March 1, 2002

Paper: AID 91
Topical Area: Research and Innovation in Reactor Technology
To be published on CD ROM

Nuclear Science and Technology Division (94)

Computational Benchmark of the 2-D Depletion Sequence SAS2D for Characterization of Spent Nuclear Fuel

Charlotta E. Sanders and Mark D. DeHart

Oak Ridge National Laboratory,*
PO Box 2008,
Oak Ridge, TN 37831-6370 USA

(865) 574-5279 (865) 576-3468
E-mail: sandersc@ornl.gov E-mail: dehartmd@ornl.gov

Submitted to the
International Youth Nuclear Congress: Youth, Future, Nuclear,
April 16–20, 2002,
Daejeon, KOREA
International Nuclear Training Center

www.iync.org
tp2002@iync.org

*Managed by UT-Battelle, LLC, under contract DE-AC05-00OR22725 with the U.S. Department of Energy.

Computational Benchmark of the 2-D Depletion Sequence SAS2D for Characterization of Spent Nuclear Fuel

Charlotta E. Sanders and Mark D. DeHart

Oak Ridge National Laboratory, PO Box 2008, Oak Ridge, TN 37831-6370 USA

Abstract

The complexity of many fuel assembly designs makes accurate depletion calculations difficult. Mixed oxide (MOX) fuels, i.e., fuel containing a mixture of uranium and plutonium oxides, presents a challenge for current generation depletion analysis codes. A comprehensive computational benchmark has been performed as part of the OECD/NEA Expert Group on Burnup Credit (EGBUC) where results have been compared for the calculation of isotopic inventories for the nuclides of interest to MOX fuel burnup credit. Two MOX compositions were considered: weapons-grade fuel (for material disposition) and first recycle MOX, using three increasingly complex models (pincell, assembly, and a mixed UO_2/MOX supercell). The results show that there is good agreement between the three modeling approaches when comparing k_{inf} and actinide concentrations. However, there were some differences of the nuclide densities for a few of the fission products, which are most likely caused by spectral differences between the models. This benchmark was designed to allow code-to-code comparisons. SAS2D has been found to be in very good agreement with a suite of independent calculations using various codes and data. Note that the results from all codes are preliminary and are subject to change. In addition, this benchmark is part of a larger program that focuses on validating SAS2D for characterization of spent nuclear fuel.

INTRODUCTION

The complexity of many fuel assembly designs makes accurate depletion calculations difficult. This complexity is exacerbated by resonance effects in fuels with significant quantities of Pu. This paper presents the results of a code-to-code comparison of depletion problems using mixed oxide (MOX) fuel loadings, and introduces a new depletion approach developed at Oak Ridge National Laboratory (ORNL).

Depletion methods used to estimate spent fuel contents to date have primarily fallen into two categories: reactor depletion codes, which are not designed for long term cooling and in general fail to track some fission products that become important only with significant cooling time; and one-dimensional (1-D) codes such as the SAS2H sequence in SCALE.[1] While the 1-D approach of SAS2H has been shown to produce remarkably good agreement with radiochemical assay measurements of PWR fuel samples,[2,3] BWR assemblies have long been a challenge for 1-D modeling because of burnable poisons, variable pin enrichments, and control blade insertion during operation. In addition, with the move toward higher initial enrichments in PWR fuels as well as the increasingly more common use of burnable poisons, the complexity of PWR fuel assembly designs has increased. Current generation depletion methods are also based on assumptions that are not always valid in MOX fuels.

ORNL has recently completed development of a two-dimensional (2-D) depletion sequence, SAS2D. This sequence uses the 2-D arbitrary geometry, S_n theory code NEWT[4] to provide 2-D fluxes for a user-specified configuration and reactor conditions. Depletion calculations are then performed for as many different materials as desired using ORIGEN-S.[5] This approach offers several advantages over the 1-D approach: assembly heterogeneities can be explicitly modeled, multiple materials can be depleted simultaneously, and cell-weighting approximations are not necessary.

An evolving challenge for depletion methods used in burnup credit analysis lies in its application to mixed oxide (MOX) fuels, i.e., fuel containing a mixture of uranium and plutonium oxides. A comprehensive computational benchmark has been performed under the auspices of the OECD/NEA Expert Group on Burnup Credit (EGBUC), [6] in which methods have been compared for the calculation of isotopic inventories for the nuclides of interest to MOX fuel burnup credit. This benchmark was designed to allow code-to-code comparisons and to allow study of potential weaknesses in methods or data relative to MOX fuel concepts.

BENCHMARK CALCULATIONS

Two MOX fuel vectors were considered for the EGBUC Phase IV-B computational benchmark: weapons-grade MOX and first recycle MOX, using three increasingly complex models to represent the depletion environment. Consequently, six calculations were performed, encompassing two initial MOX fuel compositions and three calculational models. The two initial MOX fuel compositions represent (a) a typical plutonium vector for materials derived from the reprocessing of thermal reactor UO_2 fuels (first generation MOX), and (b) a MOX fuel case appropriate to the disposition of weapons plutonium. The initial MOX fuel enrichments are presented in Table 1.

