ITER NEUTRONICS MODELING USING HYBRID MONTE CARLO/ DETERMINISTIC AND CAD-BASED MONTE CARLO METHODS

RADIATION TRANSPORT AND PROTECTION

KEYWORDS: *CAD-based Monte Carlo, ITER, hybrid Monte Carlo/ deterministic*

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The immense size and complex geometry of the ITER experimental fusion reactor require the development of special techniques that can accurately and efficiently perform neutronics simulations with minimal human effort. This paper shows the effect of the hybrid Monte Carlo (MC)/deterministic techniques—Consistent Adjoint Driven Importance Sampling (CADIS) and Forward-Weighted CADIS (FW-CADIS)—in enhancing the efficiency of the neutronics modeling of ITER and demonstrates the applicability of coupling these methods with computer-aided-design–based MC. Three quantities were calculated in this analysis: the total nuclear heating in the inboard leg of the toroidal field coils (TFCs), the prompt dose outside the biological shield, and the total neutron and gamma fluxes over a mesh tally covering the entire reactor. The use of FW-CADIS in estimating the nuclear heating in the inboard TFCs resulted in a factor of ~275 increase in the MC figure of merit (FOM) compared with analog MC and a factor of ~9 compared with the traditional methods of variance reduction. By providing a factor of ~21 000 increase in the MC FOM, the radiation dose calculation showed how the CADIS method can be effectively used in the simulation of problems that are practically impossible using analog MC. The total flux calculation demonstrated the ability of FW-CADIS to simultaneously enhance the MC statistical precision throughout the entire ITER geometry. Collectively, these calculations demonstrate the ability of the hybrid techniques to accurately model very challenging shielding problems in reasonable execution times.

I. INTRODUCTION

The neutronics modeling and simulation (M&S) of the ITER experimental fusion reactor is needed for the prediction and confirmation of the nuclear parameters that represent an essential part of the reactor design process. The immense size and complex geometry of fusion energy systems such as ITER require special techniques to perform the neutronics M&S. In this analysis the hybrid Monte Carlo (MC)/deterministic methods—Consistent Adjoint Driven Importance Sampling (CADIS) (Ref. 1) and Forward-Weighted CADIS (FW-CADIS) (Ref. 2)—were used to enhance the efficiency of the neutronics M&S of ITER. The analysis also demonstrated the applicability of coupling the hybrid techniques with computer-aided-design (CAD)-based MC methods.

In previous analyses, the CADIS and FW-CADIS methods provided a factor of >1000 increase in the MC figure of merit (FOM) for problems with physical sizes larger than ITER. These methods use approximate deterministic calculation(s), generally discrete ordinates (S_N), to create the biasing parameters needed for efficient MC. Such techniques have been shown to accelerate high-fidelity MC simulations in problems for which it would otherwise take months or even years to obtain a reasonably low level of statistical uncertainty.[3–6]

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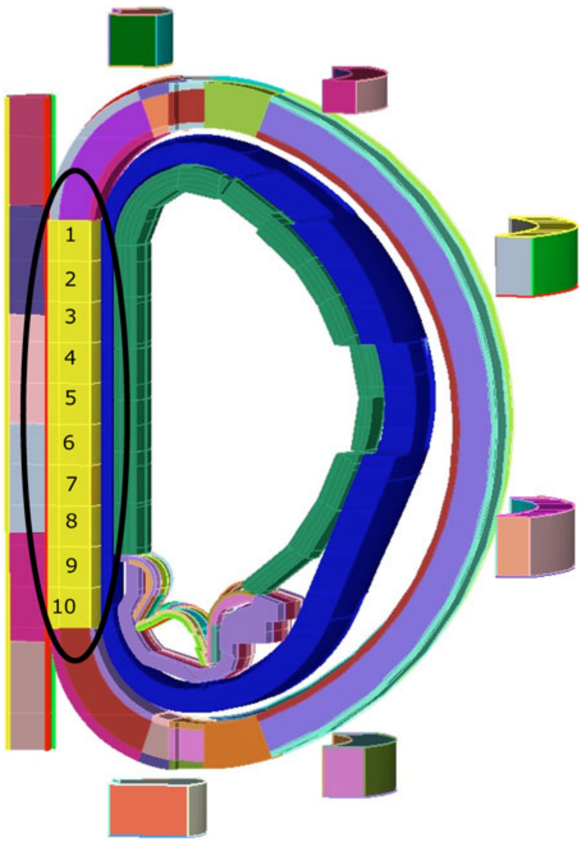

Fig. 1. Inboard TFC.

