SHUTDOWN DOSE RATE ANALYSIS USING THE MULTI-STEP CADIS METHOD

Ahmad M. Ibrahim,* Douglas E. Peplow, Joshua L. Peterson, Robert E. Grove

Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831, ibrahimam@ornl.gov

The Multi-Step Consistent Adjoint Driven Importance Sampling (MS-CADIS) hybrid Monte Carlo (MC)/deterministic radiation transport method was proposed to speed up the shutdown dose rate (SDDR) neutron MC calculation using an importance function that represents the neutron importance to the final SDDR. In this work, the MS-CADIS method was applied to the ITER SDDR benchmark problem. The MS-CADIS method was also used to calculate the SDDR uncertainty resulting from uncertainties in the MC neutron calculation and to determine the degree of undersampling in SDDR calculations because of the limited ability of the MC method to tally detailed spatial and energy distributions. The analysis that used the ITER benchmark problem compared the efficiency of the MS-CADIS method to the traditional approach of using global MC variance reduction techniques for speeding up SDDR neutron MC calculation. Compared to the standard Forward-Weighted-CADIS (FW-CADIS) method, the MS-CADIS method increased the efficiency of the SDDR neutron MC calculation by 69%. The MS-CADIS method also increased the fraction of nonzero scoring mesh tally elements in the space-energy regions of high importance to the final SDDR.

I. INTRODUCTION

Shutdown doses in fusion energy systems result from the decay of neutron-induced activation products in irradiated structural materials. A shutdown dose rate (SDDR) calculation involves three steps:

1. a neutron transport calculation to determine the space- and energy-dependent neutron flux distributions,
2. activation calculations to compute the photon source distribution, and
3. a photon transport calculation for estimating the final SDDR.

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Even without considering the second and third computational steps, SDDR calculations are much more challenging than one-step neutronics calculations, such as the calculation of the prompt dose rate during operation, because detailed space- and energy-dependent neutron flux distributions are needed from the neutron transport calculation to generate accurate radioisotopes distributions. In some applications, full-scale SDDR simulations are needed for very large systems that involve massive amounts of shielding materials in complex geometric arrangements. These simulations require calculating the distribution of radioisotopes throughout the entire system. For example, SDDR assessments are required everywhere inside the cryostat of the ITER experimental facility to evaluate the required waiting period after the shutdown of ITER and to identify the locations for which human accessibility should be prohibited. The cryostat is a large cylindrical vacuum chamber (~30 m tall and 30 m wide) surrounding the tokamak machine. Accurate determination of the effects of important factors such as the cross talk (interactions) between the different ports on the SDDR in ITER is only possible through full-scale simulations that include all the complex inner details of the ITER tokamak machine.[1]

Because the detailed space- and energy-dependent flux information are readily available in the solution of discrete-ordinates (S_N) methods, they may seem more appropriate than Monte Carlo (MC) methods for SDDR neutron transport calculations; however, the truncation errors of S_N methods can adversely affect the accuracy of SDDR predictions. Furthermore, some SDDR analyses involve radiation streaming through very narrow solid angles and very complicated pathways, which are difficult to be appropriately handled with S_N methods. The computational requirements for full-scale, structured-mesh S_N simulations of very large and complicated systems such as ITER, which are on the order of tens of processor-years, are only tractable using world-class supercomputers. Even if such supercomputers are available, some important geometric features of these complex systems can never be accurately captured using structured-mesh S_N codes. Unstructured-mesh S_N simulations have been used to calculate the SDDR at the interspaces of the ITER diagnostics ports; however, these

calculations required limited angular discretization and the use of coarse meshes with sizes on the order of tens of centimeters in some regions due to limited scaling capabilities (up to hundreds of processors) of the codes that were used. These coarse meshes cause severe discretization errors that are evidenced by the appearance of negative space- and energy-dependent neutron fluxes in the S_N solutions.[2]

