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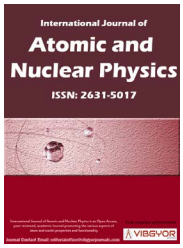
Improved MCNP Simulation Considering Neutron Angular Distribution and its Experimental Verification



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Abstract

Adeuterium-deuterium (DD) neutron generator has been simulated with MCNP 6.2. Two methods of simulating the emission of the neutrons created by the generator have been utilized: One with an isotropic emission of resultant neutrons and a second (anisotropic) accounting for the angular and energy distribution of resultant neutrons. The isotripic source was simulated using data generated by the DROSG-2000 program. A series of gold foils were irradiated at three different geometries around the neutron generator and the results compared to those produced from the two simulation methods. At zero degrees in the laboratory frame, both methods of simulation were shown to be equally valid. As the irradiation angles deviated from zero degrees, the anisotropic simulation method maintained accuracy while the isotropic simulation increased in error.

Keywords

MCNP, Simulation, Neutron activation analysis, Deuterium-deuterium generator

Introduction

Monte Carlo (MC) methods are very powerful and useful in the simulation of a variety of nuclear interactions. Simulation allows the development, optimization, and improvement of processes without having to actually operate equipment, expose people to radiation, or to allocate physical resources to these tasks. One important caveat to MC is that the simulation model must be as accurate as possible for the derived results to be worth while and meaningful. Many variables can affect the simulation model including the source specification, the description of the interaction environment, and the output data that is recorded (tally). In this work, we focus on one aspect of the model, that of the source specification.

The simulation that we have developed is of a deuterium-deuterium (DD) neutron generator. The generator works by accelerating deuteron ions to a kinetic energy of 110 keV and focusing them into a deuterium plasma that is produced on the surface of a solid target coated with titanium dioxide. Some of the ions undergo a fusion reaction (Q value = 3.2688630 MeV) that generates neutrons $\left({}^{2}\mathrm{H} + {}^{2}\mathrm{H} \rightarrow {}^{4}\mathrm{He} \rightarrow {}^{3}\mathrm{He} + n\right)$. The resultant neutrons pass through a moderator and are used for neutron activation analysis irradiations of various materials. Neutrons emitted at zero degrees in the laboratory frame from this reaction have a kinetic energy of 2.87434 MeV. However, as one deviates

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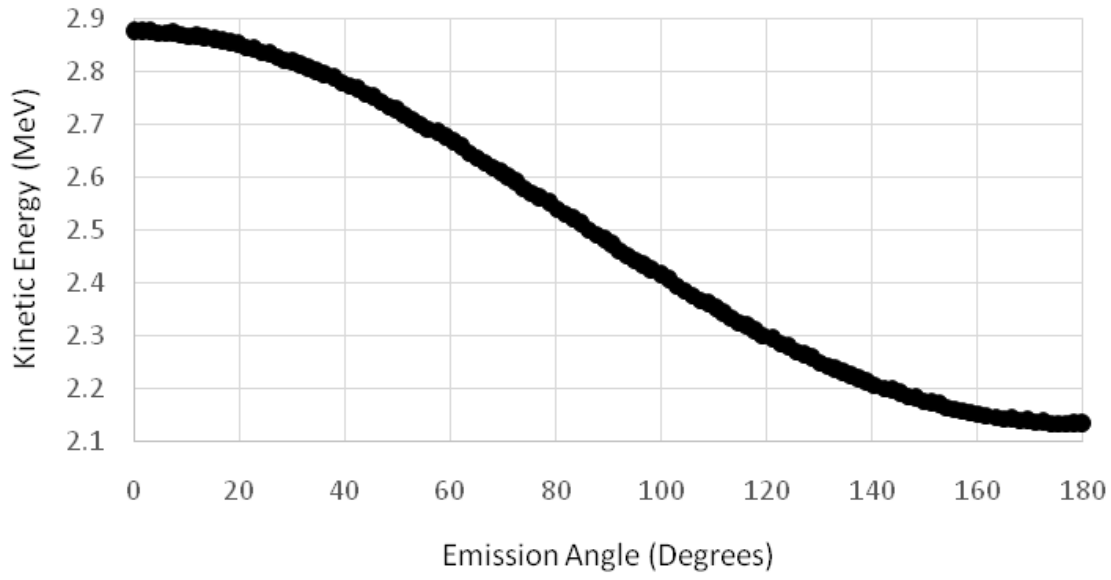

Figure 1: Neutron kinetic energy angular distribution.

