REACTOR PHYSICS METHODS AND ANALYSIS CAPABILITIES IN SCALE

REACTOR PHYSICS

KEYWORDS: *lattice physics, reactor analysis, TRITON*

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The TRITON sequence of the SCALE code system provides a powerful, robust, and rigorous approach for performing reactor physics analysis. This paper presents a detailed description of TRITON in terms of its key components used in reactor calculations. The ability to accurately predict the nuclide composition of depleted reactor fuel is important in a wide variety of applications. These applications include, but are not limited to, the design, licensing, and operation of commercial/research reactors and spent-fuel transport/storage systems. New complex design projects such as next-generation power reactors and space reactors require new high-fidelity physics methods, such as those available in SCALE/TRITON, that accurately represent the physics associated with both evolutionary and revolutionary reactor concepts as they depart from traditional and well-understood light water reactor designs.

I. INTRODUCTION

TRITON [Transport Rigor Implemented for Transient Depletion with ORIGEN (Oak Ridge Isotope Generation)] (Ref. 1) is a control module developed within the framework of the Standardized Computer Analysis for Licensing Evaluation (SCALE) code system[2] at Oak Ridge National Laboratory (ORNL). The TRITON module provides automated calculational sequences to perform depletion calculations by coupling SCALE functional modules that perform problem-dependent multigroup cross-section processing, neutron transport calculations, and isotopic depletion and decay. Neutron transport calculations can be performed by the NEWT (New Transport Algorithm)[3,4] two-dimensional (2-D) discrete ordinates code or the three-dimensional (3-D) KENO Monte Carlo code.[5] Isotopic depletion and decay are calculated by the ORIGEN point-depletion code.[6] NEWT or KENO is used to calculate weighted burnup-dependent cross sections that are employed to update ORIGEN libraries and to provide localized fluxes used for multiple depletion regions.

The rigorous treatment of neutron transport available within NEWT or KENO, coupled with the accuracy of ORIGEN depletion capabilities and SCALE resonance self-shielding calculations within TRITON, provides an accurate first-principles approach for depletion and lattice physics analysis of a wide variety of fuel designs. Next-generation reactor concepts pose a substantial departure from traditional lattice designs and will initially be built and operated without the benefit of the thousands of light water reactor (LWR) plant years of operation that serve as a basis for current design and analysis methods. Thus, high-fidelity computational methods will be necessary to better understand the physics associated with novel reactor concepts as they move from paper to reality. The TRITON/NEWT sequence is able to perform 2-D lattice calculations for nontraditional lattice designs, including hexagonal arrays, irregular-lattice configurations (e.g., CANDU fuel assemblies), and nonlattice configurations. Additionally, the TRITON/KENO sequence has the capability to perform full 3-D Monte Carlo depletion within SCALE (Ref. 7).

This paper provides a description of the SCALE 6 version of TRITON, its components, and its capabilities.

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It also presents results of calculations that demonstrate the accuracy of the TRITON methodology for reactor physics.

II. DESCRIPTION OF TRITON

TRITON is a SCALE control module that can be used for problem-dependent cross-section weighting, 2-D transport calculations with NEWT, 2-D depletion calculations through a coupling of NEWT and ORIGEN (Fig. 1), and 3-D Monte Carlo depletion calculations coupling KENO and ORIGEN (Fig. 2).

Given mixtures and lattice cell structures defined in input, TRITON controls cross-section processing operations using BONAMI to perform Bondarenko calculations for resonance self-shielding in the unresolved resonance range and using CENTRM/PMC for resolved resonance evaluation. The problem-dependent cross-section library and mixing table produced by the sequence are automatically used in the NEWT or KENO calculation so that no mixing table needs to be specified. The transport solution is followed by COUPLE and ORIGEN calculations. In depletion mode, NEWT creates a three-group weighted library based on calculated and volume-averaged fluxes for each mixture. COUPLE updates the ORIGEN-S cross-section library with cross-section data read from the weighted library. Three-group fluxes calculated by NEWT or KENO are supplied to ORIGEN for depletion calculations. COUPLE/ORIGEN calculations are repeated for each mixture being depleted, as specified by the user, using mixture-specific cross-section data and fluxes. Used in conjunction with TRITON, NEWT also can generate a library of cross sections as a function of burnup, with a branch capability that provides cross sections at each burnup step for perturbations in moderator density, fuel and moderator temperatures, boron concentration, and control rod insertion or removal.

Reactor physics problems are solved by the sequential application of the codes described above. Given the sequence for which a calculation is to be performed, TRITON is responsible for processing input, converting the input description to appropriate forms, and executing each module in sequence, with preparation and exchange of required data between modules. Sections II.A through II.E describe the key components of these analysis sequences.

II.A. Continuous-Energy Resonance Processing Via CENTRM/PMC

The CENTRM (Continuous ENergy TRansport Model)[8] module computes continuous-energy neutron spectra in zero-dimensional or one-dimensional (1-D) systems by solving the Boltzmann transport equation using a combination of pointwise and multigroup nuclear data. Several calculational options are available, including discrete ordinates in slab, spherical, or cylindrical geometry; collision probabilities in slab or cylindrical coordinates; and zonewise or homogenized infinite media. CENTRM is used primarily to calculate problem-specific fluxes on a fine energy mesh (>10 000 points), which may be used to generate self-shielded multigroup cross sections for subsequent transport calculations. The purpose of the code is to provide highly accurate angular

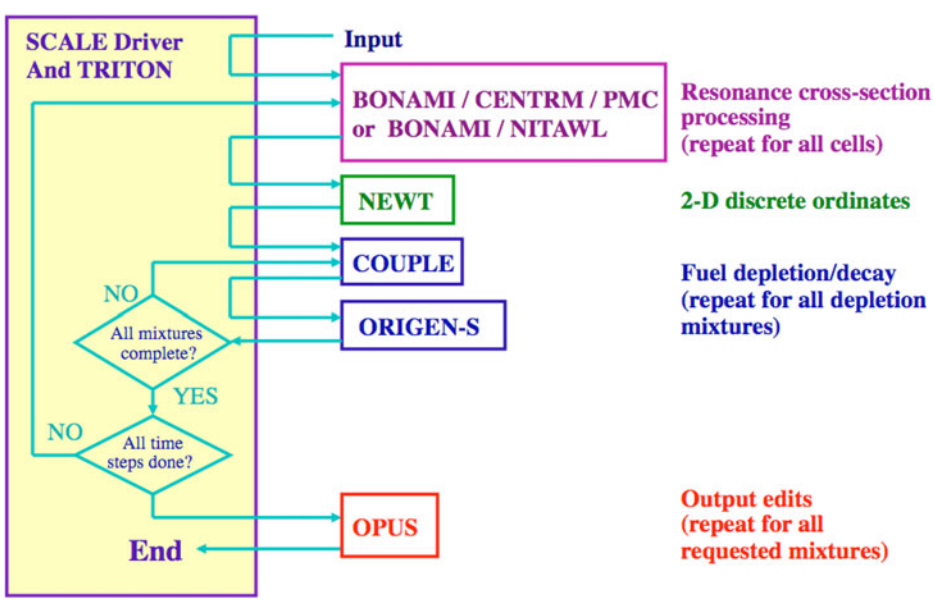

Fig. 1. Flowchart for TRITON/NEWT depletion sequence.

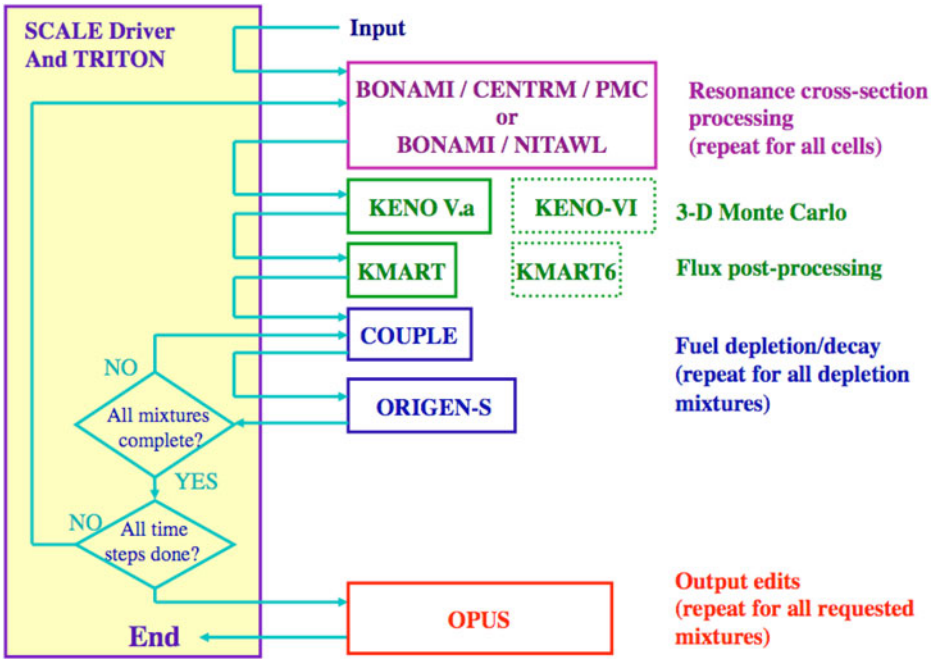

Fig. 2. Flowchart for TRITON/KENO depletion sequence.

fluxes and flux moments for applications that require a detailed description of the fine-structure variation in the neutron energy spectrum. This is accomplished by first performing a CENTRM calculation for a simplified system model (e.g., a pin cell), then utilizing the spectrum as a problem-dependent weighting function for multigroup averaging. The multigroup data processing is performed by the PMC (Produce Multigroup Cross sections) module,[9] which reads the CENTRM continuous-energy flux spectra and cross-section data; it then calculates problem-dependent, group-averaged cross sections. The resulting problem-specific multigroup cross-section library can be passed to NEWT or KENO for multigroup calculations. In this approach, the multigroup cross-section processing becomes an important component in the overall transport analysis because the resonance self-shielding and group averaging are tailored specifically to the system being analyzed.

