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MONTE CARLO ANALYSIS OF SPHERICAL SHELL TRANSMISSION EXPERIMENT WITH NEW TALLYING METHODOLOGY

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ABSTRACT

This paper discusses a new tallying methodology implemented in the Monte Carlo particle transport code MCNP for tallying a group of particles that are scattered (inelastically and elastically) in a particular region of interest and are detected at a detector. The methodology provides detailed information on the particle's energy and position. This new tally procedure has been applied to an iron, spherical-shell transmission experiment (SST) to better optimize the experimental setup. The new tallying option is used to identify particles that scattered in the iron shell and subsequently are detected at a detector. The effect of the size and location of the iron shell are analyzed. Various source energies and iron shell thickness are investigated. Note that this new tally methodology can be used in conjunction with any Monte Carlo simulation that requires such information.

1. INTRODUCTION

The Monte Carlo method is a useful tool for obtaining detailed information of a nuclear system. Available tallying options generally provide information at a point of interests; they do not provide any information on particle history. MCNP (Briesmeister, 1997), however, provides a cell-flagging option for flagging particle tracks. In this approach, particle tracks become flagged when they leave a designated region of interest. The cell-flagging option is limited in that it does not provide detailed information about the particle interactions in a volume of interest.

The Monte Carlo method has been used in the past for analyses of spherical shell systems. Early work (Everett, 1953) was done to estimate the elastic escape probability for an arbitrary one-dimensional model of a spherical shell. In this work the elastically scattered particles were tracked and tallied as they escaped the shell. A notable amount of research (Brockhoff, 1994 and Marchetti, 1998) has been done related to benchmarking previous Monte Carlo studies of a pulsed sphere experiment done at Lawrence Livermore National Laboratory. These studies were performed to reevaluate experimental configurations with new cross section data and improved Monte Carlo codes. In general, most of the prior research on this topic is related to the utilization of Monte Carlo techniques for evaluation or benchmarking of computer codes and/or cross section libraries. However, no work in public literature has proposed the use of simulation to identify inelastically scattered neutrons for improving experimental setup and interpretation.

This paper has two objectives, one of which is to develop and verify a new tallying methodology (Haghighat, 2000), which provides information on the history of "important" particles. The second objective is related to the application of this technique to the SST problem. Although this method is envisioned to be applicable to the simulation of many nuclear systems, we have applied this to this specific project.

2. OVERVIEW OF SST EXPERIMENT

The objective of this project is to accurately determine iron non-elastic scattering cross sections via a SST experiment using the time-of-flight (TOF) method. Previous studies mainly involved solid iron spheres with limited source energies (Hansen et al., 1973 and Nico et al., 1996). In this project, however, we are examining different source energy and shell thickness combinations, and we have developed a new tallying methodology in order to optimize the experimental setup and enhance experimental inference. The results of this project will be used to alleviate the well-known deficiency that exists in the iron non-elastic scattering cross-section, and thereby reduce the uncertainty in calculations involving deep penetration in iron; e.g., reactor pressure vessel neutron fluence determinations (Wagner et al., 1996).

The SST experimental setup utilizes an accelerator driven neutron source and a TOF measurement system. The target consists of multiple spherical iron shells, which enclose the neutron source. Downstream from the target is the TOF system consisting of a concrete wall and a TOF tunnel. The TOF technique is used by experimentalists to correlate a measured spectrum to different types of target interactions. The correlated spectrum is then utilized in inferring the value of the non-elastic cross-section. Figure 1 shows a schematic of the SST experimental setup prepared by MCNP.

