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TRITON: An Advanced Lattice Code for MOX Fuel Calculations

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ABSTRACT

During the past 2 years, the U.S. Nuclear Regulatory Commission (NRC) supported the enhancement of the generalized-geometry discrete-ordinates transport code NEWT, a transport module within the TRITON depletion sequence of SCALE 5, to generate burnup-dependent cross sections and other lattice physics parameters for use with the PARCS core simulator for MOX core analysis. NEWT is unique in the domain of discrete-ordinates methods because it is based on a nonorthogonal, flexible mesh scheme that allows accurate representation of complex geometric configurations that are normally impossible to model with discrete-ordinates methods without significant approximations. TRITON brings to NEWT an automated and simplified approach for setting up and performing complex sets of calculations. This paper describes the unique features and capabilities of TRITON for MOX transport calculations with depletion. Results of validation work are also presented.

1. INTRODUCTION

With the growth of spent fuel recycling internationally and weapons-grade plutonium disposition programs within the United States, the nuclear power industry is presently on the verge of a significant transformation of the nature of fuel design for reactor operation. The U.S. Nuclear Regulatory Commission (NRC) has received an application from Duke Power for a license amendment to permit the introduction of mixed-oxide (MOX)–based lead test assemblies into the McGuire and Catawba plants. This work is being done under the auspices of the U.S.–Russian Federation Plutonium Disposition Program. In addition to reactor operations, license modifications must also include provisions for the transportation, storage, and handling of such fuel.

While several European countries and the Japanese have made significant progress in the recycle of plutonium from spent fuel, including characterization of fuel performance with reactor analysis tools, the United States has not kept pace with this progress. Reactor analysis tools and data that have been heavily utilized to meet the needs of light-water-reactors (LWRs) may be inadequate to meet the challenges of significant changes in fuel composition due to the introduction of a significant plutonium component in the core design, because the nuclear analysis tools commonly employed by the commercial LWR industry were developed and refined based on extensive reactor operating experience with UO_2 fuel. Although international experience has resulted in improved data and a better understanding of analysis issues, the nature of plutonium produced by UO_2 recycle is significantly different from that of weapons-grade plutonium that would be used in U.S. disposition efforts. The weapons-grade plutonium vector has a high ^{239}Pu component, which has a large thermal resonance. Hence such a plutonium vector is potentially more sensitive to the thermal spectrum than nominal UO_2 fuel.

In response to concerns about the ability to accurately model the burnup of an LWR core containing weapons-grade MOX fuel assemblies, the NRC has supported the enhancement of the generalized-geometry discrete-ordinates transport code NEWT[1] to provide lattice physics parameters for the PARCS (Purdue Advanced Reactor Core Simulator) code[2] for the analysis of MOX-fueled LWR cores. Also supported under this work was the enhancement and formal release of TRITON (the prototypic version of which was originally named SAS2D),[3] a code that enables depletion calculations to be performed by coordinating iterative calls between cross-section processing codes, NEWT, and the ORIGEN-S point-depletion code.[4] NEWT is used to calculate weighted burnup-dependent cross sections that are used to update ORIGEN-S libraries and to provide localized fluxes used for each depletion region. TRITON uses a predictor-corrector approach to perform fuel assembly burnup and branch calculations and generates a database of cross sections and other burnup-dependent physics data that can be used by PARCS (or other nodal depletion codes) for full-core steady-state and transient analysis.

This paper provides a description of the unique capabilities of both TRITON and NEWT, especially with respect to issues potentially of concern in MOX fuel calculations. Results of calculations performed for MOX fuel lattices are also included, with code-to-code comparisons to show the behavior of TRITON relative to other industry-standard analysis tools.

2. TRITON SYSTEM DESCRIPTION

Both NEWT and TRITON are components of the SCALE (**S**tandardized **C**omputer **A**nalyses for **L**icensing **E**valuations) system,[5] developed and maintained at Oak Ridge National Laboratory (ORNL). Both codes will be publicly available with the release of version 5 of SCALE, along with several other new packages and capabilities.[6]

SCALE is a modular system comprised of numerous sets of codes and data, with a broad range of functions and capabilities. Codes are classified as *functional modules*

and *control modules*. Functional modules include the basic physics codes, such as XSDRNPM [one dimensional (1-D) discrete ordinates], KENO [three-dimensional (3-D) Monte Carlo criticality], and NEWT [two-dimensional (2-D) arbitrary geometry discrete ordinates], and many other codes applicable to criticality, shielding, depletion, radiation transport, and heat transfer. Control modules operate as sequence controllers, preparing input for functional modules, transferring data, and executing functional modules in the appropriate sequence for a particular analysis type. TRITON is a SCALE control module that is used for problem-dependent cross-section weighting, 2-D transport calculations using NEWT, and 2-D depletion calculations coupling NEWT and the ORIGEN-S point depletion code. The following subsections provide more detail on the NEWT transport solver, the TRITON sequence, and the cross-section processing options available within TRITON.