Because of the complex geometry of fusion systems, the fusion neutronics community has developed tools to combine the MCNP5 MC code[7] and CAD software. This approach preserves the complexity of the geometry, reduces human errors, and accelerates design iterations.[8]

The coupling of the hybrid techniques with CAD-based MC provides the capability to perform MC simulations with significantly enhanced computational efficiency while accurately modeling complex geometries. In addition, the time-consuming and error-prone process of manually transforming the geometry into, for example, the MCNP format can be avoided.

II. USING THE HYBRID TECHNIQUES FOR CALCULATING RELEVANT ITER PARAMETERS

The analysis calculated three quantities: the nuclear heating in the inboard straight legs of the toroidal field coils (TFCs), the prompt operational dose outside the biological shield (bioshield), and the total neutron and photon flux distributions. The first two values are needed for ITER licensing and operation, whereas the last one shows the effect of the hybrid techniques in simultaneously enhancing the efficiency of estimating mesh tallies covering the entire ITER plant.

II.A. Inboard TFC Nuclear Heating

ITER uses 18 superconducting TFCs, which operate at cryogenic temperatures. The allowable amount of nuclear heating deposited in these coils is constrained by the ability of the cryogenic cooling system to remove the heat. The thick shielding provided by the blanket and the vacuum vessel (VV) makes the calculation of the total heating in these coils a challenging problem for MC methods; therefore, reliable variance-reduction techniques are necessary. Because of the decreased thickness of the blanket and VV in front of the inboard leg, the neutron and photon heating in the inboard legs accounts for ~70% of the total TFC nuclear heating. It is therefore considered the main driver of the ITER shield design.[9] The simplified CAD model presented in Fig. 1 shows the inboard leg of one of the ITER TFCs together with the shielding layers separating it from the neutron source in the plasma region.

Each of the inboard TFC legs has a height of 8 m, a radial thickness of 70 cm, and a toroidal extent of 80 cm. For the analysis, each leg was divided into ten vertical segments, as shown in Fig. 1. Since good MC statistical precision is required for both neutrons and photons in all of the inboard TFC segments, this is considered a semiglobal problem. For global and semiglobal problems, FW-CADIS can be used to optimize one or more MC tallies on arbitrary volumes (e.g., separate cell tallies or large mesh tallies) in a single simulation. The inverse of the space- and energy-dependent fluxes calculated from a forward deterministic calculation is used to weight the source of an adjoint deterministic calculation. The adjoint fluxes are then used to calculate a biased source and weight-window parameters for the MC calculation. For this problem, the response to be optimized was specified as the total neutron and gamma heating in a rectangular parallelepiped enclosing the inboard TFC segments.

II.B. Prompt Neutron Dose

Estimates of the dose rates outside the bioshield are necessary to ensure occupational safety and to enable proper design of the reactor building. Calculating the prompt dose rate outside the bioshield during plant operation is a challenging problem because of the massive amount of shielding between the source and the exterior.[9] For this analysis, the dose rate was calculated at the point illustrated in Fig. 2.

The dose rate calculation is a classic source-detector problem for which the CADIS method was designed. CADIS optimizes the MC particle population throughout the geometry in order to improve the MC statistics of a

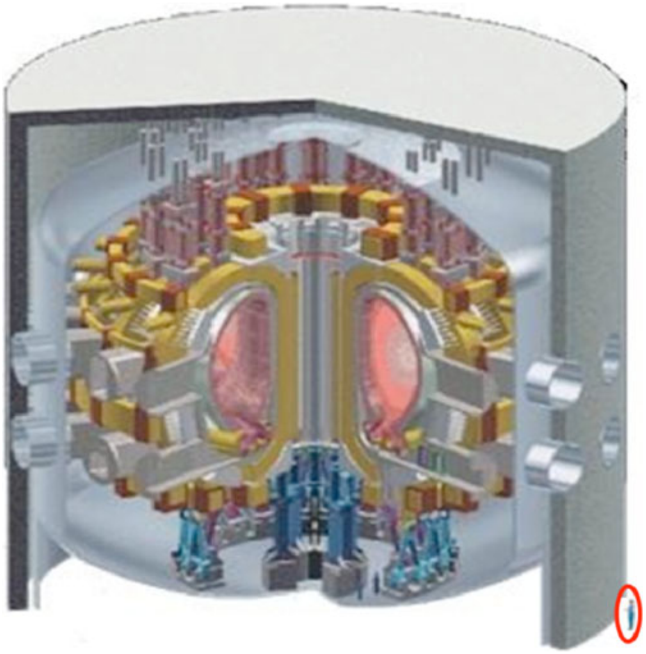

Fig. 2. Position of dose calculation.

