SIMULTANEOUS OPTIMIZATION OF TALLIES IN DIFFICULT SHIELDING PROBLEMS

RADIATION PROTECTION

KEYWORDS: *Monte Carlo, hybrid method, variance reduction*

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Monte Carlo is quite useful for calculating specific quantities in complex transport problems. Many variance reduction strategies have been developed that accelerate Monte Carlo calculations for specific tallies. However, when trying to calculate multiple tallies or a mesh tally, users have had to accept different levels of relative uncertainty among the tallies or run separate calculations optimized for each individual tally. To address this limitation, an extension of the Consistent Adjoint Driven Importance Sampling (CADIS) method, which is used for difficult source/detector problems, has been developed to optimize several tallies or the cells of a mesh tally simultaneously. The basis for this method is the development of an importance function that represents the importance of particles to the objective of uniform Monte Carlo particle density in the desired tally regions. This method utilizes the results of a forward discrete ordinates solution, which may be based on a quick coarse-mesh calculation, to develop a forward-weighted source for the adjoint calculation. The importance map and the biased source computed from the adjoint flux are then used in the forward Monte Carlo calculation to obtain approximately uniform relative uncertainties for the desired tallies. This extension is called forward-weighted CADIS, or FW-CADIS.

I. INTRODUCTION

For many years, hybrid methods that use information derived from deterministic calculations have been used to accelerate Monte Carlo calculations.[1] Consistent Adjoint Driven Importance Sampling (CADIS) is one such methodology that has been successfully applied to both MCNP with the ADVANTG patch[2,3] and MAVRIC (Refs. 4 and 5) in SCALE 6 (Ref. 6). The implementations of CADIS use an approximate adjoint discrete ordinates calculation to determine both the transport weight-window target values and the biased source distribution to optimize one tally of interest in the Monte Carlo calculation.

The needs of specific applications have recently motivated efforts to develop approaches for optimizing Monte Carlo calculations for distributions, such as flux or dose-rate distributions (e.g., mesh tallies), as well as response at multiple localized tallies. These efforts have led to the development of an extension to the CADIS method that has been demonstrated to be effective for obtaining mesh tallies with approximately uniform relative uncertainties—simultaneous optimization. The effectiveness of this new method, referred to as forward-weighted CADIS (FW-CADIS), has been demonstrated for selected applications in previous papers.[7–9] This paper demonstrates the FW-CADIS method on a difficult problem of particular interest to the radiation protection and shielding community, namely, the problem of determining the spatial dose distribution surrounding an array of commercial spent nuclear fuel casks for the determination of the site boundary dose.

II. METHODS

II.A. The CADIS Method

For a typical source-detector problem with a source emission probability distribution function $q(\vec{r},E)$, total source strength S, and detector response function $\sigma_d(\vec{r},E)$, Monte Carlo is used to find the total detector response

$$R = \int_E \int_V \sigma_d(\vec{r},E)\phi(\vec{r},E)\,dV\,dE \quad , \tag{1}$$

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which is a function of the forward scalar flux $\phi(\vec{r},E)$ integrated over the volume of the detector.

If the adjoint scalar flux, $\phi^+(\vec{r},E)$, which is the solution to the transport problem with an adjoint source $q^+(\vec{r},E) = \sigma_d(\vec{r},E)$, is known, then the total detector response can also be found by integrating the product of the forward source and the adjoint flux over the source volume,

$$R = S \int_E \int_V q(\vec{r},E)\phi^+(\vec{r},E)\, dV\, dE \quad . \tag{2}$$

Unfortunately, the exact adjoint flux may be just as difficult to determine as the forward flux. However, an approximation of the adjoint flux can still be used to form an importance map and a biased source distribution for use in the forward Monte Carlo calculation.

If an approximation to the scalar adjoint flux, $\phi^+(\vec{r},E)$, for a certain detector response function can be found, this approximation can be used as follows: First, the total detector response is computed using Eq. (2). Then a biased source probability distribution is formed by

$$\hat{q}(\vec{r},E) = \frac{q(\vec{r},E)\phi^+(\vec{r},E)}{R/S} \quad . \tag{3}$$

When sampled from this biased distribution, particles would have a starting weight of

$$w_0(\vec{r},E) = \frac{R/S}{\phi^+(\vec{r},E)} \quad . \tag{4}$$

For the weight windows used in the transport process, the target weight $\overline{w}$ as a function of position and energy would be

$$\overline{w}(\vec{r},E) = \frac{R/S}{\phi^+(\vec{r},E)} \quad , \tag{5}$$

which is the same as the starting weights for that position and energy. Source particles are born with a weight matching the weight window of the region into which they are born. This is where *consistent* comes into CADIS—the importance map and biased source work together.

