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VERIFICATION OF A DEPLETION METHOD IN SCALE FOR THE ADVANCED HIGH TEMPERATURE REACTOR*

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ABSTRACT

This study describes a new approach employing the Dancoff correction method to model the TRISO-based fuel form used by the Advanced High-Temperature Reactor (AHTR) reactor design concept. The Dancoff correction method is used to perform isotope depletion analysis using the TRITON sequence of SCALE and is verified by code-to-code comparisons. The current AHTR fuel design has TRISO particles concentrated along the edges of a slab fuel element. This geometry prevented the use of the DOUBLEHET treatment, previously developed in SCALE to model spherical and cylindrical fuel. The new method permits fuel depletion on complicated geometries that traditionally can be handled only by continuous energy based depletion code systems. The method was initially tested on a fuel configuration typical of the Next Generation Nuclear Plant (NGNP), where DOUBLEHET treatment is possible. A confirmatory study was performed on the AHTR reference core geometry using the VESTA code, which uses the continuous energy MCNP5 code as a transport solver and ORIGEN2.2 code for depletion calculations. Comparisons of the results indicate good agreement of whole core characteristics, such as the multiplication factor and the isotopics, including their spatial distribution. Key isotopes analyzed included ^{235}U, ^{239}Pu, ^{240}Pu, and ^{241}Pu. The results from this study indicate that the Dancoff factor method can generate estimates of core characteristics with reasonable precision for scoping studies of configurations where DOUBLEHET treatment cannot be performed.

Key Words: SCALE, VESTA, AHTR, salt cooled reactors, TRISO fuel, FHR.

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1. INTRODUCTION

The Advanced High Temperature Reactor (AHTR) is a 3400 MW(t) fluoride-salt-cooled high-temperature reactor (FHR) under development by the Oak Ridge National Laboratory (ORNL) [1]. The current design of this reactor uses TRISO fuel particles embedded in a slab of carbonaceous material matrix with the fuel concentrated on the surfaces of the slab, and a moderating region of carbonaceous material in the center of the slab.

The TRITON sequence in SCALE [2] can use the multigroup version of the KENO Monte Carlo transport code coupled with the ORIGEN-S fuel depletion code to perform full 3-D depletion calculations on highly heterogeneous core configurations. Although the KENO code is a Monte Carlo code, which provides the best option for modeling the transport of the particles through complicated geometries, because of the multigroup treatment of the energy variable, it is crucial for the overall accuracy to have available appropriate, problem-dependent neutronic cross sections. To deal with the double heterogeneous nature of the TRISO fuel, special "DOUBLEHET" treatments have been implemented to correctly evaluate the multigroup cross sections [3]. The DOUBLEHET feature, however, is only available in SCALE for fuel elements specific to high temperature gas reactor fuel designs, i.e. uniformly distributed TRISO grains in solid cylindrical pins or spherical pebbles typical of the NGNP design.

As expected, it was found that straightforward flux correction methods, such as volumetric fuel homogenization and explicit grain representation (similar to the continuous-energy models) of the fuel, produce grossly inaccurate depletion estimates. For one AHTR core design option the predicted fuel cycle length was 1.3 years with the homogenized fuel model and 2.2 years with the explicit grain model. Moreover, neither of these two models was able to predict the beginning of cycle (BOC) effective multiplication factor, k_{eff}. The difference in both cases was unacceptably large: k_{eff} =1.236 with the homogenized model and k_{eff} =1.361 with the explicit grain model, while the continuous energy KENO model predicted a k_{eff} =1.295. The available computation methods in SCALE account for the self-shielding effects in the fuel by considering one-dimensional, Wigner-Seitz modified cells (i.e., asymmetric plates for the volumetric-homogenized model, and spheres in a square pitch for the explicit grain model, both commonly used procedures in SCALE).

In order to accurately model the fuel depletion of these fuel plates, a method utilizing the Dancoff factor was investigated for the SCALE/TRITON multigroup depletion sequence. The method makes use of existing capabilities in the SCALE code system; in particular, it uses the ability of the cross section processing modules to accept a Dancoff factor that is calculated separately as an input parameter. The new method required verification of its accuracy by comparing its results to independent analyses where the geometry permits use of previously tested methods, or to more general approaches (e.g., continuous-energy depletion), that are assumed to be able to handle any geometric configuration.

After describing the fuel geometry specific to the AHTR design in Section 2, this paper introduces the Dancoff factor method in Section 3 and describes its preliminary verification on an NGNP-specific cylindrical fuel design. Section 4 presents the development of a continuous-

energy AHTR depletion model that uses the VESTA depletion code system, which relies on the MCNP5 code for neutron transport and ORIGEN 2.2 for depletion calculations.