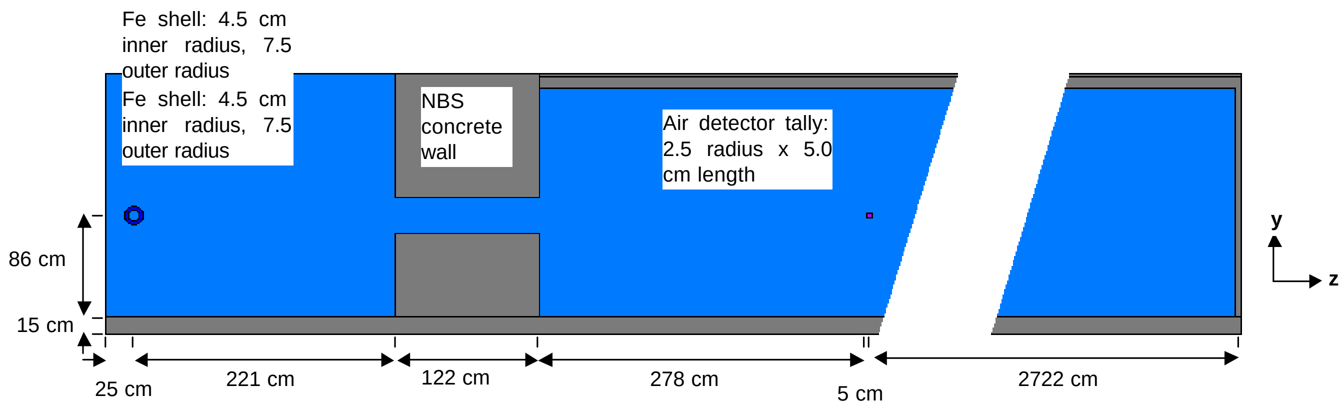


Fig. 1a Side view of full model

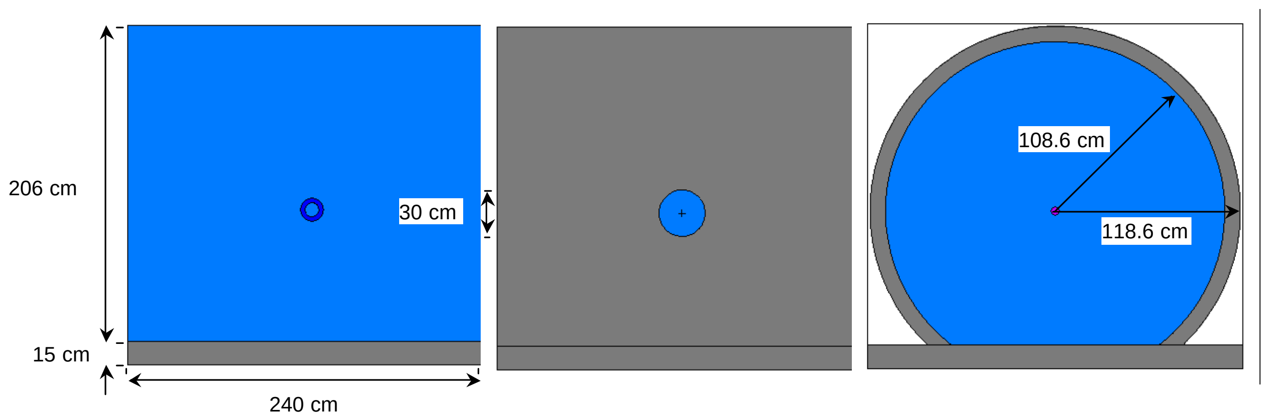


Fig. 1b Cross-sectional views through full model

The neutron source is located inside the spherical shell shown in Fig. 1a. The detector is located at ~6.2 m downstream of the source and target. For the present study, we consider neutron source energy in a range of ~1 to 8 MeV.

3. DESCRIPTION OF NEW TALLYING ALGORITHM

As previously mentioned, the new tallying algorithm has been developed to track "important" particles. For purposes of the SST experiment, these particles are neutrons that have undergone inelastic scattering in the iron target and subsequently reach the detector. While tracking these neutrons as they travel through the model, we compile a detailed array of information, including collision type, incident and emerging energy, scattering angle, position and time for the interactions in the spherical shell. This array of information is necessary for the SST experiment, however, for other nuclear systems, additional or less information may be needed. This information is then utilized to categorize the neutrons that reach the detector based on the type of interaction they have undergone within the iron shell, and then determine the components of collided and uncollided particles. The information can be used to analyze the measured flux or the overall counts in the detector volume.