II.B. 2-D Deterministic Transport Calculations Using NEWT

The NEWT transport solver provides a 2-D, unstructured-mesh discrete ordinates solution for multigroup neutron transport calculations for a wide variety of applications. NEWT employs a mesh defined by arbitrary polygons; extended step characteristic (ESC) discretization is applied to calculate transport between sides within each computational cell. Using the ESC solution method, computational cells are developed in the form of arbitrary polygons, which are further divided into trapezoids as a function of angle for a number of angles in a quadrature set. While similar in concept to the method of characteristic (MOC) class of transport solution, ESC provides a more rigorous spatial representation of bodies and allows significantly more control of spatial mesh refinement. The theory of the ESC formalism is described in detail in Ref. 10; ESC differencing is compared and contrasted with MOC methods in Ref. 3. The most significant difference, however, is that NEWT is based on short characteristics, with path lengths on the order of that of a fuel pin cell, whereas MOC methods use long characteristics, with path lengths on the order of the problem dimensions.

Using a discrete ordinates solution to the transport equation on an arbitrary grid, NEWT provides a robust and rigorous deterministic solution for nonorthogonal configurations. The arbitrary-polygon mesh developed by NEWT can be used to closely approximate curved or irregular surfaces, providing the capability to model problems that were formerly difficult or impractical to model directly with traditional finite difference 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.

Specification of the geometric configuration within NEWT is based on a combinatorial-geometry approach similar to that used in many Monte Carlo packages. In fact, the geometry package is based on the SCALE Generalized Geometry Package (SGGP), which was originally developed at ORNL for the KENO-VI Monte Carlo

code to provide the geometric flexibility necessary for extremely complex models. Although limited to 2-D analysis in an (x-y) plane in NEWT, the application of the combinatorial SGGP input structure provides the ability to easily develop models for complex configurations in two dimensions. Because it is limited to two dimensions, certain bodies (e.g., spheres) cannot be modeled; however, the input flexibility is limited only by the 2-D constraint.

SGGP input is body based, with bodies placed, rotated, translated, and cut as required for the desired configuration. Bodies are placed into "units," which are basic building blocks for model development. Units may be placed within other units, either in the form of a single placement or in the form of an array; NEWT supports both rectangular and hexagonal array structures.

In terms of body description and placement, the capabilities of the 2-D SGGP implementation in NEWT mirror the capabilities of KENO-VI. However, because the ESC methodology is in reality an advanced realization of the discrete ordinates method, a computational grid, albeit unstructured, must be introduced. Traditional discrete ordinates methods are based on a grid structure of orthogonal cells in which diamond-differencing relationships are used to estimate transport across a computational cell. The ESC method uses a short characteristics approach to calculate transport across arbitrary polygons. Diamond differencing is an approximation in which the derivatives of the flux are assumed to be linear across a computational cell, requiring cell sizes small enough to approximate this assumption. The characteristic solution is an exact representation of transport across a cell; however, approximations are introduced by the calculation of side-averaged fluxes, which limit the lengths of cell sides so that the variation of the angular flux along a side may be properly represented by an average. Both traditional and ESC discrete ordinates methods are also constrained in size by the assumption of a constant source within a computational cell. Hence, a grid structure must be introduced to further subdivide the problem domain. In NEWT, this is achieved by the introduction of a rectangular "overlay" grid; computational cells are defined by the intersection of the rectangular overlay and placed bodies. The problem domain is characterized by a largely rectangular grid, which has additional polygonal structure at the intersections of bodies and rectangular cells. The rectangular grid does not need to be continuous, however, and may be locally refined as needed to capture local effects.

NEWT may be used to model simple or complex configurations. Figure 3 illustrates a simple NEWT representation of a $\frac{1}{4}$ pin cell, in which the grid structure is easily observed. The user retains control of the number of line segments used to approximate curved surfaces; the code determines the inner radius of the regular polygon so that the volume matches the volume for the original cylinder. NEWT also provides an option to combine cells when small cells are created but are adjacent to a large cell of the same composition. In Fig. 3, each continuous region, whether rectangular or an irregular polygon, comprises a computational cell.

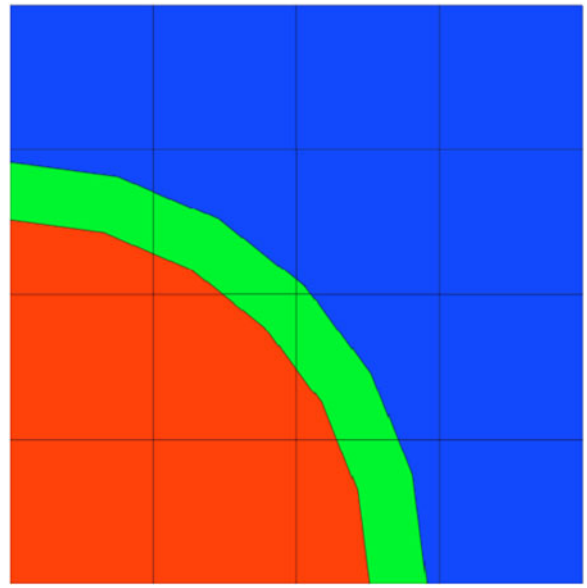

Fig. 3. NEWT model for a $\frac{1}{4}$ pin cell with an underlying 4×4 rectangular grid.

In Fig. 4, a significantly more complex model is shown, developed for a code-to-code comparison. In this

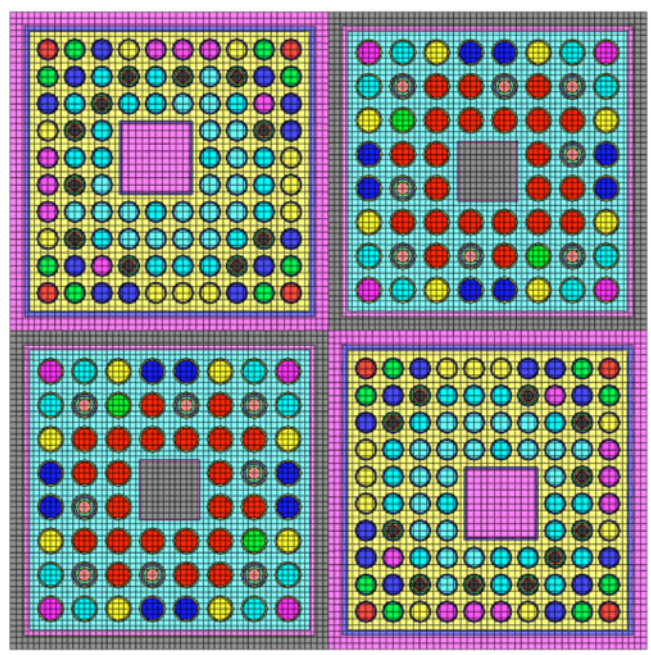

Fig. 4. Complex 2×2 configuration with ATRIUM-10 and GE-10 BWR fuel lattices.

model, a 2 × 2 fuel assembly array comprising a mixture of ATRIUM-10 and GE-10 type boiling water reactor (BWR) fuel lattices is shown. A single model (unit) for each of the two assembly designs was created; the SGGP input specification allows for rotation of units and placement using an array. In fact, this 2 × 2 array contains assemblies that themselves were developed using arrays.

Finally, Fig. 5 illustrates a model developed for a VVER-400 fuel assembly. This case was also developed using a hexagonal array. In this model, a more refined rectangular grid structure is used within each pin cell. A slightly more coarse rectangular grid is used in the vicinity of the interassembly channel and water gap.

II.C. 3-D Monte Carlo Depletion Using KENO

Despite the broad applicability of the 2-D fuel depletion analysis capability of TRITON, accurate 3-D depletion capabilities are necessary in some domains. For example, characterization of 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 2-D 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 depart from traditional design attributes to the extent that more robust 3-D methods may be required to track fuel depletion or provide reference solutions for 2-D methods. For these reasons, among others, a 3-D depletion capability has been integrated into TRITON, using the 3-D Monte Carlo KENO codes in SCALE. While Monte Carlo methods provide powerful geometric modeling capabilities in 3-D domains, such calculations typically require a large number of neutron histories to converge on an accurate system response (e.g., global neutron multiplication). Significantly more neutron histories are needed to achieve reasonably precise neutron flux and power density distributions. However, recent advances in computer hardware capabilities have made the application of Monte Carlo depletion methods a realistic and popular solution technique for complex reactor designs.

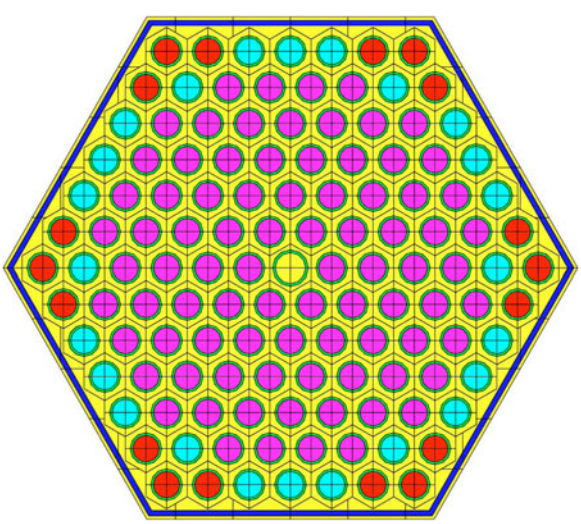

Fig. 5. NEWT representation of a full VVER-400 assembly.

