A RADIOISOTOPE DEPLETION METHOD USING MONTE CARLO TRANSPORT WITH VARIANCE REDUCTION AND ERROR PROPAGATION

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INTRODUCTION

The *NEWT* discrete ordinates package 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 named *TRITON*[3,4]. Under *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 geometry flexibility of *NEWT* to allow analysis of complex fuel lattices found in advanced commercial and research reactor designs, and even older boiling water reactor designs.

Despite broad applicability of the 2-D version 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 reactivity 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 and predict fuel depletion. For these reasons, among others, it was decided to develop a 3-D depletion capability similar in function to the 2-D capabilities currently available in *TRITON*, but based instead on the 3-D Monte Carlo-based *KENO* codes available in *SCALE*.

BACKGROUND

Deterministic solutions have long been favored over Monte Carlo simulations for the transport phase of 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 for large problem domains in three dimensions. 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 reasonable neutron fluxes or 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 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 must be recognized and addressed.

Coupled Monte Carlo-point depletion methods have been developed elsewhere with varying degrees of success. The first such implementation was the *MOCUP* package,[5] developed by INEEL based on *MCNP* and *ORIGEN2*. This analysis tool has never been fully coupled and automated, requiring limited user intervention in completing a sequence of calculations. *MOCUP* is difficult to work with, has limited applicability, and is extremely slow. An improved implementation of this code coupling was accomplished with *MONTEBURN*,[6] which uses PERL scripts to couple *MCNP* calculations with *ORIGEN2*. Both *MOCUP* and *MONTEBURN* suffer limitations due to the selection of codes. *MCNP*, although extremely robust and highly accurate, uses a continuous energy approach, which runs slower than a multigroup approach. The tracking logic in MCNP also sacrifices speed for modeling generality. However, the use of *ORIGEN2* is a far more significant limitation. Although developed in parallel with *ORIGEN-S*, both derived from the original *ORIGEN* code, *ORIGEN2* uses fixed cross-section libraries selected based on user selection appropriate for the intended application. *MONTEBURN* does provide for cross-section update of *ORIGEN2* data, but is limited to the nuclides and temperatures available within MCNP, and cannot propagate uncertainties. *ORIGEN-S* is run within *SCALE* using cross sections that are updated in each transport pass to reflect the effect of burnup, includes temperature corrections, makes no assumptions on assembly design or burnup, and is better able to track cross section effects and provide source term data not available in *ORIGEN2*.

The *KENOREST* package[7] developed by GRS in Germany corrects for both these issues to some extent. *KENOREST* is based on a coupled arrangement between *KENO V.a* from *SCALE* and the GRS *OREST* package. *OREST* is itself a coupled package using the original version of *ORIGEN* and the *HAMMER* code. *KENOREST* has been developed for LWR lattice analysis, and makes geometric assumptions that limit its general applicability. The version of *ORIGEN* in *OREST* uses older physics data (base cross sections, fission distributions, branching fractions, etc.) and lacks capabilities and development improvements added to *ORIGEN-S* in ongoing ORNL development. However, *KENOREST* has been shown to perform well relative to other codes for OECD computational depletion benchmarks.

IMPLEMENTATION OF THE 3-D DEPLETION WITHIN TRITON

None of the above implementations address the issues that are most relevant for Monte Carlo-driven depletion: determination of propagated uncertainties in *ORIGEN* results and improved performance in resolving fluxes in low-importance regions, i.e., variance reduction. Ongoing R&D work at ORNL seeks to implement the Monte Carlo transport codes *KENO V.a* and *KENO VI* within the *TRITON* driver module of *SCALE*, and to study and implement methods 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 system. ORNL possesses both adjoint and auto-differentiating versions of ORIGEN as developmental tools that have been used previously in propagating data uncertainties into the results of calculations – transition to the ability to track the effects of flux uncertainties is the next logical step.

To date, ORNL has modified the *TRITON* sequence to accept *KENO V.a* input and to perform transport solutions driven by *TRITON*. 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. *TRITON* is able to perform full *KENO V.a*-based depletion calculations for simple fuel pins, and is undergoing debugging in application to full assembly depletion analysis.

This depletion sequence is fully FORTRAN based, and can be easily installed and run on a wide variety of Unix workstations and Windows PCs within the *SCALE* system. Results of calculations demonstrating the ability to predict spent fuel isotopic inventories will be presented in the final paper. The full paper will also discuss concepts being developed to implement global variance reduction and propagation of uncertainties in the depletion sequence. Any results of such work completed by the end of 2003 will be included in the paper.

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