II.B. The FW-CADIS Method

The forward-weighted CADIS method[8,9] for calculating fluxes or dose rates everywhere with uniform relative uncertainties starts with an adjoint source $q^+(\vec{r},E)$ that is weighted inversely by the estimate of the forward quantity one wishes to calculate. For example, if the goal is to calculate a detector response function $\sigma_d(\vec{r},E)$ (such as dose rate using flux-to-dose conversion factors) over a mesh tally, then the adjoint source would be

$$q^+(\vec{r},E) = \frac{\sigma_d(\vec{r},E)}{\int \phi(\vec{r},E)\sigma_d(\vec{r},E)\, dE} \quad , \tag{6}$$

where $\phi(\vec{r},E)$ is an estimate of the forward flux. The adjoint source is nonzero only where the mesh tally is defined and its strength is inversely proportional to the forward estimate of dose.

Using this adjoint source, the standard CADIS method is used: The adjoint flux is computed, and then the importance map and biased source distribution are determined. However, in this case, the importance map represents the importance of particles to achieving uniform Monte Carlo particle density in the defined tally regions, which has been found to result in approximately uniform statistical uncertainties in these regions.

II.C. Implementation

The CADIS and FW-CADIS methods have been implemented into the MAVRIC sequence of SCALE. The MAVRIC (Monaco with Automated Variance Reduction using Importance Calculations) sequence automatically performs the necessary quick three-dimensional discrete ordinates calculations using Denovo, a newly developed S_N code, to calculate estimates of the forward and/or adjoint flux as a function of position and energy. MAVRIC then computes the biasing parameters and passes them to Monaco, the Monte Carlo code. Because the forward and adjoint deterministic solutions are being used to develop variance reduction parameters for the Monte Carlo simulation, approximate solutions from quick Denovo calculations are sufficient.

II.C.1. Denovo

Denovo is a newly developed parallel three-dimensional S_N code that is used to generate adjoint and forward scalar fluxes for the CADIS methods in MAVRIC. For usage in MAVRIC/CADIS, it is highly desirable that the S_N code be fast, positive, and robust. The phase-space shape of the forward and adjoint fluxes, as opposed to accuracy, is the most important quality for Monte Carlo weight-window generation. Accordingly, Denovo provides a step-characteristics spatial differencing option that produces positive scalar fluxes as long as the source (volume plus in-scatter) is positive. Denovo uses an orthogonal, nonuniform mesh that is ideal for CADIS applications because of the speed and robustness of calculations on this mesh type.

Denovo uses the highly robust GMRES (Generalized Minimum Residual) Krylov method to solve the S_N equations in each group. GMRES has been shown to be more robust and efficient than traditional source (fixed-point) iteration.[10] The in-group discrete S_N equations are defined as

$$\mathbf{L}\psi = \mathbf{MS}\phi + q \ , \tag{7}$$

where

$\mathbf{L}$ = differential transport operator

$\mathbf{M}$ = moment-to-discrete operator

$\mathbf{S}$ = matrix of scattering cross-section moments

q = external and in-scatter source

ϕ = vector of angular flux moments

ψ = vector of angular fluxes at discrete angles.

Applying the operator $\mathbf{D}$, where $\phi = \mathbf{D}\psi$, and rearranging terms cast the in-group equations in the form of a traditional linear system, $\mathbf{A}x = b$,

$$(\mathbf{I} - \mathbf{DL}^{-1}\mathbf{MS})\phi = \mathbf{DL}^{-1}q \ . \tag{8}$$

The operation $\mathbf{L}^{-1}v$, where v is an iteration vector, is performed using a traditional wave-front solve (transport sweep). The parallel implementation of the Denovo wave-front solver uses the well-known Koch-Baker-Alcouffe (KBA) algorithm, which is a two-dimensional block-spatial decomposition of a three-dimensional orthogonal mesh.[11] The Trilinos package is used for the GMRES implementation.[12] Since the rest of the MAVRIC sequence has not yet been parallelized, Denovo is currently used only in serial mode within MAVRIC.

II.C.2. Monaco

The forward Monte Carlo transport is done using Monaco, a fixed-source, multigroup shielding code that uses the SCALE General Geometry Package (SGGP, the same as used by the criticality code KENO-VI) and the standard SCALE material information processor. Monaco was originally based on the MORSE Monte Carlo code but has been extensively modified to modernize the coding, incorporate more flexibility in terms of sources and tallies, and read a user-friendly block and keyword style of input.

