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Title: Evaluation of Attila and MCNP computational methods for dose and exposure estimation

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Evaluation of Attila and MCNP computational methods for dose and exposure estimation

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Table of Contents

1 Introduction

Radiation transport calculations are often used to estimate dose or exposure to components and personnel surrounding a radiation source. The sources for these calculations are decaying radionuclides within various nuclear materials. Historically, dose calculations use MCNP (Monte Carlo N-Particle) transport code as the primary particle transport tool without a secondary computational tool to validate the results from the MCNP simulations [1]. The goal of this study is to make an independent check of the Monte Carlo solution from MCNP6 Version 6.2.1 with the discrete ordinates solution from Attila 10.2.0 Beta 3. As an example problem for this study, water-filled, stainless-steel vessels, modeled with an unstructured mesh (UM) with both MCNP and Attila [2], are exposed to ^{252}Cf and ^{60}Co point sources. This report also includes a discussion of the limitations of unstructured mesh in a MCNP calculation.

Attila is an unstructured mesh-based discrete ordinates solver that relies on multi-group cross sections, sources, and response functions to solve for a solution. Attila uses linear-discontinuous finite element spatial differencing to methodically calculate the same quality of solution everywhere in the model [2]. One of the advantages of using the Attila discrete ordinates solver is that it uses the same unstructured mesh as the MCNP calculation and provides a discrete ordinates solution everywhere in the model. The goal of this report is to evaluate agreement between the high-fidelity MCNP simulations with the discrete ordinates solution from Attila.

2 Model Details

This section discusses the details of the model used in both the MCNP and Attila calculations along with the assumptions made in the calculations. The geometry and materials specifications are discussed in Section 2.1. Section 2.2 discusses the sources used in the Attila and MCNP calculations. The tallies used in the Attila and MCNP calculations are detailed in Section 2.3. This section details the inputs used in the calculations.

2.1 Geometry and Materials

This example geometry uses a stainless-steel vessel with 150-mL capacity filled with 100 mL of water. The vessel used in these example particle transport models is model number 304L-05SF4-150 from Swagelok and is shown if Figure 1.

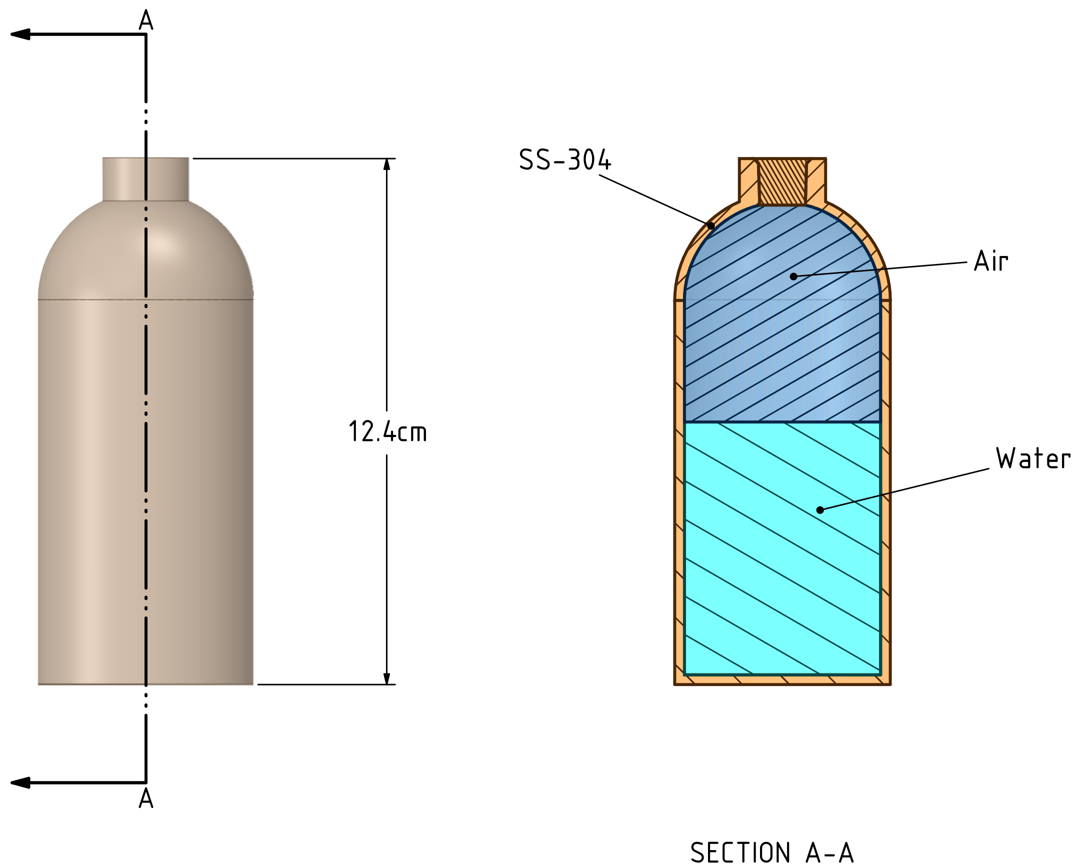

Figure 1: Overview of the cleaned vessel CAD model showing the various materials and overall dimensions.

Swagelok provides computer-aided-drafting (CAD) files for most of their products including vessel 304-05SF4-150. The CAD file imported into SpaceClaim (CAD software) cleanly and needed no "clean-up" such as repairing overlaps, gaps, ill-defined surfaces, etc. after import. The clean CAD model is then imported into Attila4MC and an unstructured mesh representation of the CAD file is generated. The meshing parameters are chosen to properly represent the original CAD geometry without significant material loss because of a coarse mesh representation. The vessel is filled with 100 ml of water, and the vessel wall and cap are SS-304. The air that fills the remainder of the vessel and surrounds the vessel and source is dry air. All material isotopic compositions and densities are from the PNNL-15870 Rev. 1 report [3]. The point source is located 10 cm and 25 cm away from the center of the vessel in separate cases, and is located on the plane with the center-of-mass of the water. Figure 2 shows a complete view of the entire model. The surrounding air shown in Figure 2 extends out by 1 m on all sides.