KENO uses the same multigroup cross-section data and interacts with ORIGEN in exactly the same manner as NEWT, and the KENO-based sequences provide a method to directly and independently assess the effect of any transport approximations made in NEWT. This has proved invaluable in testing and validation efforts related to NEWT. The converse is also true; errors associated with Monte Carlo uncertainties can be easily tested by performing 2-D analyses with NEWT. Finally, the fact that NEWT and KENO-VI share a common geometry-description paradigm makes it possible to rapidly interchange models between the two methods.

II.D. Depletion/Decay Calculations with ORIGEN

A necessary component of accurate reactor fuel calculations is the use of cross-section data libraries that correctly define nuclear reaction rates during irradiation. The cross sections used by burnup codes change as a function of burnup, enrichment, and operating conditions and depend on the fuel assembly design. It is critical to accurately characterize the cross sections for the specific fuel type being analyzed. Most reactor physics codes are not capable of analyzing the full set of fuel isotopics necessary to accurately calculate all activation and fission products and daughters thereof. ORIGEN provides the versatility to use burnup-dependent cross-section libraries produced via problem-specific transport calculations and simultaneously track every activation, fission, and decay event for which data are available.

The ORIGEN family of codes has become one of the most widely used and internationally recognized classes of depletion and decay codes in the nuclear industry for the comprehensive analysis of nuclide compositions, decay heat, and radiation sources from spent nuclear fuel. The current version is known as ORIGEN-S, developed at ORNL within SCALE (Ref. 6). ORIGEN currently tracks 1119 individual fission products generated in the fuel during irradiation, 129 actinides, and 698 isotopes associated with structural and/or activation components. The standard cross-section libraries used by ORIGEN for its depletion and decay calculations have been extensively updated as discussed in Ref. 6.

ORIGEN has been extensively validated against destructive radiochemical measurements for more than 100 spent-fuel samples from domestic and international programs involving older[11] and modern high-burnup mixed-oxide (MOX) and low-enriched uranium (LEU) fuels, decay heat measurements for more than 120 assemblies

spanning cooling times up to 30 years (Ref. 12), and neutron and gamma radiation measurements. The extensive validation of ORIGEN is a critical element in establishing the reliability of the code to support detailed lattice physics analysis with few approximations.

II.E. TRITON Depletion Algorithm

Internally, ORIGEN is designed to automatically adjust flux levels with changes in inventory to maintain a user-specified power level. However, when used as a stand-alone method, it is limited by the accuracy of the cross-section library that it reads. Within SCALE, ORIGEN reads (by default) a set of cross sections from a library created for a generic LWR fuel assembly with 33 GWd of burnup. However, because spatial fluxes are burnup dependent, changing with nuclide inventories, and because mixture cross sections also change with burnup, the TRITON depletion sequence uses a two-pass cross-section update approach to improve estimates of both fluxes and cross sections as a function of burnup. A TRITON calculation can be considered to consist of two components during this iterative phase: (a) transport calculations (cross-section processing and the neutron transport solution) and (b) depletion calculations (COUPLE and ORIGEN). COUPLE collapses the multigroup cross sections from NEWT or KENO for use in ORIGEN. Transport calculations are used to calculate fluxes and prepare weighted cross sections and other lattice physics parameters based on a given set of nuclide concentrations; depletion calculations are used to update nuclide concentrations, which are used in the following transport calculation. The TRITON/NEWT depletion sequence is illustrated in Fig. 1, while Fig. 2 shows the TRITON/KENO depletion sequence.

The cross-section update process is implemented by performing a transport solution based on anticipated concentrations at a time halfway through a given fuel cycle (or depletion period). Depletion calculations are then performed over a constant-power burn period using fluxes and cross sections predicted for mid-cycle. Depletion calculations are then extended to a point halfway through the next cycle, followed by another mid-cycle transport calculation. This process is repeated until depletion calculations are completed for all cycles in a depletion case. This process results in cross sections representative of the predicted mid-cycle burnup, which are applied in the second-pass depletion over all fuel cycles.

Figure 6 illustrates the cross-section update process for a hypothetical three-period depletion case. In this figure, transport and depletion calculations are represented by the labels "T" and "D," respectively. For this example, four sets of calculations would be necessary: one for each burn period and one for an initial case T_0/D_0 that is used to determine mid-cycle cross sections for Cycle 1 using the T_1 transport solution.

The D_1 depletion cycle restarts at time zero but performs a depletion calculation using updated cross sections provided by the T_1 transport solution. Both D_1 and D_2 depletion periods are executed in two stages, a and b. The first stage (a) performs the current burn period depletion and decay calculations and provides the isotopic concentrations for the beginning of the next burn period; the second stage (b) is used to obtain concentrations for the successive transport solution. The final depletion period, D_3, requires only a single stage, as cross sections following the final burn period are not necessary.

Cross sections produced by COUPLE and used by ORIGEN for each mid-cycle time point are saved as a library that is read by ORIGEN. Each time a new ORIGEN library is produced, the updated cross-section data are appended to the end of the existing library, resulting in a set of time-dependent cross-section libraries in a single file

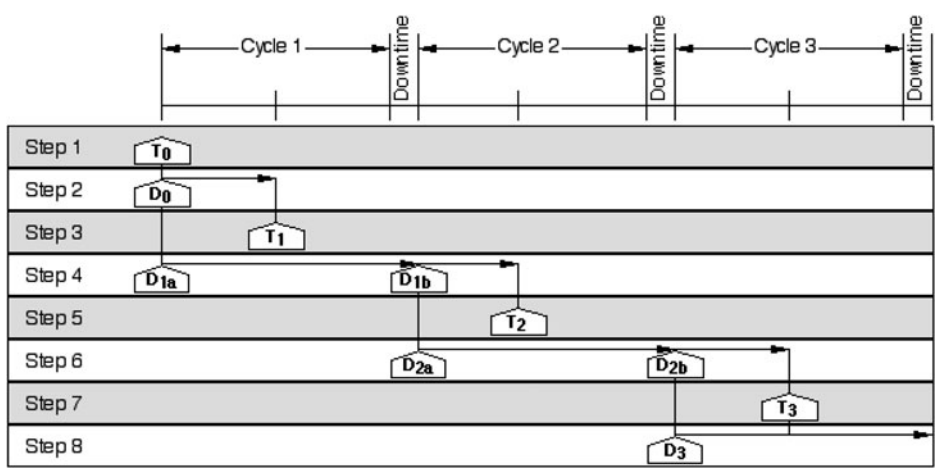

Fig. 6. TRITON transport/depletion calculation process.

for each mixture being depleted. These files can be used in other applications, e.g., for additional stand-alone ORIGEN calculations or for the creation of libraries for ORIGEN-ARP (Automatic Rapid Processing).[13]

By default, TRITON creates a single library at the midpoint of each cycle to use to approximate cross sections over the full cycle. In practice, it is often the case that a cycle (continuous operation at a given power) is long enough that significant isotopic changes do occur, and a one-step approach (i.e., a single depletion calculation based on a single set of cross sections) gives inadequate temporal discretization. The TRITON depletion sequence allows for refinement of the cross-section update time interval by allowing more intermediate steps within each cycle. The user can specify a variable number of libraries per cycle, resulting in an increased number of transport/depletion steps. For example, fuel burned at a constant power for a 1-yr burn cycle can be represented using a single cross-section library based on 6-month (mid-cycle) isotopic concentrations to approximate the average cross sections over a cycle. However, when cross sections change rapidly over a cycle (as is often the case early in life, especially with poison rods present in the assembly), this approximation is weak. In such cases, it is more appropriate to represent a single cycle with multiple subintervals. Cross-section libraries are created at the midpoint of each subinterval; because the accumulated burnup is reduced within each interval, the use of an average cross section for each interval is an improved approximation. Obviously, in the limit, as the number of intervals goes to infinity, the approximation goes to the exact solution. However, because changes in multigroup cross sections (resulting from resonance self-shielding effects) occur relatively slowly with burnup, only a minimal set of cross-section updates are generally required within a depletion cycle. The exact number of intervals that may be necessary for a given level of accuracy must be determined by the analyst. The key issue in this process is that cross sections for key burnup-dependent nuclides are being updated as a function of burnup during the depletion process.

III. TRITON CAPABILITIES

Because of the modular nature of the SCALE system, TRITON has a diverse set of capabilities. For example, because TRITON uses ORIGEN for depletion, it naturally inherits the powerful capabilities of ORIGEN for predicting isotopic inventories, decay heat, and other source terms, which are not usually possible in other reactor analysis software. Its modular nature allows the integration of KENO as an alternative to NEWT for transport solutions, providing a powerful 3-D Monte Carlo depletion capability. Sections III.A through III.E describe the capabilities of TRITON in SCALE 6.

III.A. Lattice Physics Calculations

In general, lattice physics codes are developed to model single assembly or core subregions and generate appropriately averaged homogenized cross sections for a full-core analysis package. TRITON provides this functionality, with the broad applicability of the generalized geometry capabilities and the rigorous transport solution of NEWT to generate lattice physics data for subsequent core analysis calculations using core simulator software. The NEWT solution is used to generate fluxes that are in turn employed to homogenize and collapse cross sections. Other data, such as transport-corrected total cross sections, diffusion coefficients, discontinuity factors, pin power factors, groupwise form factors, and detector responses, are also available from NEWT. Cross sections obtained in each NEWT calculation during a TRITON depletion sequence are extracted and saved in a single cross-section database file.

