Evaluation of SNS Beamline Shielding Configurations Using MCNPX Accelerated by ADVANTG

Joel M. Risner[1], Seth R. Johnson, Igor Remec, and Kursat B. Bekar
Oak Ridge National Laboratory, MS 6170, P.O. Box 2008, Oak Ridge, TN 37831 USA

Abstract

Shielding analyses for the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory pose significant computational challenges, including highly anisotropic high-energy sources, a combination of deep penetration shielding and an unshielded beamline, and a desire to obtain well-converged "nearly global" solutions for mapping of predicted radiation fields. The majority of these analyses have been performed using MCNPX with manually generated variance reduction parameters (source biasing and cell-based splitting and Russian roulette) that were largely based on the analyst's insight into the problem specifics. Development of the variance reduction parameters required extensive analyst time and was often tailored to specific portions of the model phase space.

We previously applied a developmental version of the ADVANTG code to an SNS beamline study to perform a hybrid deterministic/Monte Carlo analysis and showed that we could obtain nearly global Monte Carlo solutions with essentially uniform relative errors for mesh tallies that cover extensive portions of the model with typical voxel spacing of a few centimeters. The use of weight window maps and consistent biased sources produced using the FW-CADIS methodology in ADVANTG allowed us to obtain these solutions using substantially less computer time than the previous cell-based splitting approach. While those results were promising, the process of using the developmental version of ADVANTG was somewhat laborious, requiring user-developed Python scripts to "drive" much of the analysis sequence. In addition, limitations imposed by the size of weight-window files in MCNPX necessitated the use of relatively coarse spatial and energy discretization for the deterministic Denovo calculations that we used to generate the variance reduction parameters. We recently applied the production version of ADVANTG to this beamline analysis, which substantially streamlined the analysis process. We also tested importance function collapsing (in space and energy) capabilities in ADVANTG. These changes, along with the support for parallel Denovo calculations using the current version of ADVANTG, give us the capability to improve the fidelity of the deterministic portion of the hybrid analysis sequence, obtain improved weight-window maps, and reduce both the analyst and computational time required for the analysis process.

Introduction

Shielding analyses for the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory (ORNL) have typically been performed using MCNPX [1] with limited variance reduction (source biasing and cell-based splitting and Russian roulette) that was largely based on the analyst's insight into the problem specifics. Development of the variance reduction parameters required extensive analyst time and was often tailored to specific portions of the model phase space. The cell-based splitting parameters, which were not energy dependent, also added considerable complexity to the model geometry, as many surfaces and cells were added solely to define splitting parameters, not to describe actual geometric details. These additional surfaces and cells not only required significant analyst time to develop but also slowed the particle tracking process.

Over the past several years, ORNL has pioneered the development and application of hybrid transport methods, which utilize "moderate fidelity" discrete ordinates transport calculations to generate variance reduction parameters (weight windows and consistently biased sources) that can significantly accelerate Monte Carlo simulations. These hybrid methods have been incorporated into the MAVRIC sequence (which employs the Monaco Monte Carlo code) in the SCALE code system [2] and into the ADVANTG code [3], which generates weight windows and biased sources that can be used in MCNP [4] and MCNPX.

In a previous unpublished study, we applied a developmental version of ADVANTG to an SNS beamline study. We showed that we could substantially reduce the computational time required to achieve acceptable relative errors for specific regions of interest in the model, and furthermore, that we could obtain nearly global Monte Carlo solutions with essentially uniform relative errors for mesh tallies that cover extensive portions of the model. While those results were promising, the process of using the developmental version of ADVANTG was somewhat laborious, reducing the potential for other users to readily apply ADVANTG to applications of this type. In the current study, we applied the production version of ADVANTG, which will soon be released through the Radiation Safety Information Computational Center, to analyze radiation levels for several configurations of SNS beamline 1B. Our results again demonstrate the effectiveness of the hybrid methodology, and with this new production version of ADVANTG, the analysis process is substantially improved.

The SNS beamline 1B model

The MCNPX model that we used for this study is based on a model that has been used to evaluate dose rates for beamline 1B (BL-1B), which contains the Nanoscale-Ordered Materials Diffractometer (NOMAD) experimental arrangement. A plan view of this model at the elevation of the centerline of BL-1B is shown in Figure 1. For this study we consider three scenarios: a "white" source (neutron energies up to 300 MeV) with an open beamline, a low-energy source (primarily neutron energies from 0.009–8.17 eV) with an open beamline, and a white source with the secondary carousel rotated to a closed position. The low-energy source represents the normal operating condition for locations downstream of the T0 chopper. The white source represents an accident condition in which none of the choppers are in operation.

Figure 2 shows details of the model in the vicinity of the T0 chopper when the secondary carousel is in the open position. Figure 3 shows the same configuration for a model in which cell-based splitting and Russian roulette are used for variance reduction. Both the spatial extent of the splitting cells and the importances assigned to each of those cells require significant amounts of analyst time and experience with the model to develop. Because these cells and importances are dependent on the model geometry, the source characteristics, and the location and extent of the desired tallies, they must be developed specifically for each scenario that is analyzed. Furthermore, the cell-based importances are not energy dependent, so a single set of importances is assigned to all energies for each particle type of interest.

Generation of weight windows and biased sources using ADVANTG

For the hybrid analysis of BL-1B, we applied the Forward-Weighted Consistent Adjoint Driven Importance Sampling (FW-CADIS) methodology in ADVANTG. In the FW-CADIS approach, ADVANTG first discretizes the MCNP (or MCNPX) model based on a user-supplied spatial mesh. A deterministic forward calculation is then performed using the spatially discretized model, a user-specified multigroup cross-section library, and user-specified angular quadrature data. This forward calculation is used to generate an estimate of the flux or response of interest throughout the model phase space. For this analysis, the response of interest was the total (neutron plus photon) dose rate. An adjoint source corresponding to the Monte Carlo tallies of interest is then constructed based on the deterministic forward solution, with the adjoint source magnitude in each spatial cell being the inverse of the response, and the adjoint source spectrum being the response function of interest (e.g., the flux-to-dose-rate conversion factors). An adjoint deterministic calculation is then performed to generate particle importances as a function of space and energy. Monte Carlo target weights and a consistently biased Monte Carlo source are then constructed from the importance values. Details of the FW-CADIS method can be found in [3] and [5].

ADVANTG includes six coupled (neutron/photon) multigroup cross-section libraries, but they all have an upper neutron energy limit of approximately 20 MeV. For these beamline evaluations we required a library with neutron energies up to 300 MeV. We used a collapsed version of the HILO2K library [6] with 33 neutron groups (with an upper energy of 300 MeV) and 11 photon groups for the scenarios with the high-energy source and a collapsed HILO2K library with 5 neutron groups and 11 photon groups for the low-energy source scenario.