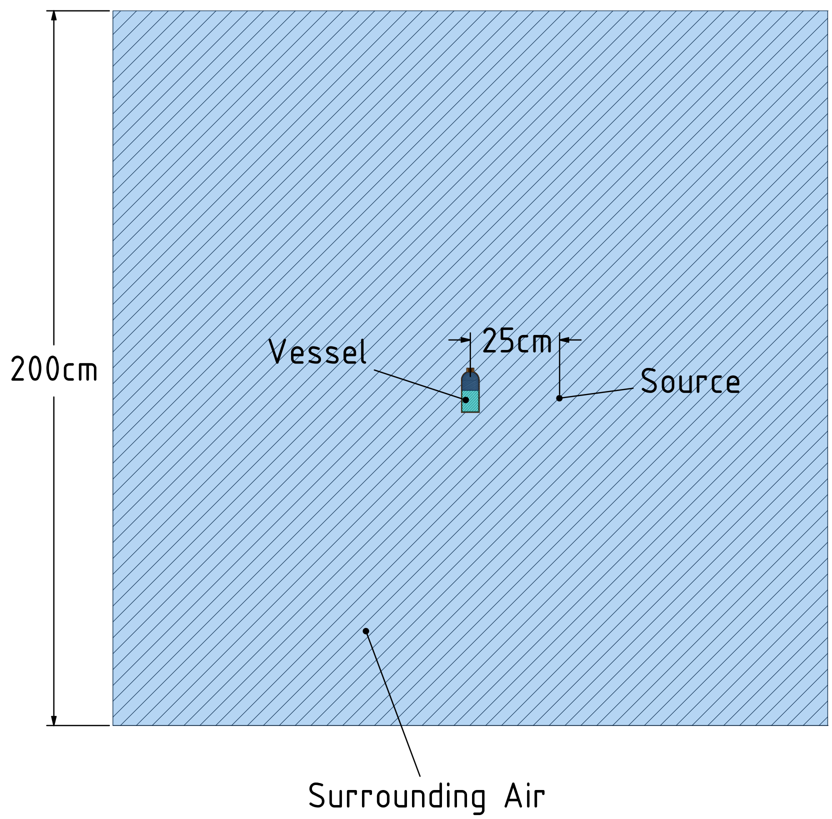

Figure 2: Overview of the CAD model used in both MCNP and Attila calculations showing the vessel and source placement as well as the surrounding air and overall dimensions.

The cross sections used in the MCNP calculations are continuous-energy ENDF/B-VIII.0 cross sections [4]. The Attila calculations use the Radion15 multi-energy group cross section set that is based on ENDF/B-VI cross section data.

2.2 Source Definition

The neutron source used in the example is an idealized Cf-252 neutron source, with the probability distribution functions shown in Figure 3. The photon source used in the example is an idealized Co-60 photon source, with the probability distribution functions for discrete gamma-ray lines shown in Figure 4. Both sources are scaled to a source strength of 1×10^6 particles/sec. The discrepancy between the Attila and MCNP ^{252}Cf is because of Attila binning the spectrum to match the energy group structure of the Radion15 cross section set. The MCNP source is continuous energy and the

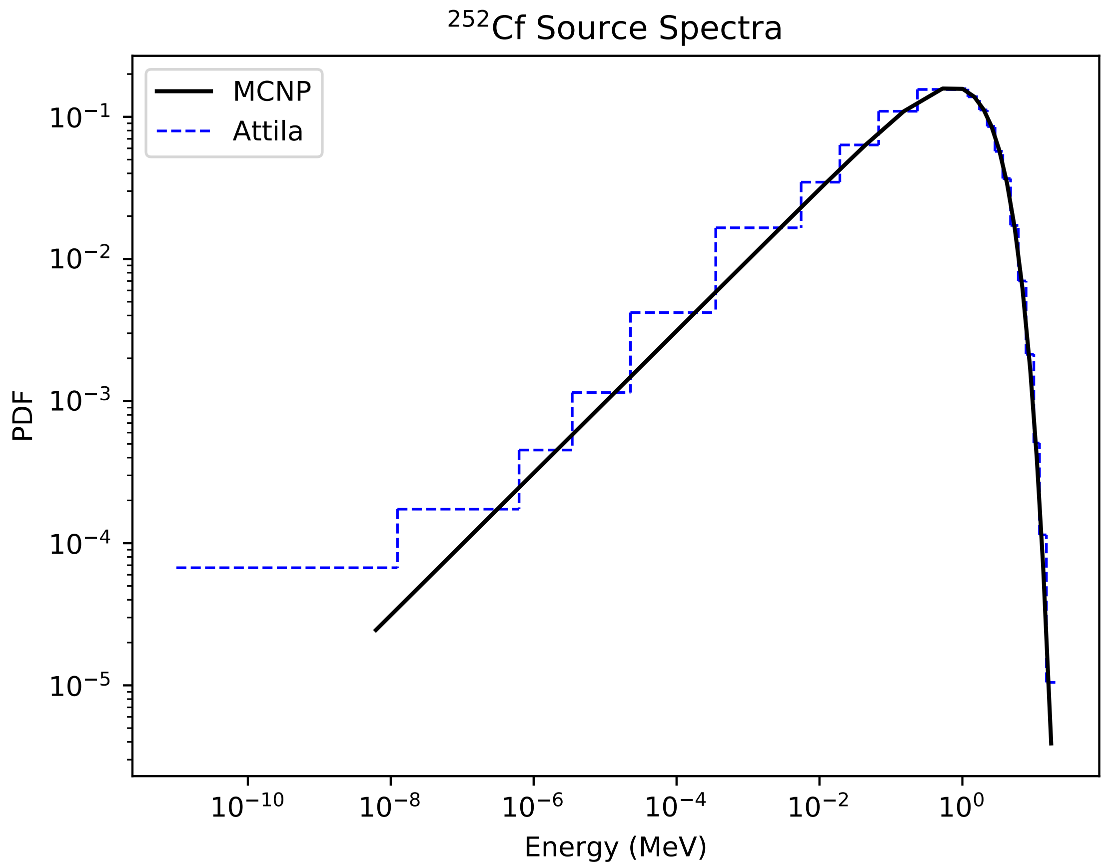

Figure 3: ^{252}Cf Source used in the MCNP and Attila calculations where the MCNP source was continuous energy and the Attila source was energy binned to match the Radion15 energy bin structure.