The rigorous 2-step (R2S) computational system entails MC neutron and photon transport calculations coupled with an activation step using a dedicated inventory code and library.[3] Accurate full-scale R2S simulations are impractical for large and geometrically complex problems because of the difficulty of calculating detailed space- and energy-dependent neutron flux distributions everywhere in the structural materials using the analog MC method, which tracks individual particles using the ordinary physical distributions. Biasing the neutron MC calculation using an importance function is not straightforward because of the difficulty of explicitly expressing the response function of the neutron calculation, which depends on the next activation and photon transport calculations. Moreover, typical R2S calculations do not consider the impact of uncertainties in the MC neutron calculation on SDDR uncertainty even though these former uncertainties usually dominate the SDDR uncertainty.

The Multi-Step Consistent Adjoint Driven Importance Sampling (MS-CADIS) hybrid MC/deterministic method has been proposed to speed up the SDDR MC neutron transport calculation using an importance function[4] that represents the neutron importance to the final SDDR. This paper describes the application of the MS-CADIS method for speeding up the SDDR MC calculations and for calculating the SDDR uncertainty due to the neutron flux uncertainties. A new proposed metric for assessing the reliability of SDDR calculations is applied in this analysis. The paper describes the feasibility of using the MS-CADIS adjoint neutron source to calculate the SDDR uncertainty resulting from uncertainties in the MC neutron calculation. The analysis performed in this paper used the ITER SDDR benchmark problem[5]. The analysis compared the efficiency of the MS-CADIS method to the traditional approach of using global MC variance reduction techniques for speeding up the SDDR neutron MC calculation.

II. PROBLEM DESCRIPTION

The model used in this analysis consists of a 7 m long cylinder with a 1 m radius. It has a central straight streaming path with a radius of 0.075 m. A 0.48 m radius stainless steel/water (80%–20%) shielding zone, which surrounds the central streaming path and has a length of 2.1 m, is included. The outer shielding zone is made of 100% stainless steel with an outer radius of 1 m. It has a rear stainless steel plate 0.15 m thick. A 0.02 m straight gap between the outer and inner shielding zones extends all the way through the model. A large, 3.25 m long cavity runs between the back of the stainless steel/water shield and the rear plate. A 14.1 MeV isotropic neutron source with a thickness of 0.01 m is represented by a disk region placed at a distance of 0.1 m from the front edge. At the other end of the geometry, the SDDR was calculated using four tallies representing four circular discs, each 0.1 m thick. Figure 1 shows the problem geometry and location of the SDDR tallies.

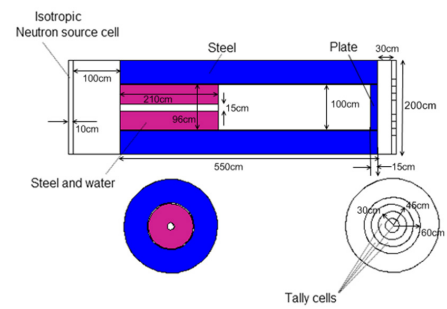

Fig. 1. ITER SDDR benchmark problem geometry.[5]

The source strength and irradiation history used in this analysis are shown in Table I.[5] SDDR was calculated at the four tallies after 10^6 sec from the last step in the irradiation scenario.

Table I. ITER Irradiation Scenario[5]

Source Strength (n/sec)	Duration	Number of times
1.0714×10^{17}	2 years	1
8.25×10^{17}	10 years	1
0	0.667 years	1
1.6607×10^{18}	1.33 years	1
0	3,920 sec	17
2.0×10^{19}	400 sec	
0	3,920 sec	4
2.8×10^{19}	400 sec	

III. METHODOLOGY

The MAVRIC shielding analysis sequence of the Standardized Computer Analyses for Licensing Evaluation (SCALE6.1) package was used for the neutron and photon transport calculations. The ORIGEN code system was used for the activation and decay calculations in this analysis.[6] MAVRIC uses the Denovo structured mesh discrete-ordinates code for deterministic calculations and the multi-group Monaco MC code for MC calculations.[6] A 200-neutron group ENDF-VII data library was used for the neutron Monaco calculations, a

27-neutron group ENDF-VII data library was used for the Denovo neutron calculations, and a 19-photon group ENDF-VII library was used for both the Monaco and Denovo photon transport calculations. All of the ORIGEN calculations used the ENDF-VII activation library.