single, localized tally. It uses one adjoint calculation to build a biased source and weight-window parameters. A point adjoint source was defined at the location of the dose rate tally. The groupwise energy spectrum of the adjoint source was defined as the flux–to–dose rate conversion factors in an energy structure equivalent to that of the multigroup data library of the deterministic calculation.

II.C. Total Neutron and Gamma Fluxes

The nuclear analysis of ITER has always depended on the analysis of each component separately using combinations of one-dimensional (1-D), two-dimensional (2-D), and three-dimensional (3-D) analyses.[9] The main reasons for the use of these approaches are the complexity of the geometry and the difficulty of obtaining good MC statistical precision throughout the entire domain. To demonstrate the effectiveness of the FW-CADIS method in obtaining approximately uniform MC uncertainties throughout the problem space, the technique was used to accelerate both total neutron flux and total gamma flux mesh tallies, each covering the entire ITER plant. The adjoint source was defined as covering the whole ITER geometry, with a spectrum that was uniform for all neutron and gamma energy groups.

III. METHODOLOGY

The ITER benchmark model[8] was used in calculating the nuclear heating in the inboard TFC. The model represents a 40-deg sector of the ITER machine with reflecting boundaries. The Oak Ridge National Laboratory (ORNL) AutomateD VAriaNce reducTion Generator (ADVANTG) code[10] was used to develop weight-window maps for the subsequent MC simulations. The ADVANTG package uses a modification of MCNP5-1.40 to map materials from the combinatorial geometry onto a user-defined orthogonal mesh. It drives the Denovo[11] 3-D S_N code to generate approximate forward and/or adjoint S_N solutions. Using the CADIS or FW-CADIS methods, ADVANTG then generates weight-window and source-biasing parameters in formats directly usable by MCNP (i.e., as a WWINP file and SDEF cards, respectively). The Karlsruhe Institute of Technology (KIT) provided the MCNP input file. This file was converted from the original ITER CAD model to the MCNP format using the McCAD translator.[12] The weight-window map created by ADVANTG was used in MC simulations with the University of Wisconsin-Madison (UW) CAD-based MC code, Direct Accelerated Geometry MCNP (DAG-MCNP) (Ref. 13). DAG-MCNP is an MC code that replaces the ray-tracing routines of MCNP with CAD routines defined in an external software library. It was extensively used in the neutronics analyses of several fusion applications such as ITER, HAPL, and ARIES (Ref. 14).

The ITER reference model, Alite03, was used for the dose and total flux calculations. This model was distributed by the ITER International Organization (ITER IO) in the form of an MCNP input file representing a 40-deg sector of ITER (Ref. 15).

For comparison purposes, Denovo was used to deterministically calculate the dose using a spatial mesh with 280 million cells. Denovo uses the Koch-Baker-Alcouffe algorithm[16] to parallelize transport sweeps on a 3-D structured grid and Krylov subspace methods to accelerate source convergence.[11] It has demonstrated excellent scaling capabilities when running very large problems with very high resolution on hundreds of thousands of cores.[11] The Denovo dose rate calculation was performed on the ORNL supercomputer Jaguar. The Denovo input file was created by ADVANTG from the Alite03 MCNP model.

Because the source particles are born in a void region with a very narrow Gaussian energy distribution centered around 14.1 MeV, preliminary analyses revealed that neither the source-biasing parameters nor the accurate representation of the ITER neutron source in the deterministic calculations of the hybrid techniques was important. An approximate source was used for the S_N calculations, and the source-biasing parameters were not used in the MC calculation. For the MC simulations, the actual ITER source was used in two equivalent forms.[17] The first representation, used in most calculations, is a source routine that is compiled with the MCNP source code. For the MCNP dose calculation without CADIS, the source distribution was defined using

TABLE I

Denovo Mesh and Run Time

	Number of Cells (millions)	Forward Calculation Time (h)	Adjoint Calculation Time (h)
Inboard TFC	0.4	1.7	2.0
Dose	0.6	—	1.9
Total flux	1.1	4.8	3.9

the generalized volume source capability internal to MCNP5 (SDEF) (Ref. 17). For the stand-alone high-resolution Denovo calculation of the dose rate, CADIS-based MCNP tests with different sources showed that the spatial distribution of the neutron source inside the plasma had minimal effect on the dose rate outside the bioshield. For simplicity, the neutron source used in this calculation was approximated by a volumetric source filling the inner half of the plasma volume.