II.C.3. MAVRIC Input

A MAVRIC input file looks very similar to an analog Monaco input: a description of the materials and physical geometry of the problem, a description of the source, and a listing of the desired tallies. For a MAVRIC calculation, the user provides two additional items. First are the mesh planes to use in Denovo, which should capture major material changes, the boundaries of the source, and the boundaries of the tallies. The other item is the specification of the adjoint source. Typically, this

TABLE I

Fresh Fuel Components for a Typical Midsized PWR Core

	Mass (kg)
U (4.2%)	
^{235}U	1 936
^{238}U	44 164
Others	
C	6
N	3
O	6 209
Al	5
Si	7
P	14
Ti	5
Cr	234
Mn	11
Fe	460
Co	3
Ni	440
Zr	10 071
Nb	33
Mo	18
Sn	165

TABLE II

Photon Source Spectra in the 19-Group Format

Energy (MeV)	Fraction
20	0.000E+00[a]
10	0.000E+00
8	0.000E+00
6.5	0.000E+00
5	0.000E+00
4	6.957E-08
3	7.989E-07
2.5	1.253E-05
2	7.508E-06
1.66	2.121E-02
1.33	4.140E-02
1	1.337E-02
0.8	7.780E-01
0.6	2.370E-02
0.4	2.341E-04
0.3	2.487E-03
0.2	1.337E-02
0.1	9.342E-03
0.045	9.690E-02
0.01	

[a]Read as 0.000×10^0.

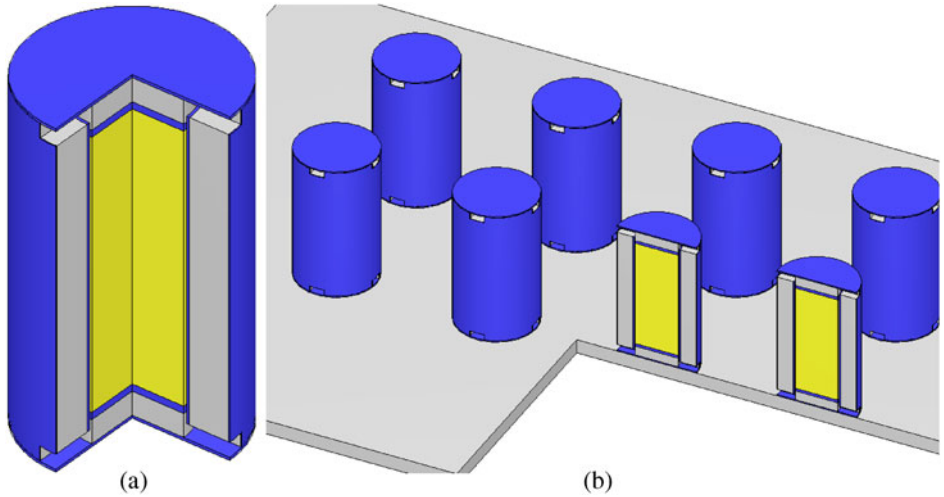

Fig. 1. Geometry of (a) a single spent-fuel cask and (b) the ISFSI model near the array.

is one or more of the tally locations and response functions. For FW-CADIS to optimize multiple tallies or a large mesh tally, the user also adds a single keyword "forwardWeighting."

III. EXAMPLE PROBLEM

As an example, consider the problem of having to determine the location for the boundary of the controlled area of an independent spent-fuel storage installation (ISFSI). Using a standard Monte Carlo code, one can calculate dose rates at specific points near the spent-fuel casks, but the direct calculation of the dose rate distribution, which may be needed to define the controlled area boundary, at large distances from an array of commercial spent-fuel casks with acceptable statistical uncertainties is computationally prohibitive with standard Monte Carlo codes. This problem requires a mesh tally over a very large area (hundreds of meters) that has reasonable statistical uncertainties for all of the meshes—both near and far from the casks.