2. AHTR FUEL STRUCTURE

The fluoride-salt-cooled high-temperature AHTR reactor design utilizes a slab fuel geometry that concentrates TRISO fuel particles on the edges of the slab for better fuel utilization and for improved cooling properties. The coated particles, while actually randomly distributed, are modeled in a regular lattice structure. In particular, we chose to use a centered cubic lattice of fuel grains (Fig. 1). The fuel plates are cooled by molten salt and are placed in hexagonal fuel block assemblies also surrounded by molten salt coolant (Fig. 2). This design requires a special treatment to account for self-shielding rather than the use of a DOUBLEHET cell in SCALE, where calculations have been designed assuming a geometry typical of the NGNP design.

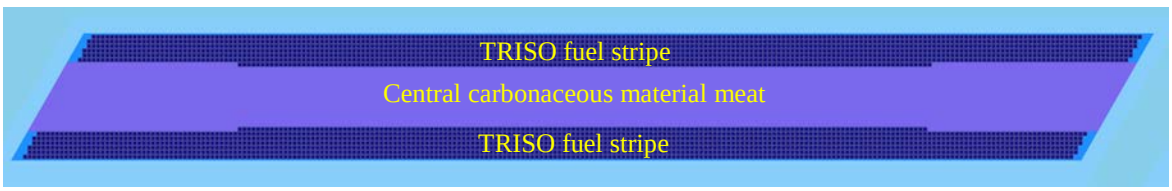

Figure 1. Fuel arrangement in an AHTR fuel slab.

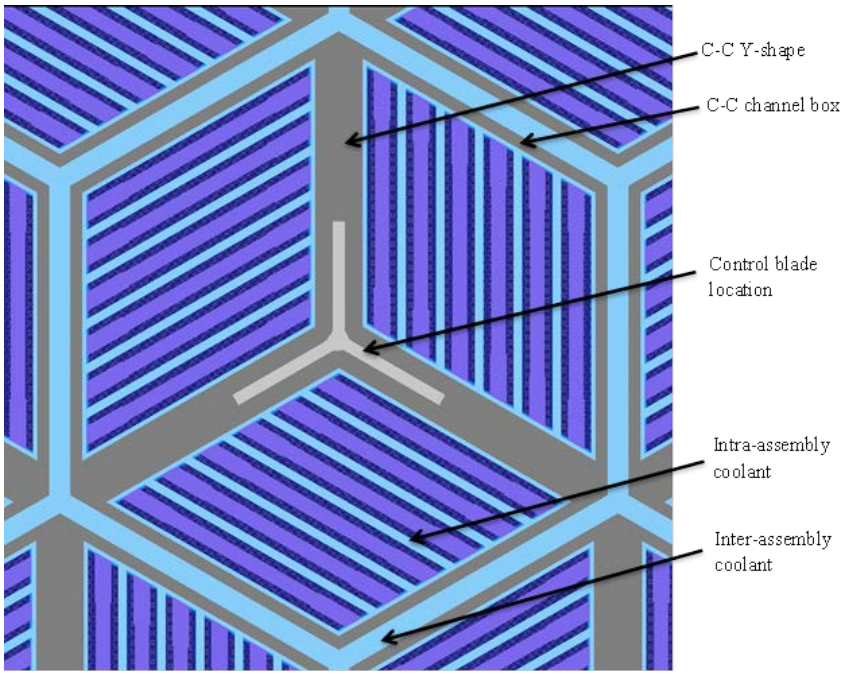

Figure 2. Fuel slab placement within AHTR fuel assembly.

3. DANCOFF FACTOR METHOD

The Dancoff factor (or Dancoff correction, or Dancoff correction factor) represents a correction to the escape probability of a neutron born in a fuel lump in order to account for the shadowing effect from other nearby absorber lumps [4]. This is an important correction for cases where a fuel lump is part of a lattice, often the case for nuclear fuel. The Dancoff factor has a clear probabilistic interpretation; it is the probability that a neutron incident on the moderator will suffer its next collision in another fuel lump. The Dancoff factor can be calculated from first principles either analytically (for simple, infinite lattice problems) or with Monte Carlo methods (for more complicated geometries). In SCALE, the MCDANCOFF module can calculate Dancoff factors for different reactor geometries using the Monte Carlo method.

The Dancoff factor can be used to correct the escape probability factor computed by the CENTRM module of SCALE [2]. It was implemented as a general capability in the TRITON depletion sequence of SCALE, and it has been recently applied to depletion in Boiling Water Reactors [5]. The Dancoff factor method proposed in this paper can use this correction to provide appropriate cross sections for an explicit grain model of the AHTR core. In its current implementation, the method assumes the following three steps:

1. A continuous energy KENO model of the problem is used to provide a reference multiplication constant at the beginning of cycle (BOC).
2. A series of calculations are conducted at BOC with the multigroup KENO model of the system utilizing different Dancoff factors to determine which Dancoff factor leads to a result for the multiplication factor of the system that matches the continuous-energy (reference) result.
3. The Dancoff factor selected from these models is then utilized in the TRITON depletion sequence.

