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Abstract. With the release of TRITON in SCALE 5.0, Oak Ridge National Laboratory has made available a rigorous two-dimensional (2D) depletion sequence based on the arbitrary-geometry 2D discrete ordinates transport solver NEWT. TRITON has recently been further enhanced by the addition of depletion sequences that use KENO V.a and KENO-VI for three-dimensional (3D) transport solutions. The Monte Carlo–based depletion sequences add stochastic uncertainty issues to the solution, but also provide a means to perform direct 3D depletion that can capture the effect of leakage near the ends of fuel assemblies. Additionally, improved resonance processing capabilities are available to TRITON using CENTRM. CENTRM provides lattice-weighted cross sections using a continuous energy solution that directly treats the resonance overlap effects that become more important in high-burnup fuel. And beginning with the release of SCALE 5.1 in the summer of 2006, point data and fine-structure multigroup libraries derived from ENDF/B-VI evaluations will be available. The combination of rigorous 2D and 3D capabilities with improved cross section processing capabilities and data will provide a powerful and accurate means for the characterization of spent fuel, making it possible to analyze a broad range of assembly designs and assay data. This in turn will reduce biases and uncertainties associated with the preduction of spent fuel isotopic compositions. This paper describes advanced capabilities of the TRITON sequence for depletion calculations and the results of analyses performed to date for radiochemical assay data.

1. Introduction

Historically, the one-dimensional (1D) SAS2H depletion sequence within the SCALE nuclear analysis suite [1] has provided a simple and rapid approach for spent fuel characterization. However, with the evolution of modern fuel assembly designs, SAS2H is often no longer an appropriate choice for spent fuel characterization. Accurate calculation of the depletion of nuclear materials requires careful determination of the neutron flux density and spectrum in the region(s) of interest. Increasing complexity in reactor designs, evolutionary concepts, and nonreactor applications such as safeguards, security, and nonproliferation require more robust geometrical modeling capabilities than those available in SAS2H in order to properly characterize neutron transport in such complex configurations.

With the release of the TRITON control module in SCALE 5.0, ORNL has made available a rigorous two-dimensional (2D) depletion sequence based on the arbitrary-geometry 2D discrete ordinates transport solver NEWT [2,3]. NEWT has continued to evolve since this initial release and will be significantly updated with the release of version 5.1 of SCALE in 2006. The update to NEWT will include a completely rewritten geometry-processing package based on the SCALE Generalized Geometry Package (SGGP) used by KENO-VI. Figure 1 illustrates the detailed modeling capabilities available within NEWT to capture the geometric detail of a boiling water reactor (BWR) fuel assembly with a control blade inserted. Also introduced with the 5.1 version of NEWT are a coarse-mesh finite-difference accelerator, pin power calculation capabilities, and an expanded set of lattice physics parameters. Minor code changes have been made to improve the accuracy of the solution and to further enhance computational performance.

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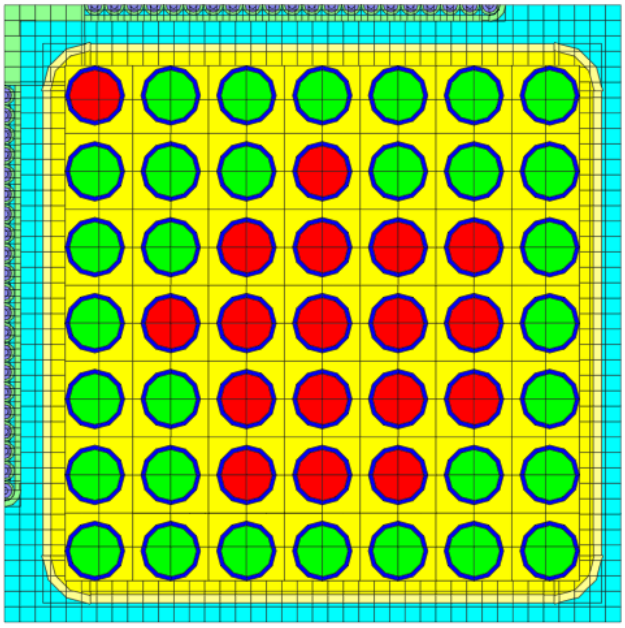

FIG. 1. NEWT model for a BWR design with control blade insertion.