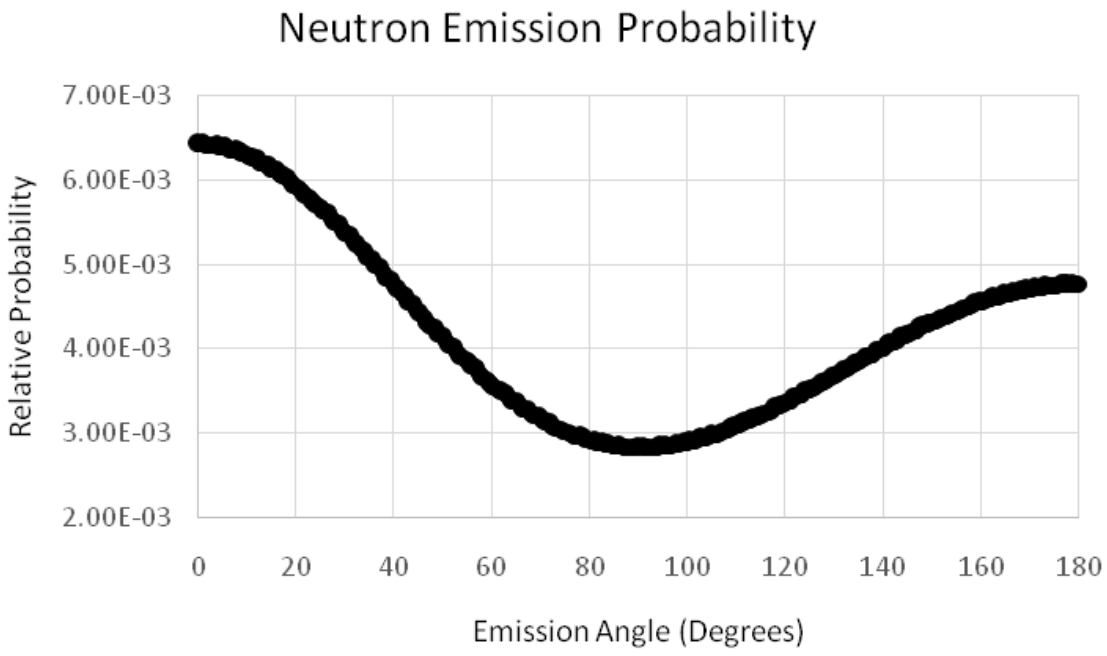

Figure 2: Relative neutron emission probability per angle.

from zero degrees, the neutron kinetic energies vary down from 2.87434 MeV and the probability of neutron emission also changes, as displayed in Figure 1 and Figure 2, respectively [1].

Understanding and accounting for neutron kinetic energy differences and emission probabilities per angle is important for simulation of the activation process. Neutron activation is strongly dependent on the kinetic energy of the interrogating neutrons. As neutrons interact with the irradiation environment, their kinetic energies change, thus affecting the probability of their capture by the material under analysis. To increase the probability of activation, neutron kinetic energies are reduced with moderating materials. Additionally, reflecting materials are placed around the irradiation chamber with the goal of scattering neutrons that have passed through, back towards the analysis sample.

Simulation allows the types, amounts, and placement of neutron moderator and reflector materials to be optimized on the computer, without the need to perform guess and check experiments. Optimal moderator and reflector materials and locations will change as different materials are analyzed with neutron activation, since neutron capture cross sections are dependent on the particular nuclide(s) under examination. Optimizations for new sample identities can be completed through simulation. Additionally, when irradiating a large volume sample, the absolute amount of activation will vary as intersecting neutrons will be incident from many angles and with a variety of kinetic energies as they emerge from moderating and reflecting materials. Simulation allows the experimenter to make predictions concerning activation, regardless of sample size or geometry. These predictions can be used to determine experimental variables such as the quantity of sample mass or volume that must be irradiated. In order to make valid predictions about the experimental setup, the simulation model must be as accurate as possible.