The 40-deg ITER model was expanded to a full 360-deg model for the Denovo calculations. This unfolding process was performed in ADVANTG using additional code that was specially written for this purpose. In CADIS and FW-CADIS, the only objective of the deterministic calculations is to provide appropriate variance-reduction parameters for the MC calculation, and hence, only approximate S_N solutions are needed. To accelerate the S_N calculations, the dimensions of the mesh used in the forward and the adjoint calculations of the hybrid sequences were nominally on the order of meters, but smaller cells were used near the tally of interest. None of the Denovo calculations took more than 5 h, and all of them used the sequential (not parallel) version of Denovo. Table I shows the number of mesh cells and the Denovo running time for each of the three quantities calculated. These running times are much smaller than those needed for MC calculations, and hence, they were not considered in the FOM analysis.

The fusion evaluated nuclear data library (FENDL-2.1) of the International Atomic Energy Agency[18] was used in this analysis. A multigroup 46-neutron/21-gamma FENDL-2.1 library was created in ANISN format for the Denovo calculation.

IV. RESULTS

IV.A. Inboard TFC Nuclear Heating

During the original benchmarking effort, the UW DAG-MCNP results for the inboard TFC nuclear heating were found to be systematically higher than those from all of the other parties contributing to the ITER benchmark.[8] The other parties were KIT with the McCad translator, the Fusion Design Study of the Chinese Academy of Sciences (FDS) with the MCAM translator,[19] and the Japan Atomic Energy Agency (JAEA) with the GEOMIT translator.[20] In Ref. 8 the discrepancy between the UW

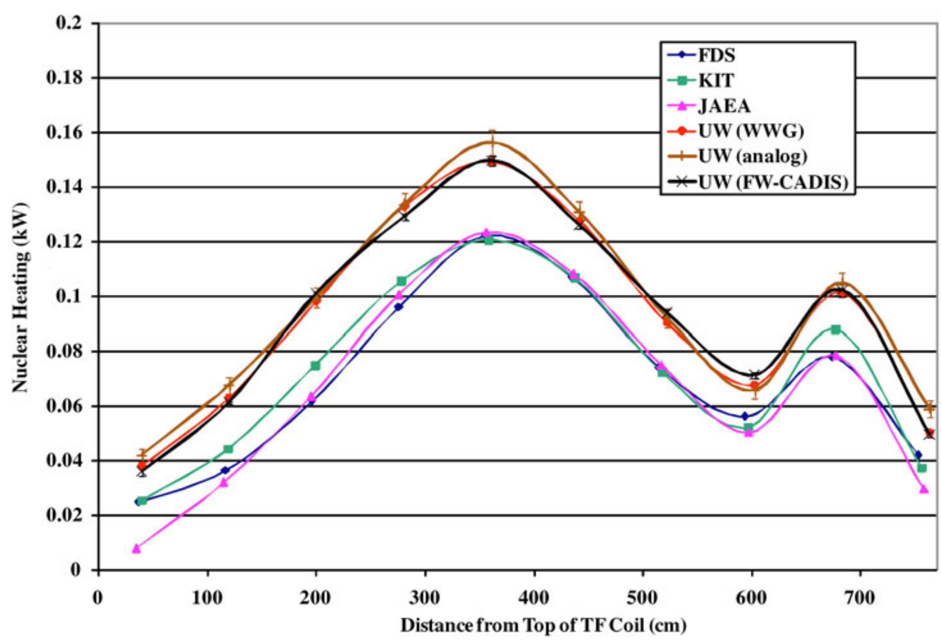

Fig. 3. Inboard TFC heating before correction of the UW CAD geometry.