Within TRITON, the T-DEPL sequence is used to perform 2D depletion analysis. This analysis sequence combines cross-section processing via BONAMI/CENTRM (or, optionally, BONAMI/NITAWL), the NEWT transport solution, and COUPLE and ORIGEN-S depletion calculations. In a calculation invoking the T-DEPL sequence, NEWT is used to create a three-group weighted cross-section library based on calculated and volume-averaged fluxes for each mixture. COUPLE is used to update the ORIGEN-S library with cross-section data read from the weighted library. Three-group fluxes calculated by NEWT are supplied to ORIGEN-S for depletion calculations. ORIGEN-S calculations are repeated for each mixture being depleted, as specified in input, using mixture-specific cross-section data and fluxes.

Because spatial fluxes are burnup-dependent, changing with nuclide inventories, and because mixture cross sections will also change with burnup, the T-DEPL sequence uses a predictor-corrector approach to update both fluxes and cross sections as a function of burnup. T-DEPL calculations can be considered to consist of two components during this iterative phase: (1) transport calculations (cross-section processing and the transport solution) and (2) depletion calculations. Transport calculations are used to calculate fluxes and prepare weighted cross sections based on a given set of nuclide concentrations; depletion calculations are used to update nuclide concentrations, which can be used in the following transport calculation.

Other SCALE 5.1 features that are available to TRITON provide additional capabilities. The use of the 1D continuous-energy discrete-ordinates transport module CENTRM within TRITON allows for the preparation of multigroup cross sections weighted with a continuous energy treatment for increased accuracy. TRITON uses ORIGEN-S to perform the depletion/decay calculations; ORIGEN-S underwent significant upgrades in the SCALE 5.0 release, including completely updated nuclear data from ENDF/B-VI, FENDL-2, and EAF-99. Nuclear data were added for hundreds of nuclides that previously were not modeled in any version of ORIGEN. The fission product yield data were increased from 5 fissile nuclides to 30. The methods in ORIGEN-S have also been upgraded to support nontraditional systems. (The more widely recognized ORIGEN2 code has not been updated in more than 10 years and is no longer supported at ORNL.)

Despite the broad applicability of the 2D fuel depletion analysis capability of TRITON, there are some domains in which accurate three-dimensional (3D) depletion capabilities are necessary. For example, criticality analysis for commercial spent fuel in transportation and storage is concerned with the positive reactivity effects of low-burnup fuel near the ends of a fuel assembly where axial leakage effects (not captured by 2D methods), may be important. Deterministic transport methods are also unable to perform full-core analysis in a practical sense because of the computational overhead of such large-scale discretization. Additionally, conceptual advanced reactor designs, such as designs for space reactors, Generation IV commercial power reactors or research reactors and other small cores, depart from traditional design attributes so that more robust 3D methods may be required to track fuel depletion or provide reference solutions for 2D methods. For these reasons, among others, a 3D depletion capability has been integrated into TRITON, using the 3D Monte Carlo–based KENO V.a and KENO-VI functional modules of SCALE [4,5]. These options are available within the T5-DEPL (KENO V.a) and T6-DEPL (KENO-VI) sequences of TRITON.

Because of the modular nature of SCALE, the process for replacing the deterministic 2D NEWT transport solution with 3D KENO solutions was relatively straightforward. However, certain functions available within NEWT (e.g., calculation of averaged three-group fluxes and fission/capture power calculations) were not readily available within either KENO module. Rather than modify KENO, the KENO postprocessing codes KMART and KMART6 (for KENO V.a and KENO-VI, respectively) have been adapted to provide collapsed cross sections and fluxes required by TRITON for setting up ORIGEN-S depletion calculations. Additionally, the restart capabilities of the KENO codes have been used to provide an improved starting source for each depletion step, further improving calculation times by reducing the number of calculations required to obtain source convergence.

Beyond these changes, however, the logical flow through TRITON in the KENO-based sequences mirrors that of the NEWT-based T-DEPL sequence. Figure 2 illustrates the computational flow through TRITON for both of the 3D depletion sequences. Because all cross-section processing and depletion processes are identical between each of the three depletion sequences, a direct comparison of results is possible, with differences attributable solely to differences in the transport solution.