2.1 Capabilities of NEWT

Using a discrete-ordinates approximation to the transport equation on an arbitrary grid, NEWT provides a robust and rigorous deterministic solution for nonorthogonal configurations. Lower-order deterministic methods typically applied in lattice analyses (e.g., integral transport and collision probability methods) do not provide the angular resolution necessary to treat strongly anisotropic fluxes, such as those in the vicinity of strong absorbers or in high-leakage cores. This limitation may be exacerbated in MOX fuels due to the increased sensitivity of such fuels to the thermal spectrum. NEWT has already been used to demonstrate the effect of minor assumptions on the thermal spectra of MOX fuels.[7]

The differencing scheme employed by NEWT, the Extended Step Characteristic (ESC) approach, allows a computational mesh based on arbitrary polygons. Such a mesh can be used to closely approximate curved or irregular surfaces to provide the capability to model problems that were formerly difficult or impractical to model directly with discrete-ordinates methods. Automated grid-generation capabilities provide a simplified user input specification in which elementary bodies can be defined and placed within a problem domain. NEWT offers several calculational options. It may be used to calculate the eigenvalue of a system, to perform a fixed-source calculation, or to calculate the critical buckling of a lattice. It allows the specification of an axial buckling or calculates an axial buckling from a specified height to account for axial leakage effects. NEWT can collapse cross sections to an appropriately weighted group structure subset in the form of an AMPX working-format library. NEWT also calculates the transport-corrected multigroup cross section and diffusion coefficients for diffusion calculations. Used in conjunction with TRITON, NEWT can generate a library of cross sections as a function of burnup, moderator density, fuel temperature, and boron concentration.

NEWT's automated grid-generation scheme, based on the placement of simple bodies within a problem domain, allows rapid development of a model without the need to manually input a complex and irregular grid structure. Figure 1 shows two computational grids generated by NEWT for a hypothetical fuel assembly; the body inputs are identical, although a more refined grid is specified for the model on the right.

Note that these models contain no curved surfaces but instead consist of arbitrary polygons computed by NEWT in which volumes are conserved. NEWT performs the task of defining polygonal shapes and boundaries to match both the body specification and that of the underlying grid. Figure 2 illustrates the grid structure for a single pin cell, in which the polygonal approximation is easier to observe.

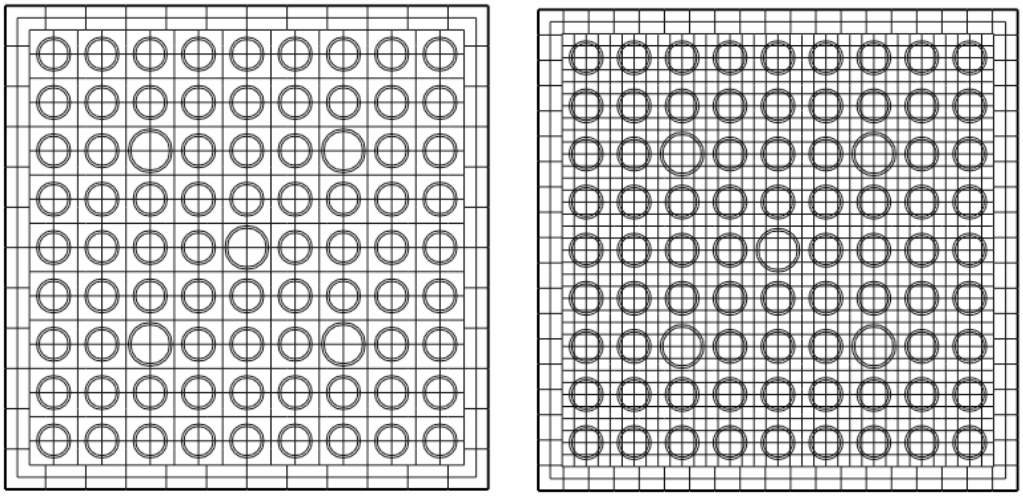

Fig. 1 Course and refined mesh models for a hypothetical fuel assembly configuration.

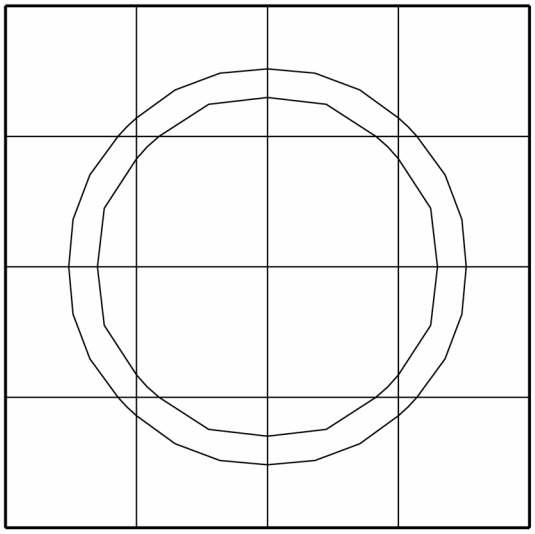

Fig. 2 NEWT pin-cell grid structure.

NEWT is able to generate a spatial flux solution for collapsing fine-group cross sections into a broad-group collapsing structure, using any homogenization instructions. However, to be of value for application in core-following nodal diffusion calculations, these cross sections must be available as a function of burnup. The TRITON sequence makes this possible by performing a time-dependent depletion calculation. Calls to NEWT as a function of burnup can be used to generate a burnup-dependent cross-section database. The approach taken in TRITON-based depletion calculations is described in the following subsection.

