HIGH-FIDELITY DEPLETION CAPABILITIES OF THE SCALE CODE SYSTEM USING TRITON

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I. INTRODUCTION

Increasing complexity in reactor designs suggests a need to reexamine methods applied in spent-fuel characterization. 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 space reactors and Generation IV power reactors also require calculational methods that provide accurate prediction of the isotopic inventory. New high-fidelity physics methods will be required to better understand the physics associated with both evolutionary and revolutionary reactor concepts, as they depart from traditional and well-understood light-water-reactor (LWR) designs. The TRITON sequence of the Standardized Computer Analyses for Licensing Evaluation (SCALE) code system [1] provides a powerful, robust, and rigorous approach to reactor physics analysis. This summary provides an overview of TRITON in terms of its key components used in reactor calculations.

In response to concerns about the ability to accurately model the burnup of an LWR core containing weapons-grade mixed-oxide (MOX) fuel assemblies, the Nuclear Regulatory Commission has supported the enhancement of the generalized-geometry discrete-ordinates transport code NEWT. [1,2] NEWT provides lattice physics parameters for a nodal core analysis code code used in the analysis of MOX-fueled LWR cores. Also supported under this work were the enhancement and formal release of TRITON [3] within the SCALE system.[4] 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. 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 for full-core analysis.

Although MOX-fueled cores may represent a challenge to existing analysis methods, next-generation reactor design concepts pose a substantial departure from traditional lattice designs and will initially be built and operated without the benefit of thousands of 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 sequence, based on the NEWT arbitrary-geometry transport solver, is able to perform two-dimensional lattice calculations for non traditional lattice designs, including hexagonal arrays, even nonirregular-lattice configurations (e.g., CANDU ACR-700 design) and non lattice configurations. 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. Additionally, the recent release of TRITON within SCALE 5.1 adds the ability to perform full three-dimensional (3-D) depletion using the KENO V.a and KENO-VI Monte Carlo packages within SCALE.

This paper provides a description of TRITON, its components, and its capabilities. It also presents results of calculations that demonstrate the accuracy of the TRITON methodology for lattice physics.

II. OVERVIEW OF TRITON

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*, *control modules*, or *utilities*. Functional modules include the basic physics codes, such as XSDRNPM (one-dimensional [1-D] discrete ordinates); KENO (3-D Monte Carlo for criticality analysis); NEWT (two-dimensional [2-D] arbitrary geometry discrete ordinates); ORIGEN-S (point depletion and decay); 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 type of analysis. TRITON is a SCALE control module that can be used for problem-dependent cross-sectional weighting, 2-D transport calculations with NEWT,[2] or 2-D depletion calculations through a coupling of NEWT and ORIGEN-S. TRITON also supports 3-D depletion calculations using either KENO V.a or KENO-VI as transport solvers.[3]

When applied in deterministic depletion calculations, the TRITON module is used to perform an iterative sequence of calculations. Given mixtures and cell structures defined in input, TRITON drives cross-section processing operations using BONAMI to perform Bondarenko calculations for resonance self-shielding in the unresolved resonance range and CENTRM/PMC for resolved resonance evaluation. The cross-section library and mixing table produced by the sequence are automatically used in the NEWT calculation so that no mixing table need be specified. The transport solution is followed by COUPLE and ORIGEN-S calculations. 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 are supplied to ORIGEN-S for depletion calculations. COUPLE/ORIGEN calculations are repeated for each mixture being depleted, as specified in input, using mixture-specific cross-section data and fluxes. Used in conjunction with TRITON, NEWT 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.

Although ORIGEN-S supports the use of time-dependent fluxes, TRITON uses a more rigorous iterative procedure. Because spatial fluxes are burnup dependent, changing with nuclide inventories, and because mixture cross sections will also change with burnup, TRITON uses a predictor-corrector approach to update both fluxes and cross sections as a function of burnup. Such calculations can be considered to consist of two components during this iterative phase: (1) transport calculations (cross-section processing and the transport solution) and (2) depletion calculations. Transport calculations are used to calculate fluxes and prepare weighted cross sections and other lattice physics parameters based on a given set of nuclide concentrations; depletion calculations are used to update nuclide concentrations, which can be used in the ensuing transport calculation.

Despite broad applicability of the 2-D fuel depletion analysis capability of TRITON, there are some domains in which accurate 3-D depletion capabilities are necessary. 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. 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–based KENO V.a and KENO-VI codes in SCALE. The TRITON sequence has been modified to accept input for either KENO module in place of NEWT input and to use the Monte Carlo codes as the transport solver component of the sequence. The SCALE utility codes KMART and KMART6, originally developed to post-process KENO V.a and KENO-VI calculations, have been adapted to provide collapsed cross-sections and fluxes required by TRITON for setting up ORIGEN-S depletion calculations.

Extensive testing has been performed to verify proper operation of TRITON and to validate its ability to predict system eigenvalues, both for critical systems and as a function of burnup; to accurately estimate spent-fuel inventories; and to provide properly weighted few-group cross sections for core simulator calculations.[5-9] Calculations have been compared with measured data when available, but code-to-code comparisons have also been used to assess certain capabilities where little or no meaningful measurements are available.[10]

III. CONCLUSIONS

The TRITON module of the SCALE code system provides a powerful and robust approach to transport and depletion 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 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 exact three-dimensional simulation possible within TRITON using KENO V.a and KENO-VI extend the capabilities of the package to practically any type of depletion environment.

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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