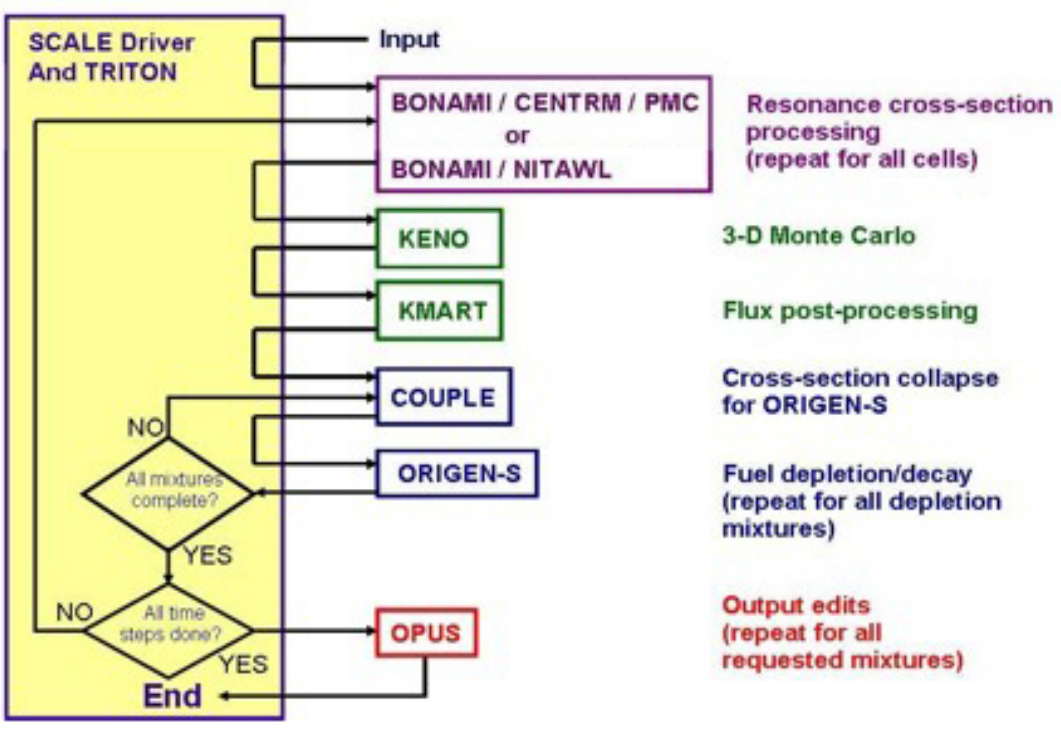

FIG. 2. TRITON sequence for KENO-based depletion.

2. Issues in Monte Carlo depletion

Use of Monte Carlo methods for depletion analyses introduces new challenges that should be addressed [6]. The Monte Carlo transport solution introduces stochastic uncertainty in fluxes. Because these fluxes are used to collapse cross sections, to estimate power distributions, and to deplete the fuel within ORIGEN-S, the predicted number densities contain random uncertainties due to the Monte Carlo solution. Depletion and decay calculations are by their nature extrapolations, so errors can be compounded with time.

Flux errors may be minimized by using very large numbers of neutron histories. Flux errors will be smallest in most reactive regions, where the greatest sampling occurs, but larger in the lower flux regions. Variance reduction will be important to force significant neutrons out to all regions of interest. Propagation of uncertainties from cross sections to isotopic concentrations will help in assessing the effect of potentially large flux variances. Both these issues will be addressed in future research at ORNL.

Nevertheless, stochastic limitations are offset by the ability to apply the power of Monte Carlo methods for complex 3D geometries. Furthermore, because of the particle tracking method of KENO V.a, it can perform extremely fast transport calculations relative to other Monte Carlo codes such as MCNP or KENO-VI. KENO-VI, on the other hand, provides complete flexibility in model development due to its combinatorial geometry input specification. Finally, because this methodology is built on the existing T-DEPL methodology in SCALE, direct benchmark comparisons can be made between the NEWT and KENO versions of TRITON for validation. The following section describes the results of such analyses.