The neutron source for the accident condition (the white source) is located 1 m from the moderator and is modeled as a plane source 12 cm high and 10 cm wide. The angular distribution is described with two angular bins, one from 0° to 1° and one from 1° to 2° with respect to the beamline axis. We used an auxiliary Python script in ADVANTG to define this anisotropic surface source for use with the Monte Carlo uncollided flux option in Denovo. This anisotropic source feature may be fully integrated in a future release of ADVANTG. The uncollided flux approach generates an accurate first-collision source which significantly reduces ray effects in the forward transport calculation. For the low-energy source (the normal operating condition), a plane source is located in the T0 chopper cavity and represents the neutrons that are transmitted through the T0 chopper. We used P_3 scattering, the default step characteristics spatial differencing scheme, and a Lobatto quadrature set with 16 “polar” angles and a triangular arrangement of azimuthal angles. Lobatto quadrature is not one of the standard options in Denovo, but it is ideally suited to this application because it provides a quadrature ordinate along the Z-axis, which, in our geometry modeling, is the axis of the BL-1B beamline. Use of the Lobatto quadrature for this application is essential, as it avoids the significant variation in target weights in the “near end” of the beamline (i.e., near the source location at 1 m) that occurs when a level symmetric S_{16} quadrature is used. This effect is illustrated in Figure 4, where target weights are shown along the beamline axis for four neutron energy groups from the deterministic calculation. Applying the weight windows developed using the S_{16} quadrature results in very poor tally convergence of the MCNPX simulation, as particles are split excessively before they have had any interaction as they are transported down the beamline.

MCNPX results

We generated weight windows and biased sources using ADVANTG for the three scenarios noted above: an open beamline with a white source, an open beamline with a low-energy source, and a white source in a configuration in which the secondary carousel is closed. We then used those weight windows and biased sources in MCNPX simulations. For the first two cases, we provide comparisons to earlier MCNPX calculations that employed cell-based splitting and rouletting. For the third case, we show only the ADVANTG results to illustrate the effectiveness of the hybrid approach in generating high-quality variance reduction parameters when significant model changes are made.

Figures 5 and 6 show mesh tally plots of the total dose rate and associated relative errors for a horizontal plane at the elevation of the beamline axis. The red contour lines on each plot are at 0.25 mrem/hr. The region outlined in blue in Figure 5 represents the “region of interest” for the original calculation, which is the portion of the model for which the cell-based splitting and rouletting parameters were developed to reduce the relative error. The hybrid results in Figure 6 show a very well-converged solution, with relative errors well under 10% over most of the solution space. The only locations for which the convergence is somewhat poor are at the beam stops for both beam lines. The beam stops are often evaluated separately, and it may be appropriate to do so with the hybrid method as well. Figures 7 and 8 show mesh tally plots for a vertical plane perpendicular to the BL-1B axis at the location of the sample position in the NOMAD detector vessel. The MCNPX run time for the original calculation was approximately 5000 CPU hours. The hybrid case used approximately 190 CPU hours for the deterministic calculations to generate the variance reduction parameters and approximately 1000 CPU hours for the MCNPX simulation.

Figures 9 through 12 show mesh tally results at the same locations as Figures 5 through 8, but for calculations with the low-energy neutron source at the T0 chopper location. Note that these results are used only for evaluation of dose rates downstream of the T0 chopper (i.e., locations beyond ~1620 cm on the Z-axis of the model). The hybrid solution again provides nearly uniform relative errors at all downstream locations except for the beam stop regions. The MCNPX run time for the original calculation was approximately 1300 CPU hours. The hybrid case used approximately 60 CPU hours for the deterministic calculations to generate the variance reduction parameters and approximately 480 CPU hours for the MCNPX simulation.

Finally, Figure 13 illustrates the total dose rate and associated relative errors for a vertical mesh tally along the BL-1B axis using the white source with the secondary carousel shutter rotated to the closed position. For the original cell-based splitting and rouletting analysis (which is not shown here), extensive model changes were required to construct splitting and rouletting regions that differed substantially between the open-shutter and closed-shutter geometries. For the hybrid case we simply applied a coordinate transformation to rotate the carousel shutter, made a simple refinement of the spatial mesh perpendicular to the beamline over the extent of the secondary shutter, and then ran the ADVANTG sequence to generate variance reduction parameters for this new configuration. No additional analyst time was required, and the variance reduction parameters again provided well-converged mesh tallies in almost all locations. This hybrid calculation used approximately 180 CPU hours for the deterministic calculations to generate the variance reduction parameters and approximately 1000 CPU hours for the MCNPX simulation.

Summary and conclusions

We have applied the ADVANTG code to perform a hybrid deterministic/Monte Carlo analysis of SNS beamline models using several combinations of beamline geometry and source energy distributions. In previous calculations that employed cell-based splitting and rouletting, each of those source/geometry combinations required extensive analyst time to modify the geometry description and develop corresponding splitting and rouletting parameters. By using the FW-CADIS hybrid method in ADVANTG, we were able to generate weight windows and consistently biased sources with very little additional analyst time required for each scenario. In addition to saving analyst time, the variance reduction parameters generated by ADVANTG provided well-converged nearly global solutions and did so with substantial reductions in the required MCNPX computational time. We also demonstrated the importance of using an appropriate quadrature for this type of application, in which particle transport is dominated by streaming along the beamline axis. For the BL-1B geometry, the use of Lobatto quadrature was crucial to the generation of weight windows that can be used with no additional user modifications. We also noted that the convergence of the ADVANTG-accelerated MCNPX calculations is somewhat poor in the beam stop area. This is probably due to target weight variations that cause rouletting followed by splitting along the beamline axis just prior to the beam stop. A separate analysis of the beam stop (rather than the essentially global approach that we used) may be a better technique for this region.

References

[1] D. B. Pelowitz, editor (April 2005), *MCNPX User's Manual Version 2.5.0*, LA-CP-05-0369, Los Alamos National Laboratory, Los Alamos, New Mexico.

[2] ORNL (June 2011), *SCALE: A Comprehensive Modeling and Simulation Suite for Nuclear Safety Analysis and Design*, ORNL/TM-2005/39, Version 6.1. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-785, Oak Ridge, Tennessee.

[3] S. W. Mosher et al. (2013), *ADVANTG – An Automated Variance Reduction Parameter Generator*, ORNL/TM-2013/416, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

[4] X-5 Monte Carlo Team (2003), *MCNP – A General Monte Carlo N-Particle Transport Code, Version 5. Volume I: Overview and Theory*, LA-UR-03-1987, Los Alamos National Laboratory, Los Alamos, New Mexico.

[5] J. C. Wagner, D. E. Peplow, and S. W. Mosher (2014), "FW-CADIS Method for Global and Regional Variance Reduction of Monte Carlo Radiation Transport Calculations", *Nucl. Sci. Eng.*, 176(1), pp. 37–57.

[6] R. A. Lillie and F. X. Gallmeier (2000), "HILO2K: A Coupled Neutron-Photon Transport Cross-Section Library for Neutron Energies up to 2000 MeV", Fourth International Topical Meeting on Nuclear Applications of Accelerator Technology, American Nuclear Society, Washington, D.C.