III.A. Source Term

Spent fuel from a typical midsized pressurized water reactor (PWR) was used to determine the source term. ORIGEN was used to deplete a full core (46.1 tonnes of uranium, 4.2% enriched) to 55 000 MWd/tonne U. The contents of the modeled fuel, shown in Table I, represent typical values for PWR fuel. ORIGEN then computed the photon spectra in a 19-energy-group structure for the fuel following a 10-yr cooling period after the last irradiation. This spectrum is shown in Table II. The total

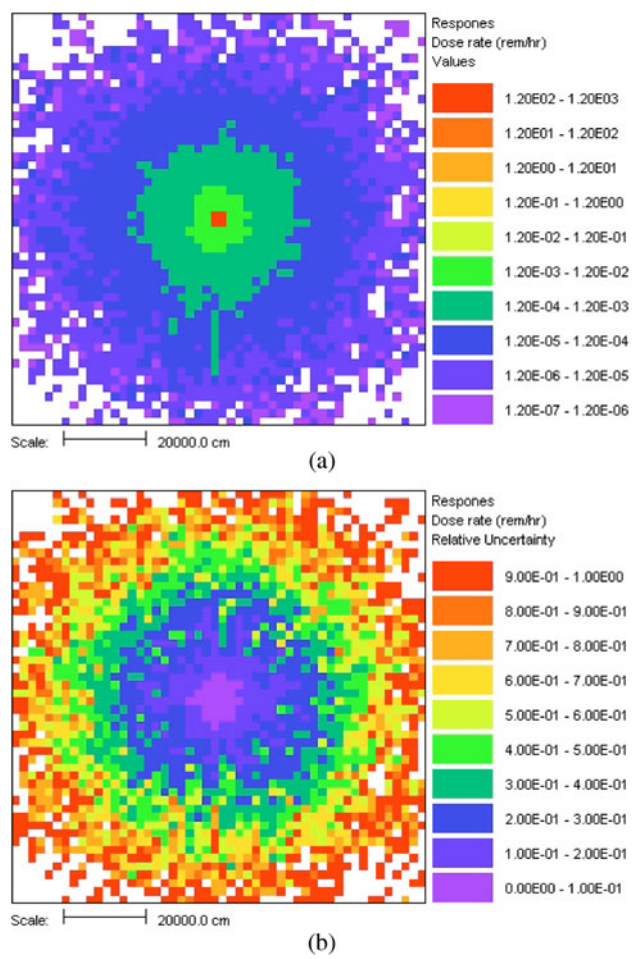

Fig. 2. Analog calculation of (a) forward dose rates (in rems per hour) at $z = 1$ m (where $z = 0$ is ground level) and (b) relative uncertainties after 560 h.

photon source strength for each cask (approximately one-sixth of a full core) was 4.7353×10^{16} photons/s. ORIGEN also calculated the neutron source, which is not used in this example problem.

III.B. ISFSI Model

A typical cask size with a 1.7-m radius and 5.7-m height was modeled. Each cask consisted of 10.63 tonnes of the fuel mixture (20 assemblies) homogenized over the 11.63-m^3 interior space. Radially, the fuel was surrounded by 0.05 m of steel, 0.68 m of concrete, and 0.02 m of steel. A 2×4 array of casks was modeled with a distance of 6.8 m between cask centers. The casks were modeled in air resting on a 0.60-m-thick concrete pad, which is on top of 5 m of soil. The square model extends from the center of the cask array out 500 m in each direction. Representations of a single cask, as well as the cask array, are shown in Fig. 1.

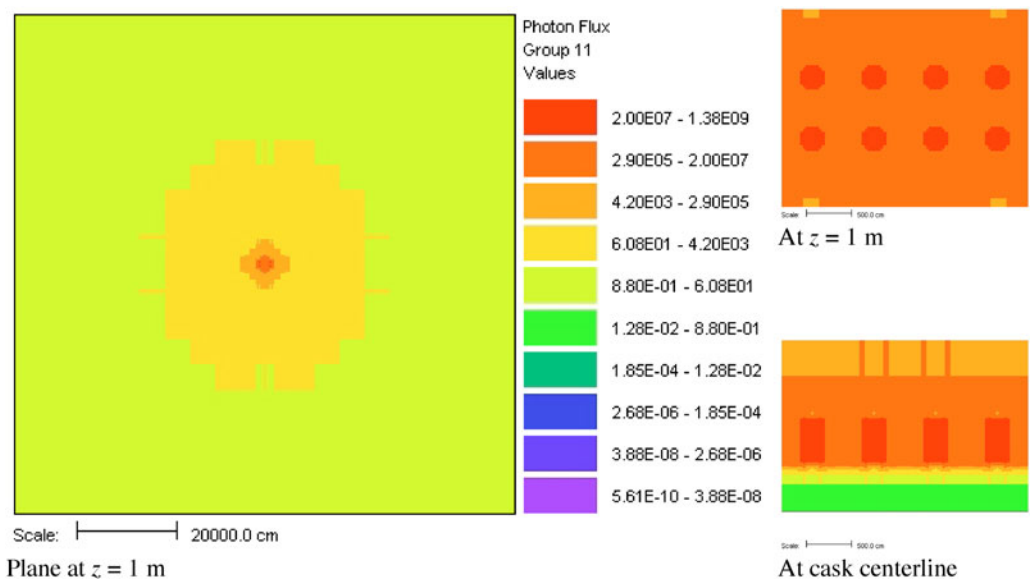

Fig. 3. Denovo-calculated flux for 1-MeV photons.

