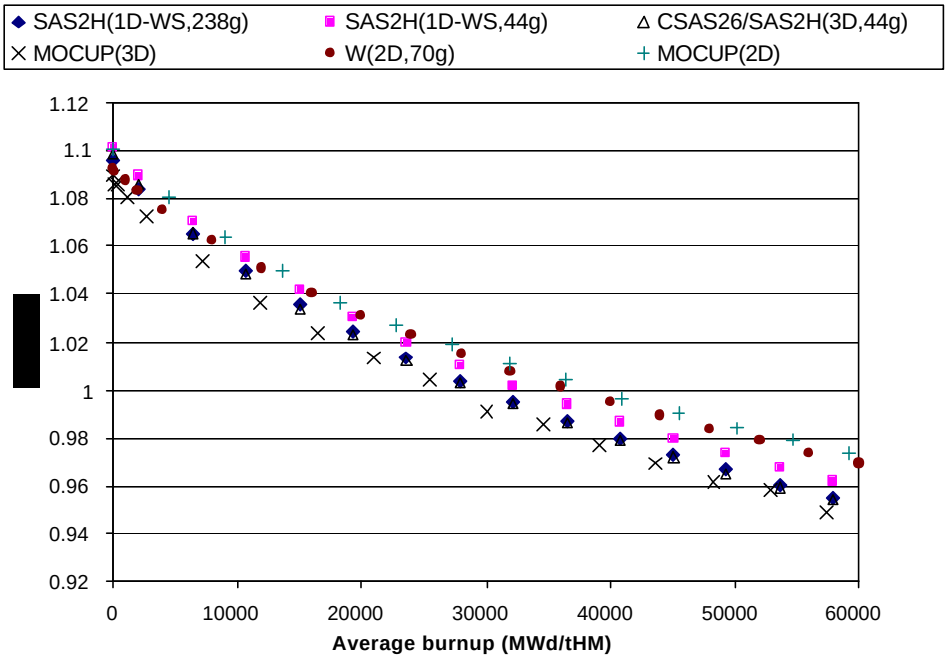


Figure 8. Comparison of *k* calculation results for unit cell of IRIS long-life core with Metallic fuel (10%w/o Pu) and H_2O coolant

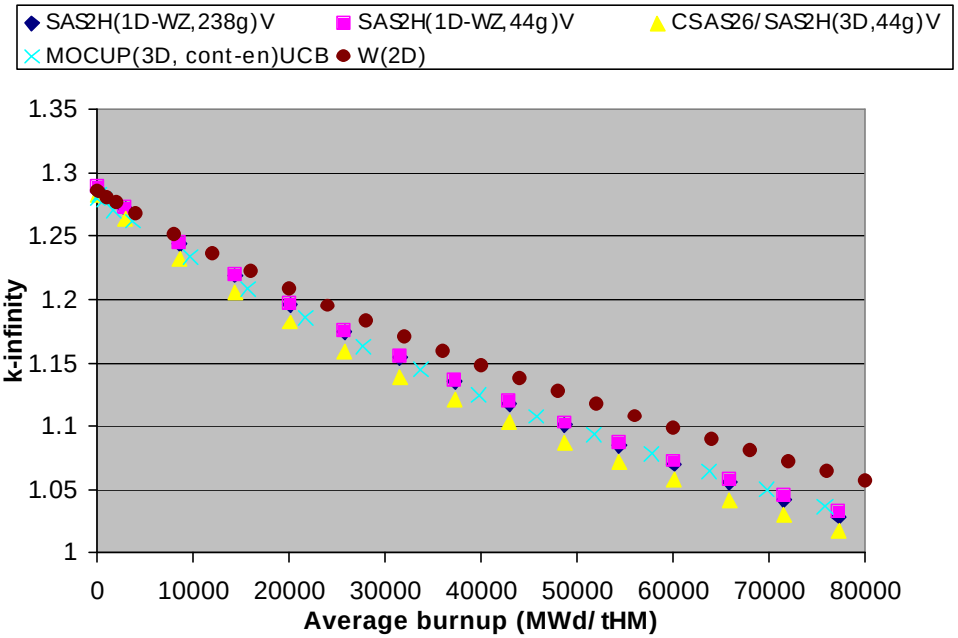


Figure 9. Comparison of *k* calculation results for unit cell of IRIS long-life core with MOX fuel (19.5%w/o Pu) and H_2O coolant