2.2 Capabilities of TRITON

The TRITON control module (originally developed as a prototype named SAS2D) performs the task of coordination of data transfer between the various physics codes and of invoking those codes in the proper sequence for a desired calculational type. TRITON brings to NEWT the automated and simplified approach for setting up and performing complex sets of calculations, a hallmark of the SCALE system. TRITON provides multiple sequence options, depending on the nature of the problem to be analyzed, for example, a single NEWT transport calculation (with problem-specific multigroup cross-section generation) or multidimensional depletion calculations that iterate between NEWT-based transport calculations and ORIGEN-S depletion calculations. TRITON also provides the capability to generate few-group cross-section data for use in subsequent nodal diffusion calculations. The rigor of the NEWT solution in estimating angular flux distributions combined with the world-recognized rigor of ORIGEN-S depletion gives TRITON the capability to perform rigorous burnup-dependent physics data with few implicit approximations. Such rigor may be necessary to capture the unique attributes of MOX fuel behavior as well as that of advanced, highly heterogeneous fuel assembly designs being deployed in current-generation reactors. TRITON supports branch calculations that allow calculation of cross sections and their first derivatives with respect to fuel and moderator temperature, moderator density, soluble boron concentration, and control rod insertion as a function of burnup. These cross sections are stored in a database format that can be retrieved and processed as appropriate for use by core analysis codes. At present, a prerelease version of TRITON is being used in conjunction with PARCS,[2] an advanced core simulator developed at Purdue University in support of NRC research.

Logical flow in a TRITON depletion calculation is illustrated in Fig. 3. Initial setup and execution of codes are performed by the SCALE driver. TRITON reads user-supplied input and is called during execution of the sequence each time data transfer or new code input is required by other functional modules. Cross-section self-shielding is performed by BONAMI and NITAWL or, optionally, by BONAMI, CENTRM, and PMC for each cell type in the problem. The following subsection provides additional detail on these cross-section processing options. These processes create a problem-specific library of weighted multigroup cross sections that is used by NEWT for a transport calculation. NEWT calculates flux distributions and generates three-group cross sections for COUPLE. COUPLE uses these cross sections to update the ORIGEN-S cross-section library. ORIGEN-S then uses localized fluxes from NEWT and cross-sections updated by COUPLE to perform depletion for a given material at a given location. The COUPLE/ORIGEN-S process is repeated for each unique material region being depleted. Once all materials are depleted, isotopic inventories are updated from ORIGEN-S results and the sequence returns to the cross-section processing step. This procedure is repeated for a user-specified number of depletion steps, using a predictor-corrector method for updating cross sections that are used to obtain isotopic concentrations. Upon completion of all depletion steps, TRITON combines all ORIGEN-S depletion libraries into a single master library. The SCALE OPUS module is then used to obtain and format user-selected data available from ORIGEN-S.

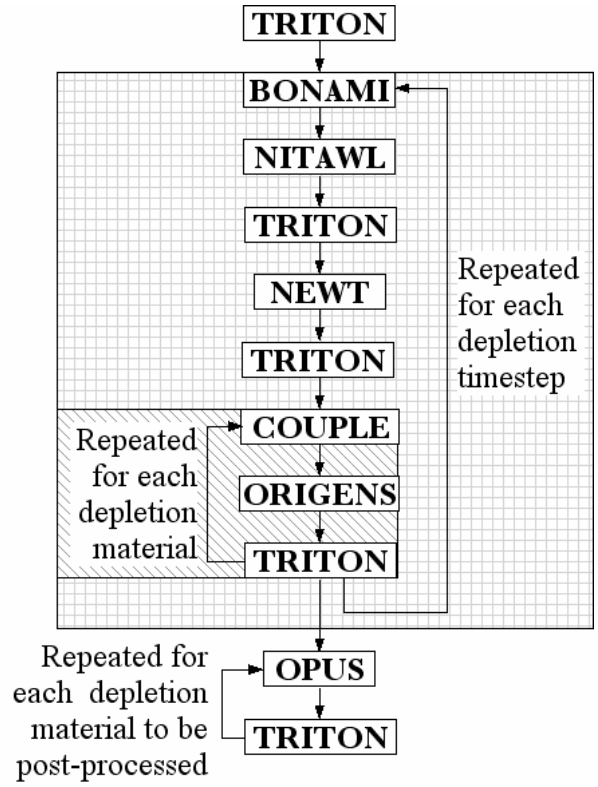

Fig. 3 Logical flow in the TRITON depletion sequence.

When used for generating few-group cross sections, NEWT prepares cross sections in a user-specified group structure and can homogenize cross sections over multiple materials/regions. If branch calculations are performed, the cross-section processing and transport solution steps are performed for nominal conditions and repeated for each branch state. Branch calculations may be performed for changes in moderator temperature, moderator density, fuel temperature, boron concentration, and control-rod insertion. Following each NEWT calculation, cross sections are archived for each branch and depletion step.