Attila source is discretely energy binned to match the Radion15 energy bin structure. Equation 1 shows the Maxwellian Fission Spectrum equation where $a = 1.18$ and $b = 1.03419$ in MCNP. The constants used to generate the Attila spectrum are not known. The points in the ^{60}Co source spectra, shown in Figure 4, are identical. The ^{60}Co source only consists of the discrete gamma emission lines.

$$p(E) = C\exp(-E/a)\sinh((bE)^{1/2}) \tag{1}$$

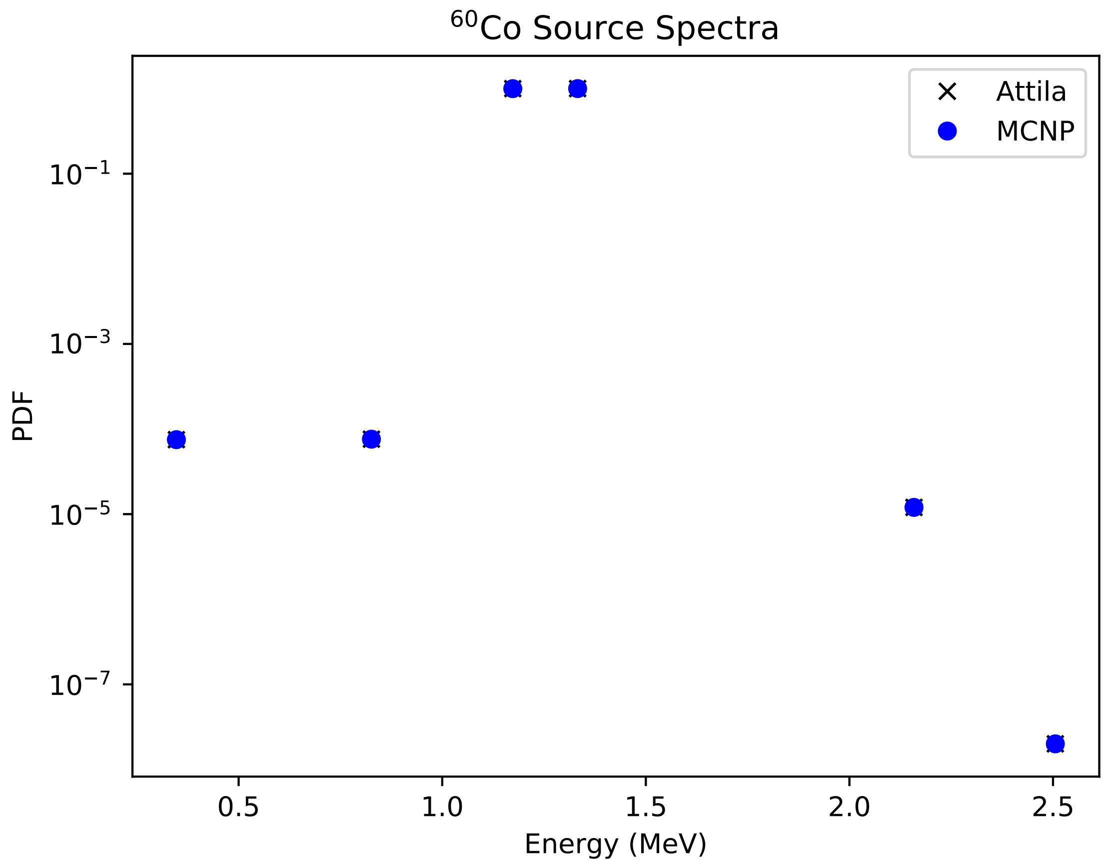

Figure 4: ^{60}Co Source probability distribution function for discrete gamma-ray energies.

2.3 Tally Definitions

To compare the MCNP and Attila calculations, three tally types were specified: 1-MeV silicon equivalent neutron fluence, silicon-equivalent ionization dose, and neutron flux. The 1-MeV silicon equivalent flux and silicon-equivalent ionization dose are calculated for the water in the vessel. Silicon-equivalent ionization dose and 1-MeV silicon equivalent flux conversion factors [5] are applied to both the MCNP and Attila calculated fluxes to produce Si-equivalent ionization dose and 1-MeV silicon equivalent neutron displacement flux, respectively. The E/EM cards in MCNP are used to apply the flux-to-dose functions to the volume-averaged flux tally on the vessel fill material. Figures 5 and 6 show the flux-to-dose conversion factors for the 1 MeV silicon equivalent neutron flux and Si-equivalent neutron dose used in both MCNP and Attila. MCNP is able to use the full fidelity flux-to-dose conversion factors, whereas the factors used in the Attila calculations must be energy binned in the Radion15 energy bin structure.