MCNP 6.2 actually contains cross section tables that include data for light ions (protons, deuterons, tritons, helions, and alphas) incident on low atomic number materials [2]. This allows the direct simulation of nuclear reactions involving light ions, such as the DD reaction. In other words, the source simulation in MCNP 6.2 could simply be a deuteron beam impinging on a deuterium target. MCNP 6.2 cross section tables would determine the resultant neutron energies at each angle of emission. Unfortunately, for bombarding ions with low kinetic energies, the fusion reaction is relatively inefficient. The number of generated neutrons produced by the simulation is a very small fraction per source particle. This means a simulation would have to run massive numbers of source particles to produce useful, significant amounts of neutrons. The neutron generator used in our laboratory typically accelerates deuterons to 110 keV. The fusion process is improbable enough at this energy that there feasibly is not enough computer time to produce a simulation result with an acceptable amount of error. The reaction is more probable at higher kinetic energies and it is possible to directly simulate it using MCNP 6.2. In the case in which direct simulation is not feasible, one must simulate the reaction after it has taken place. This means defining the simulation source not as deuterons interacting with deuterium but as neutrons being emitted from the point of generation.

The simulation of source neutrons can be performed in several different ways and we have chosen to investigate two possible specifications. The simplest method is to assume an isotropic emission of neutrons, all with the same energy and equal probabilities of emission per angle. The second, and much more complex method, is to determine the neutron yields and energies at all possible angles and to code them directly into the simulation. We refer to this second method as the anisotropic method.

In this paper we report on the ability of both methods to simulate the outcome of an actual neutron activation irradiation. An experiment in which gold foils were irradiated in three different geometries was conducted and compared to the relative amounts of activation predicted by each simulation method. Comparisons were made to determine if the two methods of source specification produced equivalent results. If a significant difference were found between the two methods, the results of the experiment would determine which is the superior method.

Materials and Methods

Monte carlo simulation

The Monte Carlo N-Particle (MCNP) Version 6.2 code, developed by Los Alamos National Laboratory (LANL) was used for simulations. MCNP Version 6.2 allows the simulation of a variety of particles, including light ions such as deuterons. For this project, a model was developed of the Adelphi DD-109 DD neutron generator in our laboratory, as shown in Figure 3. The simulation included a detailed and accurate inclusion of all reflector and moderator materials surrounding the generator as well as the support structure for these materials. Figure 4 is a visualization of a portion of the generator and surrounding materials created in the MCNP input file.

Two versions of this model were produced. The geometry of the model remained constant but two separate source specifications were developed. The first source specification was the simplest: That of an isotropic point source of neutrons, starting at the titanium target material inside the generator. The neutrons were all started with the same kinetic energy of 2.45 MeV and were emitted isotropically. The value 2.45 MeV is typically stated as the kinetic