In describing the Dancoff factor method, the “Dancoff factor correction” refers to an explicit, user-imposed correction in the CENTRM module used for cross section processing in SCALE. This correction is inferred in a separate calculation under this method. By default, the CENTRM module uses an infinite medium Dancoff factor that is internally calculated by CENTRM to account for lattice effects; this can lead to large discrepancies when compared to reference results obtained by other means.

In its current formulation, this method applies principles similar to the Reactor-Equivalent Physical Transformation (RPT) method, but instead of selecting equivalent dimensions, an equivalent Dancoff factor is generated that forces the initial critical state to match the (continuous energy) reference [6, 7]. In this regard, the method enforces the overall balance for the system in the same way the RPT does. Global quantities (e.g., the multiplication constant, the total isotopic masses) are expected to be well predicted by this method; however, it will not necessarily accurately predict the isotopic spatial distributions.

The Dancoff factor method has some advantages over the RPT method. A first advantage is that the Dancoff factor for a certain fuel region is a quantity with a very well-defined physical meaning and can be calculated explicitly from more fundamental principles for each region. Therefore, in principle there is no need to limit the method to one global parameter (Dancoff

factor), but a distribution of Dancoff factors can be calculated and used for different regions of the reactor, thus potentially improving the spatial distribution prediction of various quantities. A second major advantage is that the method, even in its current implementation, preserves the real geometry of the problem and thus can be used, for example, to perform depletion calculations for configurations where burnable poison particles are intermixed with the fuel coated particles. Finally, it was shown that this method works for configurations where the RPT method fails to find an equivalent dimension; for example, AHTR configurations with high carbon-to-heavy-metal ratios.

The initial tests of this method were conducted on an NGNP prismatic fuel block model for which the DOUBLEHET cross section treatment was available for use with the TRITON depletion sequence in SCALE. Depletion calculations were followed for 46 time steps (875 days) at constant power. Figure 3 shows a comparison between four different predictions of the multiplication factor as a function of time, while Figure 4 plots the mass of ^{239}Pu per metric ton of initial heavy metal predicted by the four methods. The plots show the large difference in predictions between the method that uses volume-homogenized fuel (labeled “Homogenized” on the plots), which always underpredicts the multiplication factor and overpredicts the amount of ^{239}Pu produced, and the method that uses the explicit grain representation but with no (explicit) Dancoff factor correction (labeled “Explicit grains”), which always overpredicts the multiplication factor and underpredicts the amount of ^{239}Pu when compared to the reference method that uses the DOUBLEHET treatment. Both the multiplication factor and the ^{239}Pu curves predicted by the explicit grains with Dancoff correction method (labeled “Dancoff factor” on the plots) almost overlap the reference curves. The average over the time steps of the difference between the multiplication factors calculated with the Dancoff factor method and the reference DOUBLEHET method is about 120 pcm (which is about one standard deviation of the difference between results), while the difference between the ^{239}Pu predictions is always less than 1% of the reference calculation. The differences can be attributed, at least in part, to the statistical precision of the Monte Carlo calculations (the typical statistical standard deviations were around 80 pcm for both methods, for each transport calculation) and the possible bias introduced by the process of matching the initial multiplication factor for the Dancoff factor method with the continuous energy reference result.

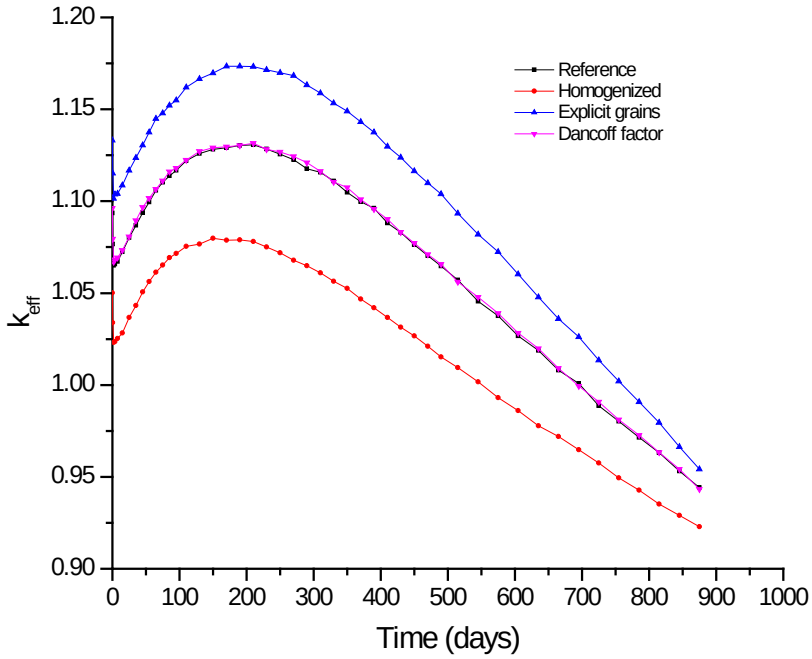

Figure 3. The evolution of k_{eff} for an NGNP fuel block.

