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Lattice Physics Capabilities of the SCALE Code System Using TRITON

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Abstract

This paper describes ongoing calculations used to validate the TRITON depletion module in SCALE for light water reactor (LWR) fuel lattices. TRITON has been developed to provide improved resolution for lattice physics mixed-oxide fuel assemblies as programs to burn such fuel in the United States begin to come online. Results are provided for coupled TRITON/PARCS analyses of an LWR core in which TRITON was employed for generation of appropriately weighted few-group nodal cross-sectional sets for use in core-level calculations using PARCS. Additional results are provided for code-to-code comparisons for TRITON and a suite of other depletion packages in the modeling of a conceptual next-generation boiling water reactor fuel assembly design. Results indicate that the set of SCALE functional modules used within TRITON provide an accurate means for lattice physics calculations. Because the transport solution within TRITON provides a generalized-geometry capability, this capability is extensible to a wide variety of non-traditional and advanced fuel assembly designs.

KEYWORDS: NEWT, lattice physics, validation, depletion, mixed oxide, MOX

1. Introduction

With the growth of spent fuel recycling programs internationally and weapons-grade plutonium disposition programs within the United States, the nuclear power industry is presently on the verge of a significant transformation in fuel design for reactor operation. The U.S. Nuclear Regulatory Commission (NRC) has received and approved an application from Duke Power for a license amendment to permit the introduction of mixed-oxide (MOX)–based lead test assemblies (LTAs) into the Catawba Unit 1 Pressurized Water Reactor. Catawba-1 began operation of the core with the LTAs present in June 2005 and is nearing the end of the first burn cycle. This work is being done under the auspices of the U.S.–Russian Federation Plutonium Disposition Program.

License applications for batch loading of MOX fuel are expected in the future. 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 Japan have made significant progress in the recycling of plutonium from spent fuel, including characterization of fuel performance with reactor analysis tools, the United States has not kept pace with this progress. The nuclear analysis tools commonly employed by the U.S. commercial light water

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reactor (LWR) industry were developed and refined based on extensive reactor operating experience with UO_2 fuel. Thus, reactor analysis tools and data that have been heavily used to meet the needs of LWRs might 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. Although international experience has resulted in improved data and a better understanding of analysis issues, the nature of plutonium produced by UO_2 recycling 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 resonance in the thermal energy range. Therefore, 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 to provide lattice physics parameters for the Purdue Advanced Reactor Core Simulator (PARCS) code for the analysis of MOX-fueled LWR cores. [1,2] The arbitrary-grid nature of NEWT is discussed further in a companion paper in this proceedings. [3] Also supported under this work was the enhancement and formal release of TRITON [4] within the Standardized Computer Analyses for Licensing Evaluation (SCALE) system. [5] TRITON is a SCALE *control module* that enables depletion calculations to be performed by coordinating iterative calls between cross-section processing codes, NEWT, and the ORIGEN-S point-depletion code. [6] NEWT is used to calculate weighted burnup-dependent cross sections that are employed to update ORIGEN-S libraries and to provide localized fluxes used for multiple depletion regions. 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 for full-core analysis. PARCS is a three-dimensional (3-D) reactor core simulator that solves the steady-state and time-dependent, multigroup neutron diffusion and Simplified P3 (SP3) transport equations in orthogonal and non-orthogonal geometries.

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

2. TRITON Description

Both NEWT and TRITON are components of the SCALE system, developed and maintained at Oak Ridge National Laboratory (ORNL). Both codes were made publicly available with the release of version 5.0 of SCALE in June 2004. However, calculations reported here were performed using the 5.1 version of SCALE, which is slated for public release in 2006.

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* or *control modules*. Functional modules include the basic physics codes, such as XSDRNPM (one dimensional [1-D] discrete ordinates), KENO (3-D Monte Carlo for criticality analysis), and NEWT (two-dimensional [2-D] arbitrary geometry discrete ordinates), and many other codes applicable to criticality, shielding, depletion, and radiation transport. 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 can be used for problem-dependent cross-sectional weighting, 2-D transport calculations with NEWT, or 2-D depletion calculations through coupling of NEWT and the ORIGEN-S point depletion code. (Additional 3-D depletion capabilities using TRITON with the KENO V.a and KENO-VI Monte Carlo codes will be available with SCALE version 5.1; these capabilities are described elsewhere in these proceedings. [7]) The following subsections provide more detail on the NEWT transport solver, the TRITON module, and the cross-sectional 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 non-orthogonal configurations. The differencing scheme employed by NEWT, the Extended Step Characteristic (ESC) method, 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. Used in conjunction with TRITON, NEWT can generate a library of cross sections as a function of burnup, with a branch capability that will provide cross sections at each burnup step for perturbations in moderator density, fuel and moderator temperatures, boron concentration, and control rod insertion or removal.