The method used for determining problem-specific multigroup cross sections for use by NEWT in a depletion sequence can be user selected. Beginning with SCALE 5, resolved-region cross sections may be processed using either NITAWL-III[8] or CENTRM.[9] Although the details of these types of analysis are beyond the scope of this paper, the nature of MOX fuel resonances is such that one must be aware of the differences between the two different cross-section processing procedures. The following subsection describes the two cross-section processing procedures available with TRITON and the relevance of each for MOX fuel analysis.

2.3 Cross-Section Processing Options

Within all SCALE cross-section processing sequences, BONAMI[10] is always called first to perform a self-shielding calculation for the unresolved resonance range based on the Bondarenko method and produces problem-dependent master data sets for nuclides with Bondarenko data, using equivalence theory to account for lattice effects. All unresolved resonances are processed by BONAMI. Following BONAMI, either NITAWL-III or CENTRM may be used to further process the resolved resonance range in SCALE master libraries.

SCALE "master format" cross-section libraries contain multigroup cross-section data processed from ENDF data using an assumed spectrum. A problem-specific, or "working" library is generated by self-shielding master library cross-sections with a problem-specific flux. The challenge is the representation of the problem-dependent fine-structure flux spectrum. The two approaches available to TRITON use completely different methods to estimate the fine spectra for resonance self-shielding.

Introduced in SCALE 5, NITAWL-III, an upgrade of NITAWL-II, has the capability to process multipole data, thus enabling it to process an ENDF/B-VI cross-section library with the Reich-Moore resonance parameters converted to multipole parameters. NITAWL uses the Nordheim Integral Treatment to self-shield cross-section data in the resolved resonance range. Each resonance is processed individually, not accounting for other overlapping resonances. Also, a flux spectrum in the fuel lump is calculated based on the moderators and absorbers in the fuel lump and assuming a 1/E flux spectrum outside the lump as well as allowing for the slowing-down source above each resonance. Because resonances are processed individually, resonance overlap effects from plutonium and uranium isotopes within a fuel lump are not captured.

The resolved resonance processor module CENTRM, to be introduced in SCALE 5, is a 1-D discrete-ordinates code that uses a pointwise continuous-energy cross-section library to produce a set of pointwise continuous-energy fluxes at discrete spatial intervals for each unit cell. Discrete-level inelastic cross-section data can also be processed by CENTRM/PMC. Down-scattering from inelastic continuum data and thermal up-scattering into the pointwise range are optionally available by a multigroup treatment. CENTRM avoids many of the inherent assumptions in NITAWL by calculating a problem-dependent flux profile, thus making it a far more rigorous cross-section treatment. Following a CENTRM calculation, the code PMC collapses the pointwise continuous-energy cross sections into multigroup cross sections for each nuclide in each material in the unit cell. The result is a multigroup library in which point cross-section data are weighted using the explicit pointwise spectrum representative of the nuclides present in a pin cell. Effects from overlapping resonances, fissile material in the fuel and surrounding moderator, anisotropic scattering, and inelastic level scattering are explicitly handled by this approach. Furthermore, CENTRM can be used to explicitly model fuel or absorber materials in subdivided regions, such as concentric rings in a fuel pin, to more precisely model the spatial effect on the flux and cross sections. This approach will provide significant improvement in the weighting of cross sections.

However, because a unique flux solution must be generated for each pin cell, depletion calculations with a large number of independently depleted materials will require a corresponding number of flux solutions. While not prohibitively expensive in a computational sense, the CENTRM approach may require additional processing time relative to NITAWL.

Finally, the choice of cross-section library can be important in MOX fuel calculations. SCALE currently provides two ENDF/B-V–based master libraries: a 238-group (fine-group) library and a 44-group (broad-group) library. The 44-group library was created by collapse of the 238-group library, assuming a spectrum computed for UO_2 fuel in an infinite pressurized-water-reactor (PWR)-type lattice. While this library has been demonstrated to perform quite well in the analysis of UO_2 fuel, the collapsed structure is not as appropriate for MOX fuel. In general, it is recommended that calculations be performed using the SCALE 238-group (fine-group) library, or to use a broad-group library collapsed using a MOX fuel spectrum. The latter approach may be inappropriate in the analysis of a supercell containing both MOX and UO_2 fuel cells.

3. TRITON VALIDATION RESULTS

Validation of TRITON for the depletion of MOX fuel presents a challenge due to the lack of publicly available experimental data. Typically, ORNL depletion methods have been validated by comparison with radiochemical assay measurements of fuel samples obtained from discharged reactor fuel. However, no such measurements are publicly available for MOX fuel. Some data are available through experimental programs in Europe, but most remain proprietary at this time. Hence, a three-pronged approach has been taken to confirm that TRITON and its constituent functional modules perform correctly. First, depletion calculations have been performed to validate the performance of TRITON for UO_2 fuel using readily available radiochemical assay data. Second, code-to-code comparisons have been made for MOX depletion calculations performed as a computational benchmark. The third validation approach has been another code-to-code comparison using cross sections prepared by two codes in nodal diffusion calculations. The following subsections provide a description of each type of analysis and the results obtained.