Because ORIGEN is a point depletion code, it is used to independently model distinct depletion regions (mixtures) instead of the fuel assembly as a whole. Coupling between these regions is achieved using the transport solution for the assembly; relative fluxes across an assembly are used to determine the local (point) flux or power in each individual ORIGEN calculation. ORIGEN supports two modes of input for depletion calculations: power or flux. When flux is input, that value is used directly in the ORIGEN solution. However, when power is input, ORIGEN will automatically adjust the flux to maintain a constant power, based on power-producing reactions to scale the flux. While depletion assuming a constant power is generally representative of a fuel element, this is not true for nonfuel elements. Targets, structural materials, and burnable poisons are generally "driven" by fluxes from neighboring fuel elements and do not contribute significantly to power production. Forcing a constant power in a burnable poison rod, for example, would result in a rapidly increasing flux due to depletion of the poison material, which is aphysical. Allowing mixed-mode depletion within TRITON better approximates the time-dependent flux behavior across an assembly.

Cross sections updated by COUPLE are first collapsed using the neutron flux obtained from the transport solution (NEWT or KENO). However, the flux spectrum calculated in a standard 2-D transport solution is typically representative of an infinite system with no leakage. Although this spectrum is often a reasonable first approximation, it is more appropriate to perform the cross-section collapse using a spectrum corrected for a finite critical system. NEWT allows for a spectral correction by performing an optional B_1 calculation for the homogenized system. This solution does a buckling search to find the buckling that represents a critical system. The buckling term represents leakage from the system and is positive for supercritical and negative for subcritical systems. The multigroup spectrum obtained from the B_1

solution is used to collapse cross sections to more properly characterize fuel burned in a critical reactor.

Because each depletion mixture is depleted independently within TRITON, cross sections are extracted from those collapsed by the transport solution for each depletion material to create a mixture-specific ORIGEN library update. Output data from ORIGEN are also mixture-specific.

III.B. Branch Calculations

The TRITON/NEWT sequence supports the calculation of branch cross sections, i.e., repeated transport calculations at one or more state points used to generate cross sections as a function of perturbations in system conditions. Currently, TRITON supports perturbations in fuel temperature, moderator temperature, moderator density, soluble boron concentration, and control rod insertion. One or more perturbations are performed at each of a set of branch states, relative to the nominal state. Macroscopic cross sections are homogenized, collapsed, and saved at the end of each branch calculation. Also included for each calculation are diffusion coefficients, discontinuity factors, pin peaking factors, fluxes, and currents that may be used in nodal core calculations, and other data processing functions.

Since TRITON separates cross-section processing, transport solutions, and depletion calculations using various functional modules, branch calculations require a number of sequenced calculations and operations for each branch state. Figure 7 illustrates a TRITON calculation with branches. Because cross-section processing can involve multiple calls to CENTRM and PMC (one for each fuel cell specification and one for all other materials), the CENTRM/PMC process for all cells is simplified and indicated by the italicized *CENTRM* box in the flowchart. Use of branch calculations in static calculations follows the same pattern, although the calculation is terminated after the last branch calculation; no depletion calculations are performed.

Because branches and depletion steps result in multiple sets of cross sections that cannot be stored in standard AMPX format, cross sections are archived in a TRITON-specific database. To date, TRITON-generated cross-section data have been used in a wide variety of applications, including generation of cross sections for core calculations with PARCS (Purdue Advanced Reactor Core Simulator)[14] for U.S. Nuclear Regulatory Commission (NRC) analyses[15]; NESTLE (Nodal Eigenvalue, Steady-state, Transient, Le core Evaluator)[16] for in-house methods development research[17]; Bold Venture for High Flux Isotope Reactor LEU conversion

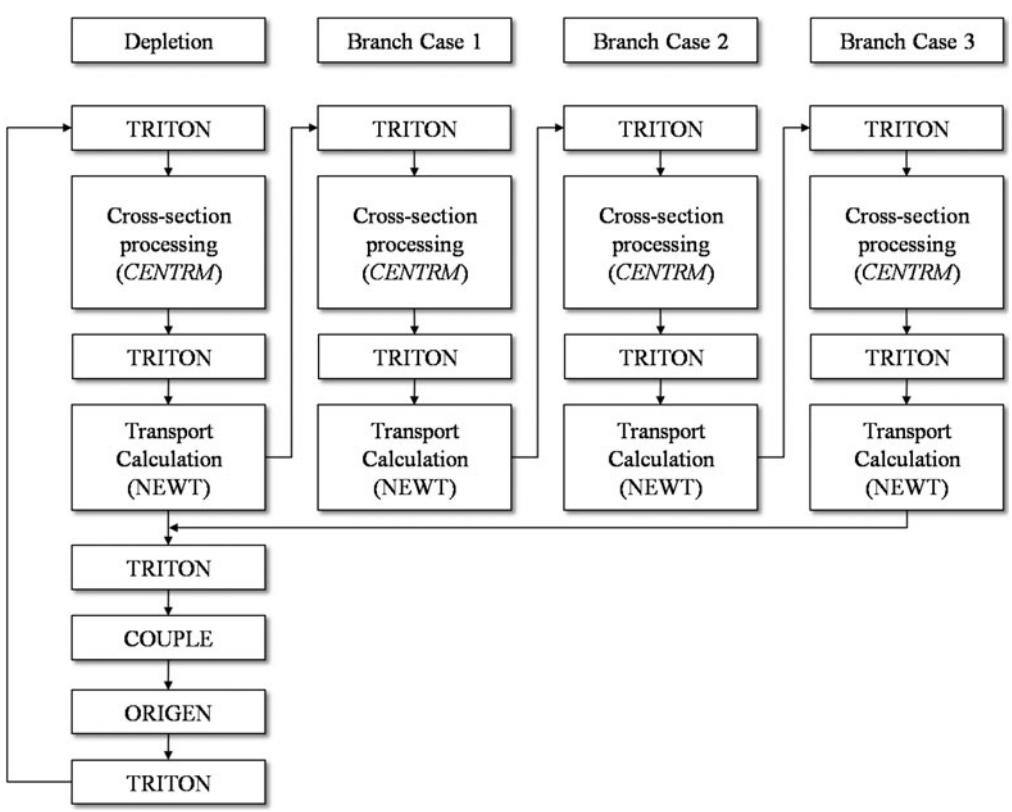

Fig. 7. TRITON code flow for branch calculations with depletion.

studies[18]; and Attila[19] for Advanced Test Reactor core calculations.[20]

III.C. HTGR and Doubly Heterogeneous Fuel Modeling

TRITON in SCALE 6 has improved support for high-temperature gas-cooled reactor (HTGR)–type fuel designs, including both geometric and cross-section processing features. Geometrically, NEWT has been updated to allow hexagonal and triangular outer boundaries, with boundary condition specifications for up to eight outer faces. A new product quadrature set has been added to NEWT to allow specification of reflective boundary conditions for outer boundaries with a 30/60-deg slope (i.e., hexagonal fuel elements). In order to perform reflective boundary treatments on sloped surfaces, the quadrature set selected must be symmetric with respect to that slope.

In terms of cross-section processing, a methodology for treating doubly heterogeneous (DH) fuel (grains of fuel within lattices or arrangements of fuel elements) has been implemented in the TRITON depletion sequences in SCALE 6. The CENTRM and PMC modules, along with special utility modules, are used to generate problem-dependent multigroup cross sections in SCALE that can accurately capture the physics of DH fuel behavior. When a DH cell type is input, pointwise flux disadvantage factors are calculated in the fuel grains (coated particles) that represent the first level of heterogeneity in HTGR fuels. Next, the disadvantage factors are used to generate cell-weighted pointwise cross sections for a homogenized fuel region that represents the fuel inside a fuel compact or pebble. Then, the spatially averaged pointwise cross sections are used to calculate the flux distribution in the fuel element. Finally, this pointwise flux is used by PMC to generate the multigroup problem-dependent cross sections with an appropriate spectrum. Only the homogenized mixture is included in the transport model; it is not necessary to explicitly model the grain level of heterogeneity. However, the ORIGEN depletion step focuses only on the contents of the fuel grain. TRITON is responsible for conversion of discrete composition number densities used in the first pass of cross-section processing.

During the depletion calculation, grain-level number densities are updated by ORIGEN calculations. TRITON is able to deplete multiple grain types within a single fuel element or separate fuel elements by independent ORIGEN cells using the flux and number densities that characterize each grain. As noted above, the cross sections used by TRITON and collapsed for use in ORIGEN have been homogenized using disadvantage factors for each grain. Hence, calculations using the homogenized cross sections and resultant homogeneous media flux will reproduce the correct reaction rates in ORIGEN to reproduce local burnup. This method has been validated by comparison with continuous-energy Monte Carlo depletion models that include explicit fuel grain representations.

III.D. Spent-Fuel Characterization

The ability to accurately predict the nuclide composition of depleted reactor fuel is important in a wide variety of applications, including the design, licensing, and operation of commercial and research reactors and spent-fuel transport/storage systems. The calculation of isotopic compositions, decay heat, radiation sources, and radiotoxicity of spent fuel has long been a capability of SCALE.