TABLE 1: Initial MOX fuel enrichments for first-recycle MOX and weapons-grade MOX fuel.

MOX Fuel Enrichment Zones	MOX Fuel Pu Content, w/o Pu_{total}/[U+Pu]	MOX Fuel Enrichment, w/o $Pu_{fissile}$/[U+Pu]
First-recycle MOX fuel		
High	8.866	5.692
Medium	6.206	3.984
Low	4.894	3.142
Average	8.000	5.136
Weapons-grade MOX		
High	4.377	4.110
Medium	3.064	2.877
Low	2.416	2.269
Average	3.950	3.709

The first model is a simplified MOX pincell, using the average MOX fuel composition, and shown in Figure 1. The second model is a 17×17 MOX fuel assembly as shown in Figure 2. The third model is a MOX-UO_2 supercell, where a 17×17 MOX fuel assembly is associated with three 17×17 UO_2 fuel assemblies in an infinite periodic lattice, as shown in Figure 3. The UO_2 fuel pins in the supercell model have an initial fuel enrichment of 4.3 wt % ^{235}U.

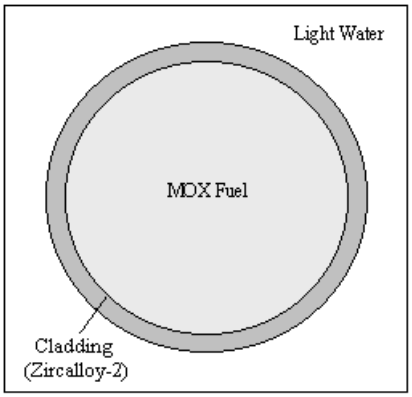

FIGURE 1: Simplified MOX pincell.

The assembly geometry is based on a typical 17×17 PWR fuel assembly. The cladding and guide tubes consist of zircalloy-2 and the moderator consists of light water with 600 ppm boron. The fuel temperature was 900 K, the cladding temperature was 620 K, and the coolant/moderator temperature was 575 K. The cladding density was 5.8736 g/cm^3 and the coolant/moderator density was 0.7245 g/cm^3. The MOX fuel assemblies were irradiated over three operating cycles, with a downtime of 30 days between each cycle, to obtain a target burnup of 48 GWd/MTU. Comparisons between the various codes were performed at 16 GWd/MTU, 32 GWd/MTU, 48 GWd/MTU, and 48 GWd/MTU after a 5-year cooling time.

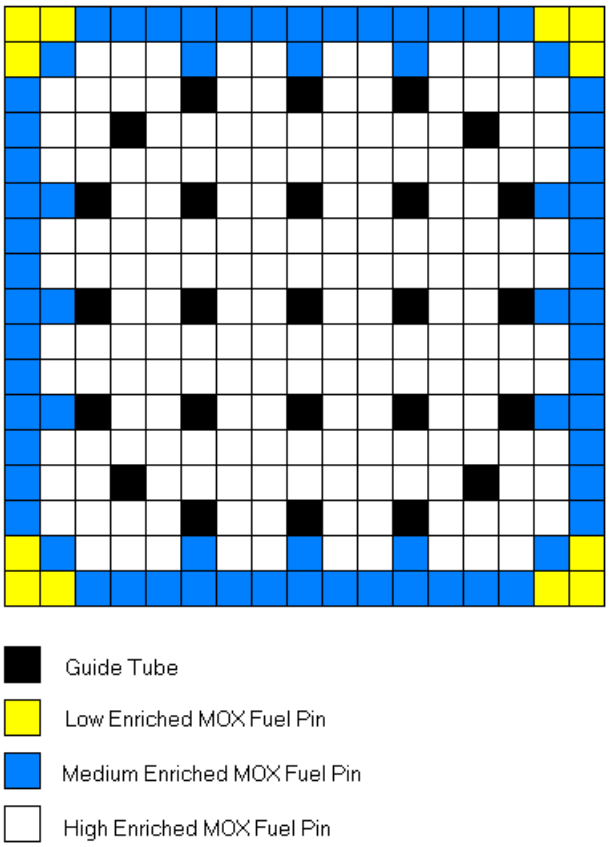

FIGURE 2: MOX fuel assembly.