Figure 1: Horizontal cut of the SNS Beamline 1B (BL-1B) MCNPX model at the elevation of the centerline of BL-1B

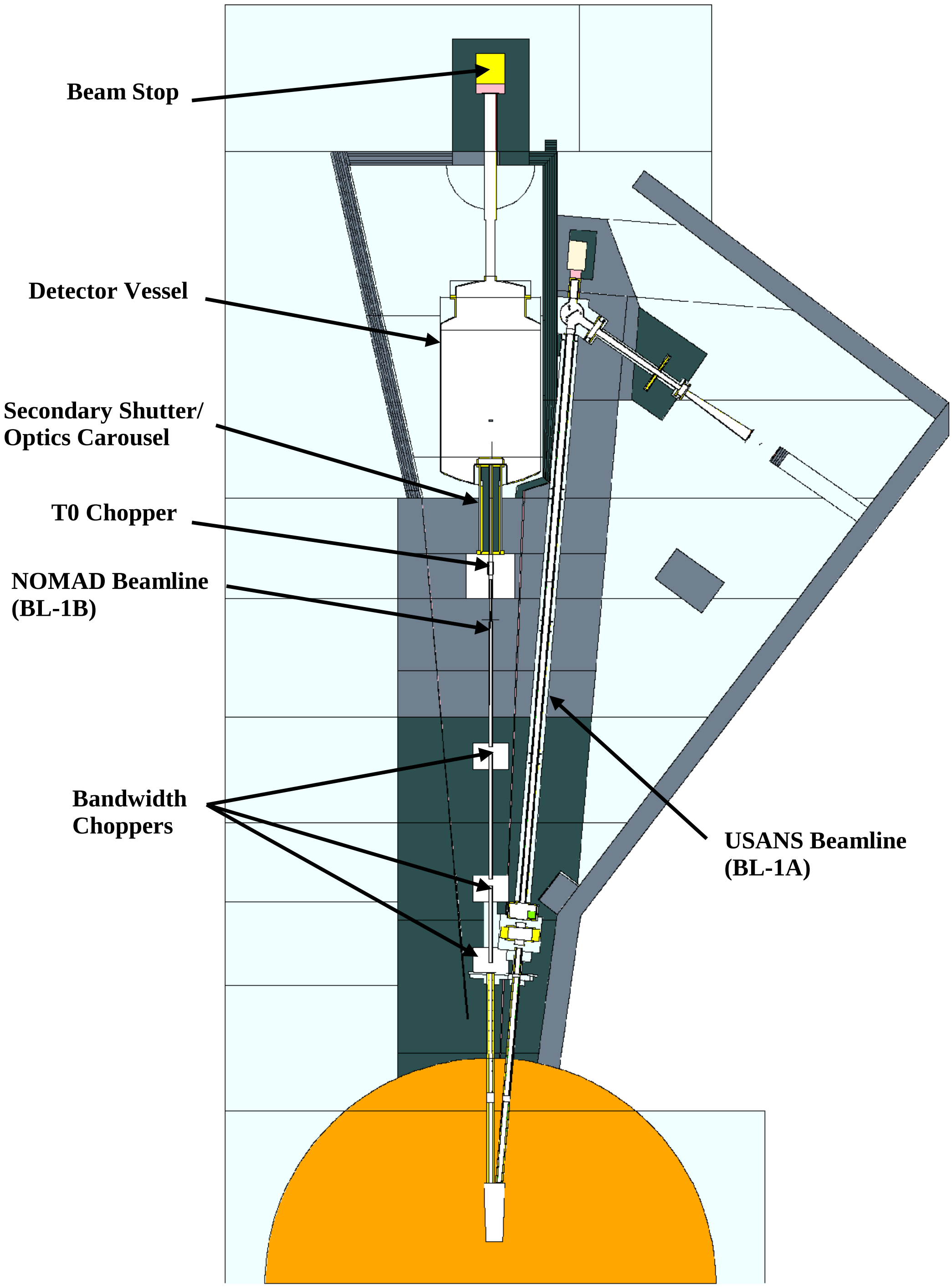


Figure 2: Horizontal cut of the SNS Beamline 1B model in the vicinity of the secondary shutter

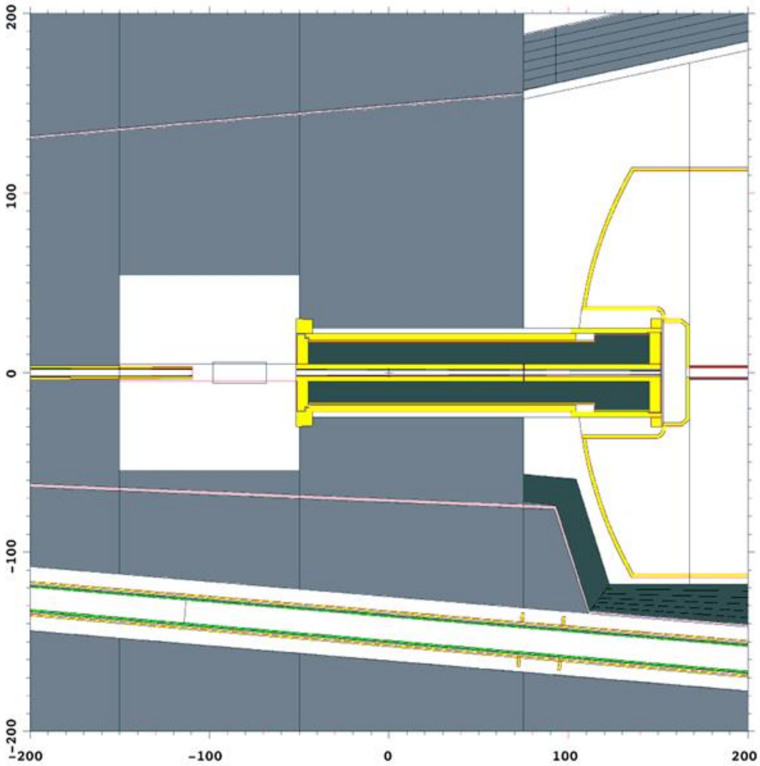


Figure 3: Horizontal cut of the SNS model in the vicinity of the secondary shutter with additional geometry details that are used only for cell-based splitting and rouletting

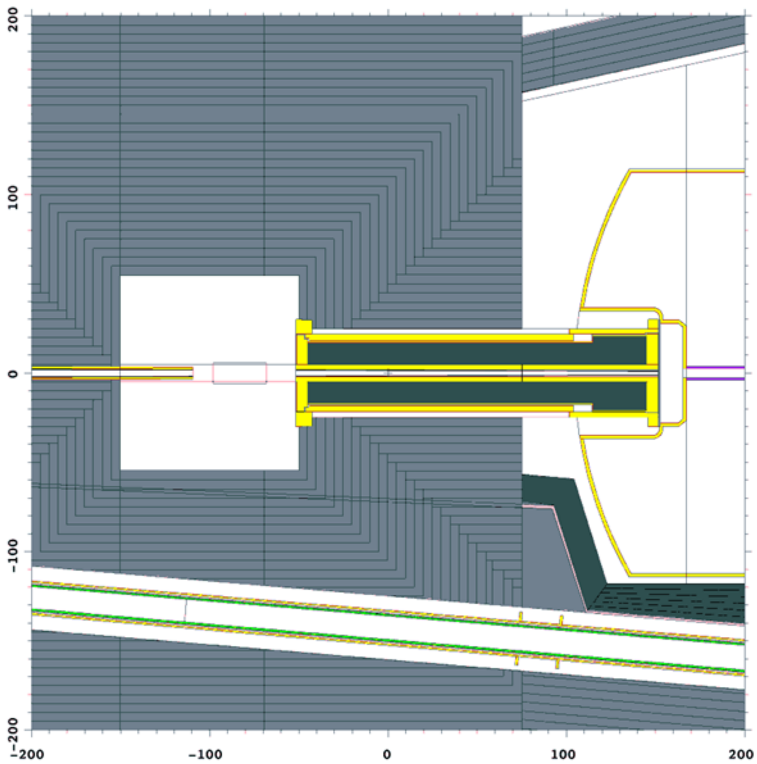


Figure 4: Neutron target weights along the beamline axis for four neutron energy groups using Lobatto-16 and level symmetric S_{16} quadrature. Note the significant variation in target weights along the "near end" of the beamline when the S_{16} quadrature is used. Use of the S_{16} target weights results in poor tally convergence in the MCNPX simulation.