Historically, the SAS2H 1-D sequence within the SCALE nuclear analysis suite provided a simple, rapid approach for spent-fuel characterization. However, because of its 1-D transport approximation, SAS2H became outdated with the evolution of modern fuel assembly designs. Increasing complexity in reactor designs, evolutionary concepts, and nonreactor applications such as safeguards, security, and nonproliferation required more robust geometrical modeling capabilities than those available in SAS2H for proper characterization of neutron transport.

With its ability to explicitly represent 2-D lattice configurations, TRITON became the logical successor to SAS2H. Since its release, TRITON and SCALE data libraries have been heavily validated against radiochemical assay data.[21,22]

As mentioned earlier, TRITON may also be used to generate cross-section libraries for the ORIGEN-ARP sequence in SCALE. This approach provides an alternative to the full TRITON sequence for spent-fuel characterization. In the ARP approach, burnup-dependent libraries are generated for a given reactor design using TRITON. These pregenerated libraries are suitable for use by the ORIGEN code. By interpolation of the cross-section data in these libraries, point-depletion ORIGEN calculations can be carried out for that particular reactor design and operating condition without requiring the full complexity of additional TRITON calculations. Depending on requirements or on the reactor design being analyzed, the libraries allow for interpolation on three variables: burnup, enrichment, and water (moderator) density.

III.E. Sensitivity/Uncertainty Analysis

Development of TRITON since the release of SCALE 6 has expanded to create a 2-D sensitivity/uncertainty analysis sequence that executes NEWT in both forward and adjoint modes. In addition, generalized perturbation theory (GPT) has been implemented for 1-D and 2-D deterministic transport calculations.[23] The 1-D and 2-D transport codes, XSDRNPM and NEWT, respectively, solve the generalized adjoint equation, an inhomogeneous form of the transport equation containing the singular Boltzmann operator for a critical system. Generalized adjoint solutions from the SCALE transport codes are used to compute sensitivity coefficients based on GPT

expressions, which consist of direct effects (from data appearing directly in response functions) and indirect effects (from data impacting the response through flux perturbations). Both direct and indirect effects may include explicit and implicit components. The explicit components describe response changes due to perturbations in multigroup cross-section data appearing in the transport equation, whereas the implicit components account for response changes caused by perturbations in cross-section self-shielding. The TRITON GPT capability provides a useful means of quantifying homogenized few-group cross-section uncertainties to facilitate reactor-core simulation uncertainty analysis. These capabilities will be available with the release of SCALE 6.1.

IV. VALIDATION OF TRITON

IV.A. Validation of Spent-Fuel Characterization

A database of isotopic measurement data has been compiled and documented at ORNL as part of a sustained validation effort to determine the biases and uncertainties in depletion calculations for the actinides and fission products of importance to spent-fuel safety applications. This database includes radiochemical assay data acquired from domestic and international experimental programs and covers a large range of burnup and fuel enrichment values. The most recent radiochemical isotopic assay data set was acquired through the international MALIBU program.[24] This program was designed to provide a large set of reliable, high-quality experimental isotopic data with low uncertainties for high-burnup commercial spent nuclear fuel. The spent-fuel measurements for the first phase of the program, which were carried out between 2004 and 2006 at three different experimental laboratories, included extensive actinide and fission product data of importance to spent-fuel safety applications. Cross-check measurements were performed for some of the analyzed spent-fuel samples to reduce the experimental uncertainties and improve confidence in the measured data. The measurement data obtained in the MALIBU program for three UO_2 spent-fuel samples are used here to demonstrate depletion analysis performance using the ENDF/B-VII library available in SCALE 6. The UO_2 samples were selected from different axial locations (and burnups) of a single fuel rod. The fuel was manufactured with 4.3 wt% initial enrichment ^{235}U and was irradiated in the Gosgen pressurized water reactor (PWR) for three fuel cycles. The samples had burnups of ~70, 51, and 46 GWd/tonne U, respectively.

These measurements were also previously analyzed with SCALE 5.1 and libraries based on ENDF/B-V data.[25] Differences in isotopic predictions result from differences in both data and cross-section processing methods. The previous calculations were performed using the SCALE 44-group ENDF/B-V cross-section library with resolved resonance processing performed using the NITAWL (Nordheim Integral Treatment And Working Library) module of SCALE; the updated calculations were performed using the 238-group ENDF/B-VII library with the CENTRM/PMC cross-section processing methodology. A set of 232 isotopes for which cross-section data are available in the ENDF libraries were applied in updating cross sections for the ORIGEN fuel depletion calculation at each depletion step.

A comparison of the calculated and measured isotopic concentrations for the three samples considered is provided in Figs. 8, 9, and 10 for both SCALE libraries used. The plotted data show, for each nuclide, the value of $(C/E - 1)$ in percentage, where C/E represents the calculated-to-experimental concentration ratio. For the uranium and plutonium isotopes, illustrated in Fig. 8, the overall agreement of calculation with measurement is similar for both SCALE libraries. On average, ^{235}U and ^{239}Pu are overestimated, respectively, by ~0.2 and 1.3%, compared with the measurement, when ENDF/B-VII (V7) is used. In the case of minor actinides (Fig. 9), a large

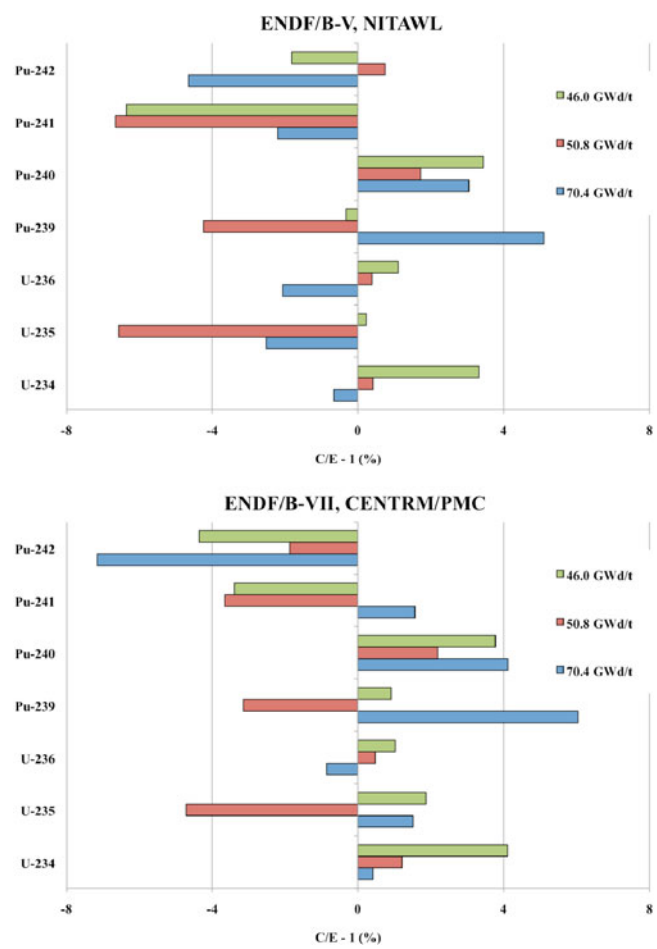

Fig. 8. TRITON calculated-to-experiment ratios for key actinides in MALIBU measurements.

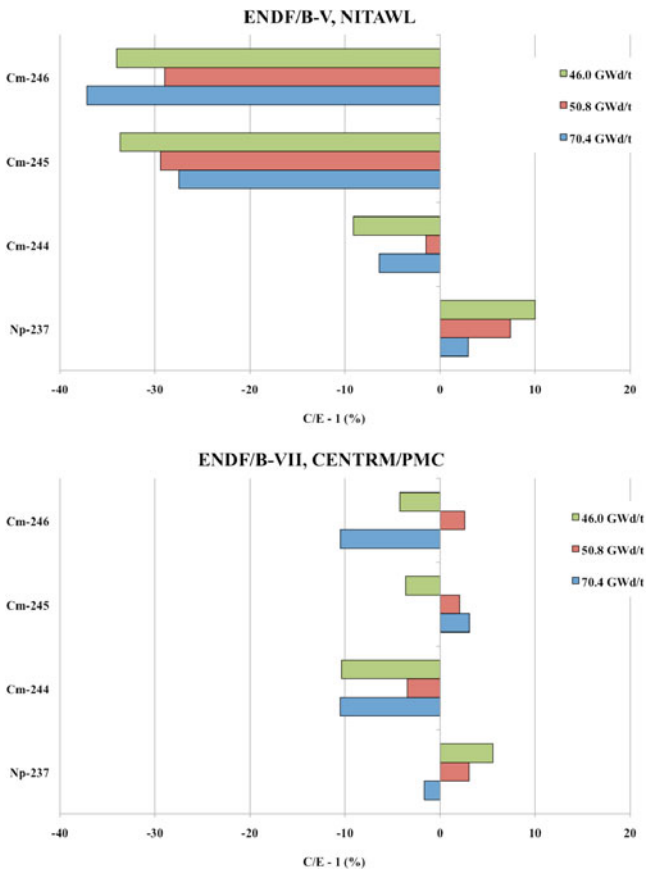

Fig. 9. TRITON calculated-to-experiment ratios for lesser actinides in MALIBU measurements.