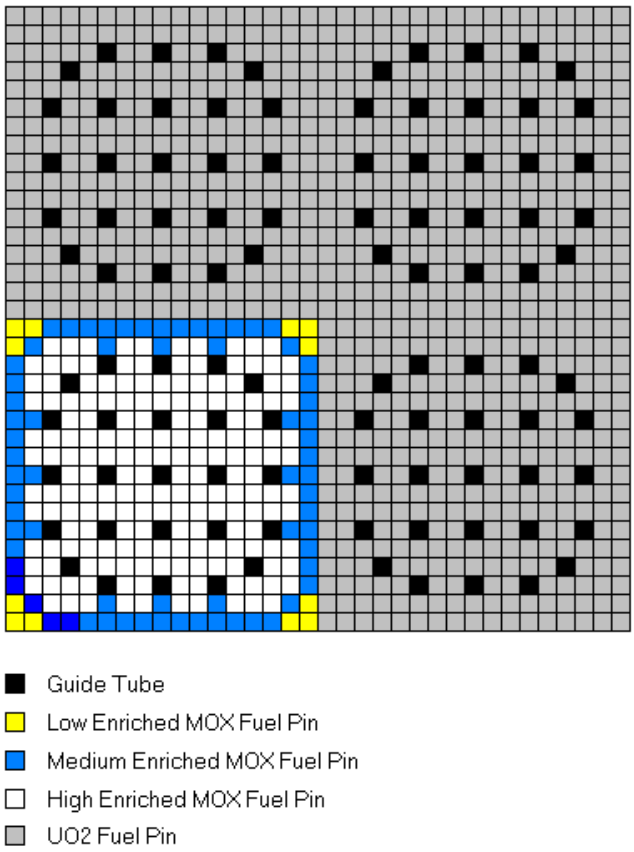

FIGURE 3: MOX-UO_2 Supercell.

CODE DESCRIPTION

As mentioned earlier, the SAS2D package is a two-dimensional (2-D) depletion sequence. Although not publicly available at the time of this writing, SAS2D will be released in SCALE 5, with availability anticipated in late 2002. SAS2D is a control module within the SCALE code system and uses the 2-D arbitrary geometry, S_n theory code NEWT to provide 2-D fluxes for a user-specified configuration. Depletion calculations are then performed for multiple materials using localized fluxes calculated within the assembly configuration provided to ORIGEN-S. For the calculations presented in this paper, SAS2D utilized a 238-group ENDF/B-V based cross-section library.

RESULTS

Comparison of number densities from calculations with the pincell model for first recycle MOX between various international codes (e.g., CASMO, MONK, WIMS, APOLLO2) and data (e.g., JEF, ENDF/B-V, JENDL) are shown in Figures 4 (U isotopes) and 5 (Pu isotopes). Note that the results from all codes are preliminary and are subject to change. Consequently, the codes have not been identified by their proper names in the graphs. Figures 4 and 5 display the ratio of each code's calculated concentration to the average of all submissions for the 48 GWd/MTU and 5-year cooling time state point. The results show that there is good agreement between the various codes when comparing nuclide concentrations. Figures 6 and 7 illustrate the code-to-average nuclide density ratio for weapons-grade MOX fuel at 48 GWd/MTU burnup and 5-year cooling time. It can be seen that the results of the various calculations are more distributed for the prediction of Pu nuclide concentrations than those of the first recycle MOX case. There are no plotted results of ^{234}U and ^{238}Pu for code 7, because these nuclides were off the scale. In addition to the U and Pu isotopes, actinide and fission products concentrations were also compared. Overall, there was good agreement between the various codes with only some differences in a few fission products concentrations (Sm isotopes and ^{155}Gd). Table 2 shows a comparison of the k_{inf} values for the various codes for first-recycle MOX and weapons-grade MOX, with variations on the order of 1–2% in k_{inf} between the codes.

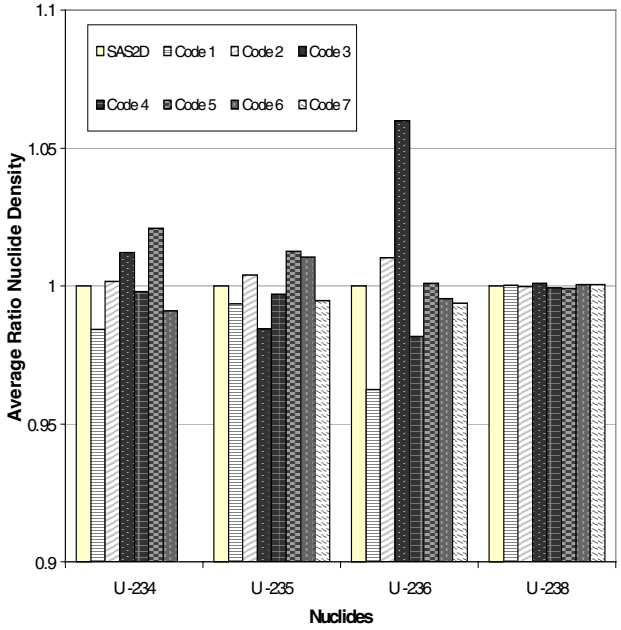

FIGURE 4: Comparison of the average nuclide density ratio for U isotopes (48 GWd/MTU burnup, 5-year cooling time, pincell model, and for first-recycle MOX).