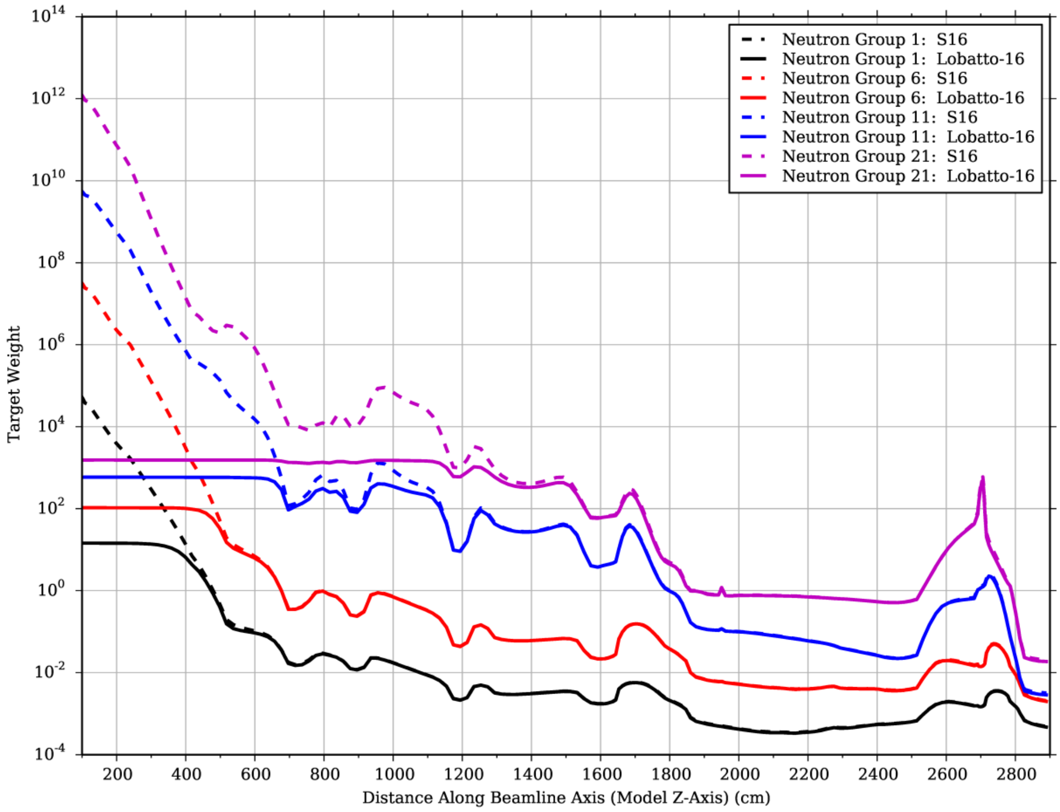


Figure 5: Total (neutron plus photon) dose rates and associated relative errors at the elevation of the centerline of SNS beamline 1B for the MCNPX cell-based splitting and rouletting solution with the white source. The "region of interest" for the calculation is outlined in blue.

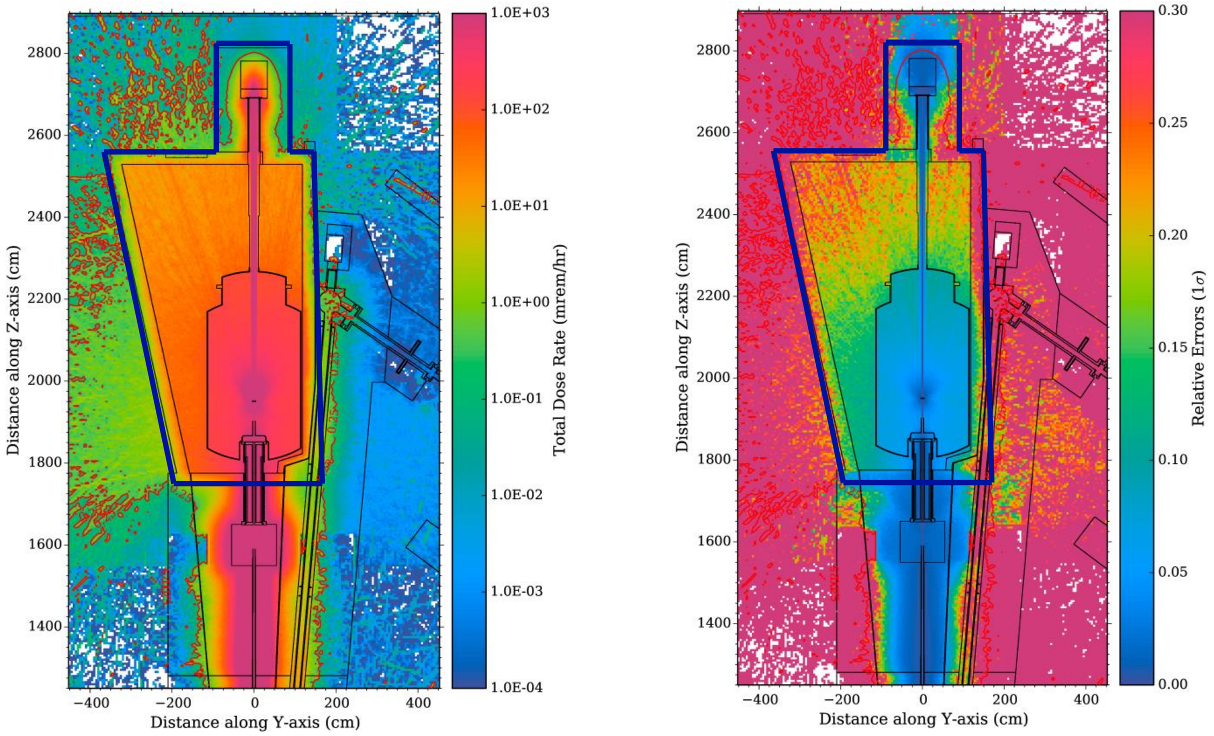


Figure 6: Total (neutron plus photon) dose rates and associated relative errors at the elevation of the centerline of SNS beamline 1B for the hybrid ADVANTG/MCNPX solution with the white source