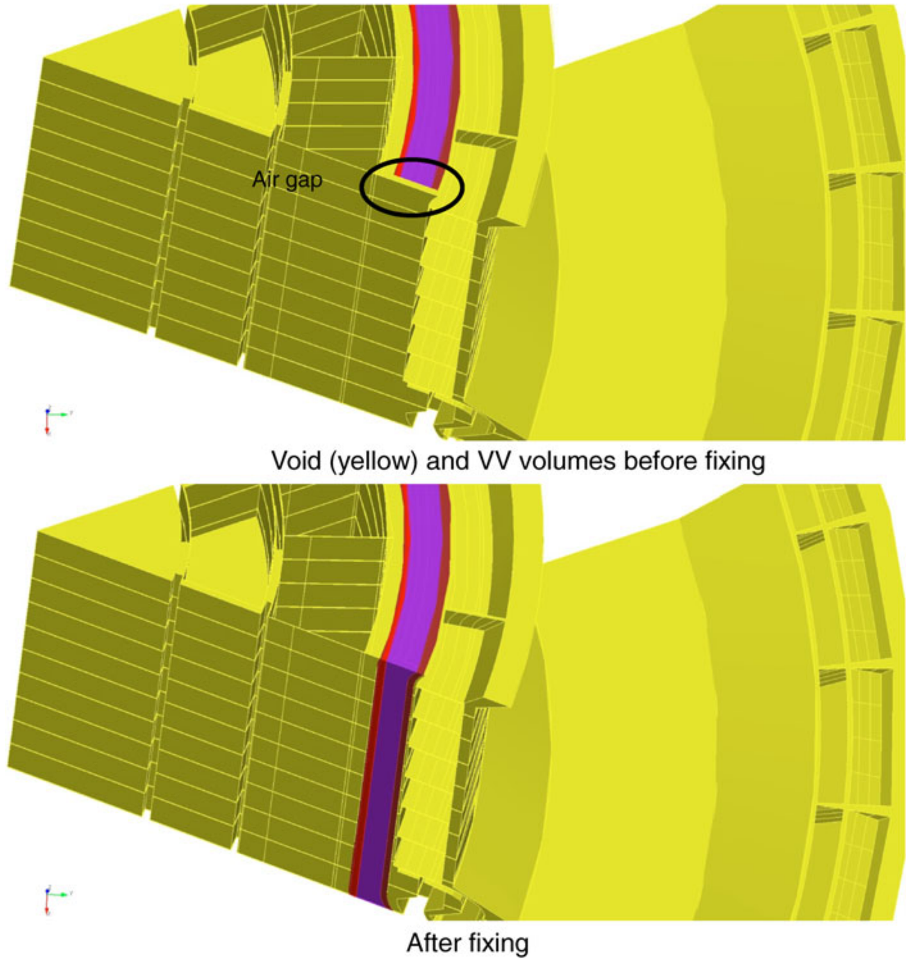

Fig. 4. UW CAD geometry before and after replacement of the void with VV materials.

results and those of the other parties was attributed to a bias introduced by the use of the MCNP weight-window generator (WWG) to automatically generate mesh-based weight windows for DAG-MCNP. The calculation was repeated with FW-CADIS, and the results, shown in Fig. 3, were found to align with the original UW results reported in Ref. 8. To verify that no bias is introduced by any kind of variance reduction, an analog DAG-MCNP calculation was performed on 32 processors.[a] The analog results shown in Fig. 3 were found to agree with both the UW WWG and FW-CADIS results.

Because the MCNP computation time T is controlled by the inboard TFC segment with the maximum statistical uncertainty R_{max}, the FOM can be defined as

$$\text{FOM} = \frac{1}{R_{max}^2 \times T} \ .$$

[a] All MCNP5 and DAG-MCNP5 simulations that are identified as "analog" or "without variance reduction" still include the standard implicit capture method.

As a result of the occasional appearance of histories with abnormally high tally contributions, difficulties were encountered while analyzing the FW-CADIS effects on the FOM. These occurrences, which appeared approximately once every 2 million histories, caused significant increases in the relative uncertainties and variances of the variance. The increase in the relative uncertainty caused by one of these particles was 13%, while the increase in the variance of the variance was >75%. The fluctuation in the variance of the variance prevented the FOM from converging when FW-CADIS was used. While investigating the behavior of one of these particles, a geometry error was discovered in the CAD model used by UW for its ITER benchmark. The 40-deg sector ITER model had a 5-cm gap at each side of the VV in the toroidal direction. The gap extended all the way through the 35-cm-thick inboard VV. Particles streaming through this gap caused the systematically high heating results for UW compared with the other parties participating in the benchmark. These particles were noticed only with FW-CADIS because the ADVANTG weight-window map was based on the KIT native MCNP model, which did not have the geometry error. The low-energy particles in front of the VV were assigned high weights because without the gap, they have a very low probability of reaching the inboard TFC without splitting. The streaming of these particles through the gap to the inboard TFC regions with the very low weights was not taken into account in the weight-window map. To correct the UW CAD model, the VV cells were extended toroidally to fill the gap. Figure 4 shows the VV and the surrounding void regions before and after correction of the UW CAD model.