2.2 Capabilities of TRITON

The TRITON control module performs the task of coordination of data transfer between various physics codes available within SCALE and of invoking those codes in the proper sequence for a desired type of calculation. TRITON provides the capability to generate few-group, cross-sectional data for use in subsequent nodal diffusion calculations. The high-fidelity nature of the NEWT solution in estimating angular flux distributions combined with the rigor of the ORIGEN-S depletion solver gives TRITON the capability to perform precise burnup-dependent physics calculations with few implicit approximations, and limited primarily by the accuracy of nuclide cross-sectional data. 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. Cross-sectional self-shielding is carried out by BONAMI for unresolved-range resonance data; the resolved resonance processor module CENTRM performs a 1-D discrete-ordinates code that uses pointwise cross-section data to produce a set of continuous-energy fluxes at discrete spatial intervals for each unit cell. Following a CENTRM calculation, the code PMC uses the resulting flux to collapse the pointwise continuous-energy cross sections into multigroup cross sections for each nuclide in each material in a unit (e.g., pin cell). The result is a multigroup library in which point cross-sectional 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.

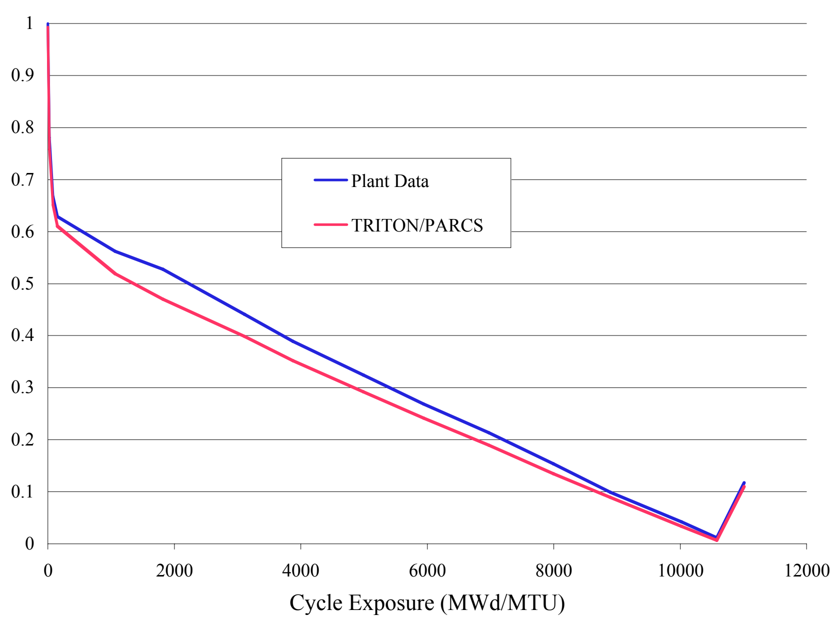
3. Validation of TRITON/PARCS

Validation of the coupled TRITON/PARCS sequence of calculations has been completed, in part by using proprietary data from Electricite de France's St. Laurent Unit 1 core. Physics data are available for Cycles 1–10; beginning with Cycle 5, the core was partially loaded with MOX-bearing fuel assemblies. In simulating the reactor's operation, TRITON was used to perform depletions calculations with branches for standard UO_2 fuel along with three different MOX fuel assembly designs. The cross sections were translated to the format used by PARCS, which was used in the performance of core-follow calculations. Four-group cross sections were prepared—earlier analyses based on a two-group structure were found to be inadequate to capture key effects in the nodal calculations. Comparisons were made between plant data and PARCS predictions for assembly powers and critical boron calculations for Cycle 10, after following the core over previous cycles. Figure 1 illustrates the relative differences between the reported and predicted assembly powers in the lower-right quadrant of the core at the end of Cycle 10. Actual assembly peaking factors are not given to protect proprietary information. Nevertheless, the figure clearly shows excellent agreement between predicted and measured data. The net root mean square (RMS) difference is 1.26%. For the UO_2 fuel assemblies, the RMS agreement is 1.20%, and 1.38% for the MOX fuel assemblies. The slightly higher differences for MOX assemblies is more likely due to the positions of the MOX fuel in the core than to issues in the transport solution. Figure 2 illustrates the predicted critical boron concentration relative to actual operational concentrations and shows good agreement over the entire cycle.

Figure 1: Relative error between reported and predicted assembly powers using TRITON/PARCS for St. Laurent Unit 1 at the end of Cycle 10.