3. Validation

Benchmark calculations have been performed using pressurized water reactor (PWR) fuel assembly data provided in validation reports of the 1D SAS2H depletion sequence in SCALE [7-9]. Benchmark models of the spent fuel assemblies have been developed with both T5-DEPL and T6-DEPL. Calculated results have been compared with the measured radiochemical spent fuel assay data given in the reports and with previously calculated SAS2H and T-DEPL results. Benchmark calculations have been performed for a wide variety of fuel assemblies; additional validation work is ongoing at ORNL. This paper provides results obtained from four PWRs:

- Calvert Cliffs
- Obrigheim
- San Onofre
- Trino Vercelles

3.1. Calvert Cliffs 14 × 14 fuel

The Calvert Cliffs fuel assembly is a Combustion Engineering (CE) 14 × 14 fuel assembly design. The fuel assembly modeled was D047. The specific location in the assembly of the measured sample was rod MKP109 at an elevation of 165.22 cm with a burnup of 44.34 GWd/MTU [7]. Measured data were obtained for the major actinides, cesium isotopes, and other fission products of importance to burnup credit (i.e., strong neutron absorbers). A comparison of the calculated results from SAS2H, T-DEPL, T5-DEPL, and T6-DEPL with measured data are presented in Table I and Figs. 3 (actinides) and 4 (fission products).

These results demonstrate consistency between the 1D, 2D, and 3D SCALE depletion sequences. The comparisons with the measured data show errors of generally 10% or less for the actinides and most fission products. Results for six of the fission products deviate from the measured data by approximately 20%. More importantly, results are generally consistent among the various codes. Differences are seen between the 1D and multidimensional results for those nuclides that are most

sensitive to the thermal spectrum (i.e., ^{235}U and Pu isotopes), indicating the possibility of inadequate characterization of the thermal spectrum in the 1D model.

Table I. Calvert Cliffs fuel assembly D047, rod MKP109 (44.34 GWd/MTU)

Nuclide	Measured (g/gUO2)	SAS2H %Diff.	T-DEPL (NEWT) %Diff.	T5-DEPL (KENO V.a) %Diff.	T6-DEPL (KENO-VI) %Diff.
U-234	1.20E–04	1.40	1.14	1.16	1.14
U-235	3.54E–03	–8.70	–5.05	–5.44	–5.40
U-236	3.69E–03	1.90	–1.81	1.81	1.80
U-238	8.25E–01	–0.10	–0.16	–0.16	–0.18
Pu-238	2.69E–04	–5.00	–6.63	–6.56	–6.59
Pu-239	4.36E–03	–1.50	6.26	4.96	5.00
Pu-240	2.54E–03	–3.90	–0.17	–0.70	–0.96
Pu-241	1.02E–03	–2.40	–0.71	–1.30	–1.14
Pu-242	8.40E–04	4.10	–0.90	–0.65	–0.49
Np-237	4.68E–04	7.20	7.25	7.13	7.25
Cs-133	1.24E–03	3.40	3.47	3.47	3.46
Cs-134	3.00E–05	–18.60	–19.45	–19.45	–19.43
Cs-135	4.30E–04	1.70	3.42	3.20	3.22
Cs-137	1.25E–03	1.20	–0.40	–0.40	–0.41
Nd-143	7.63E–04	0.50	1.63	1.47	1.48
Nd-144	1.64E–03	0.20	–0.07	0.03	0.02
Nd-145	7.44E–04	–0.60	–0.39	–0.34	–0.31
Nd-146	8.30E–04	1.30	1.74	1.74	1.72
Nd-148	4.28E–04	0.30	0.60	0.64	0.61
Nd-150	2.08E–04	4.20	4.71	4.71	4.68
Pm-147 + Sm-147	2.68E–04	–4.80	–5.88	–5.80	–5.76
Sm-148	2.22E–04	–18.20	–17.98	–17.98	–17.99
Sm-149	4.70E–06	–49.10	–51.18	–51.55	–51.39
Sm-150	3.61E–04	–5.60	–6.03	–6.03	–5.99
Sm-151 + Eu-151	9.78E–06	38.50	N/A	35.18	34.62
Sm-152	1.21E–04	22.00	20.99	20.68	20.89
Eu-153	1.48E–04	2.50	0.54	0.79	0.75
Sm-154 + Eu-154 + Gd-154	8.42E–05	–3.40	–3.73	–3.94	–4.01
Eu-155 + Gd-155	9.82E–06	–25.30	–23.96	–24.16	–24.17