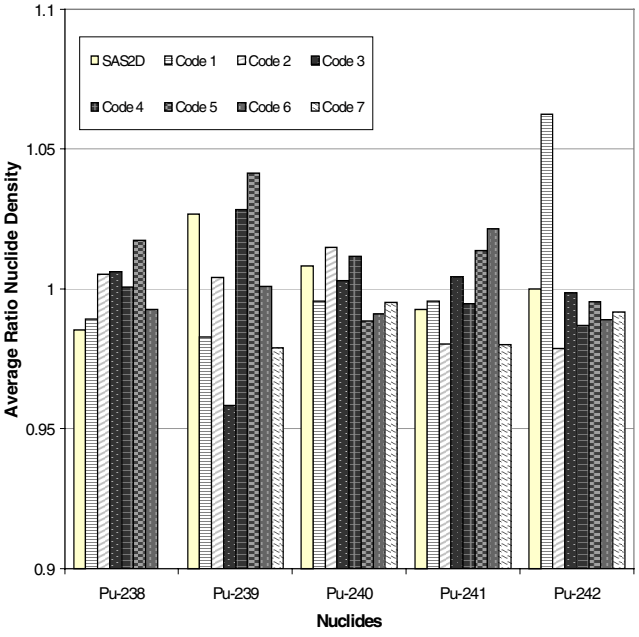

FIGURE 5: Comparison of the average nuclide density ratio for Pu isotopes (48 GWd/MTU burnup, 5-year cooling time, pincell model, and first-recycle MOX).

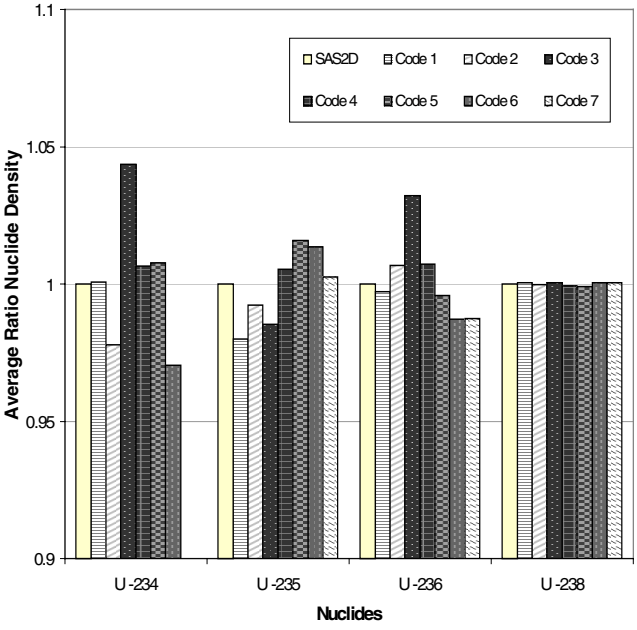

FIGURE 6: Comparison of the average nuclide density ratio for U isotopes (48 GWd/MTU burnup, 5-year cooling time, pincell model, and weapons-grade MOX).

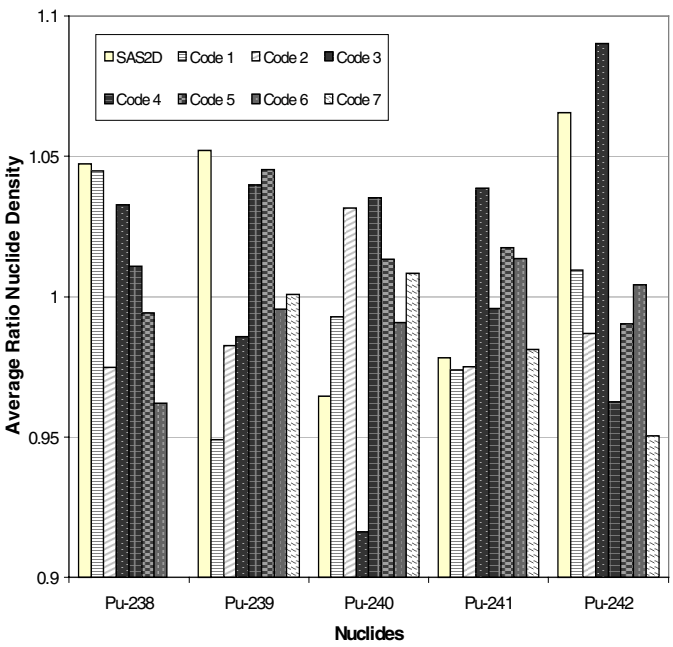

FIGURE 7: Comparison of the average nuclide density ratio for Pu isotopes (48 GWd/MTU burnup, 5-year cooling time, pincell model, and weapons-grade MOX).