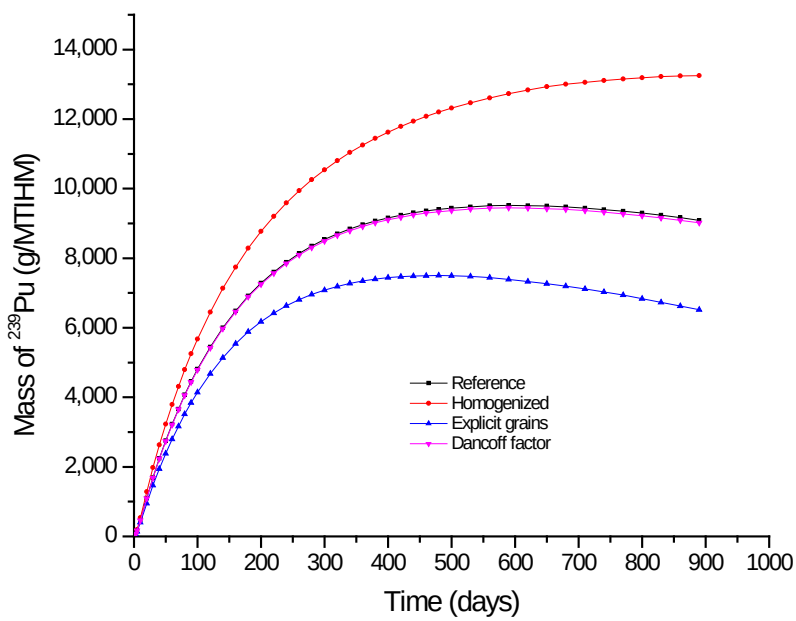

Figure 4. The evolution of ^{239}Pu concentration for an NGNP fuel block.

4. AHTR MODELS AND RESULTS

After confirming the feasibility of the method on the NGNP fuel, the technique was applied to the AHTR reference design.

4.1. SCALE/TRITON AHTR Model

As in the Dancoff factor method description provided in Section 3, the baseline AHTR fresh core [1] was first modeled using the continuous-energy SCALE/KENO transport solver, and the reference $k_{eff,CE}$ value was calculated to be 1.32609±0.00038. Then, a series of multigroup KENO calculations were performed using different values for the Dancoff factor. Figure 5 shows a graphical representation of the k_{eff} values obtained with the multigroup KENO calculation for different Dancoff factors (black dots, with error bars) and the corresponding fitting curve (blue curve, third degree polynomial). The intersection of the fitting curve with the continuous energy value (red, continuous line) gives the Dancoff factor for use in the TRITON depletion calculations. This value for the Dancoff factor is affected by an uncertainty caused by the uncertainties in both the continuous energy reference and the multigroup values for the multiplication factor. The red dashed lines in Figure 5 represent the $k_{eff,CE} \pm 1\ \sigma$ values.

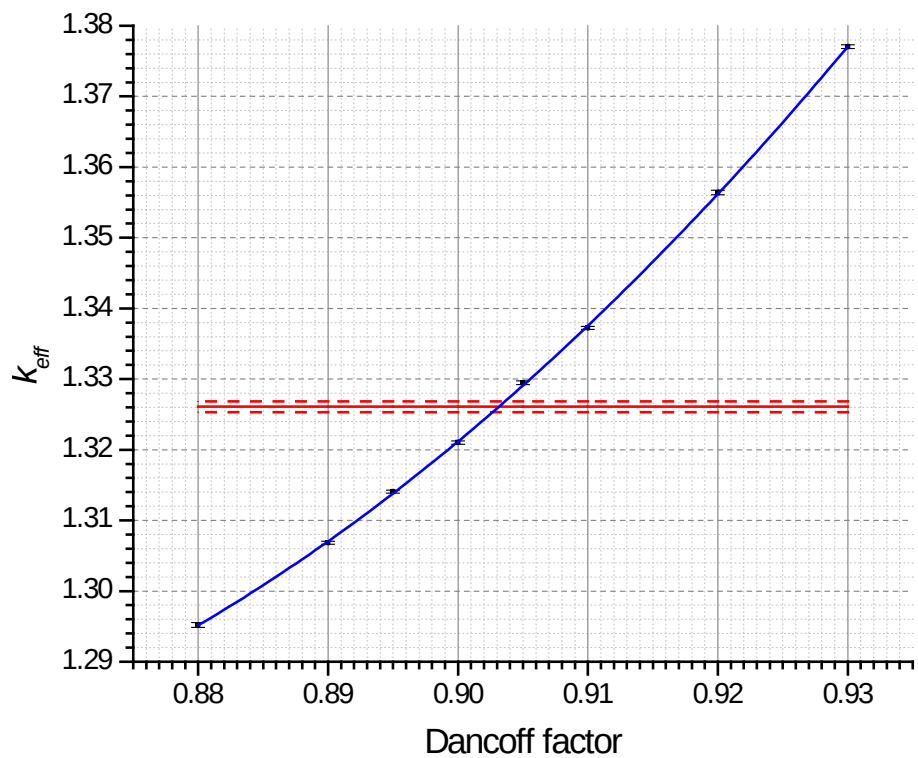

Figure 5. Evaluation of Dancoff factor for TRITON depletion.