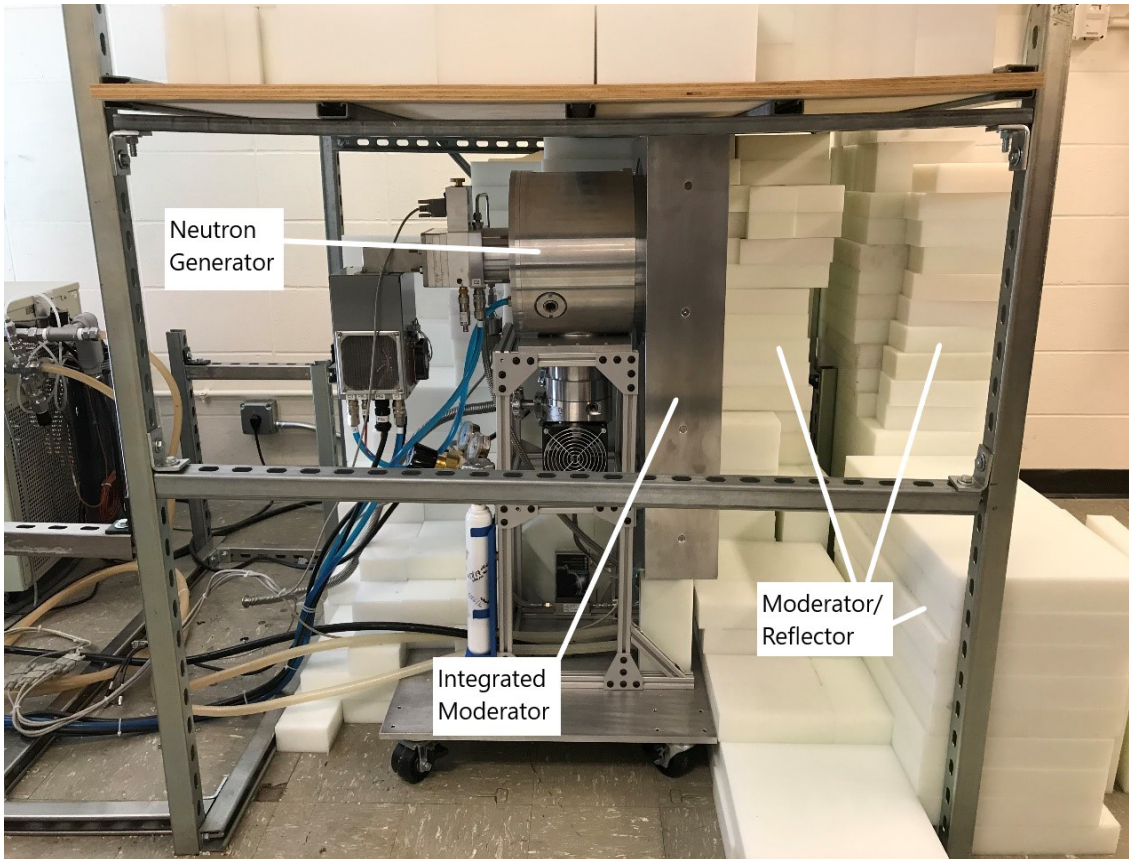

Figure 3: Adelphi DD-109 neutron generator (moderator/reflector partially removed).

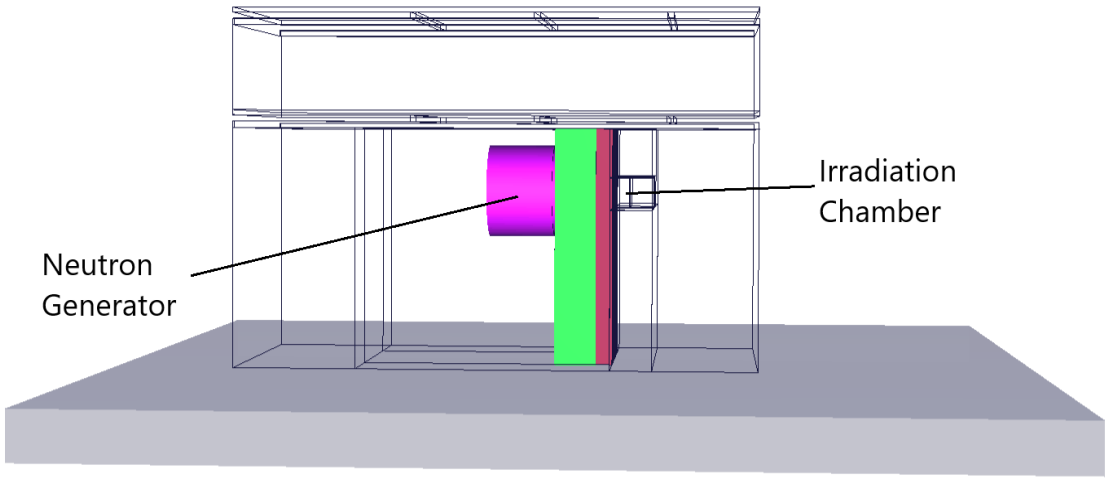

Figure 4: Simulated neutron generator.

energy of the resulting neutron from the DD fusion reaction [3].