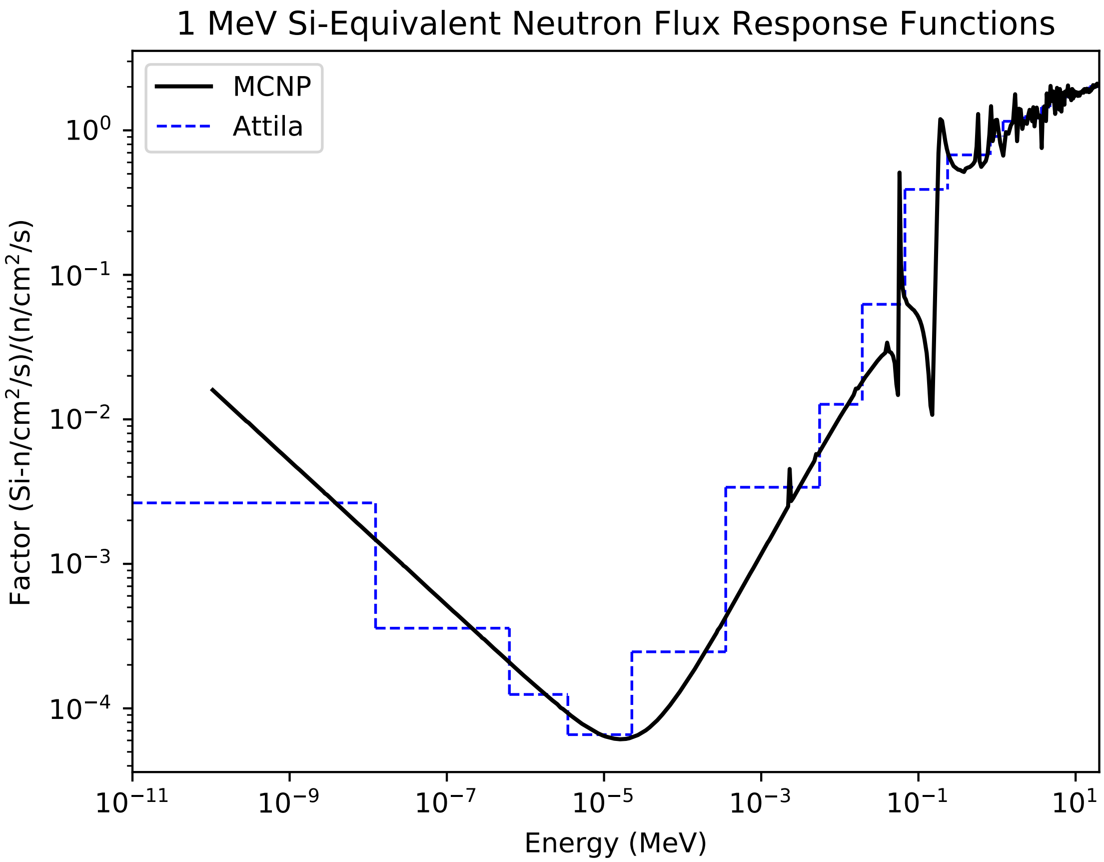

Figure 5: 1-MeV silicon equivalent neutron displacement flux response function comparison. The MCNP response function has relatively fine binning, whereas the Attila function was energy binned to match the Radion15 energy bin structure.

Silicon equivalent gamma dose is calculated in the water for the ^{60}Co. The flux-to-dose conversion factors applied to the gamma flux is based on ENDF/B-VII-1.0. Figure 7 shows the Si-Equivalent gamma flux response function used in both MCNP and Attila.

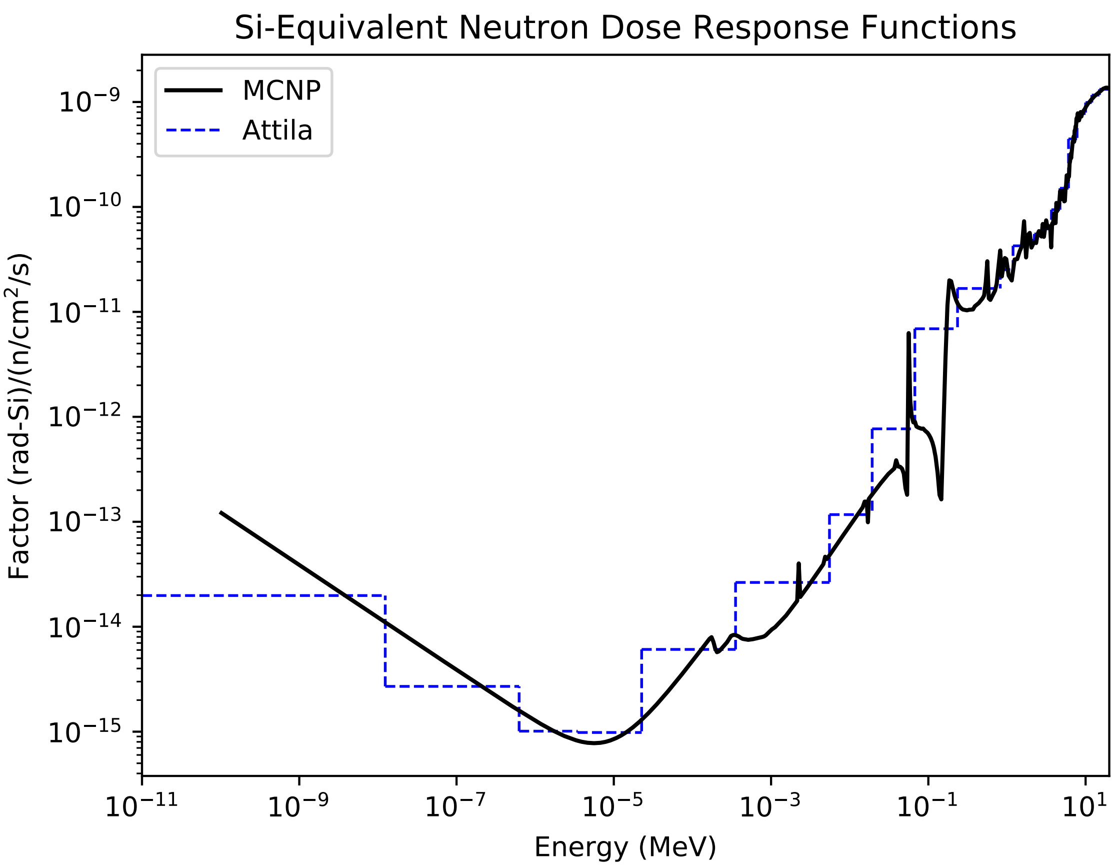

Figure 6: Silicon equivalent neutron dose response function comparison. The MCNP response function has relatively fine binning, whereas the Attila function was energy binned to match the Radion15 energy bin structure.