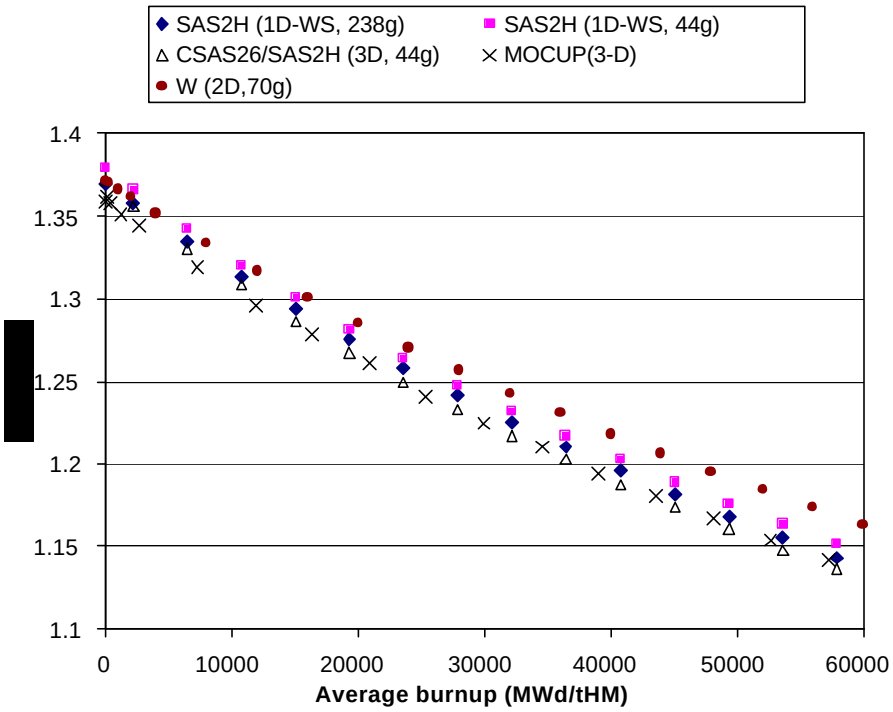


Figure 10. Comparison of *k* calculation results for unit cell of IRIS long-life core with Metallic fuel (19.5%w/o Pu) and H_2O coolant

While we needed to use up to 14 UltraSparc 10 workstations in order to reduce the running time to about one day for MOCUP, the new CSAS26/SAS2H methodology allowed us to run the same depletion problem on a single Pentium III PC (866 MHz) for less than 15 hours. For example, one time step takes approximately 2 hours and 25 minutes on 11 Ultra-10s (UltraSparc II, 333MHz, 128MB RAM, 2MB cache) using PVM. Therefore, it takes about 34 hours to finish a 14-timesteps problem. The possible reason for this extensive CPU requirement for MOCUP are large MCNP cross-section libraries that take much more space than the SCALE4.3 libraries. The MCNP cross section library may require more than 50 MBytes. The memory bus speed can be important since the cross-section data will not fit into the cache memory. Thus, it should not be a surprise that three or four Pentium III PCs may outperform 11 Ultra-10 workstations due to a faster access to memory data.

5. CONCLUSIONS

Our desire to avoid CPU-intensive Monte Carlo based depletion analysis (MOCUP), forced us to look for alternative methodologies that could account for the axially varying compositions. The new methodology based on the combination of CSAS26 and SAS2H within SCALE 4.3 has shown to be fast while accounting for the axial variation in depletion and effective cross sections. The results of SCALE 3-D calculation are in good agreement with MOCUP in evaluation of multiplication factor for the unconventional designs shown here. When the system has a hard neutron energy spectrum, the number of nuclides being accounted for becomes important. We also compared results of IRIS unit cell analysis for different 1D, 2D, and 3D methodologies. Having in mind

differences in cross section libraries, differences in the number of actinides and/or fission products, and unconventional design with harder spectrum, we got reasonable agreements.

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