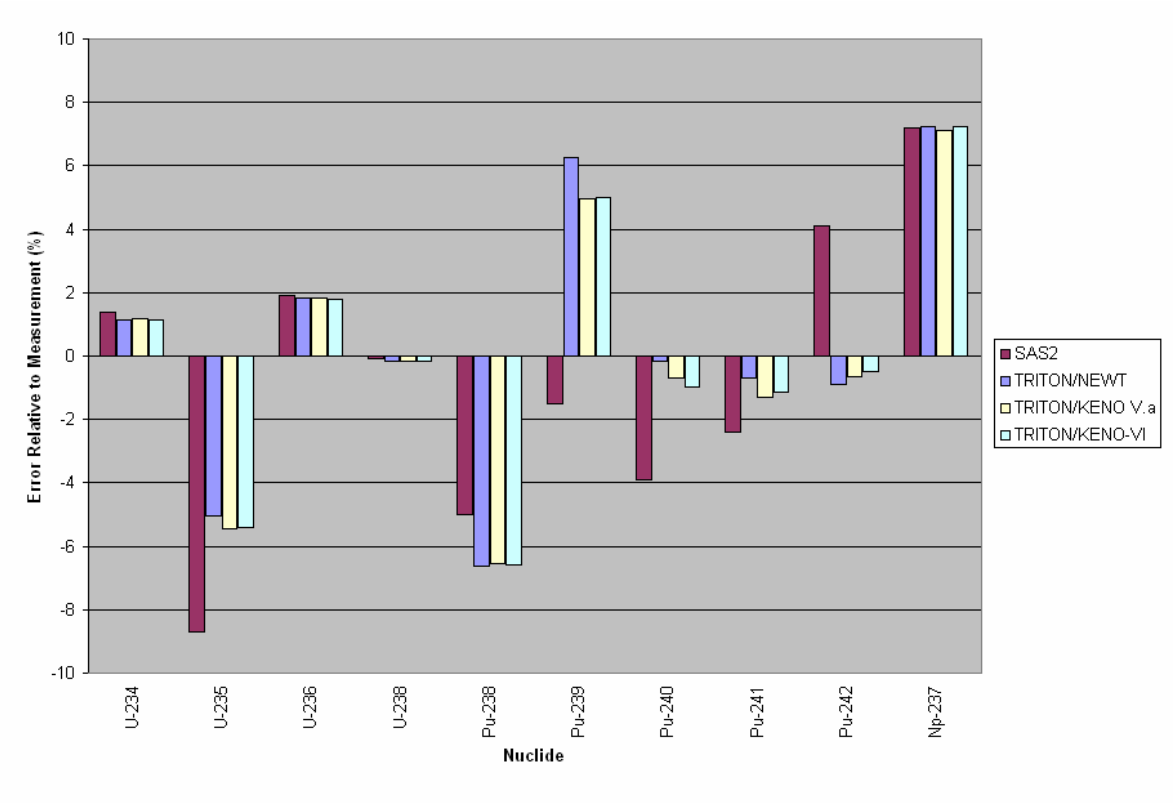

FIG. 3. Calvert Cliffs calculated results vs measured data for actinides.