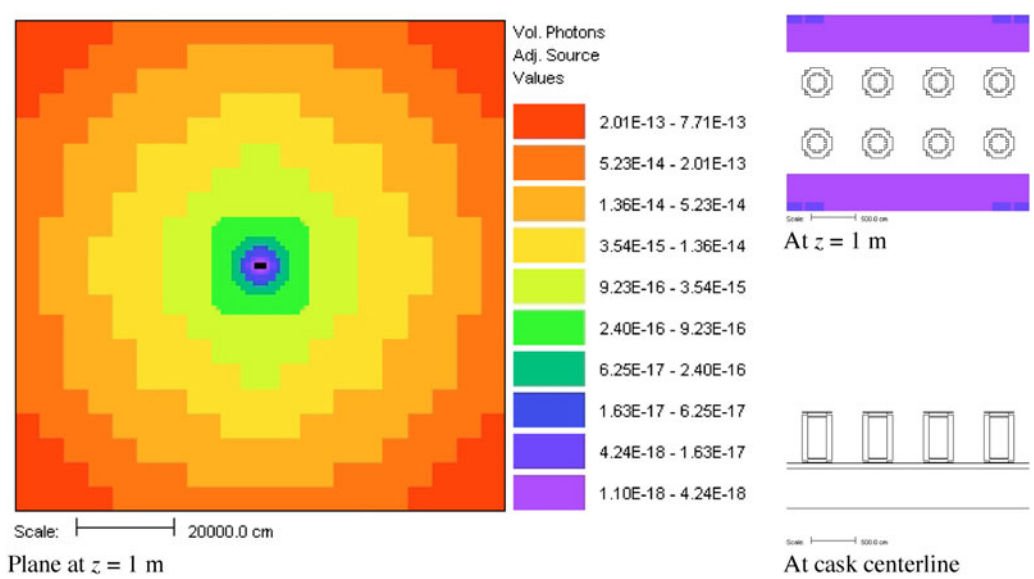

Fig. 4. Adjoint source that has been weighted by the forward dose rates. Note that there is only adjoint source away from the cask array—where the dose rates are desired.

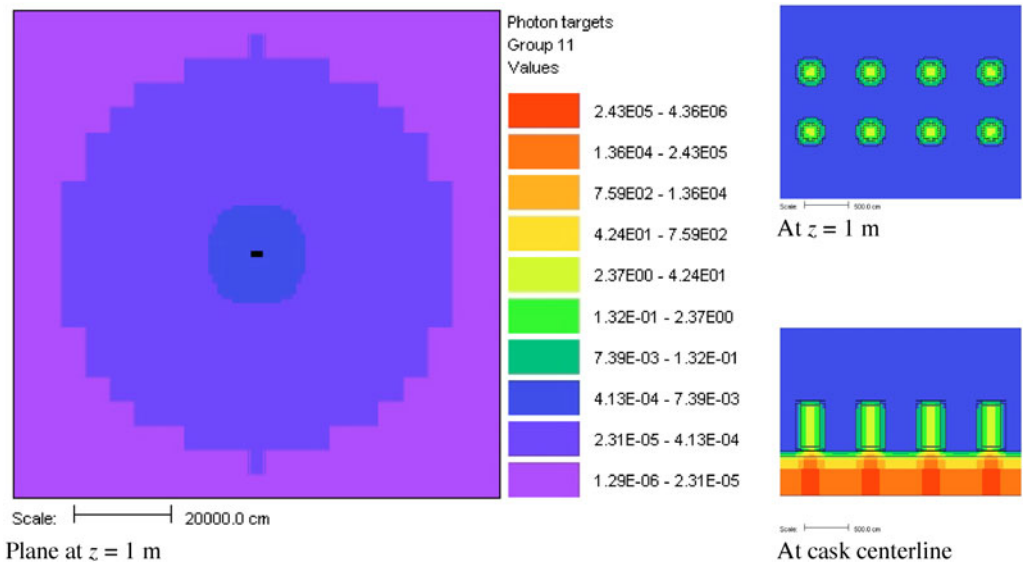

Fig. 5. Importance map target weights for 1-MeV photons.