The second source specification incorporated anisotropy for the emission of the neutrons. The source specification accounted for both neutron yield and energy, over all angles. To determine the yield and energy per angle, the DROSG-2000 program (http://www-nds.iaea.org) was utilized. DROSG-2000 is a Microsoft Windows or LINUX freeware program available through the International Atomic Energy Agency that contains reaction data for 60 accelerator reactions that produce neutrons [1]. The program contains three separate codes, named neuyie, whiyie and timrev. The codes allow for the generation of accelerator reaction pro-

duced neutron energies, differential cross sections, yields, and spectra. We used the code neuyie to generate neutron energies and cross sections at various angles. In executing the code, one selects the type of nuclear reaction, the kinetic energy of the bombarding particle, and the number of angles that data is desired for. The program then produces a data table based on the known double differential cross section for the selected reaction. The data table lists the emission angle, neutron energy, and cross section in both the center of mass and laboratory reference frames.

The neutron emission data was directly coded into MCNP for the anisotropic simulation. The neutron source was specified as a surface source with a radius of 2.0 centimeters, adjacent to and directed towards the titanium target material. In the source definition (sdef), a distribution was set up for neutron energies that were given by DROSG-2000. The distribution was specified as a dependent source variable (ds) that depended on values contained on the source information (si) card. The source information card listed all the possible angles of emission from cos(Θ) = 1 to cos(Θ) = -1. Paired with the source information card was a source probability (sp) card, which gave the probability that a neutron would be emitted at a given angle. The neutron emission angle probabilities were determined by dividing each individual angular cross section specified in DROSG-2000 by the sum of the cross sections of all the angles.

Both the isotropic and anisotropic source specifications were simulated with a model constructed of our Adelphi DD-109 neutron generator and surrounding moderator/reflector. The model included an irradiation chamber located at the face of the generator. In the irradiation chamber, gold foils were simulated at three different angles and distances. The gold foils were 1.27 centimeters in diameter, 5.08×10^{-3} centimeters thick, and possessed a density of 1.93×10^{1} grams/cm^3. Foil location A was on the side of a polyethylene block (not displayed in Figure 5 for clarity), 2.05×10^{1} centimeters off the midline of the generator. The edge of the foil was facing the generator. Foil location B was 5.85 centimeters off the midline of the generator and was 7.5 centimeters from the face of the generator. It was positioned behind a polyethylene block (1.02×10^{1} cm × 2.05×10^{1} cm × 5.5 cm, 9.3×10^{-1}g/cm^3) with a 4×10^{-1}-centimeter sheet of lead (1.135×10^{1} g/cm^3) adjacent, both of which were included in the simulation. Foil location C was at the midline of the generator head, immediately adjacent to the lead sheet. All three foil locations were at the same elevation. Figure 5 shows the relation of the three foils to each other in the irradiation chamber and was produced from the MCNP input using the Visual Editor program. The location of the irradiation chamber relative to the neutron generator is noted in Figure 4.