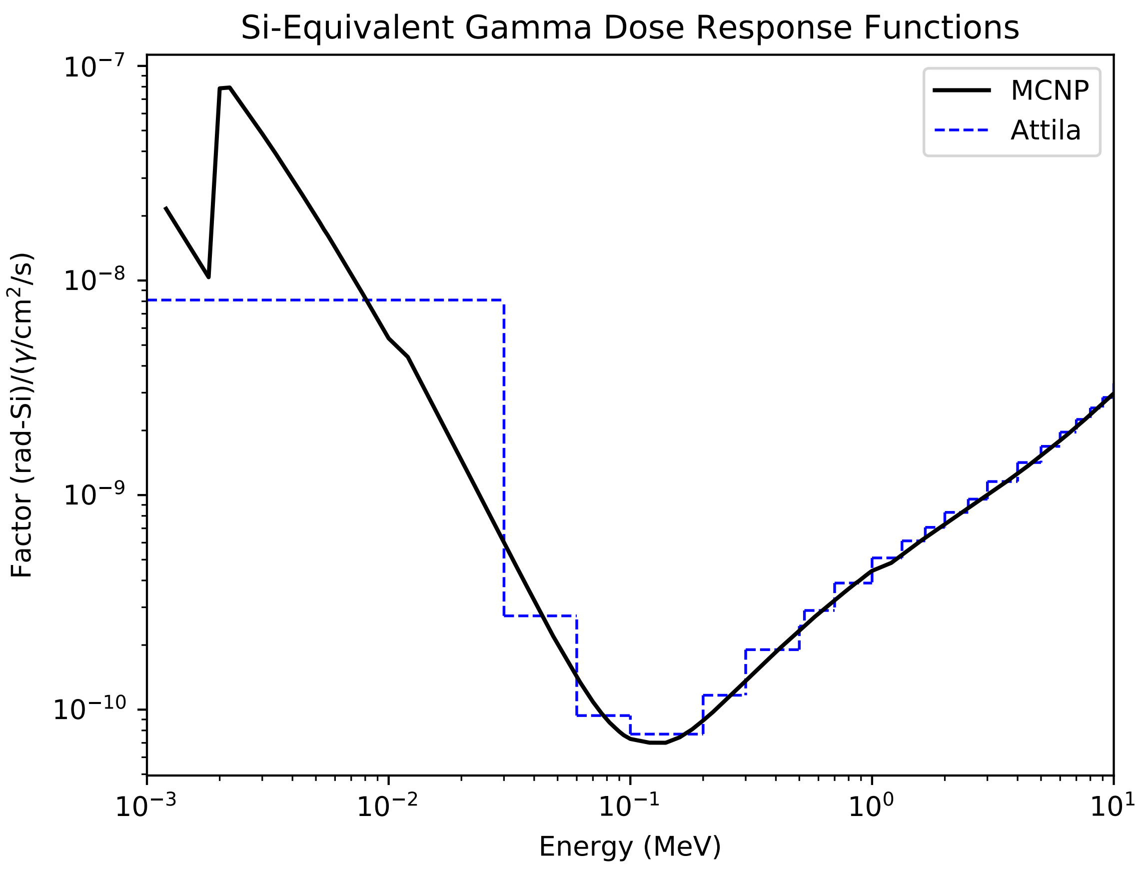

Figure 7: Si-Equivalent Gamma Dose Response Function Comparison. The MCNP response function has relatively fine binning, whereas the Attila function was energy binned to match the Radion15 energy bin structure.

3 Attila Calculation Details

This section describes the procedure for calculating the quantities of interest with the Attila discrete ordinates solver. The purpose of using this solver in conjunction with the MCNP calculations is to provide independent confirmation of the MCNP results.

In order to use a point source in the Attila solver, the first scatter distributed source (FSDS) methodology was implemented. The FSDS methodology executes an analytic ray-tracing routine from the source point to each node of the unstructured mesh to calculate both the uncollided flux and the first scattering source distribution for each mesh element. This first scattered source is then used as the source term in a normal discrete ordinance calculation, which will account for the downstream scattering components of the radiation field. Finally, these two solutions, uncollided flux (from the analytical ray trace routine) and collided (from the Sn solver), are summed using super position to arrive at the final directed flux solution for each particle type. Note that unlike MCNP, Attila solves the linear time-independent version of the Boltzmann transport equation deterministically for each particle type as a function of space (resolution dependent on the UM), angle (dependent on quadrature set and Pn order) and energy using the multi-group approximation.

The Radion15 cross sections, which were developed to be a general purpose shielding cross section set and was based on ENDF-VI [6] generation of cross section data, were used for both neutrons and photons. Radion15 includes 22 neutron groups and 25 photon groups for a collection of 44 common engineering elements and isotopes. The presented calculations use P5 scattering order for both neutrons and photons, which is the maximum order supported by the Radion15 cross section set. The Attila default of Triangular Chebychev Legendre quadrature specified with S24 (624 angles uniformly distributed over the unit sphere) was selected for both calculations. The combination of the specified unreconstructed geometry mesh, multi-group cross section set, the P5 scattering treatment, and the S24 quadrature set converged in a reasonable amount of time.

4 Simulation Results

This section contains the results from the MCNP and Attila calculations where the inputs to these calculations are detailed above. The results related to the neutron and photon sources are split into two separate subsections. Section 4.1 details the results using the neutron source and Section 4.2 includes the photon source results. Several of the figures in this section include "MCNP," "MCNP_Detailed," and "Attila" spectra. The dataset labeled "MCNP_Detailed" is tallied with a higher-fidelity energy bin structure. The datasets labeled "MCNP" and "Attila" are energy binned in the Radion15 energy group structure for direct comparison between MCNP and Attila. Both MCNP use the same fidelity of transport, but are tallied on different bin structures.

4.1 Cf-252 Spontaneous Fission Neutron Results

Table 1 shows the results of the ^{252}Cf neutron point source incident on the water inside the vessel and compares the results from MCNP and Attila. The quantities in Table 1 are energy-integrated quantities. The errors shown in Table 1 are the errors associated with the statistical nature of the Monte Carlo Method used by MCNP and do not account for systematic errors associated with the calculations. Systematic errors should be quantified in future work Based on the MCNP-calculated silicon equivalent neutron dose value, the time it would take a 1×10^6 n/s ^{252}Cf source located 25 cm away to achieve 1 mrad(Si) in the water inside the vessel is 41.5 hours.