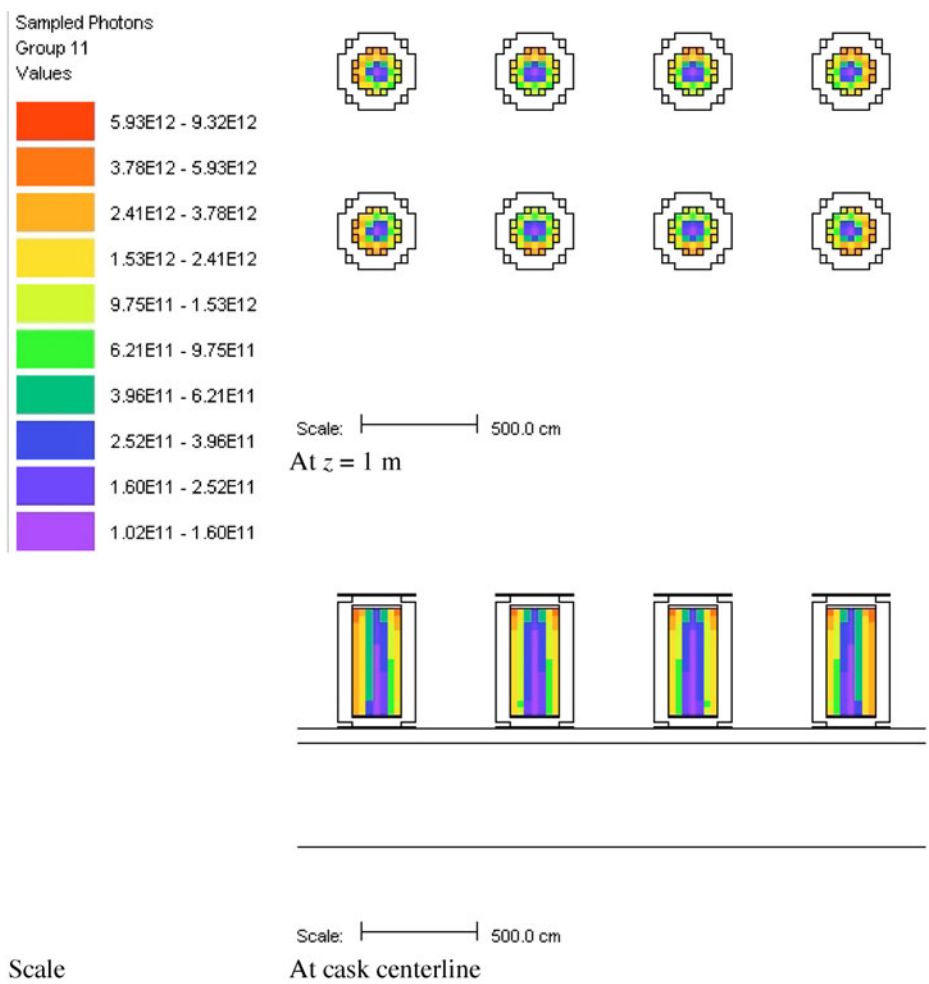

Fig. 6. Biased source strength.

III.C. Calculations

To establish a reference for comparison, an analog Monaco calculation was done. Because implicit capture is always on in Monaco, lower-weight windows were set to 0.0001 everywhere. The analog calculation was allowed to run for 560 h on a single Linux processor. The mesh tally of dose-rate results near the ground surface and the relative uncertainties are shown in Fig. 2. Each voxel in the figure is an area of 20×20 m extending over the first 2 m above the ground. Note that the areas of high dose rate (near the casks) are the only portions of the mesh tally with reasonable relative uncertainties (e.g., $<10\%$). Due to the high uncertainties, it is difficult to determine where the contour of 1.2×10^{-5} rem/h (the 25 mrem/yr limit for a 2000-h working year) lies. Some voxels of the mesh tally indicate a zero dose rate, since no photons reached them during the simulation. After 560 h of simulation, a reliable estimate of dose rate at any significant distance from the cask array is not achieved.