TABLE 2: Calculated pincell k-infinity values for first-recycle MOX and weapons-grade MOX.

Code	End of Cycle 1	End of Cycle 2	End of Cycle 3	5 Years Cooling
k-infinity values for first-recycle MOX				
SAS2D	1.0608	1.01035	0.96541	0.92808
Code 1	1.05958	1.00783	0.96162	0.91903
Code 2	1.05638	1.00028	0.94969	0.90789
Code 3	1.07077	1.0143	0.96157	0.91923
Code 4	1.05824	1.00469	0.95812	0.91803
Code 5	1.04636	0.99422	0.94853	0.90233
Code 6	1.05829	1.00398	0.95731	0.9194
Code 7	1.0561	1.0016	0.9517	0.9112
k-infinity values for weapons-grade MOX				
SAS2D	1.09625	1.00144	0.92543	0.90483
Code 1	1.09068	0.99041	0.90879	0.87288
Code 2	1.08089	0.98056	0.89916	0.87082
Code 3	1.08553	0.98856	0.90566	0.87657
Code 4	1.08547	0.98849	0.91182	0.88549
Code 5	1.07194	0.97580	0.90020	0.87016
Code 6	1.09004	0.98782	0.9045	0.88175
Code 7	1.0843	0.9847	0.9044	0.8765

Comparisons of number densities from calculations with the assembly model for first recycle MOX between various codes are shown in Figures 8 (U isotopes) and 9 (Pu isotopes). Figures 8 and 9 illustrate the code-to-average nuclide number density ratio for 48 GWd/MTU burnup and 5-year cooling time. Even though the complexity of the model has increased in comparison to the pincell model, the nuclide concentrations are still very accurately predicted by the various codes. Figures 10 and 11 display the average nuclide density ratio versus nuclide for weapons-grade MOX at the same state point. Upon comparing the figures, note that there is greater variation between the various codes for the prediction of Pu nuclide concentrations, especially for the weapons-grade MOX case. Relative to the pincell model, the variation among the predicted nuclide concentrations are more pronounced in the assembly model. These variations are also shown in Table 3 where comparisons of the k_{inf} values for the various codes for first recycle MOX and weapons-grade MOX are displayed. Compared to the pincell, the variations in the k_{inf} values for the assembly model are about 1% larger resulting in a 2–3% spread among the various codes.

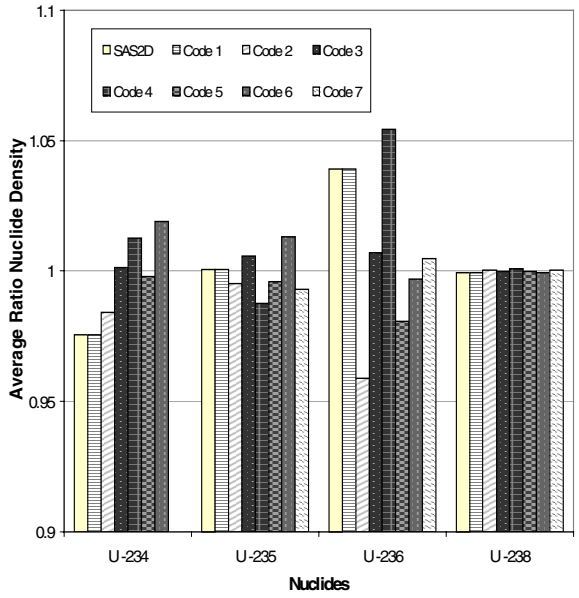

FIGURE 8: Comparison of the average nuclide density ratio for U isotopes (48 GWd/MTU burnup, 5-year cooling time, assembly model, and first-recycle MOX).

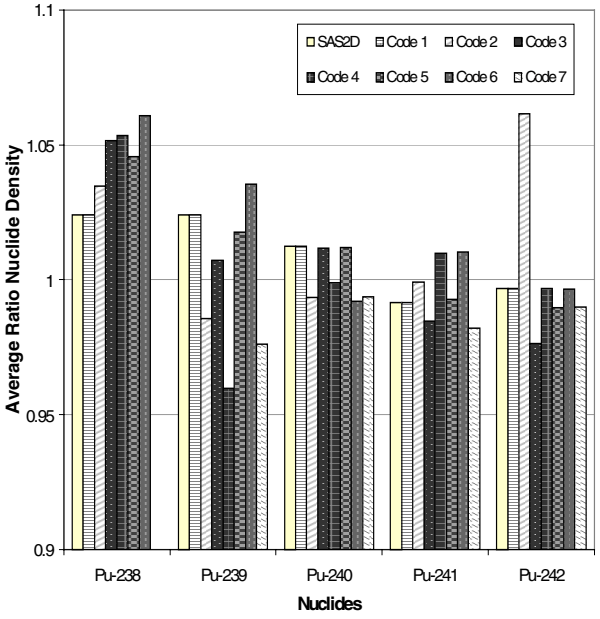

FIGURE 9: Comparison of the average nuclide density ratio for Pu isotopes (48 GWd/MTU burnup, 5-year cooling time, assembly model, and first-recycle MOX).