3.1 Depletion of UO_2 Fuel—Radiochemical Assay Data

Post-irradiation fuel samples obtained from the Calvert Cliffs Unit 1 PWR under the PNL Approved Testing Material program represent one of the best publicly available data for chemical assays from a PWR.[11] Assembly D047, Rod MKP109, had three samples taken from axial heights of 13.20, 27.70, and 165.22 cm. Chemical assays were performed for 10 actinides, 15 individual fission products, and 4 fission product mass chains. The third sample had a total burnup of 44.34 GWd/MTU. These assay data were selected for depletion analysis using TRITON. The pin was selected for assay because of its location on the interior of the assembly distant from any water holes, which could be accurately modeled using a simple 1-D transport approximation. Reference 11 also reports results obtained using the SCALE SAS2H module (based on 1-D XSDRNPM

transport calculations) and the SCALE ENDF/B-V 44-group cross-section library. TRITON analyses were performed using the same 44-group data library; CENTRM cross-section processing was used in TRITON.

Figure 4 shows the results of calculations for this fuel pellet sample. SAS2H and TRITON show good agreement for most nuclides. Similar trends in error relative to measurement indicate that most discrepancies are likely due to measurement error or cross-section data error rather than code or modeling errors. TRITON does a better job in predicting ^{235}U concentration; this is consistent with results seen in other radiochemical assay comparisons for other samples, and is felt to be due to a more accurate estimate of local fluxes in the pin of interest by TRITON. TRITON predicts ^{152}Sm inventories much more accurately than SAS2H; the exact reason for this is not clear. Overall, however, the results indicate that TRITON is able to accurately perform its general fuel depletion function.

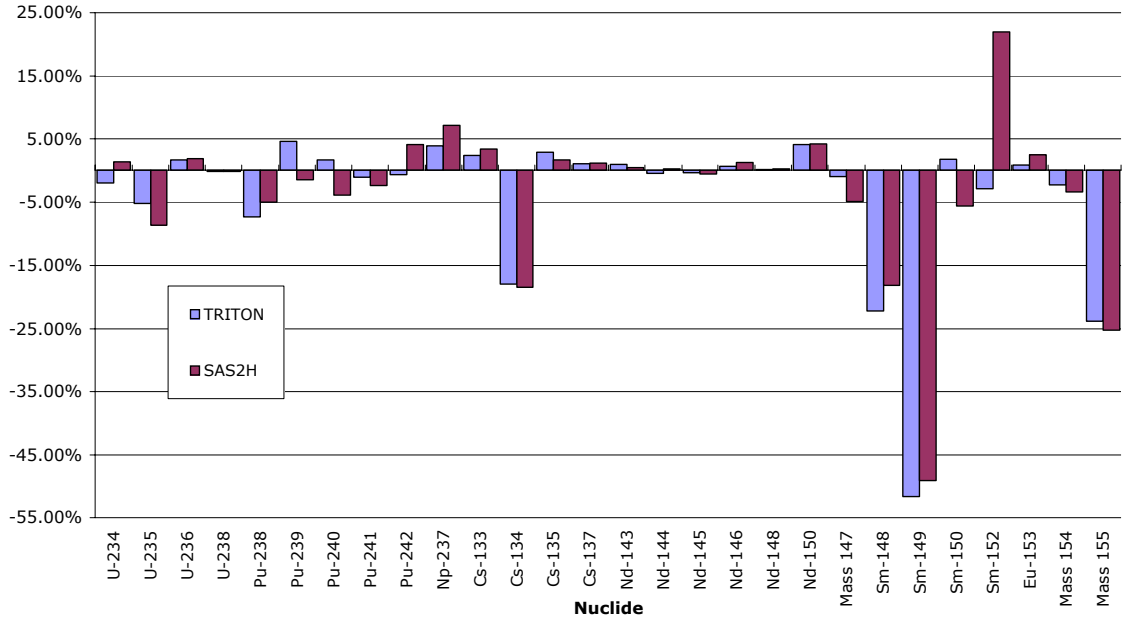

Fig. 4 Error in prediction of isotopic inventories for the Calvert Cliffs Assembly D047, Rod MKP109, 44.34 GWd/MTU sample.

3.2 Depletion of MOX Fuel—Computational Benchmark

The Expert Group on Burnup Credit of the Nuclear Energy Agency (NEA) of the Organization for Economic Cooperation and Development (OECD) has recently published the results of an international collaboration to compare the ability of various codes and data in the analysis of different MOX fuel configurations.[12] Models included an infinite lattice MOX pin cell, an infinite lattice of MOX-fueled assemblies with three MOX enrichments in a Westinghouse 17×17 design, and a supercell calculation using one MOX assembly and three UO_2 assemblies in a repeating pattern. Two different MOX fuel vectors were applied in each model—the first based on plutonium obtained

from UO_2 recycle and the second based on weapons-grade plutonium. TRITON calculations were performed as part of this benchmark, using the SCALE 238-group ENDF/B-V library and BONAMI/NITAWL for cross-section processing. (CENTRM processing was not yet functional at the time the calculations were performed.) The results for Case 2 (MOX supercell, weapons-grade fuel) are shown in Fig. 5. The codes used by other participants are as follows: NUPEC–CASMO-4, CEA–DARWIN (APOLLO2/PEPIN2), GRS–KENOREST (KENO V.a/ORIGEN2), PSI–BOXER, BNFL–WIMS8A, JAERI–SWAT (SRAC95/ORIGEN2), DTLR–MONK8A, ORNL–TRITON (NEWT/ORIGEN-S).