MAVRIC with FW-CADIS was then used to compute the same mesh tally of dose rates. The first step used Denovo to estimate the forward fluxes, shown in Fig. 3, and compute an estimate of the dose rates. The adjoint is defined where we want to most accurately compute the final dose rates—at ground level, where the boundary of the controlled area would be located, far from the cask array. The dose rate very close to or between the casks is not needed. Therefore, the adjoint source covering just the first 2 m above the ground everywhere except near the casks was constructed using the conversion factors for flux-to-dose rate as the energy spectra and the inverse of the forward flux as the spatial function, as is shown in Fig. 4. Denovo then calculated the adjoint flux, and MAVRIC built the importance map, shown in Fig. 5, and the biased source, shown in Fig. 6. The mesh used by Denovo and the importance maps had only $90 \times 70 \times 56$ cells over the entire model, which represents a very coarse mesh for a deterministic model. Cell sizes ranged from centimeters in the soil to 50 m in the air far from the array. Denovo calculation times were 17 and 21 min for the forward and adjoint problems, respectively. Monaco was allowed to run for 108 h. Figure 7 shows the dose rates, along with the relative uncertainties for each voxel. Note that the 1.2×10^{-5} rem/h contour is located ~360 m from the center of the cask array.

The mesh tally relative uncertainties for the FW-CADIS calculation are nearly uniform, with 80% of the mesh tally cells having $<5\%$ statistical uncertainty and 97% of the cells having $<10\%$ uncertainty—even though the dose rates ranged over 10 orders of magnitude. The relative uncertainties for the entire mesh tally can be plotted as a cumulative distribution function (CDF), showing what fraction of cells had less than a specified amount of relative uncertainty. This is done in Fig. 8 for the FW-CADIS calculation as well as a similar distribution for the longer analog calculation. Note here that in the analog calculation, only 1.3% of the voxels had $<10\%$ relative uncertainty. (These were the voxels near the cask array.)

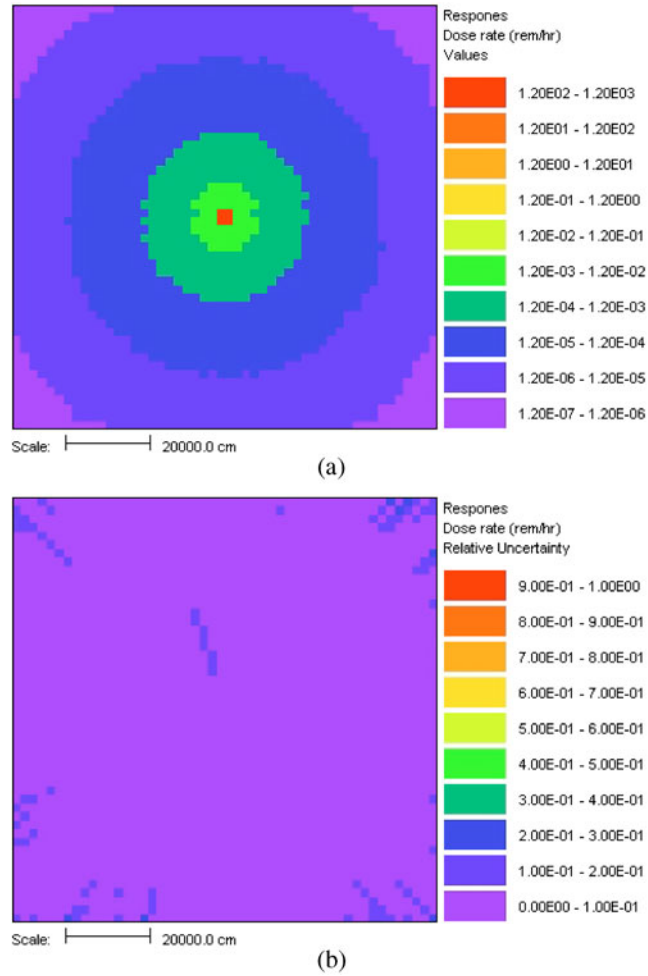

Fig. 7. Final results for (a) dose rates at $z = 1$ m and (b) relative uncertainties after 108 h.