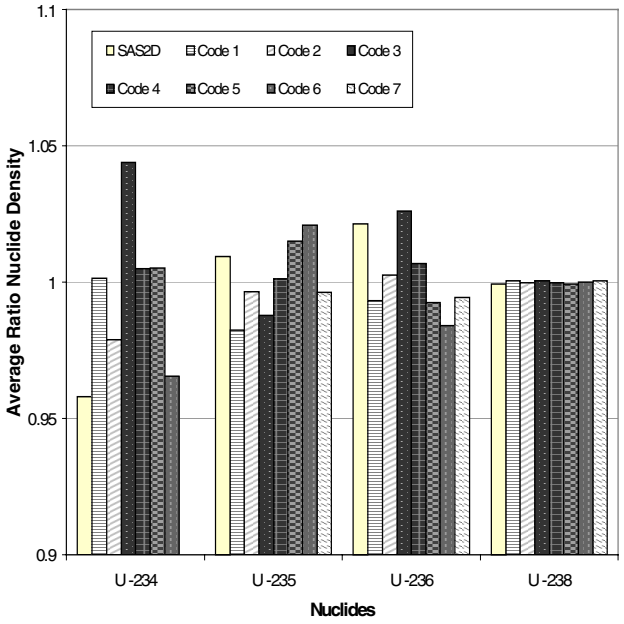

FIGURE 10: Comparison of the average nuclide density ratio for U isotopes (48 GWd/MTU burnup, 5-year cooling time, assembly model and weapons-grade MOX).

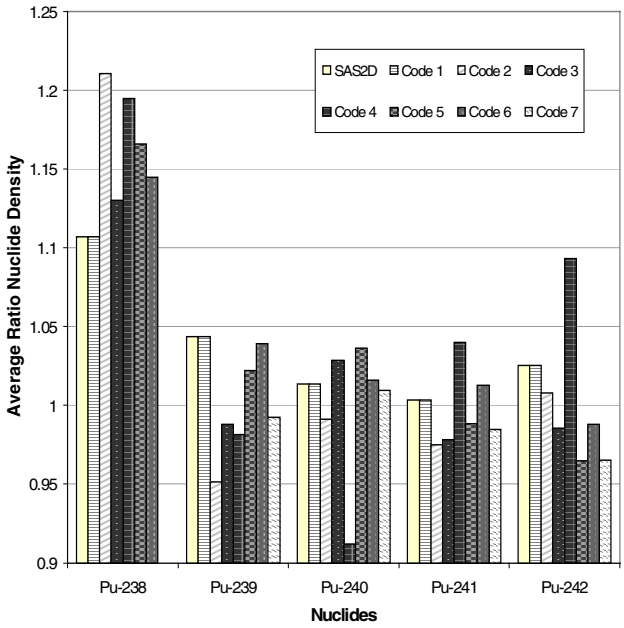

FIGURE 11: Comparison of the average nuclide density ratio for Pu isotopes (48 GWd/MTU burnup, 5-year cooling time, assembly model, and weapons-grade MOX).

TABLE 3: Calculated assembly k-infinity values for first-recycle MOX and weapons-grade MOX.

Code	End of Cycle 1	End of Cycle 2	End of Cycle 3	5 Years Cooling
k-infinity values for first-recycle MOX				
SAS2D	1.06269	1.01166	0.96610	0.92842
Code 1	1.05978	1.00753	0.961	0.91857
Code 2	1.05624	0.99968	0.94869	0.90715
Code 3	1.07123	1.01355	0.96253	0.91972
Code 4	1.06088	1.00618	0.95837	0.91826
Code 5	1.04976	0.99654	0.94974	0.90409
Code 6	1.05541	0.99749	0.95292	0.91676
Code 7	1.0590	1.0046	0.9510	0.9108
k-infinity values for weapons-grade MOX				
SAS2D	1.09673	1.00114	0.92477	0.90447
Code 1	1.08996	0.98919	0.9067	0.87071
Code 2	1.07981	0.97923	0.89724	0.86897
Code 3	1.08385	0.98618	0.90313	0.87344
Code 4	1.08652	0.9878	0.9089	0.88219
Code 5	1.07323	0.97602	0.89903	0.86913
Code 6	1.0833	0.98167	0.90121	0.87964
Code 7	1.0821	0.9835	0.9009	0.8744

Comparison of number densities from calculations with the supercell model for first recycle MOX between various codes are shown in Figures 12 (U isotopes) and 13 (Pu isotopes). Like before, the figures illustrate the code-to-average nuclide number density ratio for 48 GWd/MTU burnup and 5-year cooling time. While the complexity of the model has further increased in comparison to both the pincell model and assembly model, the predictions of the nuclide densities are still remarkably good. Figures 14 and 15 displays the average nuclide density ratio versus nuclide for weapons-grade MOX of each code at 48 GWd/MTU burnup and 5-year cooling time. The trends are similar here to those of the pincell and assembly model in that the codes are more spread out in their predictions of the Pu nuclide concentrations, especially for the weapons-grade MOX case. Table 4 displays a comparison of the k_{inf} values for the various codes for first recycle MOX and weapons-grade MOX. The concurrence between the codes is not as good as observed for the previous models. The differences in the k_{inf} values are on the order of 3–4%.