As shown in Fig. 5, after the CAD geometry was corrected, the UW results agreed with those of the other parties. With 18-h MCNP simulations, the ten inboard TFC segments had nearly uniform statistical uncertainties between 3 and 4.5%. With the exception of the Pareto slope,[21] which was 2.4, the first inboard TFC segment passed all the MCNP statistical checks. Table II compares the FOM of DAG-MCNP runs in analog mode, with the MCNP WWG, and with FW-CADIS. The geometry error was corrected only in the last case.

TABLE II

Inboard TFC FOM Comparison

	Time (days)	Maximum Uncertainty (%)	Normalized FOM
Analog	121	5.9	1
UW (WWG)	11	3.6	30
UW (FW-CADIS)	0.77	4.5	275

TABLE III

Prompt Dose Rate Outside Bioshield

	Dose Rate (mrem/h)	Relative Uncertainty	Time (day)	Normalized FOM
MC (No CADIS)	0.48	76.7%	610.0	1
MC (CADIS)	0.30	4.80%	7.6	20 956
Denovo	0.18	280 million cells 1 h, 14 400 cores = 600 processor-days		

IV.B. Prompt Dose Rate During Operation

A point detector tally was used for calculating the prompt operational dose outside the bioshield. Table III shows the dose and the FOM of the point detector tally with and without the use of CADIS and the dose calculated deterministically with Denovo.

The point detector MC calculation without CADIS showed the extreme difficulty in obtaining reliable MC results without additional types of variance reduction. Even after 610 processor-days of computational time, the statistical uncertainty was 77%. The CADIS-based simulations achieved a statistical uncertainty of $<5\%$ and passed all of the MCNP statistical checks in $\sim$8 processor-days. Because of the high variance of the variance ($\sim$100%) of the MC calculation without CADIS, it is difficult to

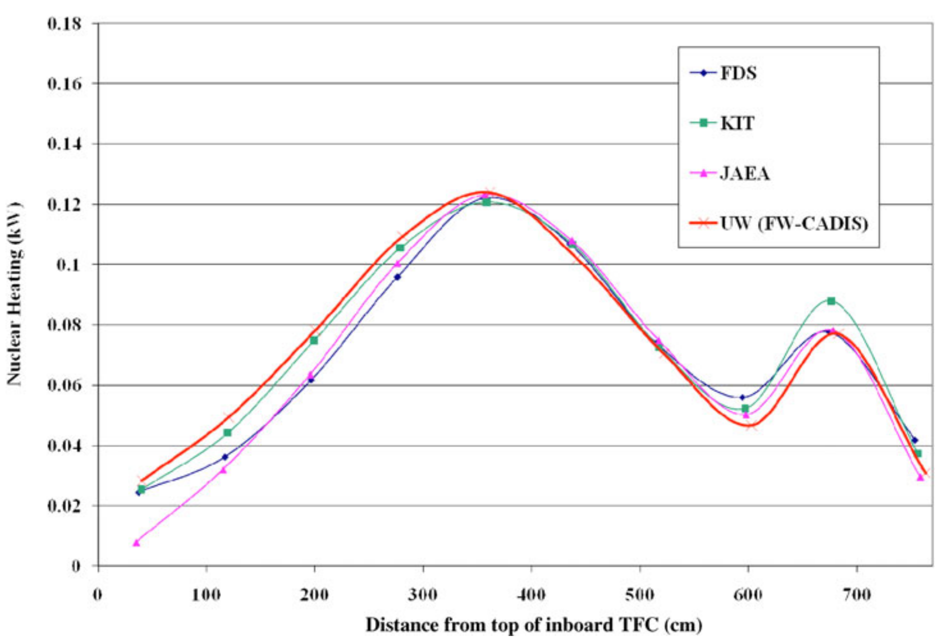

Fig. 5. Inboard TFC heating after correction of the UW CAD geometry.

calculate a reliable FOM for this case. However, the results suggest an improvement of approximately 21 000 because of the use of CADIS. The results of the MCNP simulation with CADIS and the very fine mesh Denovo calculation differ by a factor of 1.7. Discrepancies of this magnitude are not unusual—considering the 14 orders-of-magnitude total neutron flux attenuation, the discretized geometry model, the different solution methodology, and the use of a 46-neutron/21-gamma FENDL-2.1 multigroup library in Denovo versus the continuous-energy FENDL-2.1 library in MCNP.

