

# INTEGRATED KENO V.a MONTE CARLO TRANSPORT FOR MULTIDIMENSIONAL DEPLETION WITHIN SCALE

Mark D. DeHart and Lester M. Petrie

Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831-6170

[dehartmd@ornl.gov](mailto:dehartmd@ornl.gov)

## INTRODUCTION

This paper describes a new three-dimensional (3-D) Monte Carlo-based depletion sequence that is being developed as part of the SCALE code system and presents some initial comparisons of results. The sequence couples the KENO V.a Monte Carlo code and the ORIGEN-S depletion code, both functional modules within the SCALE system.

The *NEWT* discrete ordinates package code developed at ORNL[1,2] has significantly extended the capabilities of discrete ordinates transport calculations due to its completely arbitrary grid discretization approach. A significant application of *NEWT* in nuclear systems analysis has been as the radiation transport solver in a new two-dimensional (2-D) depletion package sequence named *TRITON*[3,4]. Within *TRITON*, *NEWT* is used to calculate spatial flux distributions and to collapse nuclide cross sections for use in the *ORIGEN-S* depletion code. *TRITON* uses a predictor-corrector method, iteratively calling *NEWT* and *ORIGEN-S* to track changing flux and power distributions with burnup, matching time-dependent power to user-specified operating histories. *TRITON* allows the depletion of multiple independent mixtures in a nuclear system, and uses the geometric flexibility of *NEWT* to allow analysis of complex fuel lattices found in advanced commercial and research reactor designs.

Despite broad applicability of the 2-D version fuel depletion analysis capability of *TRITON* to fuel depletion analysis,[3] there are some domains in which accurate three-dimensional (3-D) depletion capabilities are necessary. For example, criticality analysis for commercial spent fuel in transportation and storage is concerned with the positive reactivity effects of low-burnup fuel near the ends of a fuel assembly where axial leakage effects, not captured by 2-D methods, may be important. Deterministic approaches based on Boltzmann 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, development of a 3-D depletion capability has been initiated integrated to *TRITON*, using the 3-D Monte Carlo-based *KENO-V.a* and *-VI* codes available in *SCALE*.

## BACKGROUND

Deterministic solutions methods have advantages over Monte Carlo methods simulations for the transport solutions used in coupled depletion analyses because of their ability to generate an accurate spatial distribution of fluxes over a complete problem domain. On the other hand, Monte Carlo methods provide powerful geometric modeling capabilities in three dimensional domains. Monte Carlo calculations must perform a large number of neutron particle simulations to converge on an accurate system response (e.g., global neutron multiplication). In order to obtain achievable reasonable neutron fluxes and power density distributions, significantly more computational effort must be invested. This computational effort is compounded in a depletion calculation, where transport solutions must be repeated in an iterative sequence alternating with depletion calculations to update isotopic cross sections and inventories. And while deterministic solutions are based on fluxes that are converged to a specified degree over the full problem domain, the nature of Monte Carlo simulations makes it extremely difficult to obtain accurate fluxes in locations that are far removed from the most reactive region of an analysis domain. Since the accuracy of the neutron flux is therefore a function of position in a Monte Carlo simulation, the accuracy of the depletion solution is likewise spatially distributed. If effective depletion based on Monte Carlo transport is to be successfully implemented, these deficiencies difficulties must be recognized and addressed.