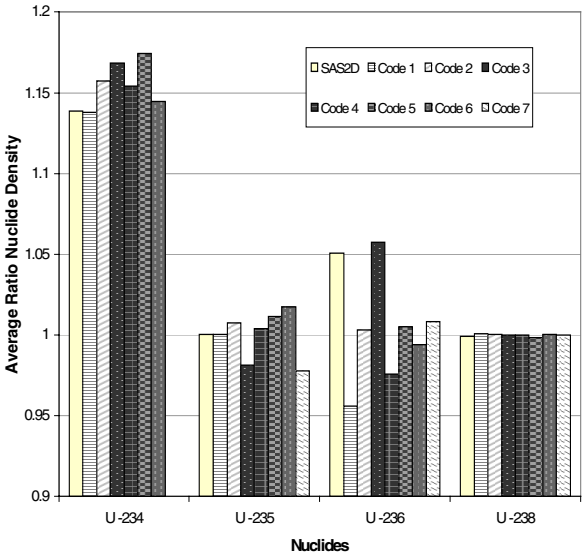

FIGURE 12: Comparison of the average nuclide density ratio for U isotopes (48 GWd/MTU burnup, 5-year cooling time, supercell model, and first-recycle MOX).

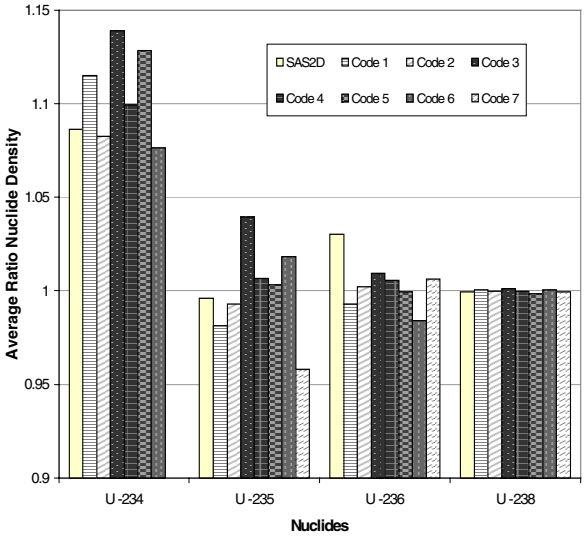

FIGURE 14: Comparison of the average nuclide density ratio for U isotopes (48 GWd/MTU burnup, 5-year cooling time, supercell model, and weapons-grade MOX).

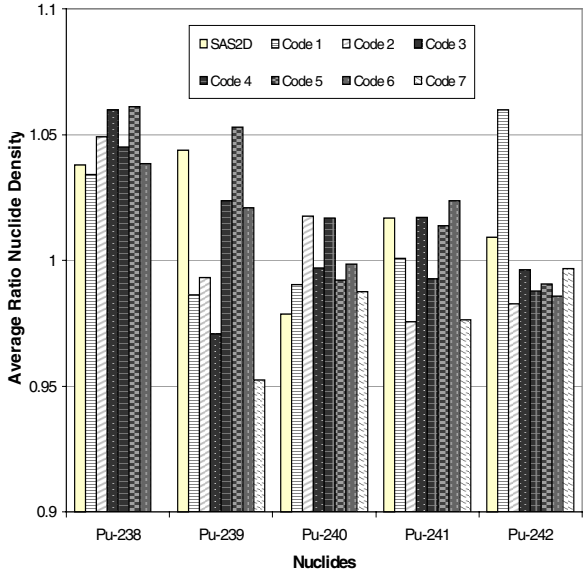

FIGURE 13: Comparison of the average nuclide density ratio for Pu isotopes (48 GWd/MTU burnup, 5-year cooling time, supercell model, and first-recycle MOX).