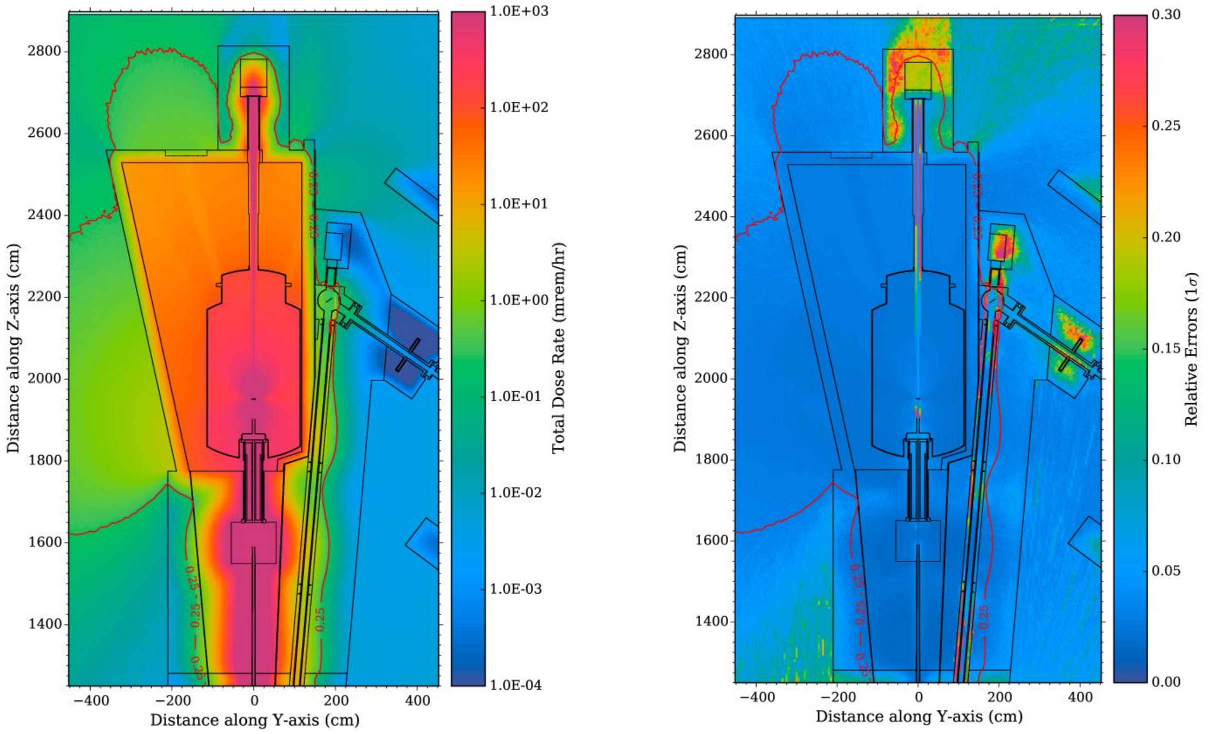


Figure 7: Total (neutron plus photon) dose rates and associated relative errors for a vertical mesh tally perpendicular to the SNS BL-1B axis for the MCNPX cell-based splitting and rouletting solution with the white source. The "region of interest" for the calculation is outlined in blue.

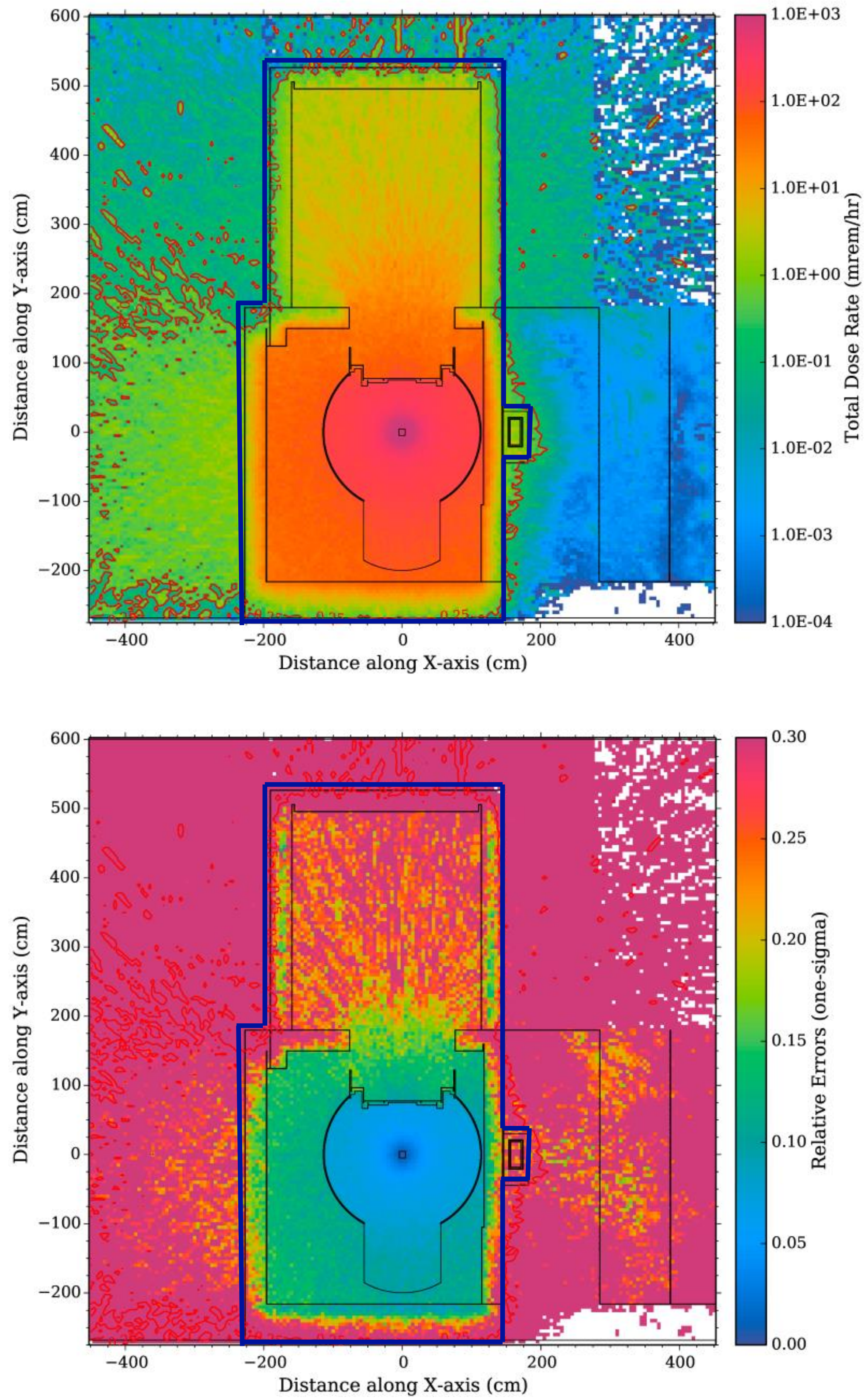
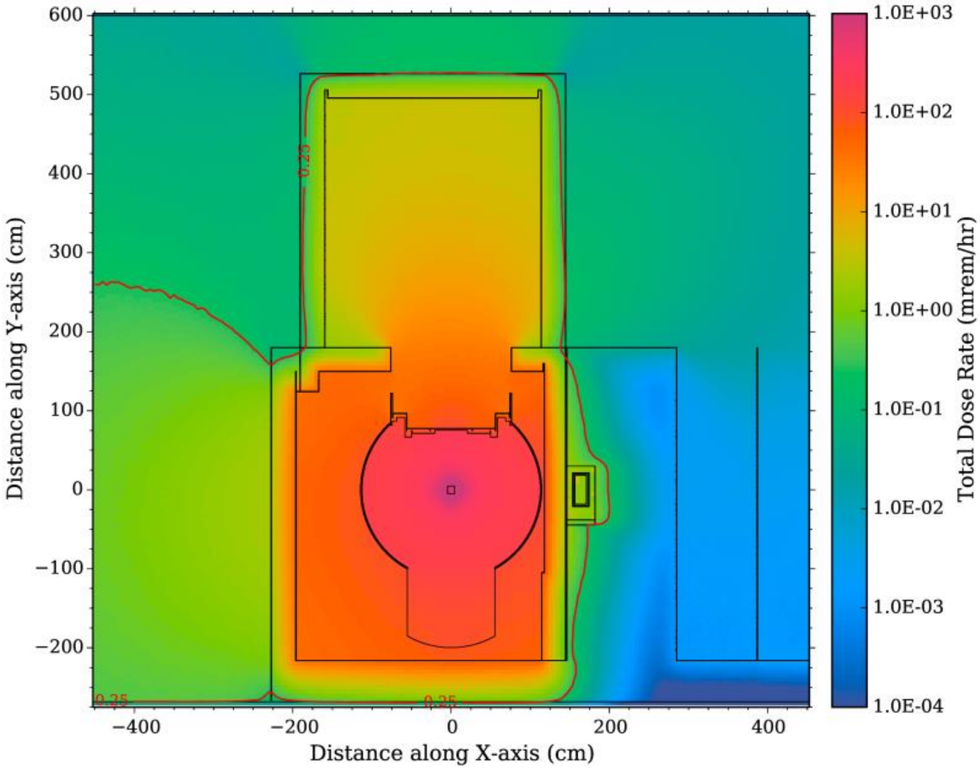