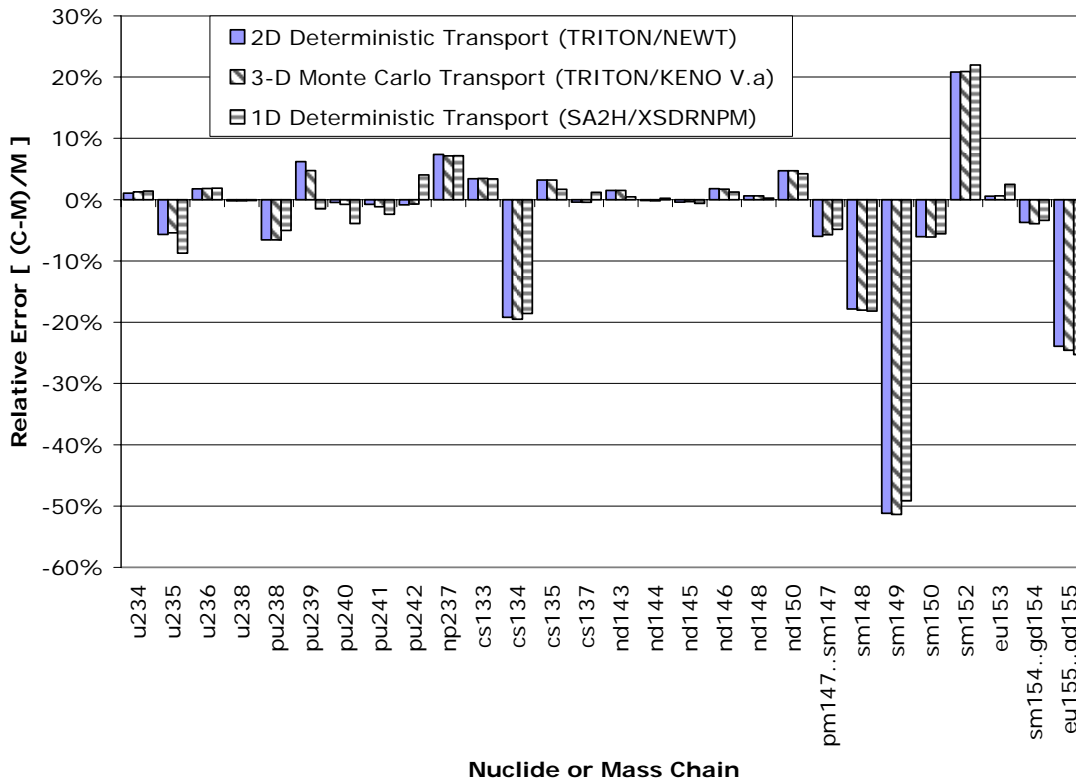


Figure 1. Comparison of results relative to measured isotopic data for spent fuel.

## RESULTS

The *KENO V.a* Monte Carlo transport code has been integrated within the *TRITON* driver control module of *SCALE*. The *TRITON* sequence has been modified to accept *KENO V.a* input in place of *NEWT* input and to use *KENO V.a* to perform transport solutions driven by *TRITON* as a transport solver. The *SCALE* utility code *KMART*, originally developed to post-process *KENO V.a* calculations, has been adapted to provide collapsed cross-sections and fluxes required by *TRITON* for setting up *ORIGEN-S* depletion calculations. Ongoing R&D work seeks to study and implement methods using variance reduction techniques to improve the efficacy of iterative depletion based on Monte Carlo transport solutions. Error propagation from the results of Monte Carlo simulations will become a key attribute of such a this system. ORNL possesses both adjoint and auto-differentiating versions of *ORIGEN-S* as developmental tools that have been used previously in propagating data uncertainties into the calculation results. Transitioning this capability to track the effects of flux uncertainties is the next logical step.

Calculations have been performed for a number of different configurations. Figure 1 shows the measured to computed error for each of three computational methods relative to measured data for a 44 GWd/MTU sample burned in the Calvert Cliffs Unit 1 PWR.[5] The first column in each set shows results obtained using *TRITON* with the deterministic *NEWT* solution; the second column shows the relative isotopic prediction using *KENO V.a* within *TRITON* for the same configuration. The *KENO V.a* model was treated as axially infinite. Finally, for reference, results obtained using a one-dimensional (1-D) homogenized-assembly approach are show in the third column. Isotopic comparisons are made for all nuclides for which measured data were available. The plot shows excellent agreement between *NEWT* and *KENO*-based transport calculation. Even the 1-D approximation does a reasonable job, but does most poorly for nuclides most sensitive to spectral effects.

## CONCLUSIONS

The updated version of *TRITON* that supports Monte Carlo depletion based on *KENO V.a* shows

tremendous potential for application in three-dimensional configurations. The addition of error propagation analysis and variance reduction methods will provide simple and straightforward analysis capabilities for a wide variety of applications.

## REFERENCES

1. M. D. DeHart, "An Advanced Deterministic Method for Spent-Fuel Criticality Safety Analysis," *Trans. Am. Nucl. Soc.* 78, 170-172 (June 1998).
2. M. D. DeHart, "NEWT: A New Transport Algorithm for Two-Dimensional Discrete Ordinates Analysis in Non-Orthogonal Geometries," Vol. II, Sect. F21 of SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation, NUREG/CR-0200, Rev. 7 (ORNL/NUREG/CSD-2/R7), Vols. I, II, III, to be published in 2003.
3. DeHart, M.D., Zhong, Z., and Downar, T. J., to appear. "TRITON: An Advanced Lattice Code for MOX Fuel Calculations," in *Proc. of American Nuclear Society, Advances in Nuclear Fuel Management III*, October 5–8, 2003, Hilton Head Island, SC, USA.
4. M. D. DeHart, "TRITON – A Multidimensional Depletion Sequence For Characterization Of Spent Nuclear Fuel" Vol. I, Sect. T1 of SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation, NUREG/CR-0200, Rev. 7 (ORNL/NUREG/CSD-2/R7), Vols. I, II, III, to be published in 2004.
5. O. W. Hermann, S. M. Bowman, M. C. Brady, and C. V. Parks, *Validation of the SCALE System for PWR Spent Fuel Isotopic Composition Analyses*, ORNL/TM-12667, Martin Marietta Energy Systems, Inc., Oak Ridge National Laboratory, March 1995.