This procedure yields a Dancoff factor value of 0.90315. This value was used for all depletion steps in the TRITON model for the baseline AHTR design.

4.2. VESTA AHTR Model

Because experimental data is unavailable for the AHTR fuel plates, a code-to-code comparison with a continuous energy depletion code was undertaken. The continuous energy method avoids potential issues related to the correct treatment of self-shielding and provides an alternative methodology that should generate the same conclusion in order to test the viability of the approximations. In order to accomplish this, the VESTA depletion code, which utilizes MCNP5 and ORIGEN 2.2, depleted the system over the same time scale, and the k_{eff} results were compared to the results of an AHTR SCALE/TRITON model that used the Dancoff factor method. In addition, key isotopic inventories, including ^{235}U, ^{239}Pu, ^{240}Pu and ^{241}Pu, and their masses were compared to the results of the TRITON calculations. The middlestep depletion methodology was used in VESTA, since this most closely corresponds to the process utilized by TRITON, thus simplifying comparisons. In this method, k_{eff} is determined from transport calculations at the start of a time step, the mixture is depleted to the center of the time step, and the transport calculation is repeated using the information from this intermediate step. Only the composition data at the end of each full step is recorded.

The VESTA case was designed to match the TRITON model as closely as possible, including the use of a cubic lattice structure to model the randomly distributed TRISO grains. Both the VESTA and TRITON simulations used nuclear data based on the ENDF/B-VII.0 library. Both MCNP and SCALE used a fuel temperature of 1200 K, but the coolant temperature, which is 948 K in the SCALE model, was approximated with a temperature of 900 K in MCNP, the closest temperature available for the cross section libraries distributed with the MCNP code. The multigroup version of SCALE can interpolate the cross sections for temperatures that are different from the temperatures for which the libraries were generated. The transport calculations for this model used sufficient accuracy to generate a standard deviation of less than 100 pcm in k_{eff} for each time step, similar to the accuracy for the SCALE/TRITON model. The primary difference between the models included the continuous energy spectrum used by MCNP for transport calculations, and the 44,000 energy group tally structure utilized by VESTA, compared to the 238 groups used in TRITON. Both in SCALE/TRITON and in VESTA simulations for AHTR core models, the region-wise comparisons have been performed on two radial regions and two axial regions for a total of four regions, using the axial symmetry of the models. These are coarse spatial regions but can still provide an indication of the agreement for the spatial distributions. Using more regions would increase the already long computational time.

4.3. Comparison Results

VESTA and TRITON (with Dancoff factor correction) results were compared for various characteristics to determine the degree of agreement. The comparison of the multiplication factor over time is shown in Fig. 6. The average eigenvalue generated by TRITON is, in general, lower than the VESTA value during the depletion process, on average by approximately 275 pcm. The initial eigenvalue has a difference of approximately 72 pcm. The apparent bias between the TRITON and VESTA code systems could be due to the difference in the methodologies used by the two codes (including the depletion modules, ORIGEN-S and

ORIGEN2.2, respectively), differences in the libraries used by KENO and MCNP, and the possible bias introduced by the Dancoff factor method in TRITON as a result of the calibration to the continuous energy case output. The 275 pcm bias was acceptable for the current scoping studies for AHTR. From these results, the core lifetime was estimated to be 2.12 years in TRITON and 2.13 years in VESTA.