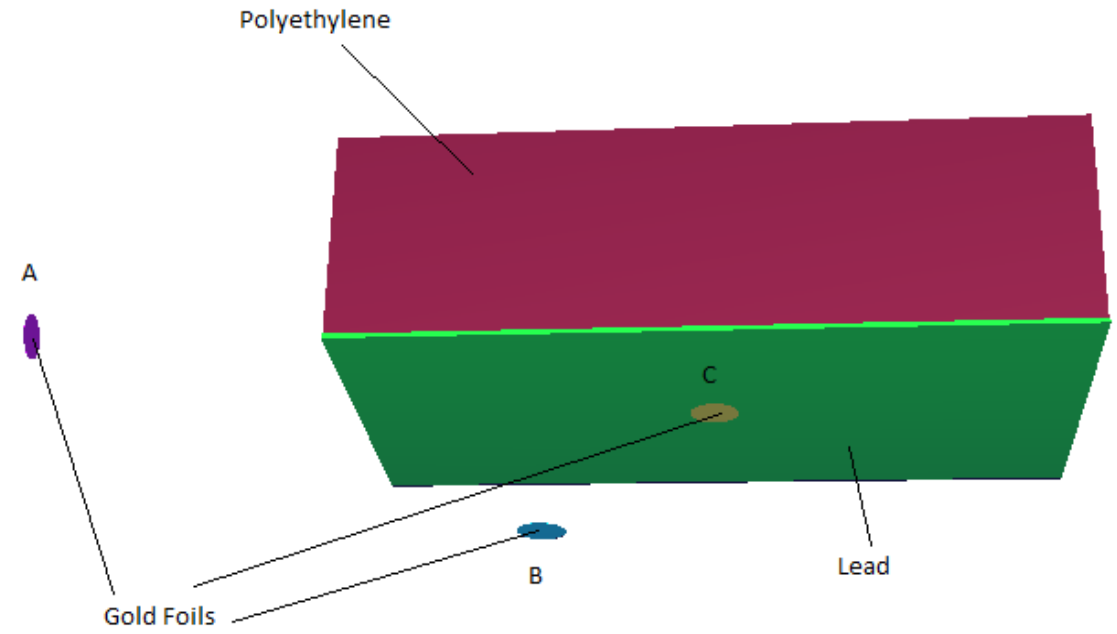

Figure 5: Gold foil geometry.

An F4 tally was set up for each of the foils to simulate the production of ^{198}Au from activation of ^{197}Au in the foils. The F4 tally by itself represents the particle flux (neutrons/cm^2) average over a cell [4]. Through the use of a tally multiplier (FM), the tally can be modified to record the number of ^{198}Au atoms produced. The tally multiplier consists of a normalization factor, the material number for gold specified in the MCNP input, and the ENDF reaction number for radiative capture. The normalization factor is calculated by multiplying Avogadro's Constant, the isotopic mass of ^{197}Au, the density of gold, and a conversion factor for cm^2 to barn. The tally multiplier will compute the number of ^{198}Au atoms per cm^3 produced. A segment divisor (sd) with a specification of unity (1) is added, resulting in the total number of ^{198}Au atoms produced in the cell to be given by the tally.

Isotropic simulation was executed with 1×10^7 source particles and the anisotropic simulation with 4×10^7 source particles. These numbers ensured that all tally relative errors were maintained below 0.05, a value considered generally reliable.

Gold foil irradiation

A set of six gold foils were used for the irradiation. All foils were weighed prior to irradiation. Two foils each were irradiated at locations A, B, and C. The locations were set dimensionally to match those of the MCNP simulations. Each foil was irradiated for a period of three minutes with the generator operated at 110 keV. Following irradiation, the foils were transferred to a high purity germanium (HPGe) detector where a spectrum was acquired for a period of five minutes. A total of two minutes was allotted for transfer from the irradiation cavity to the detector. Spectra were analyzed and the number of events falling around the 411.8 keV photo peak were counted as evidence of ^{198}Au formation. ^{198}Au emits a 411.8 keV gamma ray in 95.62% of decays [5].

Results

The F4 tally results for each location from both the anisotropic source simulation and the isotropic source simulation are given in Table 1. The tally results represent the number of ^{198}Au atoms formed per source particle. Both simulations showed a distribution in the number of ^{198}Au atoms formed, with the anisotropic simulation resulting in the greatest rate of formation at location C and the isotropic simulation resulting in the greatest rate of formation at location A.

Each of the ^{197}Au foils was weighed prior to irradiation and counted on a high purity germanium (HPGe) detector after irradiation. The spectra generated by the HPGe were analyzed and the number of counts falling around the 411.8 keV photo peak counted. The number of 411.8 keV gamma rays detected were divided by each foil's mass to normalize for the number of atoms present. The normalized number of counts were averaged for each of the two foils at locations A, B and C. Results are displayed in Table 2. The highest rate of ^{198}Au formation was measured to be at the center point of the irradiation cavity (location C), followed by location B, and finally location A. Location A demonstrated a large fall off of formation as expected, as it was to the side of the center point and the foil was not facing the neutron source.

The relative rate of ^{198}Au formation at each of the three locations was described by dividing the rate of formation at one by another and is summarized in Table 3. The differences in placement as well as

Table 1: Simulation results.

Location	Anisotropic simulation (atoms/source particle) [Relative Error]	Isotropic simulation (atoms/source particle) [Relative Error]	Simulation result percent difference
A	2.417×10^{-6} [4.97×10^{-2}]	1.248×10^{-5} [3.00×10^{-2}]	-416.44%
B	1.235×10^{-5} [1.84×10^{-2}]	7.386×10^{-6} [3.03×10^{-2}]	40.20%
C	1.381×10^{-5} [1.93×10^{-2}]	8.466×10^{-6} [2.65×10^{-2}]	61.29%

Table 2: Irradiation results.