A semiautomated coupling between Monaco and Denovo on one side and ORIGEN on the other side was implemented using Python scripts. The mesh consisted of approximately 250,000 elements with varying sizes of 1.5–5 cm in the radial directions, x and y and 5–10 cm in the axial direction, z. For the Denovo and ORIGEN calculations, each mesh element was made up of the material present at the center of the element in the Monaco model.

The SDDR calculations were performed using three approaches. The first approach used analog Monaco neutron calculations, the second used the standard forward-weighted CADIS (FW-CADIS) (Ref. 7) method for speeding up the Monaco neutron calculations, and the third used the MS-CADIS method. All of these calculations used the same running time (1 h) for the Monaco photon calculations and used the same photon importance map (weight windows) generated with the CADIS method. The adjoint photon source for this CADIS calculation was defined as a rectangular parallelepiped surrounding the four tally regions with the adjoint source spectrum set equal to the photon flux-to-dose-rate conversion factors. The side length of the CADIS adjoint photon source was 1.2 m and the height was 0.1 m. The only difference between the three approaches was the method used to speed up the Monaco neutron calculation.

It is necessary to mention that the absolute values of the SDDR tallies were not compared to the published results of the ITER benchmark problem because they depend on the mesh and the nuclear data libraries. For unbiased comparison of the effectiveness of the three approaches, the Monaco and the Denovo calculations and the importance maps of all the approaches used the same mesh and neutron and photon energy group structure.

III.A. Assessing the Degree of Undersampling

A new metric was used to assess the reliability of each SDDR calculation in this analysis. When calculating the energy-dependent neutron flux throughout the problem geometry, the Monaco neutron calculation used a mesh tally with 4.844×10^7 space-energy elements. In the Monaco neutron simulations, not all the space-energy tally elements received scores. In fact, the maximum fraction of the elements with nonzero MC scoring, which indicates calculating a tally result in those elements, was only 50.5% for all these Monaco neutron calculations. However, not all of the zero-scoring elements are important to the SDDR. Elements with energies at which the cross sections of the radioisotopes producing neutron transmutation reactions are very low and elements that are very far from the SDDR detectors are not expected to have radioisotopes that heavily contribute to the SDDR at the detectors. A deterministic approximation for the contribution of each space-energy element to the SDDR at a certain detector can be estimated by multiplying the MS-CADIS neutron adjoint source strength at this element by the deterministic neutron (forward) flux estimate at this element. The fraction of nonzero scoring elements important to a detector SDDR can be determined by adding the SDDR contribution of all nonzero scoring elements and dividing this sum by the total deterministic estimate of the detector SDDR. This deterministic estimate of the fraction of the SDDR response that exists in nonzero scoring space-energy elements was used as a metric to determine the degree of undersampling in the SDDR calculation at a certain detector.

III.B. Uncertainty Propagation

A method that uses a single deterministic photon adjoint calculation has been developed to estimate the lower bound of the SDDR uncertainty resulting from uncertainties in the photon source.[8] This method cannot be used directly in R2S calculations without propagating the uncertainties in the neutron fluxes into the activation calculations. However, using quantities generated during the implementation of the MS-CADIS method, an extension of this method can be derived to calculate the SDDR uncertainties resulting from stochastic uncertainties in the neutron fluxes.