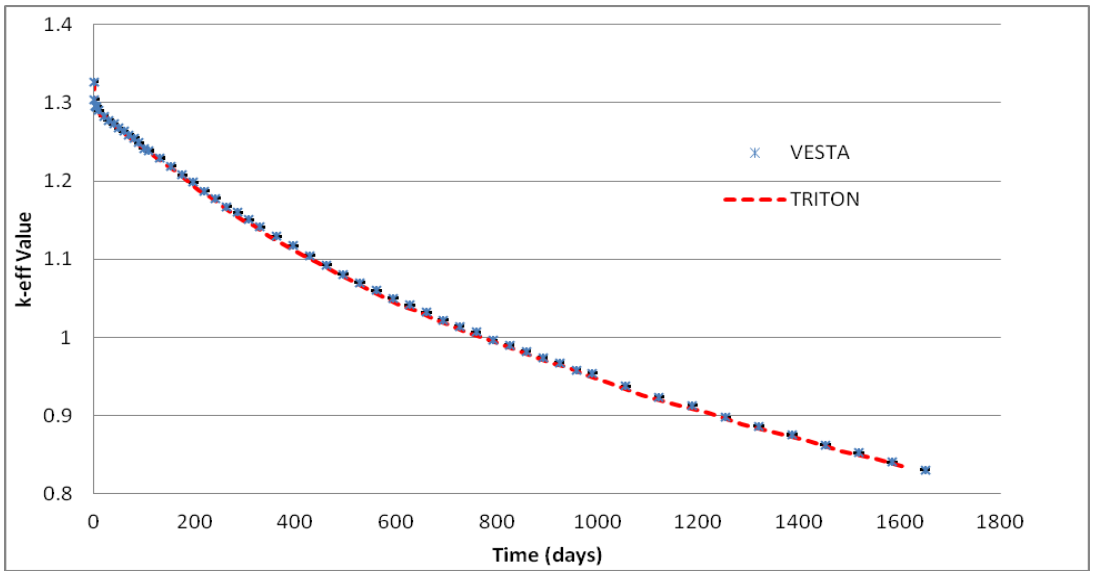

Figure 6. Evolution of k_{eff} vs. time for TRITON and VESTA depletion calculations.

The various isotopic data were also tracked throughout the core lifetime. Figure 7 shows the percent difference of TRITON and VESTA ^{235}U masses for various regions of the core over time. ^{239}Pu, ^{240}Pu, and ^{241}Pu masses are shown in Fig. 8, Fig. 9, and Fig. 10, respectively. Many other nuclides (not shown) generated a pattern similar to the trends seen in the plutonium isotopes, demonstrating good whole core agreement, with moderate differences in spatial distribution. The initial differences at the BOC are not meaningful due to the small quantities of plutonium generated; even slight differences generate very large relative errors. The divergence above 1% of the spatial distribution of ^{235}U occurs after the end of cycle (EOC, defined as the time when the system's multiplication factor becomes smaller than 1.0) for the single fuel batch. These results indicate that the Dancoff factor approach can generate isotopic composition predictions representative of the spatial distribution with a sufficiently detailed input at the level of accuracy necessary for the scoping study. It should be noted, however, that some nuclides, particularly americium and curium isotopes, have larger disagreements. At EOC, where agreement was typically highest, the ^{243}Am concentration was over 15% higher in the TRITON case, as were multiple curium isotopes, while ^{242m}Am was over 40% lower. These results will require further analysis to determine the causes of these discrepancies.

The comparison of the runtime between TRITON and VESTA shows that the TRTION run uses only a fraction of the total time needed by VESTA to complete similar depletion calculations. The TRITON case required approximately 17 days of processor (cpu) time to run, while the

VESTA case needed approximately 136 days. While some of this difference can be attributed to other uses of the cluster used for the VESTA case, it is large enough to indicate a significant advantage for TRITON. The VESTA runs could be completed faster when multiple processors are available, but the Dancoff factor method drastically shortens the amount of time, an advantage that will be a benefit when parallel TRITON development is completed.

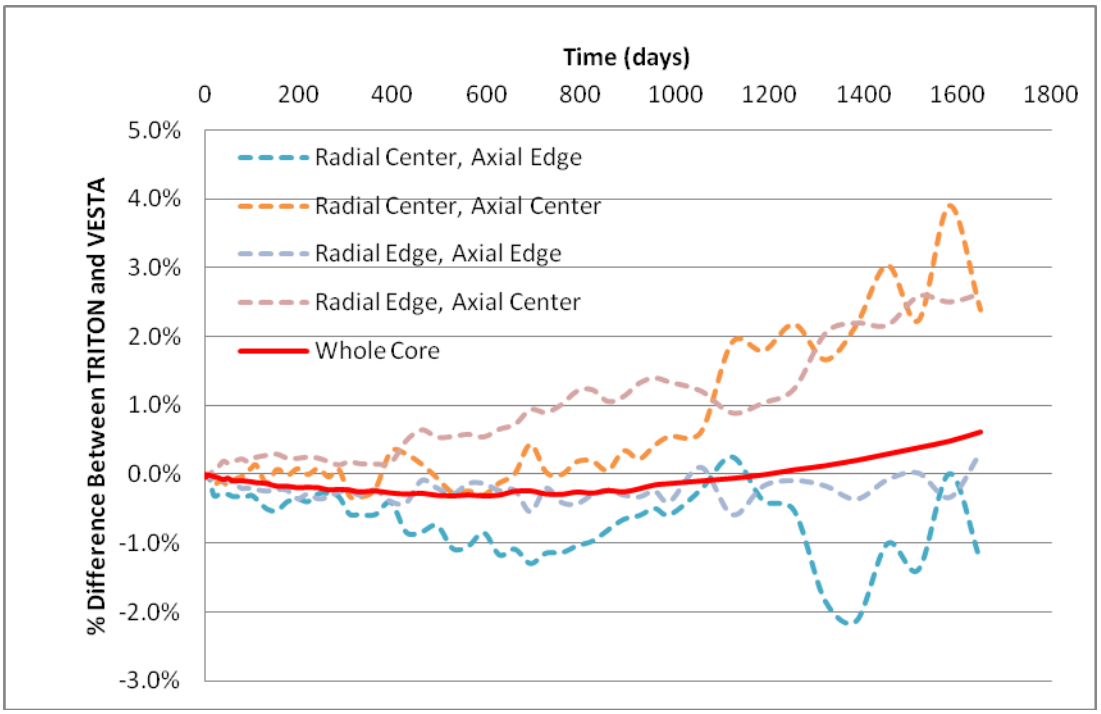

Figure 7. Evolution of percent difference between mass of ^{235}U for TRITON and VESTA depletion calculations vs. time in various regions of the AHTR.