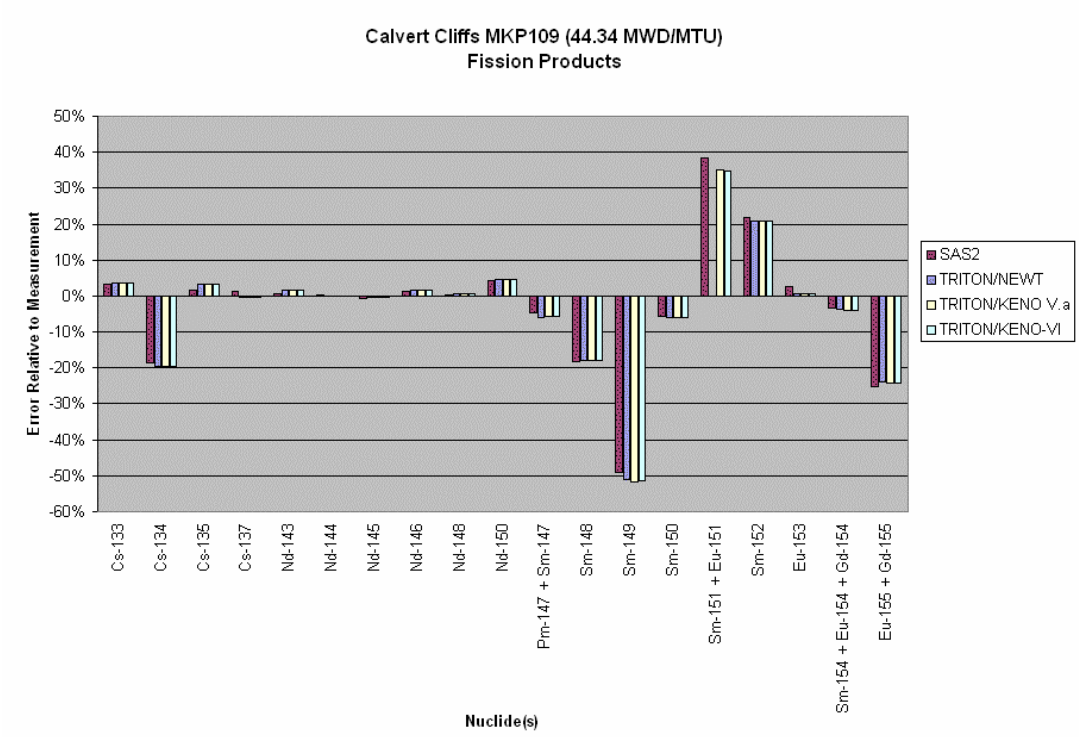

FIG. 4. Calvert Cliffs calculated results vs measured data for fission products.

3.2. Obrigheim

Isotopic measurements of the Obrigheim German PWR 14 × 14 assemblies were performed in Europe. For these measurements, each assembly was cut in half lengthwise and dissolved. The radiochemical analysis for a number of actinide and fission products was subsequently carried out by four independent institutes. The Obrigheim measurements thus provide "assembly average" isotopic values that, in comparison with individual pellet measurements, are more consistent with the spatially independent (i.e., assembly average) point-depletion techniques typically used to characterize spent fuel for away-from-reactor applications.

The assembly modeled in this study was assembly 176, batch 90, with an enrichment of 3.1 wt % and a burnup of 29.52 GWd/MTU [7]. The comparison of results in Table II shows good agreement between measurements and calculations, except for ^{242}Cm, one of the lesser actinides for burnup credit applications. Because of the isotopic homogenization of this assembly, the homogenization approximation applied by SAS2H yields exceptionally good results relative to multidimensional methods.

Table II. Obrigheim fuel assembly 176 (29.52 GWd/MTU)

Nuclide	Measured (mg/gU)	SAS2H %Diff.	T-DEPL (NEWT) %Diff.	T5-DEPL (KENO V.a) %Diff.	T6-DEPL (KENO-VI) %Diff.
U-235	9,180.00	-2.0	-2.0	-0.2	-0.3
U-236	3,810.00	1.2	0.7	0.2	0.3
Pu-238	107.1	3.0	-2.2	-2.6	-2.5
Pu-239	4,943.00	< 0.1	-0.2	1.1	1.1
Pu-240	2,040.00	-0.1	1.1	1.0	0.9
Pu-241	1,128.00	0.5	-0.9	-0.4	-0.4
Pu-242	438	-4.7	-8.1	-9.3	-9.2
Cm-242	21.8	-23.1	-27.1	-27.3	-27.2
Cm-244	19.2	-9.1	-9.9	-11.6	-11.2

3.3. San Onofre mixed oxide (MOX) fuel

The EEI-Westinghouse Plutonium Recycle Demonstration Program—sponsored by Edison Electric Institute, Westinghouse Electric Corporation, and the Atomic Energy Commission—was conducted between 1968 and 1974. A significant part of the program involved the measurement of isotopic compositions of uranium, plutonium, and a few other actinides in irradiated MOX fuel from the San Onofre PWR Unit 1, a reactor with a Westinghouse design and operated by Southern California Edison and San Diego Gas & Electric companies. Four MOX fuel assemblies were loaded at the start of Cycle 2 at the San Onofre Nuclear Generation Station Unit 1 and irradiated during both Cycles 2 and 3. Isotopic composition analyses were conducted by Westinghouse Electric Corporation on six sample pellets from four fuel rods of the MOX test assembly D51X. The measured actinide inventories have been used to benchmark the use of SAS2H depletion calculations for MOX fuel [8].