3.03%	–0.14%	–1.19%	–0.38%	–0.87%	–1.56%	–1.37%	0.98%
–0.16%	–1.67%	–1.32%	–0.19%	0.37%	0.93%	–2.17%	–1.30%
–1.23%	–2.14%	0.35%	0.91%	–0.65%	0.75%	1.55%	
0.74%	–1.86%	0.52%	–0.08%	1.60%	1.10%	1.60%	
–0.88%	0.09%	–1.08%	1.39%	0.66%	0.32%		
–0.74%	0.58%	0.63%	1.11%	–0.57%		RMS	1.26%
–1.39%	–2.29%	1.41%	2.05%			RMS (UO_2)	1.20%
1.99%	–2.05%					RMS (MOX)	1.38%

Figure 2: Relative critical boron concentration for St. Laurent Unit 1, Cycle 10.



4. Comparison of TRITON to Other Codes

TRITON was selected by the NRC because of the rigor of the transport solution of NEWT; however, TRITON is clearly not limited to MOX fuel analysis. Ongoing validation analyses have included a suite of code-to-code comparisons initiated by the Japan Atomic Energy Research Institute (JAERI) for LWR Next Generation fuels. [8] The benchmark report features results for a variety of analysis codes, methods, and data for pin cells and for both PWR and boiling water reactor (BWR) fuel assemblies, each with both UO_2-only and MOX fuel loadings. Reported results include k_{eff}, pin powers, and reactivity calculations. TRITON calculations have recently been completed for the UO_2 BWR benchmark. Figure 3 shows the performance of TRITON depletion calculations relative to other depletion approaches. TRITON results deviate from the other codes at high burnup by over-predicting reactivity. It is believed that this is due to the inclusion of insufficient numbers of fission products in the transport model. Nevertheless, TRITON results are in excellent agreement with the results submitted by other participants. Void reactivity calculations performed as part of the benchmark are illustrated in Fig. 4. Again, TRITON shows excellent agreement with the results of other participants.

Figure 3: K-infinity predictions as a function of burnup for the JAERI BWR-UO_2 assembly benchmark.

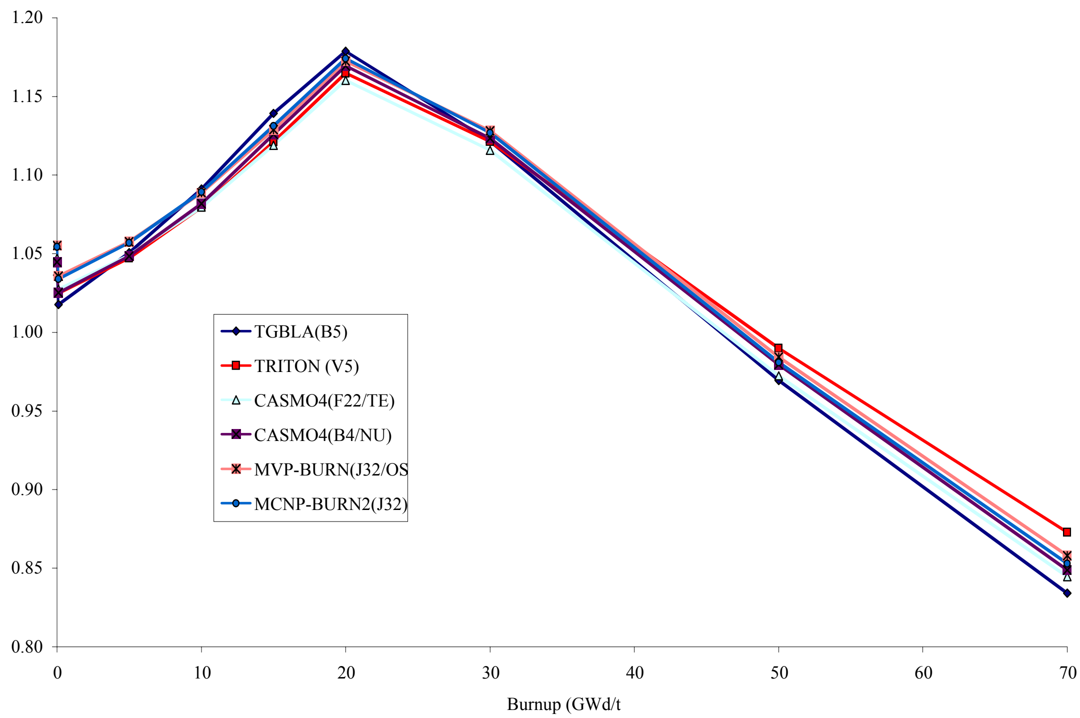
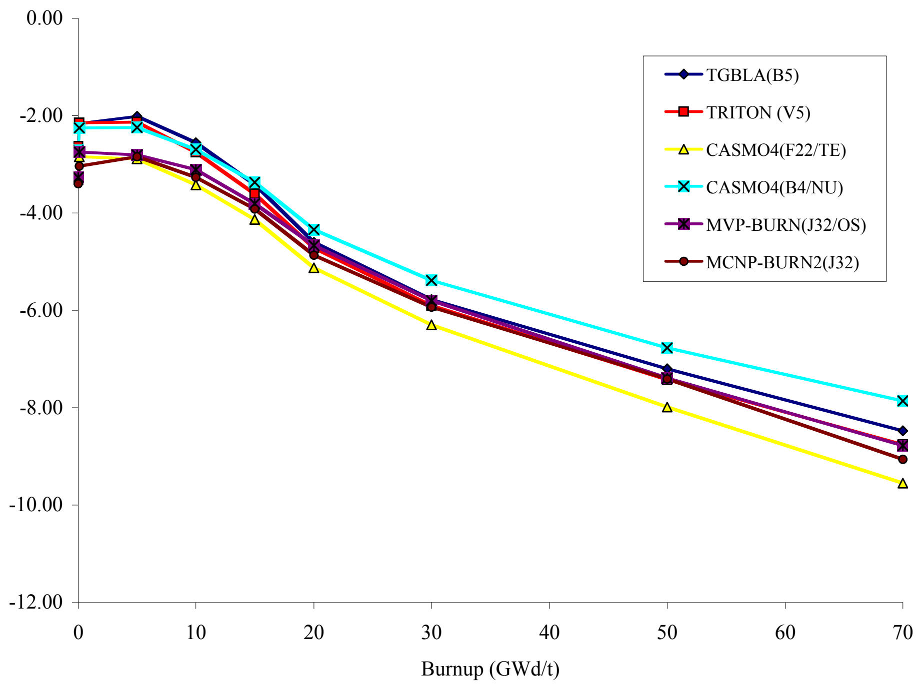