Table 1: Volume-averaged Neutron Tallies on Water

Tally Name	MCNP 6.2.1	Attila	%-Difference $\frac{MCNP-Attila}{MCNP}\times 100$
Scalar Flux	$(1.410\pm0.003)\times10^2$ n/cm^2/s	1.399×10^2 n/cm^2/s	0.80%
Si-equiv. Ionization Dose	$(6.692\pm0.003)\times10^{-9}$ rad(Si)/s	7.169×10^{-9} rad(Si)/s	-7.1%
1-MeV Si-equiv. Flux	$(1.194\pm0.003)\times10^2$ n/cm^2	1.200×10^2 n/cm^2	-0.54%

MCNP and Attila agree within 7.1% for all tallies in the calculations. The scalar flux is within 0.8%, while the silicon equivalent Dose tally is 7.1%. Figure 8 shows the differential energy neutron flux spectra as calculated by MCNP and Attila, where the black spectrum labeled "MCNP Detailed" has very fine energy bins to capture the details of the energy dependent neutron flux, and the red and blue spectra labeled "MCNP" and "Attila," respectively, are binned to the same Radion15 cross section energy bin structure. The "MCNP" and "Attila" spectra are mostly in agreement for each energy bin. Perfect agreement is not expected because one method is continuous in energy and one is discretized.

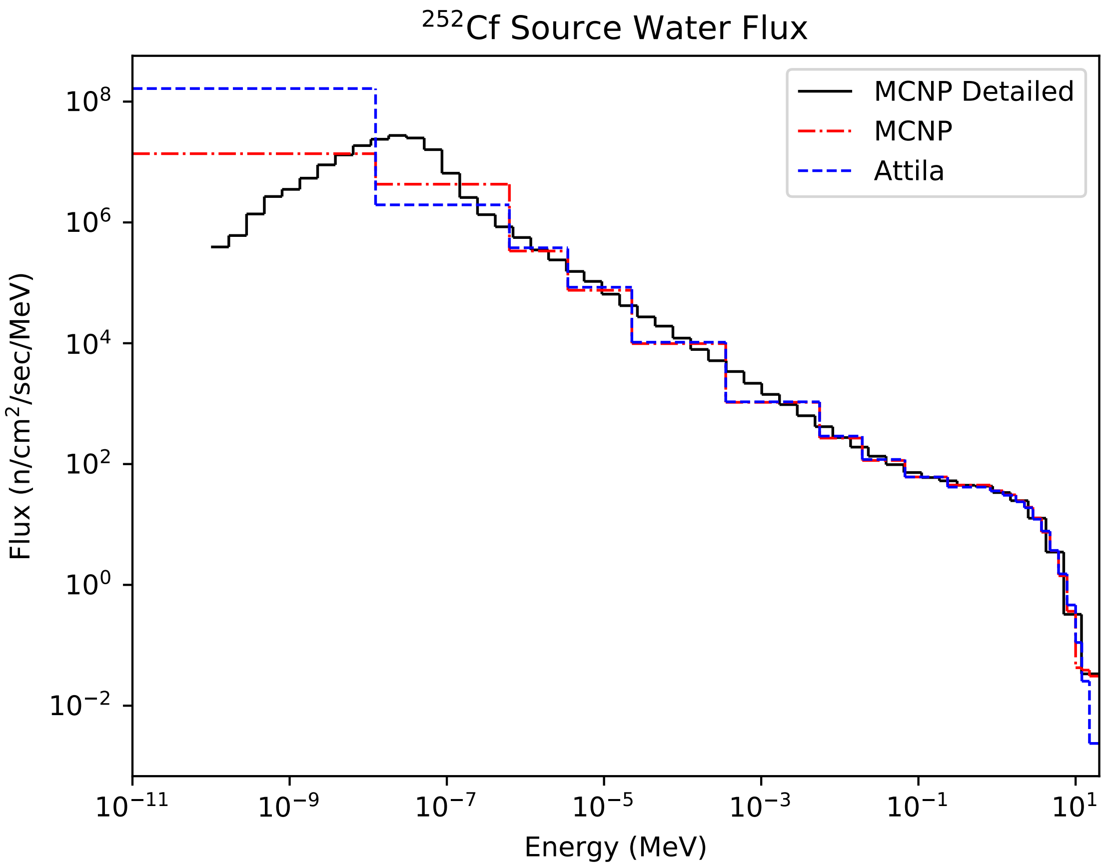

Figure 8: Differential neutron flux spectra results from MCNP and Attila. The MCNP results are shown for fine binning and for binning on the Radion15 structure.

Figure 9 shows the differential energy neutron dose spectra with the three spectra presented in the same way as Figure 8. The 7.1% difference in the energy-integrated dose values can be attributed to the discrepancy in the lowest energy bin dose values between MCNP and Attila.