As part of the current validation, the sample pellet from pin 079 at an elevation of 49 in. with a burnup of 20.89 GWd/MTU was modeled. Comparisons of the calculated results from SAS2, T-DEPL, T5-DEPL, and T6-DEPL with the measured data are presented in Table III. Once again, the calculated results are consistent and generally agree well with the measured data. The two nuclides with poor results, ^{234}U and ^{238}Pu, have relatively low concentrations and importance.

Table III. San Onofre MOX fuel assembly DX51, pin 079 (20.89 GWd/MTU)

Nuclide	Measured	SAS2H %Diff.	T-DEPL (NEWT) %Diff.	T5-DEPL (KENO V.a) %Diff.	T6-DEPL (KENO-VI) %Diff.
U-234	4.66E-02	-13.1	-13.4	-13.7	-13.5
U-235	4.40E+00	-2.0	0.8	1.1	1.0
U-236	4.89E-01	6.6	2.6	2.6	2.4
U-238	9.43E+02	<0.01%	<0.01%	<0.01%	<0.01%
Pu-238	2.82E-01	-36.3	-35.4	-34.8	-35.1
Pu-239	1.65E+01	5.2	3.0	4.0	3.8
Pu-240	7.68E+00	-3.3	2.6	1.9	2.3
Pu-241	3.66E+00	1.5	0.1	1.6	1.1
Pu-242	8.97E-01	5.9	3.6	3.2	3.4
Nd-148	2.27E-01	0.1	0.6	0.6	0.6

3.4. Trino Vercelles

Trino Vercelles is a 825-MW Westinghouse PWR in Italy. The reactor is based on one of the earlier Westinghouse designs and is unlike most PWR designs in the United States, but similar to that of the Yankee Rowe PWR. Use of this uncommon design will serve to demonstrate the modeling capabilities of KENO for non-uniform fuel assembly designs. The fuel assembly design is based on a 15 × 15 lattice of fuel pins with 16 of the outer pins excluded to accommodate cruciform positions, as illustrated in the 2D plot of the KENO V.a model in Fig. 5.

Radiochemical assay data obtained from assembly 509-069, irradiated during both the first and second fuel cycles, were used for benchmarking in this validation [9]. Comparisons of the calculated results from the four depletion options of SCALE with the measured data are presented in Table IV. Once again, the calculated results are consistent and, except for ^{134}Cs and ^{154}Eu, generally agree well with the measured data. The Cs-134 error is known to derive from weaknesses in ENDF/B data.