Benchmark case 2 represents the greatest challenge for analysis methods and showed the greatest variation among the participants. The legend indicates the organizations submitting each set of results. Figure 5 shows eigenvalues predicted for selected burnups. These results indicate reasonable agreement early in life, but with disagreement increasing with increasing burnup. For all cases, results reported included not only eigenvalues but also assembly-averaged isotopic concentrations. These results show a similar trend with increasing burnup, indicating that additional work is necessary to better understand the depletion process in MOX fueled cores. Reference 11 provides a limited discussion of effects observed among participants' calculations, but additional work is indicated. Nevertheless, the findings also show that TRITON results (ORNL) are within the spread of results of other participants. It is believed that a repeat of these calculations with CENTRM-based cross-section processing would improve the TRITON results and perhaps bring them in closer agreement with other participants. However, as a computational benchmark, there is no “correct” answer, and no indication of which direction is an improvement.

3.3 Steady-State Comparisons for MOX Fuel

In evaluation of NEWT for cross-section processing for PARCS, Purdue University has worked with a pre-release version of TRITON and the commercial code HELIOS[13] to prepare cross sections for PARCS and to compare results The OECD/NEA VENUS-2 MOX benchmark was selected as a starting point to compare code performance. VENUS-2 is an international benchmark with both 2- and 3-D exercises.[14] The VENUS facility is a zero-power critical reactor located at SCK CEN in Belgium. The core consists of four central assemblies of 3.3 w/o UO_2 fuel pins, with 10 Pyrex pins each, and eight assemblies on the periphery of the core comprised of UO_2 and MOX fuel. The seven internal rows contain 4.0 w/o UO_2 fuel pins, and eight external rows contain MOX fuel with 2.0/2.7 w/o high-grade plutonium. A quarter-core diagram of VENUS-2 is shown in Fig. 6.