3.1 Uncertainty Estimation

We calculate the relative error in the estimation of the counts or tally by considering a general statistical process. For a large number of trials, the variance in x_i outcomes is given by:

$$S_x^2 \cong \overline{x^2} - \bar{x}^2 \tag{1}$$

The relative error may then be determined in the usual way by dividing the standard deviation by the mean:

$$R_x = \frac{S_x}{\bar{x}} = \sqrt{\frac{\overline{x^2}}{\bar{x}^2} - 1} \tag{2}$$

By considering the Central-Limit Theorem to be valid for large n, the above formula may be reduced to the following form:

$$R_{\bar{x}} = \sqrt{\frac{\sum_{i=1}^{n} x_i^2}{\left(\sum_{i=1}^{n} x_i\right)^2} - \frac{1}{n}} \tag{3}$$

Thus far, the above equation provides the relative error associated with a mean of any general distribution of outcomes x_i. For simplicity, we consider that the distribution x_i is a Bernoulli process, wherein the possible outcomes of x_i are either 1 or 0. In this approach, we assume that each history counted at the detector location is an outcome of 1 and those not reaching the detector are 0. It is important to note that for Monte Carlo simulation where the particle weights are not 1 (i.e. with variance reduction techniques) this approach is not valid. For a Bernoulli process, the above formulation reduces to:

$$R_{\bar{x}} = \sqrt{\frac{1}{c} - \frac{1}{n}} \tag{4}$$

where c is the total number of counts at the detector, i.e. the sum of the x_i values equal to 1.

3.2 Estimation of Flux

The above formulations may be utilized for estimating the variance or relative error for the particle counts and the fluxes. Typically, for the present application of the SST experiment optimization we do not necessarily need the flux values. The neutron counts are sufficient for parametric studies related to optimization. However, for purposes of verification of the tallying methodology, a procedure for estimating scalar flux is warranted. To estimate the scalar flux at the detector we use the path-length estimator technique. The general form of the path-length estimator for the scalar flux is given by:

$$f = \frac{\sum_{i=1}^{H} p_i}{H \Delta V \Delta E} \tag{5}$$

where p_i is the length of the i^{th} particle trace (path length), ΔV is the tally volume, ΔE is the energy interval of the tally and H is the number of histories. For the present configuration of the SST experiment, we can simplify the estimate given above. Because the detector is located at such a long distance and is very small, it is reasonable to assume that all particles have path-lengths equal to the length of the detector, hence Eq. 5 reduces to:

$$f \cong \frac{c}{H \Delta A} \tag{6}$$

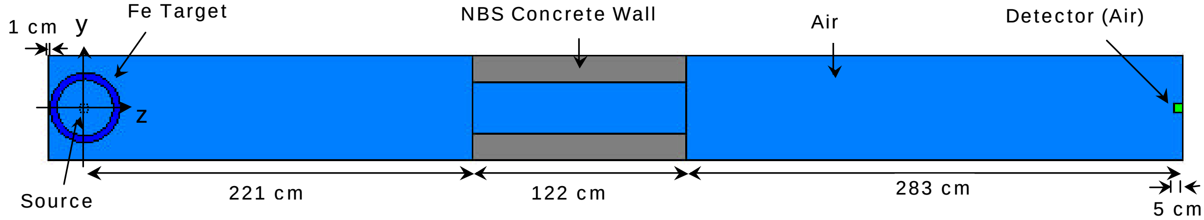
where ΔA is the surface area of the detector. Effectively, since the neutron tracks are nearly perpendicular to the face of the detector, the path-length estimator reduces to the surface-crossing estimator.

3.3 Verification of the New Tallying Algorithm

The new tallying methodology is currently used with MCNP. The analysis of the tally data is done by using a post-processing procedure, however, this process also may be integrated into MCNP. It has been verified based on a comparison with the standard volume flux tallying option in MCNP (i.e., F4). In this comparison the information regarding the neutrons that have collided with the target is used to separate components of the flux at the detector region. The particles that have not collided are also tallied. The F4 tally in MCNP is used to generate a reference scalar flux at the detector region.

A test model, which is a reduced size of the full SST experiment, has been constructed for this verification. The overall model boundaries are 60 x 70 x 647 cm^3. The neutron source considered is a uniform source of size 4 x 4 x 4 cm^3 placed at the left-hand-side of the model, and centered about the origin. The source is modeled as an isotropic source of 8 MeV neutron energy. A cylindrical detector of radius 2.5 cm radius and length 5.0 cm is positioned at 621 cm from the origin. The target shape is a spherical shell of inner radius of 16 cm and outer radius of 20 cm centered at the origin. The collimator (within the concrete wall) is 122 cm long and has a 30 cm diameter. The test model is shown in Figure 2.