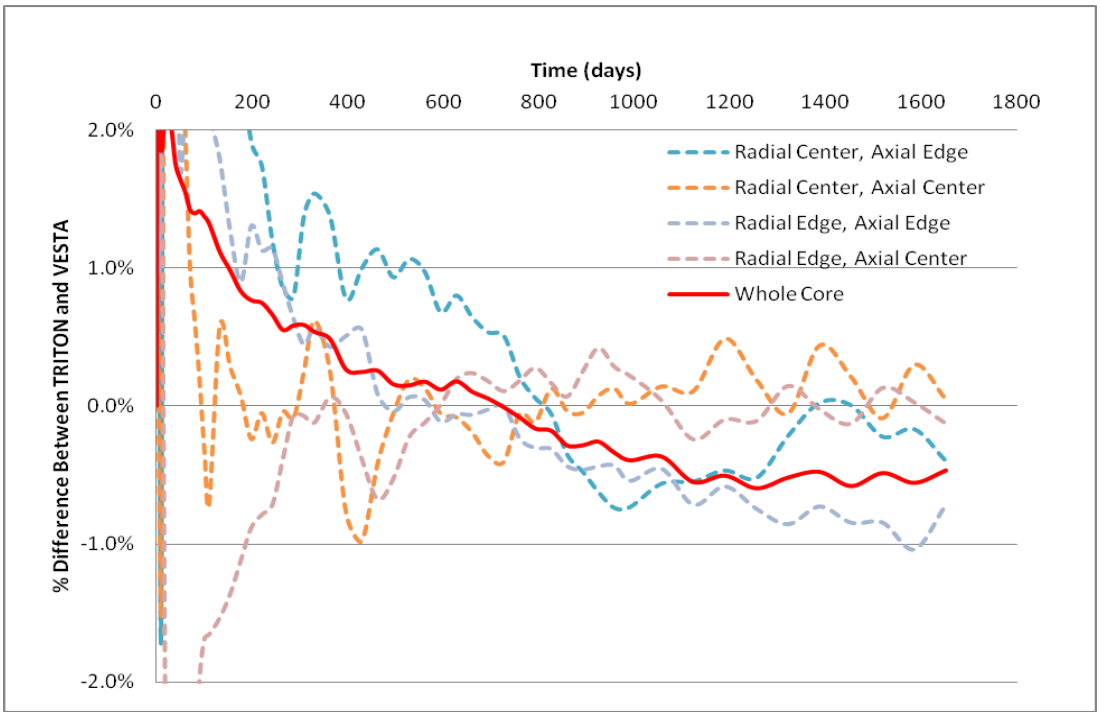

Figure 8. Evolution of percent difference between mass of ^{239}Pu for TRITON and VESTA depletion calculations vs. time in various regions of the AHTR.