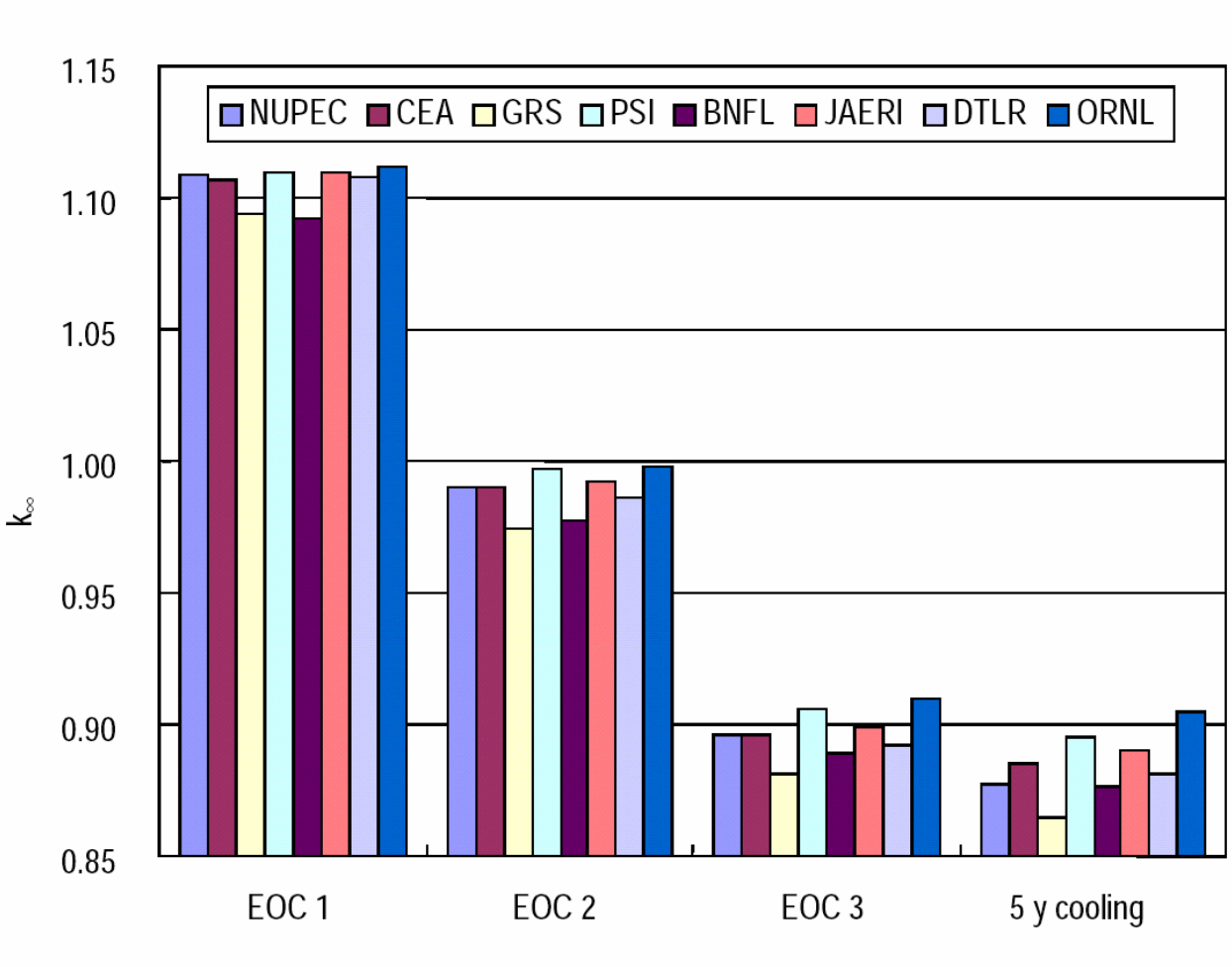

Fig. 5 Results of OECD Phase 4B MOX Benchmark—Case 2: supercell with weapons-grade MOX fuel and UO_2 (Ref. 11).

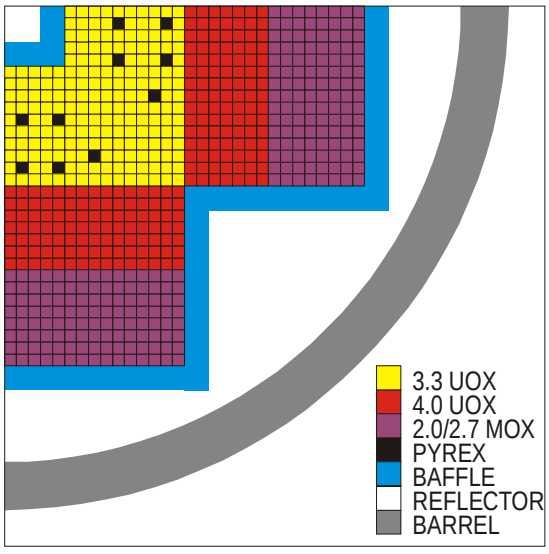

Fig. 6 VENUS-2 core configuration.

Several studies were performed in the analysis of VENUS-2. First, pin-cell calculations were performed to ensure that all codes behaved as expected. Eigenvalue calculations were performed for the three fuel types; results are given in the first three columns of Table 1 for multiple codes used in these analyses. The MCNP result for the 3.3% UO_2 pin cell is anomalous and may be in error. With this exception, all codes tested are in good agreement. Differences between HELIOS results and SCALE (TRITON and XSDRNPM) results are probably primarily due to differences in data libraries. Homogenized cross sections prepared using both HELIOS and TRITON were used in PARCS calculations, and PARCS was able to reproduce the results of the code from which cross sections were obtained. (These results are not shown.)

Calculations were also performed for subregions of the VENUS-2 core. This was done in preparation of assembly-averaged cross sections for PARCS. Calculations were performed for the UO_2 assembly with its corner water region, baffle, and Pyrex rods; for the mixed UO_2/MOX assembly; and for a region comprised of the UO_2/MOX assembly, baffle, and exterior reflector. These results are shown in the next three columns of Table 1. A 1% difference that was noted between HELIOS and TRITON results for the two MOX assembly cases was cause for concern. Additional calculations performed using KENO V.a and MCNP were found to be in better agreement with the eigenvalue calculated by NEWT within TRITON, indicating a potential problem with HELIOS for MOX fuel. However, this issue is apparently minor in a full-core calculation (results given in the last column of Table 1), as both TRITON and HELIOS calculations are in good agreement for the system eigenvalue.

Table 1 VENUS-2 Eigenvalue calculations for various codes and configurations.

	3.3% UO_2	4.0% UO_2	MOX	UO_2 assm.	UO_2/MOX assm.	UO_2/MOX assm. + refl.	Full core
HELIOS 1.7 (190g)	1.4085	1.34331	1.26339	1.17477	1.29886	1.15295	1.08969
HELIOS 1.7 (45g)	1.40691	1.34189	1.26332	1.17502	1.29843	1.1542	
TRITON (44g)	1.40385	1.33303	1.25345	1.17309	1.28986	1.14419	1.08829
XSDRNPM (44g)	1.40385	1.33366	1.25345				
MCNP 4B	1.38087	1.33775	1.25769		1.29478 (0.04%)	1.14637 (0.05%)	
KENO V.a (44g)					1.29179 (0.04%)	1.14655 (0.05%)	
Benchmark ave.	1.40593	1.33726	1.25673				

The same assembly and full-core calculations were also performed using PARCS with cross sections generated by both HELIOS and TRITON's transport solver NEWT. Table 2 shows the performance of PARCS with both sets of cross sections. The reflected assembly causes problems in the PARCS two-group solution using either cross-section

source, but the eight-group solution is consistent with the solution of the parent code for all cases.

Table 2 VENUS-2 Eigenvalue calculations using PARCS with HELIOS and TRITON cross sections.