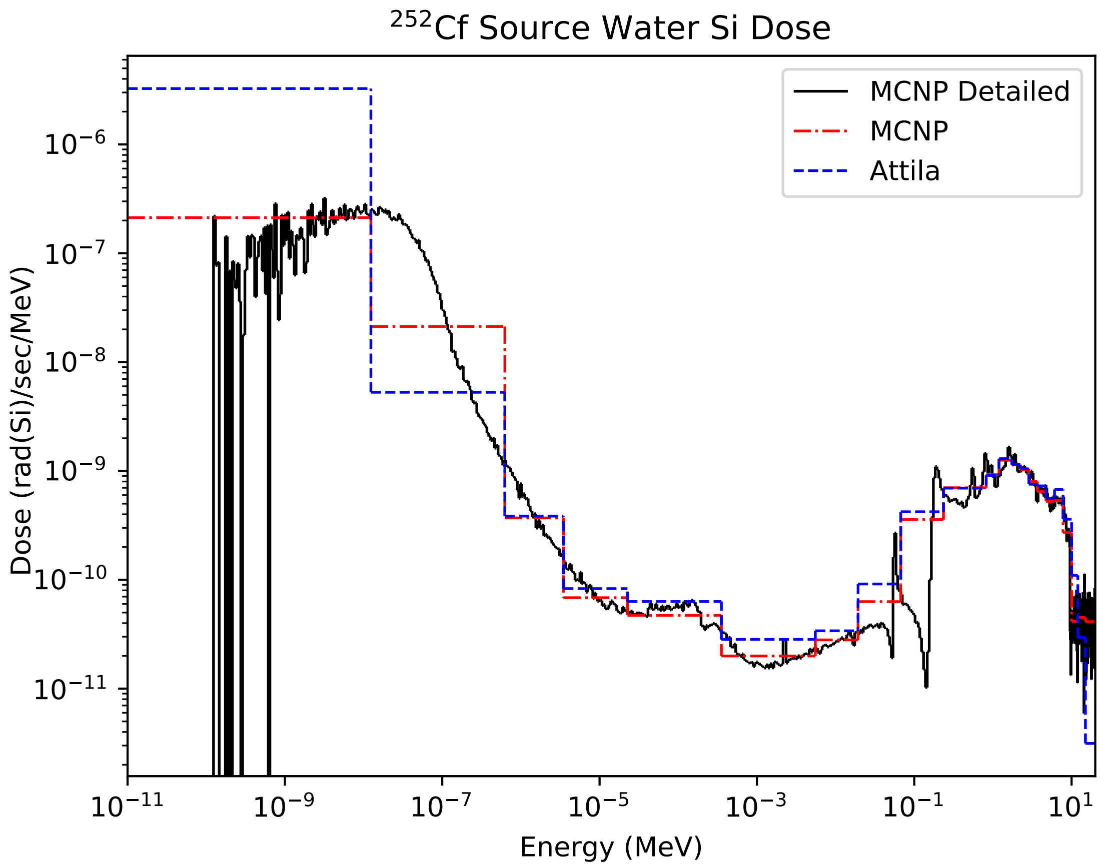

Figure 9: Differential Si-equivalent neutron dose spectra results from MCNP and Attila. The MCNP results are shown for fine binning and for binning on the Radion15 structure.

4.2 ^{60}Co Gamma-ray Results

Table 2 shows the results of the ^{60}Co gamma-ray point source incident on the water inside the vessel and compares the results from MCNP and Attila. The quantities in Table 2 are energy-integrated quantities. The scalar flux agrees to $\approx$0.51% while the Si-Equivalent Dose has a discrepancy of $>$10%. Based on the MCNP-calculated Si-equivalent gamma dose value, the time it would take a 1×10^6 n/s ^{60}Co source located 25 cm away to achieve 1 mrad(Si) in the water inside the vessel is 4.72 hours.

Table 2: Volume-averaged Gamma Tallies on Water

Tally Name	MCNP 6.2.1	Attila	%-Difference $\frac{MCNP-Attila}{MCNP} \times 100$
Scalar Flux	$(1.332 \pm 0.003) \times 10^2$ γ/cm^2/s	1.326×10^2 γ/cm^2/s	0.51%
Si-Equivalent Dose	$(5.88 \pm 0.01) \times 10^{-8}$ rad(Si)/s	6.52×10^{-8} rad(Si)/s	-10.9%

Figure 10 shows the gamma flux spectra for MCNP and Attila. The "MCNP" and "Attila" spectra agree except for the lowest and highest energy bins. These differences may be attributed to a difference in cross sections. The Radion15 cross sections are fission-spectrum weighted and are derived from ENDF/B-VI.1 cross sections. ENDF/B-VIII.0 is used to calculate the "MCNP" and "MCNP Detailed" spectra shown in Figure 10.