IV.C. Total Flux

For this analysis, two Cartesian mesh tallies of uniform cubical mesh elements 20 cm on a side covering the whole 40-deg sector of the Alite03 model were used to tally both the total neutron and gamma fluxes. Figures 6 and 7 show the cumulative distribution functions (CDFs) of the neutron and gamma mesh tally uncertainties with and without FW-CADIS for 50-day MCNP runs. For the total neutron flux mesh tally, 99% of the voxels had nonzero values, and 78% had relative uncertainties <10% with FW-CADIS. In the analog case, only 59% of the voxels had nonzero values, and 10% had relative uncertainties <10%. For the total gamma flux mesh tally, 95% of the voxels had nonzero values, and 60% had relative uncertainties <10% with FW-CADIS. In the analog case, only 30% of the voxels had nonzero values, and 10% had uncertainties <10%.

V. CONCLUSIONS

Hybrid MC/deterministic and CAD-based MC techniques have been applied to calculate the total nuclear heating in the inboard leg of the TFCs, the prompt dose outside the bioshield, and the total neutron and gamma fluxes over a mesh tally covering the entire reactor. These problems that have always been viewed as too challenging to be addressed with either of the two approaches individually and required combinations of 1-D, 2-D, and 3-D analyses. The coupling of the hybrid with CAD-based MC has been demonstrated to significantly increase the efficiency of the neutronics M&S of complex geometries for which CAD-based MC methods are needed. It is reasonable to expect that these techniques can be successfully applied to other challenging simulation problems in ITER and other fusion systems.

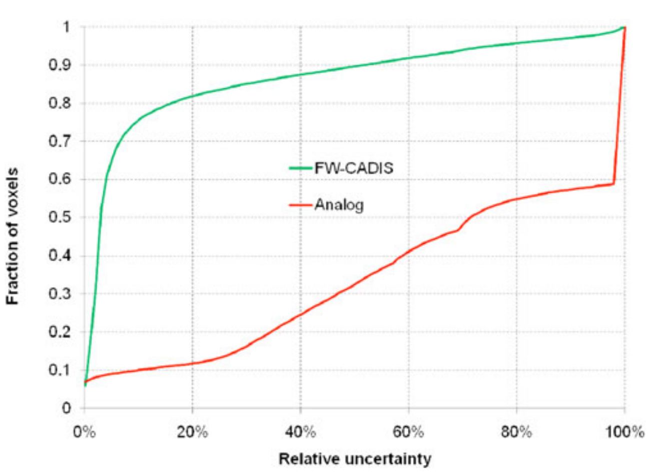

Fig. 6. Total neutron flux mesh tally CDF (50 days).

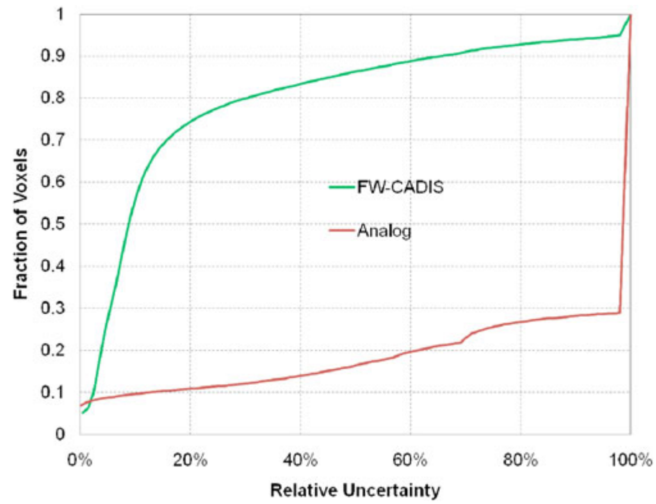

Fig. 7. Total gamma flux mesh tally CDF (50 days).

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