In the R2S computational system, the statistical uncertainty in the MC calculations of the SDDR can be expressed as

$$\sigma_{SDDR}^2 = \sigma_n^2 + \sigma_p^2, \tag{1}$$

where the standard deviation σ_p reflects the stochastic uncertainty of the MC photon transport simulation and σ_n is the SDDR uncertainty due to the neutron MC calculation, and σ_{SDDR} is the total SDDR uncertainty. σ_p can be calculated during the MC photon transport calculation, but σ_n cannot be easily calculated. If the neutron fluxes are calculated using a mesh tally with many space-energy elements, the total SDDR uncertainty due to the uncertainty in the neutron MC calculation can be expressed as

$$\begin{aligned}\sigma_n^2 = &\sum_{ijkg}\left(\frac{\partial SDDR}{\partial \phi_{n_{ijkg}}}\right)^2 \sigma_{ijkg}^2 \\ &+2\sum_{ijkg<l}\left(\frac{\partial SDDR}{\partial \phi_{n_{ijkg}}}\right)\left(\frac{\partial SDDR}{\partial \phi_{n_l}}\right)\rho_{ijkg,l}\sigma_{ijkg}\sigma_l,\end{aligned} \tag{2}$$

where $\rho_{ijkg,l}$ is the correlation coefficient expressing the correlation or uncorrelation of fluxes at the space-energy elements $ijkg$ and l. Space-energy elements farther away from each other are most likely uncorrelated ($\rho_{ijkg,l} = 0$), but it is unlikely that any pair of elements have any degree of anticorrelatation ($\rho_{ijkg,l} < 0$) (Ref. 8). A lower bound for σ_n can be found by setting $\rho_{ijkg,l} = 0$, and an upper bound can be found by setting $\rho_{ijkg,l} = 1$ for all space-energy elements in Eq. (2).

In a discretized form, the SDDR can be expressed in terms of the neutron flux and the MS-CADIS adjoint source as

$$SDDR = \sum_{ijkg} \phi_{n_{ijkg}} q^{+}_{n\,ijkg}, \tag{3}$$

where the MS-CADIS adjoint neutron source $q^{+}_{n\,ijkg}$ represents the SDDR due to the neutron flux at space-energy element $ijkg$. Substituting this discretized form into Eq. (2), the lower bound of σ_n can be found from

$$\sigma^2_{n_{lower}} = \sum_{ijkg} \left(q^{+}_{n\,ijkg}\right)^2 \sigma^2_{ijkg}, \tag{4}$$

and the upper bound of Eq. (2) can be expressed as

$$\sigma_{n_{upper}} = \sum_{ijkg} q^{+}_{n\,ijkg} \sigma_{ijkg}. \tag{5}$$

Equations (4) and (5) represent only lower and upper bounds for the real uncertainty that lies between these limits. Future work will explore the degree to which the neutron flux space-energy elements are correlated.

IV. RESULTS

To assess the ability of each approach to reliably calculate the SDDR, the time of the Monaco neutron calculations was varied and the SDDR was computed at the four tally regions using each approach outlined in the Sect. III. The activation and the photon transport calculations were fixed in this analysis. Figure 2 shows the SDDR values in the four tally regions as a function of the running time of the Monaco neutron calculation.

For each approach individually, the differences between the fluctuations in the SDDR values did not exceed 12% after 2 days of running time for the neutron Monaco calculations. However, SDDRs of the analog cases were clearly undersampled even after 32 days of running time for the neutron Monaco calculation. The calculated SDDR values were significantly undersampled with the analog cases because the analog Monaco neutron calculations could not score in space-energy elements that are considered very important to the SDDR.

For the Monaco neutron calculations with running times greater than 4 days, the fractions of space-energy elements in which Monaco calculated a non-zero flux value are shown in Fig. 3. The SDDR response fractions that exist in nonzero scoring elements are also shown in Fig 3. The latter fractions were calculated by multiplying the MS-CADIS adjoint neutron source strength at each space-energy element that had an MC scoring by the forward flux value in the element.