	UO_2 assm.	UO_2/MOX assm.	UO_2/MOX Assm. + refl.	Full core
*TRITON 44g**	*1.17309*	*1.28986*	*1.14419*	*1.08829*
PARCS 2g (TRITON XS)	1.17492	1.28956	1.17620	
PARCS 8g (TRITON XS)	1.17307	1.28946	1.14772	1.08108
*HELIOS 45g**	*1.17477*	*1.29886*	*1.15295*	*1.08969*
PARCS 2g (HELIOS XS)	1.16891	1.29742	1.16689	
PARCS 8g (HELIOS XS)	1.17447	1.29744	1.16558	1.08561

*Results from Table 1.

To further study the behavior of TRITON and HELIOS for MOX fuel depletion, Purdue University is using both TRITON and HELIOS in the analysis of the transient response of a MOX-fueled core defined as a computational benchmark. Although the transient calculations have not yet been completed, additional fresh-fuel calculations have been performed that help to shed some light on differences between HELIOS and TRITON results. By using the DECART code[15] it becomes possible to isolate differences between codes. DECART calculations were run using cross sections from the SCALE 44-group library and the HELIOS 45-group library. The computational benchmark is based on a Westinghouse 17×17 assembly design. The lattice supercell consists of assemblies loaded with 4.5 w/o UO_2 fuel and MOX assemblies loaded with 2.5, 3.0, and 5.0 w/o plutonium MOX rods. The reactivity of the MOX assembly is controlled by 24 Westinghouse Annular Burnable Absorber (WABA) rods.

The first comparisons were made by calculating eigenvalues for infinite lattice pin-cell models for each fuel type. Table 3 shows the results for all calculations. Two DECART calculations were performed for each pin type—one using HELIOS cross sections and the other using the SCALE cross sections used by TRITON. Results are generally in very good agreement among the three codes. Furthermore, differences between TRITON and HELIOS results are primarily due to differences in cross-section libraries, as seen by similar differences between otherwise identical DECART calculations performed using the two cross-section libraries. Interestingly, unlike the VENUS-2 analyses, the largest differences are noted for the UO_2 rod rather than the MOX rods. Again, as a computational benchmark, there is no "correct" answer. However, the TRITON results may be improved using the SCALE 238-group library, because, as noted earlier, the SCALE 44-group library is more appropriate for a UO_2-fueled LWR spectrum. No doubt HELIOS results would improve with the use of a fine-group library. Broad-group libraries were chosen in this case to facilitate the extraction of cross sections for use by DECART.

Table 3 Pin-cell problem benchmark results.

	UOX 4.5%	MOX 2.5%	MOX 3.0%	MOX 5.0%
TRITON 44g	1.48009	1.37514	1.39270	1.42960
HELIOS 45g	1.48373	1.37740	1.39482	1.43009
DECART 45g	1.48429	1.37659	1.39409	1.43039
DECART 44g	1.47843	1.37408	1.39159	1.42915

A second set of analyses was performed using an infinite lattice of MOX-fueled assemblies. The WABA positions in the core were replaced with a representative B_4C control rod mixture, and calculations were performed with and without control rods present to obtain the control rod worth. Again, calculations were performed with TRITON, HELIOS, and DECART, using both sets of cross sections with DECART. Results of these calculations are tabulated in Table 4. As indicated, there is reasonably good agreement between the codes in the prediction of both the value of k_{inf} for the assembly, as well as the prediction of the control rod worth. DECART calculations indicate a 124-pcm difference in results between the two cross-section libraries. However, TRITON and NEWT agree to within 40 pcm in prediction of control rod worth. In fact, TRITON and HELIOS are in better agreement with each other than either is with DECART.

Table 4 Assembly benchmark problem results.

	Without control rod	B_4C CR inserted	
		k_{inf}	CR value (pcm)
TRITON 44g	1.44196	1.05750	38446
HELIOS 45g	1.44493	1.06007	38486
DECART 45g	1.44267	1.06054	38213
DECART 44g	1.44313	1.05976	38337

4. SUMMARY

The neutron physics of MOX fuels may represent a challenge to existing analysis approaches. The more rigorous treatment of neutron transport available within NEWT, coupled with the accuracy of ORIGEN-S depletion and SCALE self-shielding calculations within TRITON-driven lattice physics analysis, provides a first-principles approach for calculation of cross sections for such fuel designs. Although not initially developed or intended to be a general production tool for MOX analyses, the TRITON sequence allows a closer inspection of the physics of MOX fuel transport and burnup, providing improved insight to the physics of such systems. It is anticipated that this knowledge will allow improvement in other analysis methods and/or data to help meet the needs of future MOX-fueled cores.

The NRC plans to use cross sections generated using TRITON with the PARCS nodal diffusion code in the analysis of reactor cores containing MOX fuels, as confirmatory calculations for those accompanying license submittals. Work is ongoing to demonstrate the validity and accuracy of TRITON in its ability to perform depletion calculations and to generate appropriate cross sections for PARCS. The work reported here represents a sampling of test calculations completed toward this end. Additional calculations are planned in the near future using radiochemical assays from MOX fuel pins, along with core-follow calculations to predict actual core data taken from France's St. Laurant reactor, which has been operated using MOX-fueled assemblies. However, both sets of measured MOX data remain proprietary and will not become publicly available for some time. Additional tests using publicly available data will also be performed.

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