Figure 8: Total (neutron plus photon) dose rates and associated relative errors for a vertical mesh tally perpendicular to the SNS BL-1B axis for the hybrid ADVANTG/MCNPX solution with the white source



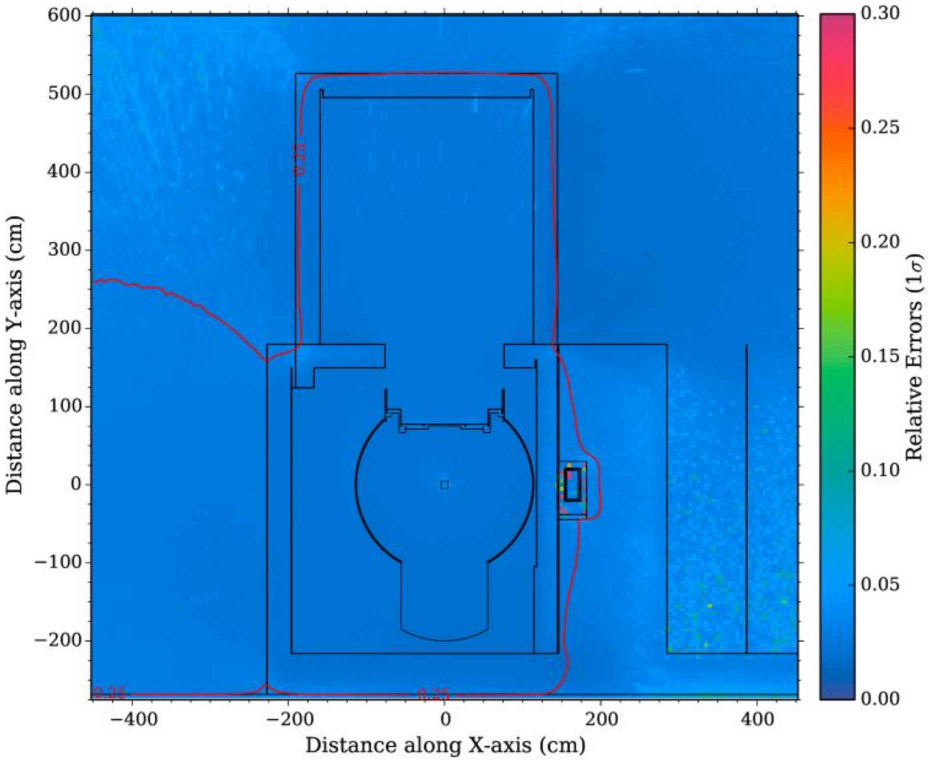


Figure 9: Total (neutron plus photon) dose rates and associated relative errors at the elevation of the centerline of SNS beamline 1B for the MCNPX cell-based splitting and rouletting solution with the low-energy source. The "region of interest" for the calculation is outlined in blue.

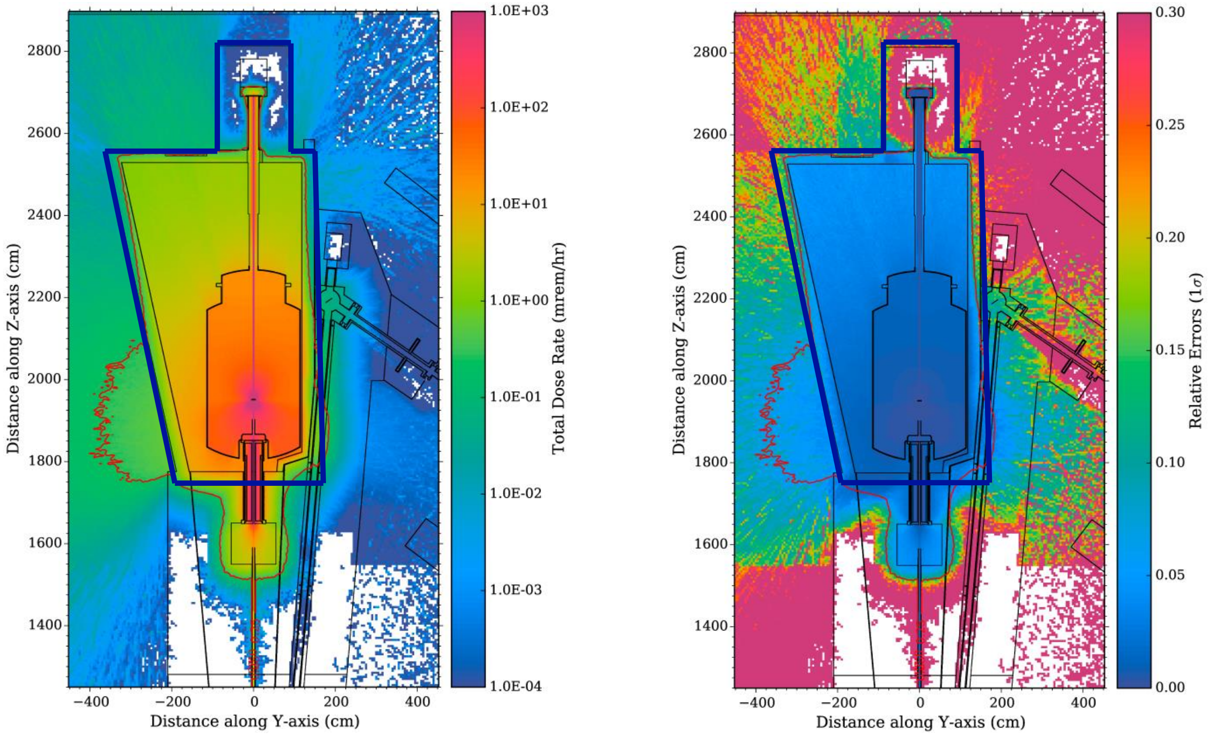


Figure 10: Total (neutron plus photon) dose rates and associated relative errors at the elevation of the centerline of SNS beamline 1B for the hybrid ADVANTG/MCNPX solution with the low-energy source