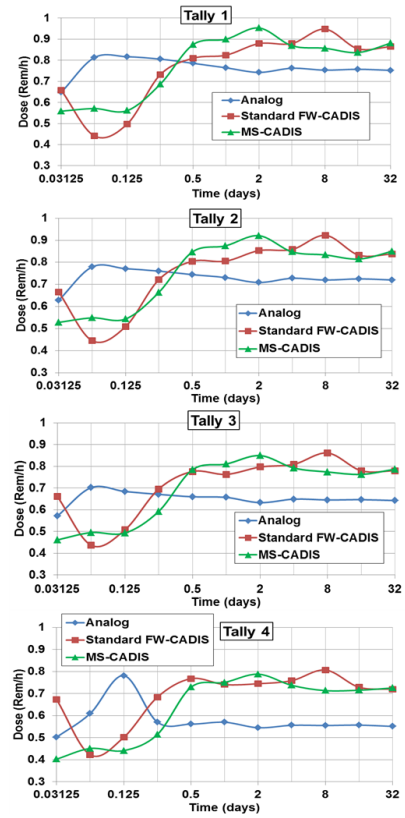

Fig. 2. SDDR estimates at the four tally regions shown in Fig. 1 as a function of time of Monaco neutron calculations.

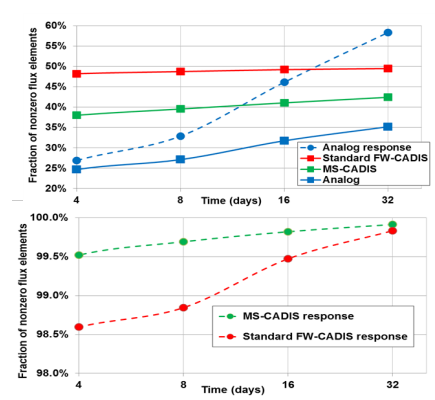

Fig. 3. Fractions of nonzero scoring space-energy elements and fractions of SDDR responses in nonzero scoring space-energy elements in the Monaco neutron calculations.

The fraction of nonzero scoring elements was about 15%–20% less with the MS-CADIS approach than with the standard FW-CADIS approach. However, the response fraction in the nonzero scoring elements was greater by a factor of 0.3%–0.9% with the MS-CADIS approach. For all the analog cases with different running times, the fractions of non-zero-scoring elements were less than 35% and the fractions of the responses in non-zero-scoring elements were less than 60%.

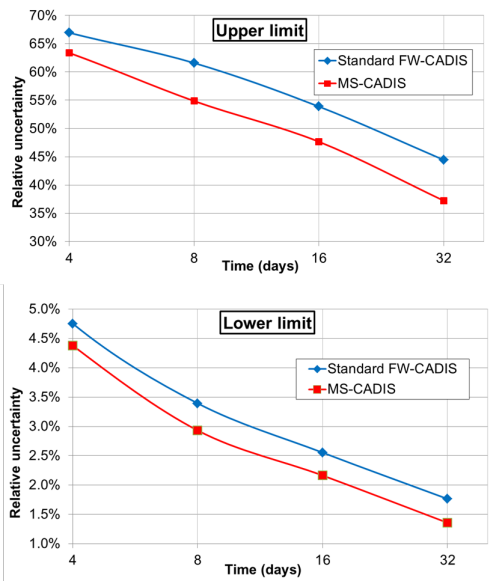

Fig. 4. Upper and lower limits of relative uncertainties in SDDR calculations.

Figure 4 shows the upper and lower limits of the uncertainties in the SDDR calculations for both the standard FW-CADIS and the MS-CADIS approaches. These upper and lower limits used Eqs. (4) and (5) to propagate the uncertainties in the neutron fluxes to the uncertainties in SDDR. Because the estimates of uncertainties are meaningless for undersampled MC simulations, the relative uncertainties were not calculated for the analog cases and for the standard FW-CADIS and MS-CADIS cases with Monaco neutron calculations that ran for less than 2 days. With a Monaco neutron calculation that ran for 32 days, where the response fraction in the nonzero scoring elements was greater than 99.5% for both the FW-CADIS and MS-CADIS cases, the upper limit of the uncertainty was 15% less with the MS-CADIS method than with the FW-CADIS method and the lower limit was less by 23%. These correspond to increases in the MC figure of merit (FOM) of 38% and 69% if the times of the activation calculations and the photon transport calculations are disregarded.