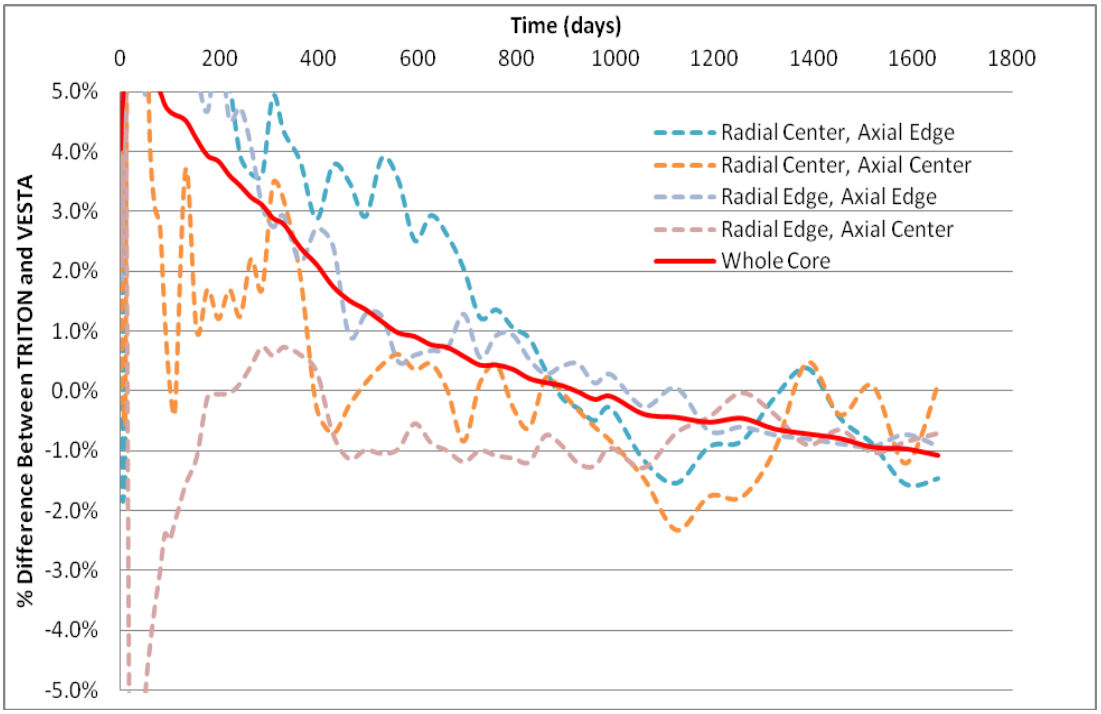

Figure 9. Evolution of percent difference between mass of ^{240}Pu for TRITON and VESTA depletion calculations vs. time in various regions of the AHTR.

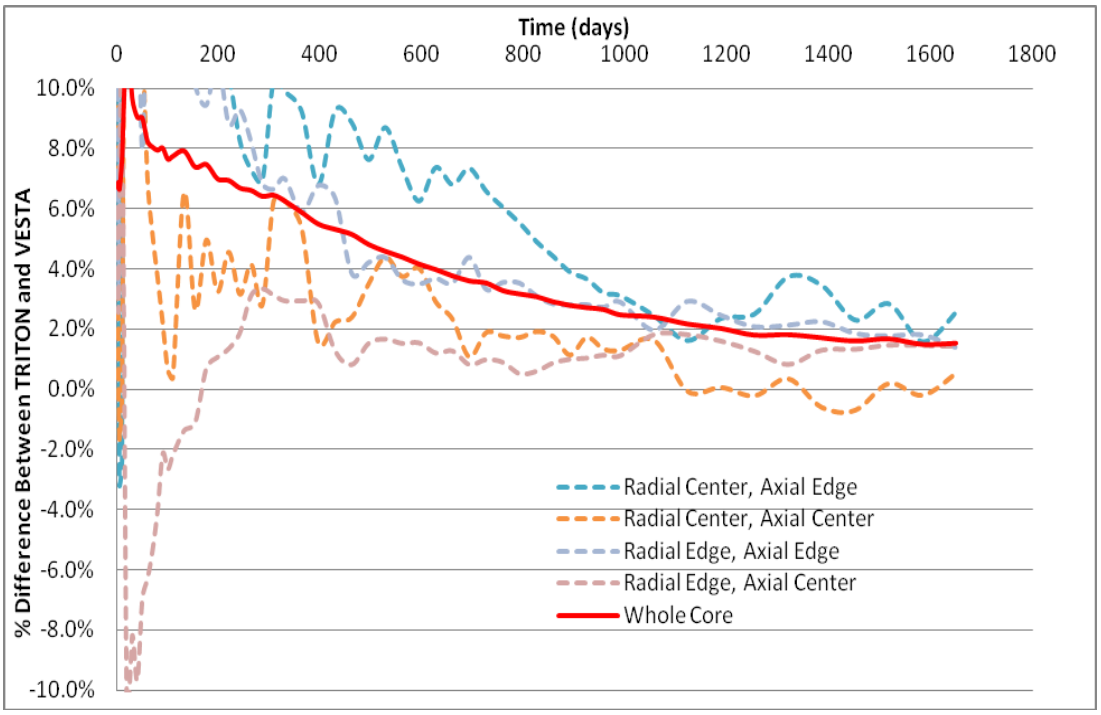

Figure 10. Evolution of percent difference between mass of ^{241}Pu for TRITON and VESTA depletion calculations vs. time in various regions of the AHTR.

5. CONCLUSIONS

The Dancoff factor correction method provides a reasonably accurate, more rapid technique for performing global characteristic analysis on arbitrary fuel geometries. The method uses existing capabilities in the SCALE code system and, in its current formulation, is similar to the RPT method. Among its advantages, this method is capable of modeling detailed geometry configurations at the same level of detail as a continuous energy depletion method. Because of the detailed geometry description, its main disadvantage is the long computational time required, although it still compares favorably with the continuous energy depletion method used in VESTA. The Dancoff factor method was verified by code-to-code comparisons with predictions on configurations where DOUBLEHET treatment can be reliably applied and with a continuous energy VESTA calculation. Additional studies will be needed to determine whether applying a distribution of user-calculated Dancoff factors will improve the spatial accuracy; however, the current results indicate that a global factor can provide sufficient accuracy to determine whole core characteristics for scoping studies.

ACKNOWLEDGMENTS

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