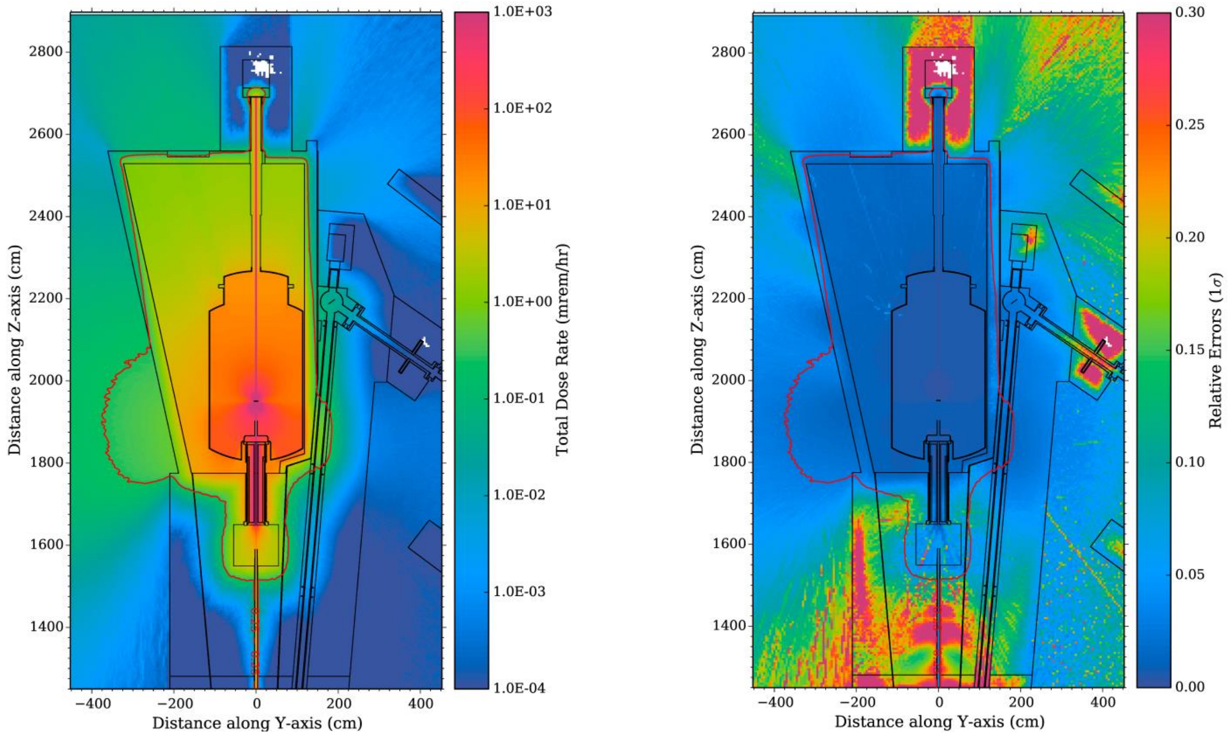
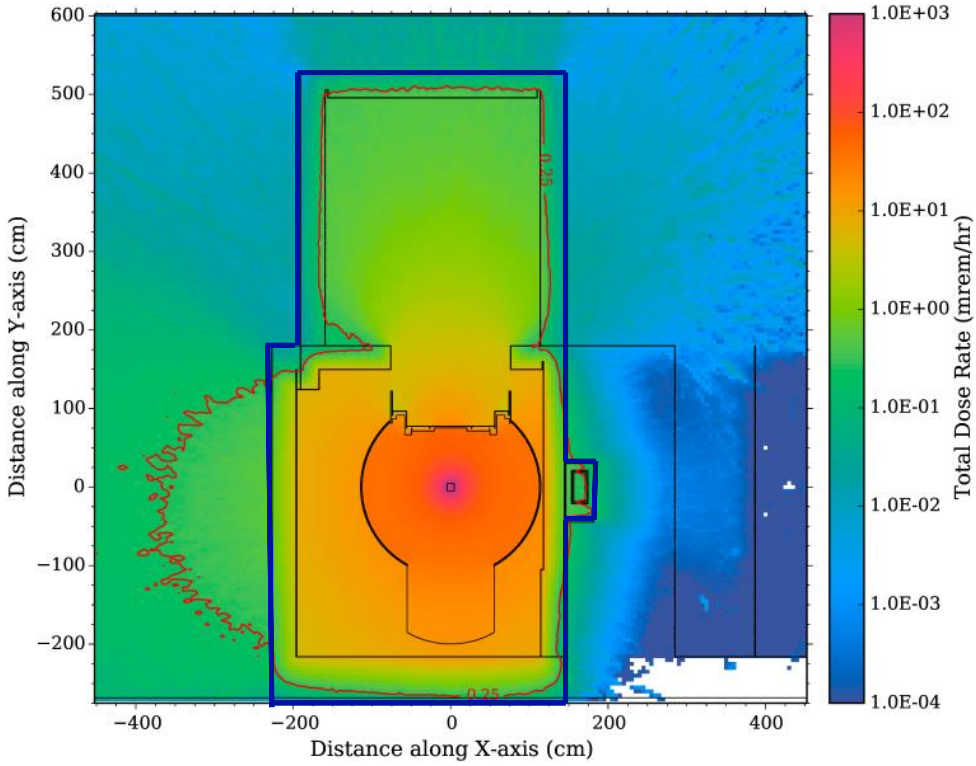


Figure 11: Total (neutron plus photon) dose rates and associated relative errors for a vertical mesh tally perpendicular to the SNS BL-1B axis for the MCNPX cell-based splitting and rouletting solution with the low-energy source. The "region of interest" for the calculation is outlined in blue.