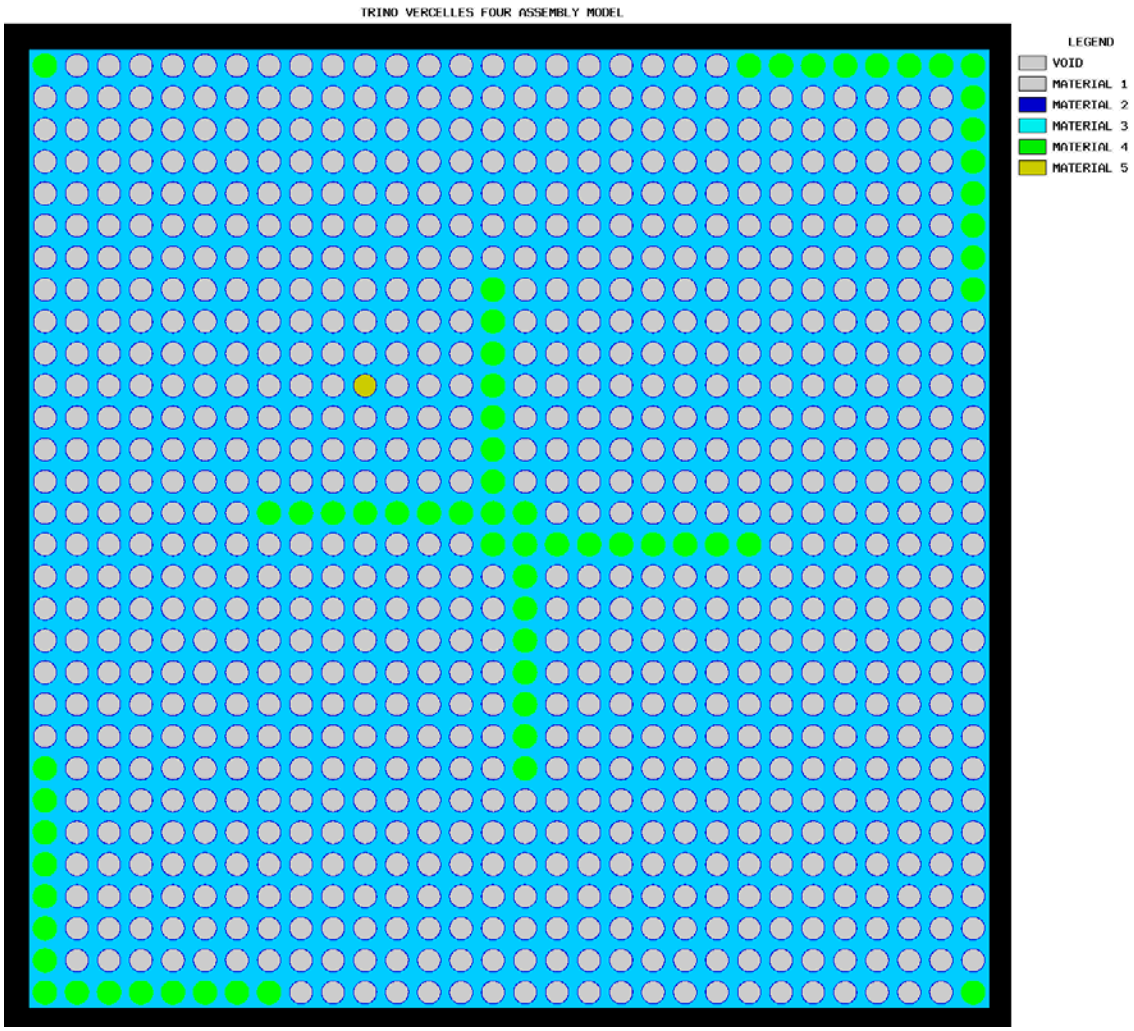

FIG. 5. 2-D plot of KENO V.a model for Trino Vercelles assembly 509-069.

Table IV. Trino Vercelles fuel assembly 509-069, rod E11 (12.859 GWd/MTU)

Nuclide	Measured (mg/g U)	SAS2H %Diff.	T-DEPL (NEWT) %Diff.	T5-DEPL (KENO V.a) %Diff.	T6-DEPL (KENO-VI) %Diff.
U-235	1.95E+01	0.51	0.46	0.49	0.53
U-236	2.45E+00	-5.75	-6.77	-6.85	-6.87
U-238	9.59E+02	-0.05	-0.01	-0.01	-0.05
Pu-239	4.58E+00	-1.51	-1.60	-1.69	-1.85
Pu-240	8.40E-01	8.20	8.90	8.28	8.97
Pu-241	4.00E-01	3.62	-3.14	-2.84	-3.51
Pu-242	4.60E-02	10.26	1.53	1.62	1.45
	(Curies/g U)				
Cs-134	2.49E-02	-25.94	-27.87	-27.90	-27.97
Cs-137	3.94E-02	0.71	-0.88	-0.88	-0.86
Eu-154	1.37E-03	-25.62	-23.33	-23.63	-23.48

4. Conclusions

The updated TRITON depletion sequences using NEWT and the 3D Monte Carlo codes KENO V.a and KENO-VI show tremendous potential for application in 3D configurations. Performance of both Monte Carlo depletion sequences has been assessed by comparison with 1D and 2D results obtained using deterministic transport methods and by direct comparison to measured spent fuel data. Results show excellent agreement with other codes and data. These calculation sequences provide simple and straightforward analysis capabilities for a wide variety of applications. Planned future work includes implementation of variance reduction techniques to improve computational efficiency and statistical uncertainty propagation from the Monte Carlo calculations to the predicted isotopic concentrations.

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