IV. CONCLUSIONS

This paper highlights the benefits of the FW-CADIS method in the MAVRIC sequence of SCALE for optimizing mesh tallies for a difficult shielding problem (i.e., dose rates at a significant distance from an array of commercial spent nuclear fuel casks). The method has also been successfully applied to other problems, including the calculation of dose rates throughout an entire PWR facility[7] and nuclear well-logging problems.[13] In all applications to date, excellent results have been achieved. The method requires two approximate discrete ordinates calculations (one forward and one adjoint) to generate consistent source biasing and weight-window parameters

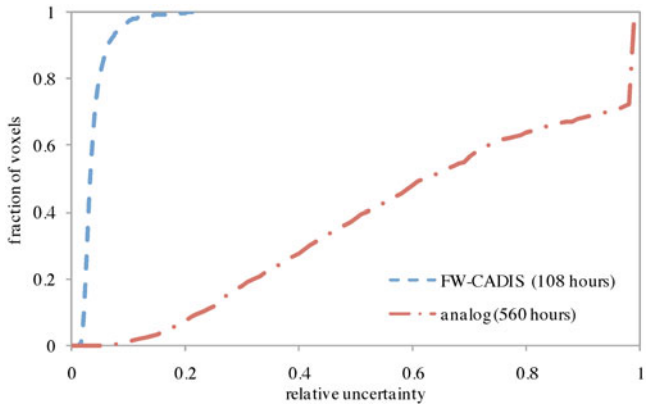

Fig. 8. Relative uncertainty CDF histogram for the FW-CADIS calculation and the analog calculation.

for the subsequent Monte Carlo simulation and does not require any modifications to existing Monte Carlo codes. Although more testing and thorough analysis of results continue, the potential of this method for optimizing global distributions, including energy-dependent flux distributions, as well as semiglobal distributions, such as response at multiple localized detectors or spectra, appears very promising.

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REFERENCES

1. A. HAGHIGHAT and J. C. WAGNER, "Monte Carlo Variance Reduction with Deterministic Importance Functions," *Prog. Nucl. Energy*, **42**, *1*, 25 (2003).

2. J. C. WAGNER, "Acceleration of Monte Carlo Shielding Calculations with an Automated Variance Reduction Technique and Parallel Processing," PhD Dissertation, Pennsylvania State University (1997).

3. J. C. WAGNER, "An Automated Deterministic Variance Reduction Generator for Monte Carlo Shielding Applications," *Proc. 12th Biennial Radiation Protection and Shielding Division Topl. Mtg.*, Santa Fe, New Mexico, April 14–18, 2002, American Nuclear Society (2002).

4. D. E. PEPLOW and J. C. WAGNER, "Automated Variance Reduction for SCALE Shielding Calculations," *Proc. 14th Biennial Radiation Protection and Shielding Division Topl. Mtg.*, Carlsbad, New Mexico, April 2–6, 2006, p. 391, American Nuclear Society (2006).

5. D. E. PEPLOW, S. M. BOWMAN, J. E. HORWEDEL, and J. C. WAGNER, "Monaco/MAVRIC: Computational Resources for Radiation Protection and Shielding in SCALE," *Trans. Am. Nucl. Soc.*, **95**, 669 (2006).

6. "SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluations," ORNL/TM-2005/39, Version 5.1, Vols. I–III (Nov. 2006); available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-732.

7. E. D. BLAKEMAN, D. E. PEPLOW, J. C. WAGNER, B. D. MURPHY, and D. E. MUELLER, "PWR Facility Dose Modeling Using MCNP5 and the CADIS/ADVANTG Variance-Reduction Methodology," ORNL/TM-2007/133, Oak Ridge National Laboratory (Sep. 2007).

8. J. C. WAGNER, E. D. BLAKEMAN, and D. E. PEPLOW, "Forward-Weighted CADIS Method for Global Variance Reduction," *Trans. Am. Nucl. Soc.*, **97**, 630 (2007).

9. D. E. PEPLOW, E. D. BLAKEMAN, and J. C. WAGNER, "Advanced Variance Reduction Strategies for Optimizing Mesh Tallies in MAVRIC," *Trans. Am. Nucl. Soc.*, **97**, 595 (2007).

10. J. S. WARSA, T. A. WAREING, and J. E. MOREL, "Krylov Iterative Methods and the Degraded Effectiveness of Diffusion Synthetic Acceleration for Multidimensional S_N Calculations in Problems with Material Discontinuities," *Nucl. Sci. Eng.*, **147**, 218 (2004).

11. R. S. BAKER and K. R. KOCH, "An S_n Algorithm for the Massively Parallel CM-200 Computer," *Nucl. Sci. Eng.*, **128**, 312 (1998).

12. M. A. HEROUX and J. M. WILLENBRING, "Trilinos Users Guide," SAND2003-2952, Sandia National Laboratories (2003).

13. J. C. WAGNER, D. E. PEPLOW, and T. M. EVANS, "Automated Variance Reduction Applied to Nuclear Well-Logging Problems," *Nucl. Technol.*, **168**, 799 (2009).