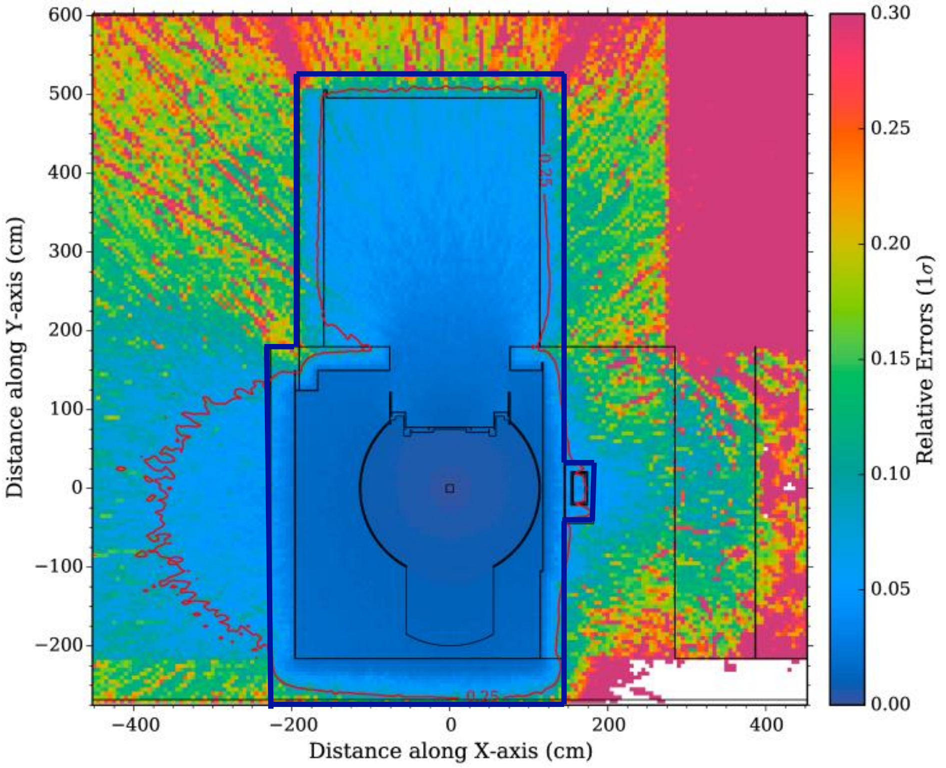
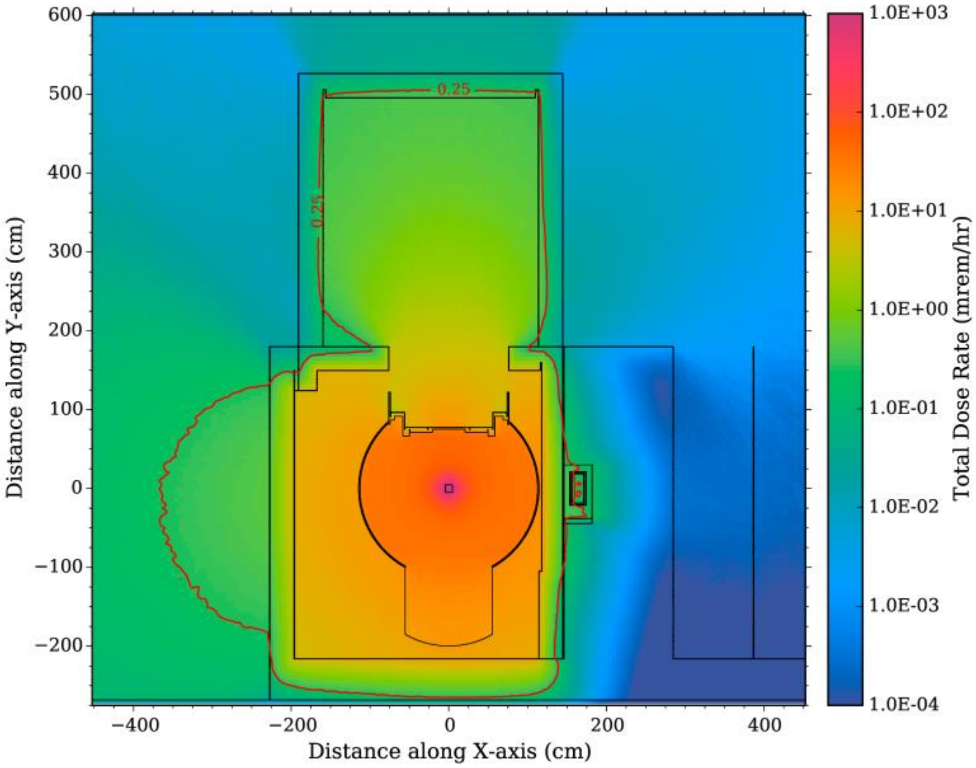


Figure 12: Total (neutron plus photon) dose rates and associated relative errors for a vertical mesh tally perpendicular to the SNS BL-1B axis for the hybrid ADVANTG/MCNPX solution with the low-energy source



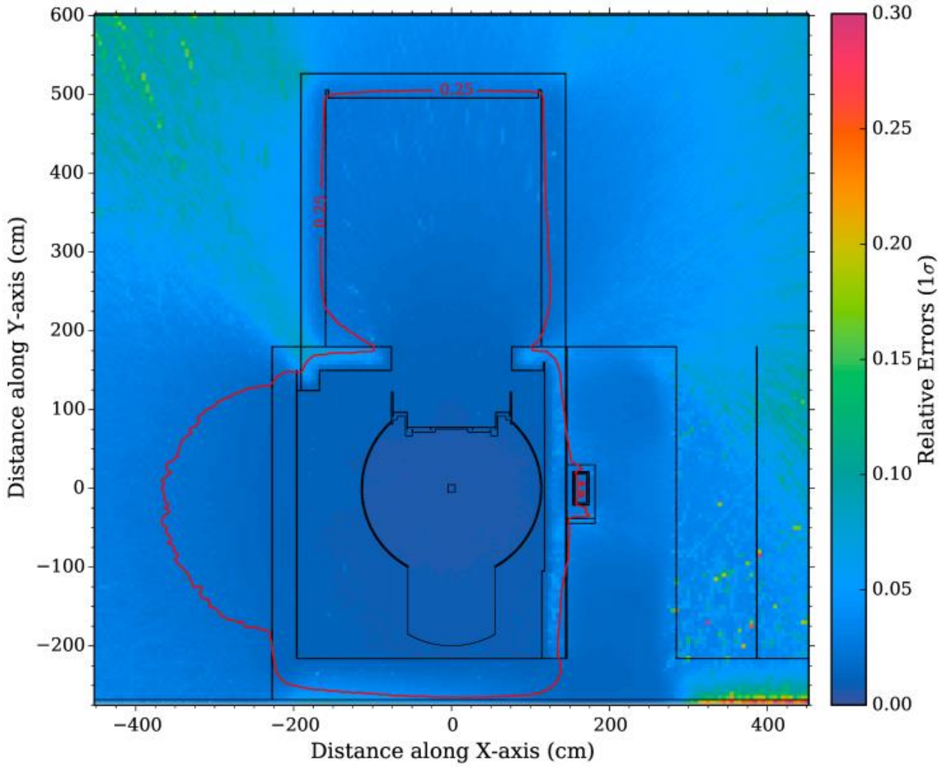


Figure 13: Total (neutron plus photon) dose rates and associated relative errors for a vertical mesh tally at the centerline of SNS beamline 1B for a hybrid ADVANTG/MCNPX solution with the white source and the secondary carousel closed