The MS-CADIS approach was previously shown to enhance the efficiency of SDDR calculations by a factor of 500 compared to the standard FW-CADIS approach.[4] However, the standard FW-CADIS approach, which tends to spend more computational effort in simulating particles in low flux regions, is specifically well suited for this problem because the tallies are located at the regions of the lowest flux values. Additionally, the cross sections of the transmutation reactions with the highest contribution to SDDR, namely, ^{59}Co (n,γ) ^{60}Co, ^{181}Ta (n,γ) ^{182}Ta, and ^{58}Fe (n,γ) ^{59}Fe, are highest at low energies, where the neutron flux values are the lowest.

V. CONCLUSION

Application of the MS-CADIS method to SDDR calculations in fusion energy systems was tested using the ITER benchmark problem. Compared to the standard FW-CADIS method, the increase in the FOM of the SDDR neutron MC calculation due to the use of the MS-CADIS method was between 38% and 69%. The MS-CADIS method also increases the fraction of nonzero scoring mesh tally elements in the space-energy regions of high importance to the final SDDR.

Implementation of the MS-CADIS method in the SCALE and the ADVANTG (Ref. 9) code systems is currently under way.

REFERENCES

1. R. PAMPIN, R. JUAREZ et al., "Investigation of Radiation Cross-Talk Effects on Biological Dose Rates in Maintenance Areas Inside the ITER Tokamak," *ANS RPSD 2014 - 18th Topical Meeting of the Radiation Protection & Shielding Division of ANS Knoxville, TN, Sept. 14 – 18, 2014,* American Nuclear Society, LaGrange Park, IL (2014).
2. R. PAMPIN, M. J. LOUGHLIN et al., "Radiation Transport Analyses for Design Optimisation of the ITER Core LIDAR Diagnostic," *Fusion Sci. Technol.*, **56**, 751 (2009); http://dx.doi.org/10.13182/FST56-751.
3. Y. CHEN, U. FISCHER, "Rigorous MCNP Based Shutdown Dose Rate Calculations: Computational Scheme, Verification Calculations and Application to ITER," *Fusion Eng. Des.,* **63**, 107 (2002); http://dx.doi.org/10.1016/S0920-3796(02)00144-8.
4. A. IBRAHIM, D. PEPLOW et al., "Novel Hybrid Monte Carlo/Deterministic Technique for Shutdown Dose Rate Analyses," *Fusion Eng. Des.*, **89**, 1933 (2014); http://dx.doi.org/10.1016/j.fusengdes.2014.03.014.
5. M. LOUGHLIN, "Conclusions of Shutdown Dose Rate Benchmark Study," *6th ITER Neutronics Meeting*, Hefei, China, June 17–24, 2011 (2011).
6. S. BOWMAN, "SCALE 6: Comprehensive Nuclear Safety Analysis Code System," *Nucl. Technol.*, **174**, 126 (2011); http://dx.doi.org/10.13182/NT10-163.
7. J. WAGNER, D. PEPLOW et al., "FW-CADIS Method for Global and Regional Variance Reduction of Monte Carlo Radiation Transport Calculations," *Nucl. Sci. Eng.*, **176**, 37 (2014); http://dx.doi.org/10.13182/NSE12-33.
8. D. PEPLOW, A. IBRAHIM et al., "Propagation of Uncertainty from a Source Computed with Monte Carlo," *Trans. Am. Nuc. Soc.*, **108**, 643 (2013).
9. S. MOSHER, A. BEVILL et al., *ADVANTG—An Automated Variance Reduction Parameter Generator*, ORNL/TM-2103/416, Oak Ridge National Laboratory (2013); http://dx.doi.org/10.2172/1105937.