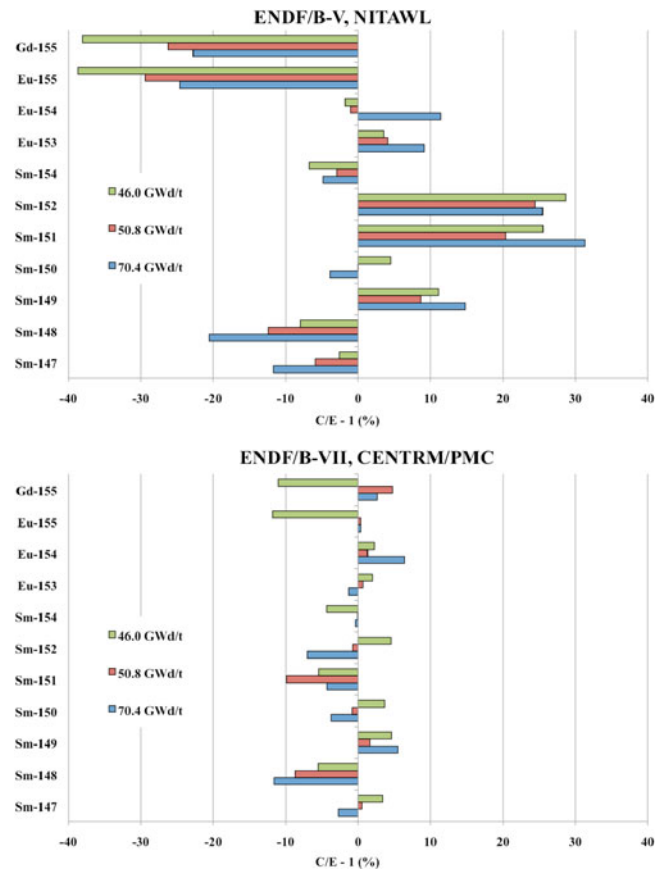

Fig. 10. TRITON calculated-to-experiment ratios for fission products in MALIBU measurements.

improvement in the agreement of calculation with measurement for V7 data relative to ENDF/B-V (V5), by ~30% on average, is seen for ^{245}Cm and ^{246}Cm, isotopes important for source term calculations.

The samarium isotopes (Fig. 10) are much better estimated with V7 than with V5, notably ^{147}Sm, ^{149}Sm, ^{151}Sm, and ^{152}Sm; these are fission products with large absorption cross sections that are important to burnup credit criticality calculations. The ^{149}Sm isotope, a key fission product absorber, is calculated on average within 4% of measured data with V7; with V5, it is calculated within 12%. Large improvements, with differences of ~20% between V7 and V5 results, are also seen in the estimation of ^{151}Sm and ^{152}Sm. Figure 10 also shows a large improvement in the C/E ratios for europium and gadolinium with V7. For example, in the case of ^{153}Eu and ^{155}Gd, both fission products important to burnup credit, the average C/E decreases from 5.6 to 0.4% and from −29 to −1%, respectively, with V7.

Although these results show a clear improvement in spent-fuel inventory prediction with V7 data, they also illustrate the accuracy of TRITON in prediction of isotopic depletion and decay. This is important not only for spent-fuel safety applications but also for lattice physics calculations, where late-in-life assembly cross sections are heavily influenced by accumulated activation and fission products.

IV.B. Validation of Monte Carlo Depletion

Validation of the TRITON/KENO Monte Carlo depletion capability has been performed with benchmark calculations using LWR fuel assembly data provided in validation reports of the SAS2H 1-D depletion sequence in SCALE (Ref. 22). Benchmark models of the spent-fuel assemblies were developed and calculated with TRITON/KENO using CENTRM/PMC and the 44-group ENDF/B-V cross-section library in SCALE 5.1. Results were compared with the measured radiochemical spent-fuel assay data given in the original validation reports and previously calculated SAS2 and TRITON/NEWT results. Benchmark calculations were performed for 29 samples taken from the following LWR fuel assemblies:

1. Calvert Cliffs Unit 1 PWR fuel assemblies D047, D101, and BT03

2. Obrigheim PWR fuel assemblies 168, 170, 171, 172, and 176
3. San Onofre Unit 1 PWR MOX fuel assembly D51X
4. Gundremmingen BWR fuel assemblies B23 and C16.

A composite plot of the actinide results for all 29 samples is shown in Fig. 11. The fission product results are plotted in Fig. 12. Figures 11 and 12 show the average percent differences and the standard deviations from all cases. The calculated results for most actinides and fission products are within 10% of the measured data.

IV.C. Critical Benchmark Validation

Because early development work with NEWT was in support of MOX fuel analysis, one of the first lattice criticals adopted for validation of NEWT criticality capabilities was the VENUS-2 MOX benchmark, developed by the Nuclear Energy Agency of the Organisation for Economic Co-operation and Development.[26] VENUS-2 is an international benchmark with both 2-D and 3-D exercises. The VENUS facility is a zero power critical reactor located at SCK/CEN in Belgium. For the VENUS-2 experiment, the core consisted of four central assemblies of 3.3 wt% ^{235}U enrichment UO_2 fuel pins, with ten Pyrex pins each, and eight assemblies on the periphery of the core made up of UO_2 and MOX fuel. The seven internal rows contain 4.0 wt% UO_2 fuel pins, and eight external rows contain MOX fuel with 2.0/2.7 wt% high-grade plutonium. A diagram of the 2-D VENUS-2 core is shown in Fig. 13. The 2-D benchmark specification provided a measured axial buckling of 0.00239 cm^{-2}. A NEWT model for the VENUS core was developed based on the benchmark specification; a one-quarter core model was developed to take advantage of symmetry. Using SCALE 6 and the 238-group ENDF/B-VII cross-section library, NEWT calculated a k_{eff} value of 1.0011. Benchmark solutions provided in Ref. 26 include both deterministic and Monte Carlo solutions from DORT (2), HELIOS (2), BOXER (1), GNOMER (2), MCNP (4), and MCU (1). The 12 submitted solutions had a mean calculated k_{eff} value of 0.9980 ± 0.0043. The NEWT eigenvalue solution lies within 1σ of the mean. A number of other partial-core calculations were

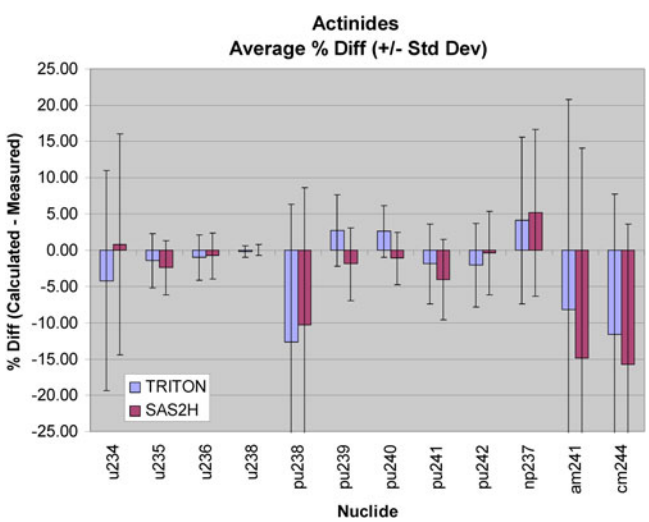

Fig. 11. Comparison of TRITON/KENO results with measured actinide data.

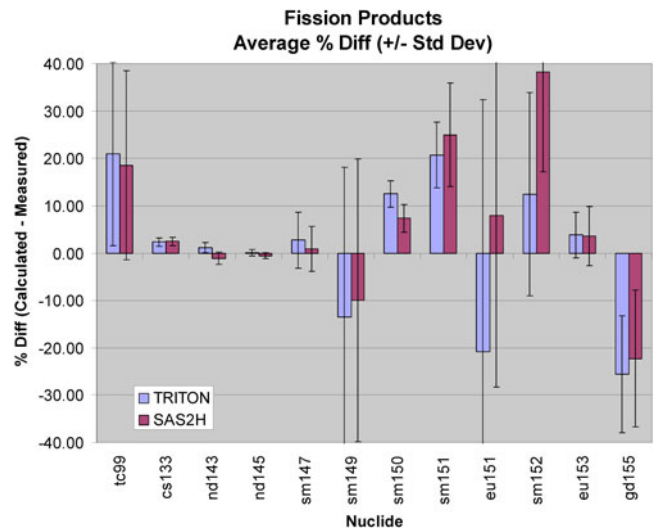

Fig. 12. Comparison of TRITON/KENO results with measured fission product data.

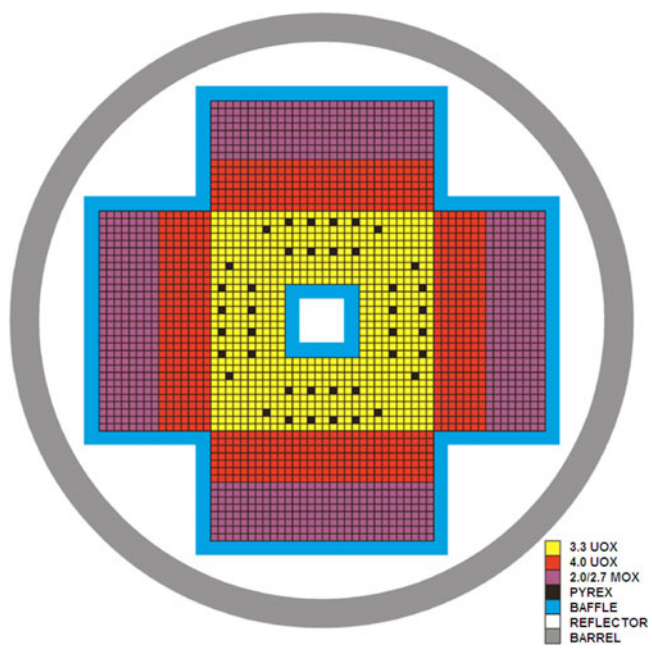

Fig. 13. VENUS-2 core configuration.

performed as part of the benchmark, and TRITON-generated cross sections were used in PARCS calculations with homogenized cross sections. The results of these analyses are reported in Ref. 1.