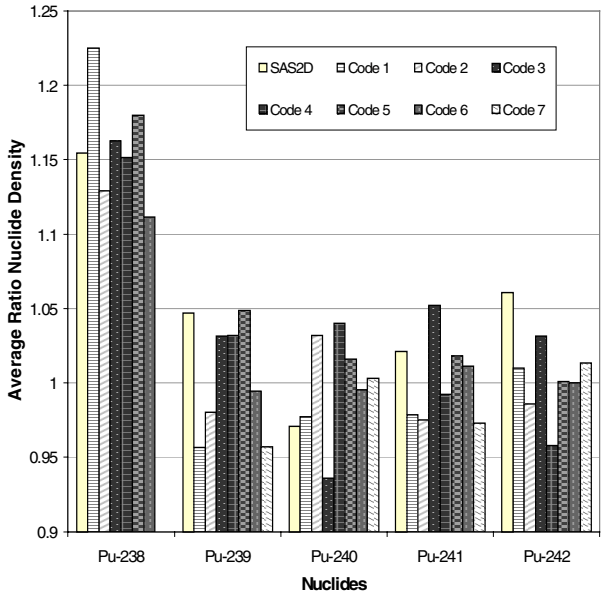

FIGURE 15: Comparison of the average nuclide density ratio for Pu isotopes (48 GWd/MTU burnup, 5-year cooling time, supercell model, and weapons-grade MOX).

TABLE 4: Calculated supercell k-infinity values for first-recycle and weapons-grade MOX.

Code	End of Cycle 1	End of Cycle 2	End of Cycle 3	5 Years Cooling
k-infinity values for first-recycle MOX				
SAS2D	1.09382	0.99992	0.93210	0.92098
Code 1	1.07342	1.01526	0.96472	0.92115
Code 2	1.10154	1.00401	0.92554	0.91255
Code 3	1.10808	1.00307	0.91973	0.90405
Code 4	1.07511	1.01464	0.96277	0.92247
Code 5	1.07571	0.98225	0.91344	0.89595
Code 6	1.09525	0.99587	0.92144	0.91134
Code 7	1.0988	0.9991	0.9198	0.9082
k-infinity values for weapons-grade MOX				
SAS2D	1.11129	0.99815	0.91021	0.90466
Code 1	1.09488	0.98782	0.90318	0.8665
Code 2	1.10649	0.99022	0.89605	0.88515
Code 3	1.11317	0.99613	0.90148	0.89068
Code 4	1.09262	0.98825	0.90646	0.87929
Code 5	1.09188	0.97718	0.88947	0.87658
Code 6	1.11003	0.99169	0.8989	0.89068
Code 7	1.1077	0.9866	0.8919	0.8809

CONCLUSIONS

SAS2D has been found to be in very good agreement with a suite of independent calculations using various codes and data. The results show that there is good agreement between the three modeling approaches when comparing k_{inf} and actinide concentrations. However, there were some differences of the nuclide densities for a few of the fission products (Sm isotopes and ^{155}Gd), which are most likely caused by spectral differences between the models. Also, the k_{inf} values shows that there is a clustering of results. Whether this is due to data problems or modeling inconsistencies is currently unknown. The weapons-grade MOX cases are a more severe test of Pu data, which has not been extensively investigated previously. Note that the results from all codes are preliminary and are subject to change. In addition, it should also be pointed out that this benchmark is part of a larger program that focuses on validating SAS2D for characterization of spent nuclear fuel.

REFERENCES

1. Hermann, O. W., and C. V. Parks, "SAS2H: A Coupled One-Dimensional Depletion and Shielding Analysis Code," Vol. I, Sect. S2 of *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*, NUREG/CR-0200, Rev. 6 (ORNL/NUREG/CSD-2/R6), Vols. I, II, and III, May 2000. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-545.

2. Hermann, O. W., S. M. Bowman, M. C. Brady, and C. V. Parks, *Validation of the SCALE System for PWR Spent Fuel Isotopic Composition Analyses*, ORNL/TM-12667, Martin Marietta Energy Systems, Inc., Oak Ridge National Laboratory, March 1995.

3. DeHart, M. D., and O. W. Hermann, *An Extension of the Validation of SCALE (SAS2H) Isotopic Predictions for PWR Spent Fuel*, ORNL/TM-13317, Lockheed Martin Energy Research Corp., Oak Ridge National Laboratory, September 1996.

4. DeHart, M. D., "An Advanced Deterministic Method for Spent-Fuel Criticality Safety Analysis," *Trans. Am. Nucl. Soc.,* **78**, 170–172 (June 1998).

5. Hermann, O. W., and R. M. Westfall, "ORIGEN-S: SCALE System Module to Calculate Fuel Depletion, Actinide Transmutation, Fission Product Buildup and Decay, and Associated Radiation Source Terms," Vol. II, Sect. F7 of *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*, NUREG/CR-0200, Rev. 6 (ORNL/NUREG/CSD-2/R6), Vols. I, II, and III, May 2000. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-545.

6. Thorne, P. R., G. J. O'Connor, and R. L. Bowden, "Problem Specification for the OECD/NEANSC Burnup Credit Benchmark Phase IV-B: Mixed Oxide (MOX) Fuel," http://www.nea.fr/html/science/wpncs/buc/specifications/4b.pdf (February 2002).