Figure 4: Void reactivity (0% – 70%) as a function of burnup for the JAERI BWR-UO_2 assembly benchmark.



5. Additional Validation of TRITON

Development and testing of both NEWT and TRITON continue to expand the variety of problems analyzed for lattice physics applications. Pre-application analysis for the Advanced CANDU Reactor ACR-700 design was successfully performed in 2005 in studies of void reactivity coefficients, together with a comparison with other methods, including Monte Carlo calculations. [9] Researchers in several countries in Eastern Europe have used the SCALE version 5.0 of TRITON for Russian pressurized water reactor (VVER) calculations. Improvements made in the SCALE version 5.1 within NEWT for hexagonal arrays and a general rewriting of input processing algorithms have made the package much more efficient, with significantly simplified model development requirements for hexagonal assembly lattice calculations. This new development allows improved modeling of VVER fuel assemblies.

Validation efforts are ongoing in a collaborative task with ORNL, Purdue University, and the NRC for coupled core-follow calculations for the Peach Bottom BWR using TRITON and TRACE. [10] TRACE calculations will be used to predict core power and void fractions as a function of burnup for core-follow calculations using TRITON-calculated cross sections. Results of these calculations will be published when analyses are complete.

Because TRITON performs depletion calculations via ORIGEN-S, substantial amounts of data beyond time-dependent number densities are available from such calculations. ORIGEN-S provides information including shielding source terms, gamma line data, particle production rates, and decay heat. Recent calculations using TRITON have been used to validate its ability to calculate decay heat sources for BWR relative to 45 full-assembly calorimeter measurements, and these have been shown to be in excellent agreement, within the range of measurement error. [11]

6. Conclusions

The TRITON module of the SCALE code system provides a powerful and robust approach for transport and depletion analysis of reactor fuel assemblies. Coupled with PARCS, accurate core simulation calculations can be performed for complex fuel designs. Results shown here demonstrate the validity of calculations used to generate lattice physics parameters for core analyses. Stand-alone TRITON calculations also show good agreement with other widely used analysis methods.

The arbitrary-geometry features of NEWT and the high-fidelity of the combined CENTRM/NEWT/ORIGEN-S sequence provide a powerful tool for the study of advanced designs and nontraditional fuel bundle concepts. The input geometry specifications for NEWT, based on the SCALE Generalized-Geometry Package (SGGP) combinatorial-geometry format of the KENO-VI Monte Carlo code with SCALE, provide a simple means for rapid model development, ranging from simple pin cells and regular lattices to irregular arrangements of nuclear materials. Additionally, the similarity of the geometry model allows simple translation to and from KENO-VI calculations, in which independent transport solutions can be compared for code-to-code validation.

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