IV.D. Coupling with Reactor Core Simulators

Early development with NEWT and TRITON had as a goal the preparation of few-group lattice physics parameters for core analysis with the PARCS nodal code. Specifically, cross sections were prepared for use in PARCS core analysis, using proprietary data from Electricite de France's St. Laurent Unit 1 core,[27] which contained MOX fuel. Core-follow calculations were performed for Cycle 1 of the Peach Bottom Unit 2 BWR as part of a validation project for the NRC (Ref. 28).

A simplified pin-cell model was developed for NEWT based on the Japanese High-Temperature Test Reactor (HTTR) fuel design.[29] The fuel consists of TRISO fuel particles embedded in annular graphite compacts, which are in turn loaded into sleeves and centered in a coolant channel. The coolant channel is centered within a hexagonal zone representing a single fuel cell. The NEWT model developed to represent this pin cell is illustrated in Fig. 14. TRITON depletion calculations were performed to generate cross sections as a function of burnup for 1750 days irradiation time at 30 MW/tonne U. Cross sections were collapsed into 2, 4, and 8 energy groups in separate calculations to evaluate the effect of the group structure on solution accuracy. A single hexagonal lattice model with reflective boundary conditions was developed for PARCS, which was then run to solve the hexagonal geometry diffusion problem with fresh fuel and no depletion to verify that it was able to reproduce the eigenvalue predicted by NEWT for the various few-group sets. The value of k_{eff} calculated by PARCS was found to be in agreement within 10 pcm of the NEWT fresh fuel state. PARCS was then rerun for depletion calculations using its macro-depletion option. Figure 15 provides a comparison of k_{eff} as a function of burnup calculated directly by TRITON relative to those calculated by PARCS using TRITON cross sections. PARCS solutions are in excellent agreement with TRITON over the entire burnup range. Because the two curves essentially lie on top of one another, a plot of the difference between the two (in pcm) is also shown. Agreement remains within 13 pcm over the entire burnup cycle, with no observable trend as a function of burnup.

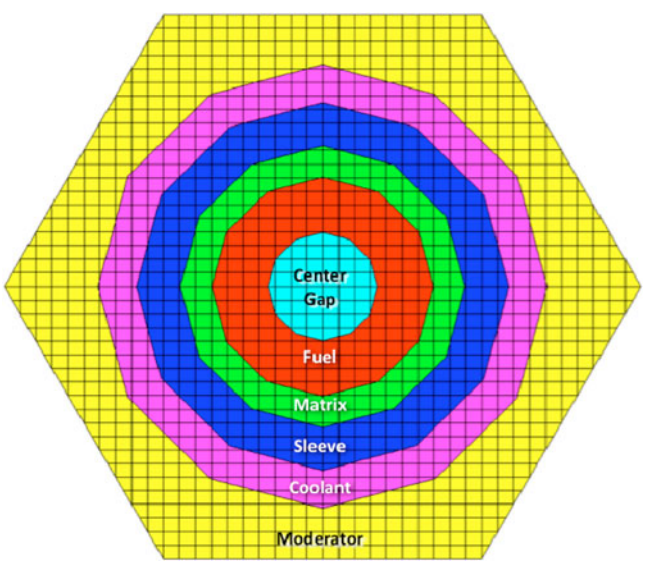

Fig. 14. Simplified HTTR pin cell modeled with TRITON to generate a set of cross sections for PARCS.

Recent work at ORNL has involved adoption of the NESTLE (Ref. 16) core analysis package for in-house application. The original NESTLE code, written in Fortran 77, has been fully converted into Fortran 90 and has been significantly modularized into functional components. During this process, several code issues were identified and rectified. NESTLE has also been enhanced to include a drift-flux solver for BWR simulation. Similar in function to GenPMAXS, a cross-section converter named T2N (TRITON to NESTLE) has been developed. Comparisons between TRITON and NESTLE calculations using TRITON-generated cross sections have been performed based on a simplified PWR model, as shown in Fig. 16. Results of depletion calculations are shown in Fig. 17; errors are generally on the order of 1 to 2 pcm over most of the burnup range.

The coupling of TRITON and NESTLE has been validated using a coupled neutronics and thermal-hydraulics benchmark of the Peach Bottom Unit 2 Cycle 1 core.[30,31] The benchmark performed was a test of initial conditions at startup. The calculated k_{eff} and the radial and axial power distributions showed good agreement with measured data. In addition, core depletion calculations were performed and showed excellent agreement between the codes.

IV.E. Validation of Core-Follow Calculations Using TRITON and PARCS

As discussed previously, a coupled TRITON/PARCS sequence of calculations was performed by using proprietary data from Electricite de France's St. Laurent Unit 1 core. Physics data are available for Cycles 1 through 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 depletion 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 using GenPMAXS. Brookhaven National Laboratory used these cross sections with PARCS in the performance of core-follow calculations. Comparisons were

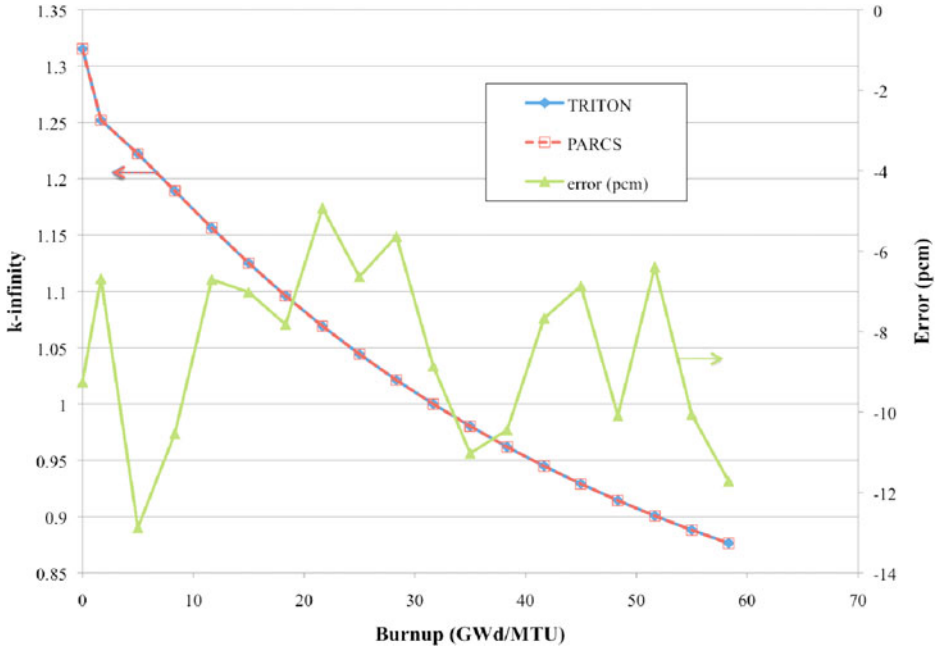

Fig. 15. Comparison of TRITON and PARCS depletion calculations for an HTTR pin-cell model.

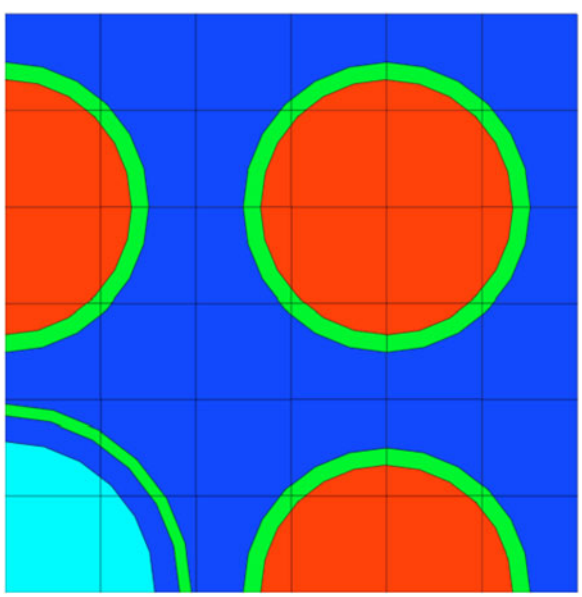

Fig. 16. NEWT model of a simplified PWR assembly used for NESTLE calculations.

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 18 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, Fig. 18 clearly shows excellent agreement between predicted and measured data. The net root mean square difference is 1.26%. For the UO_2 fuel assemblies, the root mean square agreement is 1.20%; it is 1.38% for the MOX fuel assemblies. The slightly higher differences for MOX assemblies are more likely due to the positions of the MOX fuel in the core than to issues in the transport solution. Figure 19 illustrates the predicted critical boron concentration relative to actual operational concentrations and shows good agreement with actual plant data over the entire cycle.