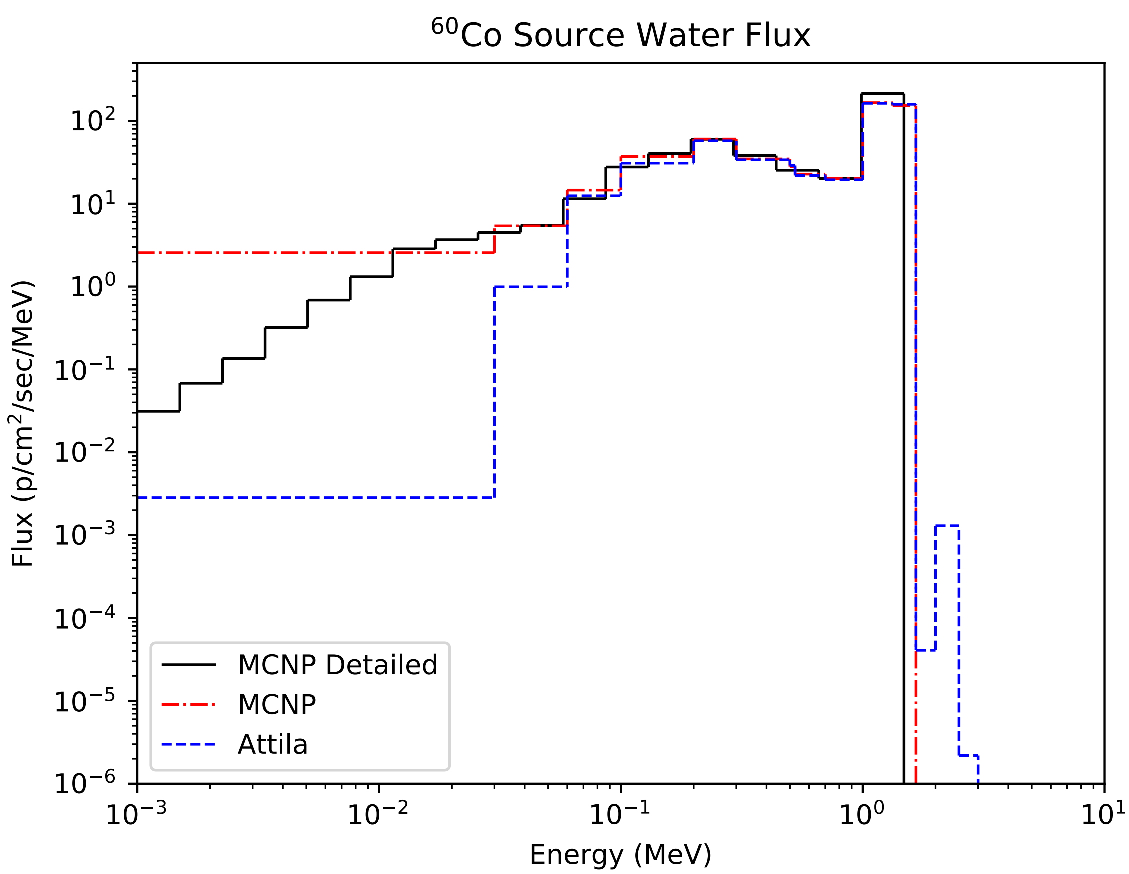

Figure 10: Differential gamma-ray flux spectra results from MCNP and Attila. The MCNP results are shown for fine binning and for binning on the Radion15 structure.

The differences in the differential gamma flux spectra shown in Figure 10 manifest themselves in the discrepancies between the “MCNP” and “Attila” spectra shown in Figure 11. The “MCNP Detailed” spectrum shows the resonances in the gamma spectrum that the coarse energy bin structure of the “MCNP” and “Attila” spectra average. At first glance, the reader may suspect that the energy-integrated Si-equivalent dose as calculated by MCNP would be larger than the Attila-calculated value. However, the slight discrepancy in the higher energy bins leads the Attila-calculated energy-integrated Si-equivalent dose to be higher than the MCNP-calculated value by 11%.

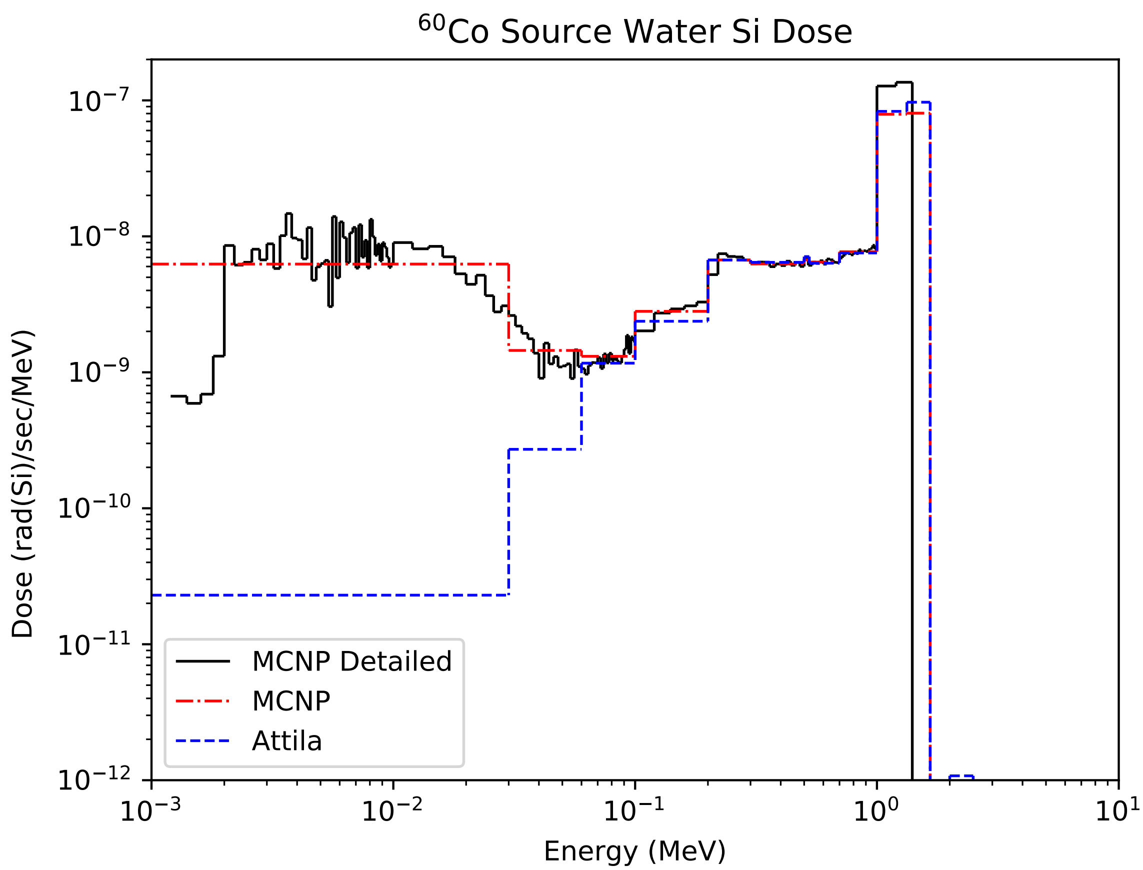

Figure 11: Differential Si-equivalent gamma dose spectra results from MCNP and Attila. The MCNP results are shown for fine binning and for binning on the Radion15 structure.

5 Conclusions

A vessel from the Swagelok Company filled with 100 ml of water is used to compare the dose results between MCNP V. 6.2.1 and Attila discrete ordinates solver. This work showed that the

Attila discrete ordinates solver agrees reasonably with the MCNP calculation, serving as an independent check on the MCNP calculations. The scalar flux values for both neutrons and gammas as calculated by MCNP and Attila agreed within 1%. However, when a flux-to-dose conversion factor is applied to the Attila-calculated flux, the discrepancies between the MCNP and Attila-calculated values exceeded 10% for the photon source and 7.1% for the neutron source. The discrepancies between MCNP and Attila are attributed to the coarse binning of the response functions and a difference in cross sections. Based on the discrepancies between MCNP and Attila, Attila is suitable for a rough independent check of the MCNP calculation.

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