Location	Counts	Foil weight (g)	Counts per gram	Location average (Counts per gram)
A	1.73×10^{2}	1.269×10^{-1}	1.36328×10^{3} +/- 1.038×10^{2}	1.37754×10^{3}
A	1.73×10^{2}	1.243×10^{-1}	1.39179×10^{3} +/- 1.060×10^{2}	+/- 1.049×10^{2}
B	6.86×10^{2}	1.243×10^{-1}	5.51891×10^{3} +/- 2.119×10^{2}	5.75306×10^{3}
B	7.49×10^{2}	1.251×10^{-1}	5.98721×10^{3} +/- 2.201×10^{2}	+/- 2.160×10^{2}
C	8.55×10^{2}	1.294×10^{-1}	6.60741×10^{3} +/- 2.274×10^{2}	6.27668×10^{3}
C	7.70×10^{2}	1.295×10^{-1}	5.94595×10^{3} +/- 2.155×10^{2}	+/- 2.215×10^{2}

Table 3: Relative amounts of simulated and measured au-198 activation.

Location	Measured data	Anisotropic simulation	Isotropic simulation
A/B	0.24 +/- 0.02	0.20 +/- 0.01	1.69 +/- 0.07
A/C	0.22 +/- 0.02	0.18 +/- 0.01	1.47 +/- 0.06
B/C	0.92 +/- 0.05	0.89 +/- 0.02	0.87 +/- 0.04

orientation of the foils in the neutron field resulted in significant differences in both the measured as well as simulated ^{198}Au formation rates. The anisotropic source simulation was able to closely match the measurement results, at all three locations. It showed the greatest amount of activation to occur at location C, followed closely by location B, and then location A. The difference between locations B and A was large, similar to what was found by measurement. The isotropic source simulation on the other hand demonstrated the highest rate of ^{198}Au formation to be at location A, which was closest to the generator. The second greatest amount of activation was at location C and the least amount at location B.

Discussion

In this project, we compared two different methods of MCNP simulation with measurement data. Simulating an isotropic source of neutrons is relatively simple to perform where as simulating a source that accounts for the distribution of both neutron kinetic energy and yield at different angles requires additional effort. An anisotropic source requires that the double differential cross section be known and coded into the source definition. The method we used for the anisotropic source definition was described in this work and the actual input is given in Appendix A.

Comparing the two simulation methods to the measured data, we found that the anisotropic method closely followed actual measurements. The anisotropic simulation resulted in the greatest amount of activation being found at location C. Location B was simulated to result in 89% of the activation at location C. Location A, which was offset significantly from the irradiation cavity center was simulated to only have 20% of the activation of location C. The actual measurements found the greatest amount of activation to occur at location C, followed by location B with 92% of the relative activations of location C. Location A found a significantly reduced activation with only 24% of what resulted at location C. The isotropic simulation did not yield results that matched the measurements. Isotropic source specification simulated the greatest amount of activation to be at location A, which in measurement found the least amount of activation. Location B was isotropically simulated to have the least amount of activation where as in measurement, the activation here was only slightly less than the greatest amount.

One could expect either simulation method to be useful for irradiations of small samples close to the center point of the irradiation cavity, especially if not attempting to quantify the absolute amount of activation. For simulations of irradiations of relatively large samples, or for more complicated tasks such as optimizing moderator and reflector materials, the extra effort to account for anisotropy in the source definition should be expended. The quantification of absolute activation or metrics such as radiation dose necessitates the more accurate description of the source. The spectrum of kinetic

energies of neutrons will vary significantly as they pass through moderator, reflector and the sample. These changes in kinetic energies will ultimately affect quantities that are energy dependent, such as the activation rates and radiation weighting factors (for Equivalent Dose calculations).

Conclusion

Two different methods of specifying a neutron source when developing MCNP simulations have been described and performed. The results of both methods were compared to an actual measurement experiment. It was determined a source definition that accounted for neutron anisotropy matched the experimental results much more closely than those found assuming an isotropic source of neutrons. The simpler isotropic simulation method may be adequate when conducting simple irradiations involving relatively small samples. Optimization of the irradiation environment, irradiations involving complex geometries or large samples, and simulations requiring a higher degree of accuracy should employ a more detailed source specification that includes neutron angular and energy distributions.

Acknowledgement

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