IV.F. Validation of DH Fuel Depletion

As discussed earlier, the ability to perform depletion of DH fuel designs was introduced in the release of SCALE 6. Although the DH cross-section processing methodology has been tested in criticality calculations for code-to-code benchmarks,[32,33] the nature of the depletion process introduces additional complexities that must be validated. A lack of experimental measurements for the depletion of HTGR fuel elements makes direct validation difficult at present; however, a computational benchmark has been developed to prescribe simple infinite-lattice fuel configurations for code-to-code testing.[34] This benchmark consists of three configurations: an infinite lattice of fuel grains (in which there is no DH effect), an infinite lattice of pebbles prototypic of PBMR fuel, and an infinite-lattice supercell of hexagonal lattice fuel compacts and coolant in a graphite media. All three configurations have been analyzed and compared with

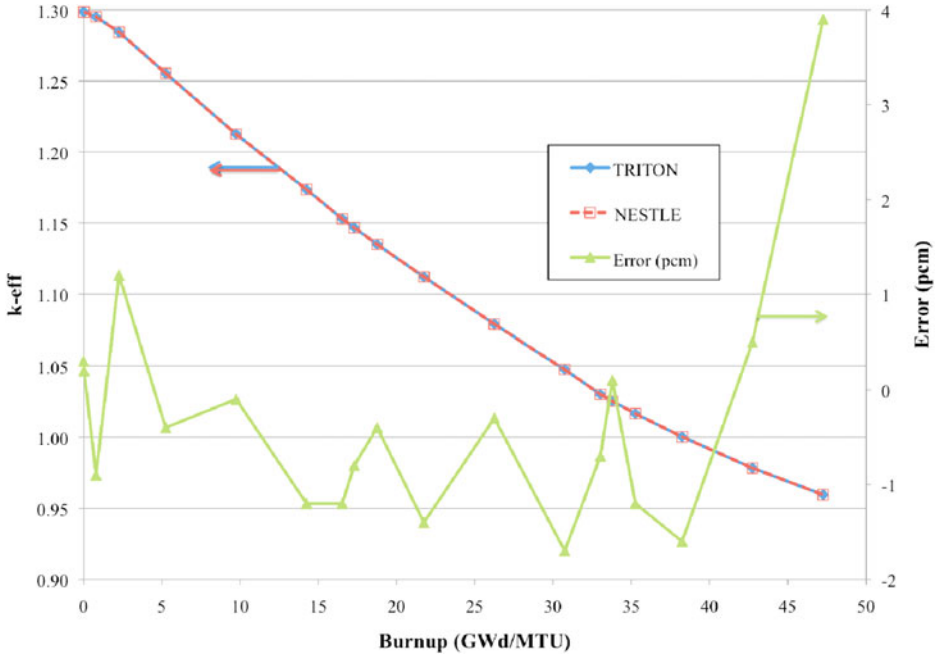

Fig. 17. Comparison of TRITON and NESTLE depletion calculations for a simplified UO_2 assembly model.

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%

Fig. 18. Relative error between reported and predicted assembly powers using TRITON/PARCS for St. Laurent Unit 1 at the end of Cycle 10.

results calculated using the continuous-energy Monte Carlo code Serpent.[35] TRITON calculations were performed using the two-pass homogenization approach described earlier. Serpent calculations used an explicit representation of randomly dispersed particles and represent the best-estimate simulation of fuel-particle interactions. Figure 20 shows the results of TRITON (NEWT and KENO) depletion calculations for the hexagonal lattice supercell phase of the benchmark, relative to Serpent calculations; both used ENDF/B-VII cross-section data. TRITON's cross sections were processed by AMPX, while Serpent's cross sections were processed by NJOY (Ref. 36). Small differences are seen between the two codes, but overall the agreement is very good over the entire depletion cycle. KENO depletion calculations within TRITON are essentially the same as the NEWT-calculated results. In the absence of qualified experimental data for spent-fuel samples burned in a prototypic environment, this close agreement of completely independent methods and data provides a great deal of confidence in the capabilities of both methods to represent the physics of HTGR fuel depletion. Completion of a broad code-to-code comparison for this benchmark is expected in 2011 and will provide a number of independent solutions for comparison of various methods.

V. CONCLUSIONS

The TRITON module of the SCALE code system provides a powerful and robust approach for 2-D discrete ordinates or 3-D Monte Carlo transport and depletion

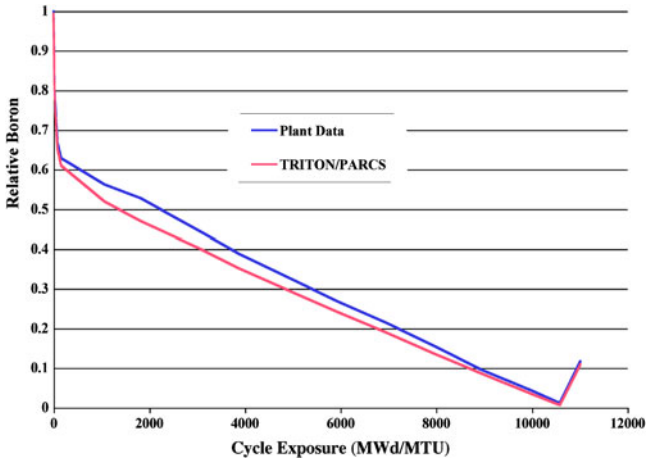

Fig. 19. Relative critical boron concentration for St. Laurent Unit 1, Cycle 10.

analysis of reactor fuel assemblies. Coupled with a core simulator, accurate core-follow calculations can be performed for complex fuel designs. The arbitrary-geometry features of NEWT provide a powerful tool for 2-D studies of advanced designs and nontraditional fuel assembly concepts. The input geometry specifications for NEWT, based on the SCALE Generalized-Geometry Package combinatorial-geometry format of the KENO-VI Monte Carlo code in 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 input for 3-D Monte Carlo depletion calculations.

As a part of the SCALE code system, TRITON uses a set of special-purpose functional modules that have been developed to solve specific classes of problems. CENTRM and PMC provide the capability to perform continuous-energy resonance self-shielding and multigroup cross-section processing. ORIGEN performs detailed nuclide depletion and decay calculations. NEWT affords a deterministic approach for detailed 2-D lattice transport calculations, and KENO gives the ability to perform 3-D Monte Carlo depletion. TRITON uses SCALE cross-section data, validated through extensive application. TRITON is validated, configured, controlled, and tested within the SCALE software quality assurance system.

The NEWT 2-D discrete ordinates solver has been validated against UO_2 and MOX critical benchmarks. For the VENUS-2 MOX critical benchmark, TRITON/NEWT calculated a k_{eff} value of 1.0011.

TRITON 2-D discrete ordinates and 3-D Monte Carlo depletion sequences have been validated for spent-fuel inventory prediction by comparison with measured spent-fuel assay data from a large number of LWR spent-fuel assemblies. The latest results using SCALE ENDF/B-VII cross-section data agree within 10% on average for most actinides and fission products.

The TRITON 2-D depletion sequence has been coupled with both the PARCS and NESTLE reactor core simulators. These methods have been validated by performing

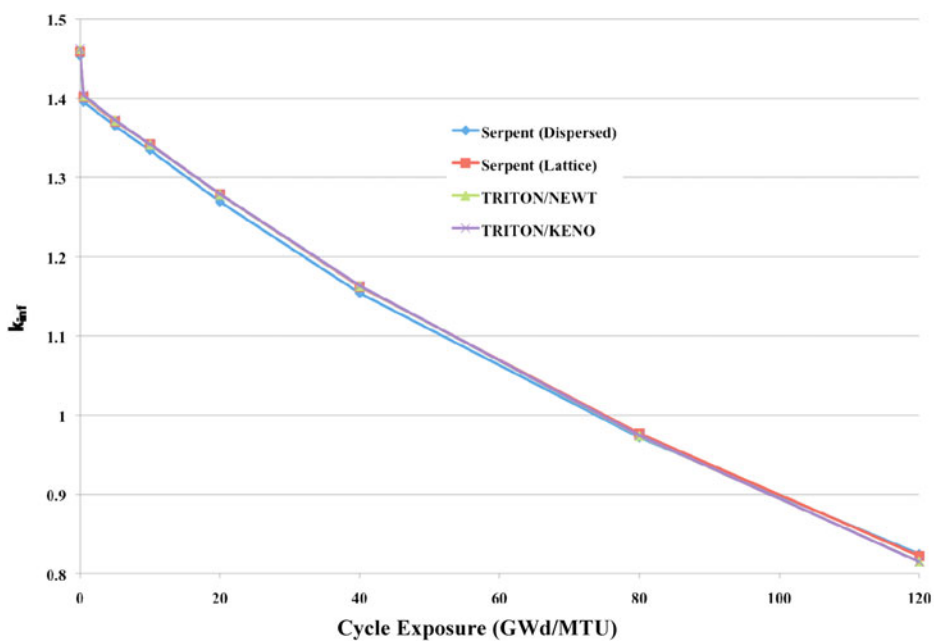

Fig. 20. Comparison of TRITON and Serpent results for DH fuel depletion.

core-follow calculations for St. Laurent Unit 1 and depletion calculations for Peach Bottom Unit 2 Cycle 1, respectively.

TRITON has been validated for depletion of DH fuels, such as fuel grains in pebble bed or prismatic fuel blocks. Because of a lack of experimental data, TRITON results were compared with the Serpent continuous-energy Monte Carlo depletion code, which has the capability to explicitly represent randomly dispersed particles. Both NEWT and KENO multigroup depletion calculations performed for pebble bed fuel and hexagonal lattice fuel compacts in a graphite media showed good agreement with Serpent.

TRITON is currently limited to multigroup analysis. Continuous-energy Monte Carlo depletion capability with KENO is currently under development. SCALE 6 has a limit of approximately 2100 mixtures in its automated sequences, including TRITON. Removal of this limit in SCALE is in progress. Both of these enhancements are expected to be released in SCALE 6.2. In addition, significant speedup of TRITON's input/output processing of cross-section data will be available in SCALE 6.1. Development of a parallel computing architecture for release in SCALE 7 is also underway, and this version will include a fully parallel TRITON depletion sequence.

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