Fig 2a Side-view of the test model



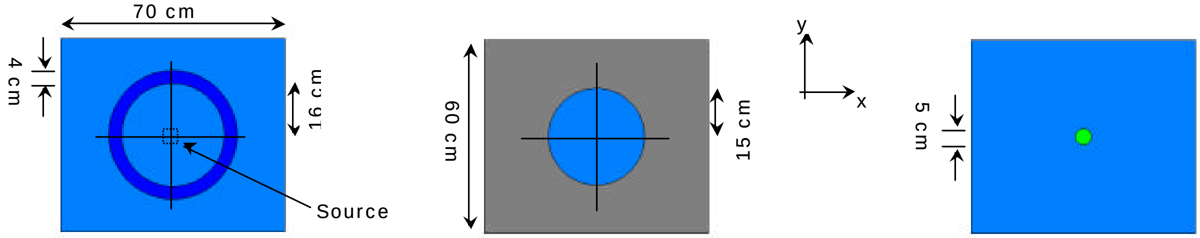


Fig 2b Cross-sectional view of the test model

Table 1 gives the total flux and its uncollided component at the detector. Further, it partitions the flux according to the type of scattering interaction that particles had experienced while traveling through the target. The energy bins are selected in order to achieve a statistical error of =5% for the total counts within each bin.

Table 1 Detailed Breakdown of Normalized Flux Values at the Detector

Normalized Flux Values	Energy Bin (MeV)					
	1.003 to 1.873	1.873 to 4.444	4.444 to 7.947	7.947 to 7.980	7.980 to 7.99999	7.99999 to 8.000
New Tally Algorithm						
S_1[(a)]	0	4.67E-11 (100%)	1.47E-08 (5.64%)	2.03E-08 (4.80%)	2.24E-08 (4.57%)	8.41E-10 (23.57%)
S_2[(b)]	5.38E-09 (9.33 %)	6.73E-09 (8.33%)	2.62E-09 (13.36%)	0	0	0
S_3[(c)]	1.54E-08 (5.50%)	1.67E-08 (5.29%)	4.49E-09 (10.21%)	0	0	0
uncollided	---	---	---	---	---	5.90E-08 (2.81%)
TOTAL	2.08E-08 (4.74%)	2.35E-08 (4.46%)	2.18E-08 (4.63%)	2.03E-08 (4.80%)	2.24E-08 (4.57%)	5.99E-08 (2.79%)
MCNP F4 Tally Algorithm						
uncollided	---	---	---	---	---	5.86E-08 (%2.82)
TOTAL[(d)]	2.00E-08 (4.80%)	2.29E-08 (4.50%)	2.10E-08 (4.70%)	1.99E-08 (4.82%)	2.36E-08 (4.44%)	5.86E-08 (2.82%)

(a) S_1: elastic only
(b) S_2: inelastic only
(c) S_3: combination of inelastic and elastic
(d) CPU time ˜ 16 hrs., number of histories ~ 1 billion

The total flux determined via the new tally methodology is in good agreement with that determined by the conventional method of the MCNP F4 tally; i.e., within the statistical uncertainty. It is also interesting to note that the inelastically scattered particles (S2 and S3) contribute significantly to the total particle flux within the energy range of ~1.0 to 4.4 MeV, while the elastically scattered particles contribute to higher energies. This type of information will be very helpful for analyzing experimental results.

4. UTILIZATION OF NEW TALLYING ALGORITHM

The sensitivity of the SST experiment is determined by several design parameters. These parameters include the shell thickness and position, and the source energy. It is desirable to optimize the sensitivity of the experiment by selecting appropriate source/shell combination(s). The sensitivity of the detector response is most influenced by the number of inelastic neutrons at the detector. Another significant effect is the neutrons that interact with the surrounding materials such as the concrete and contribute to the detector response. These neutrons are effectively the background in the response.

The new tallying methodology has been utilized to quantify the inelastic neutrons at the detector. A significant modeling effort using this new tally methodology has been performed to analyze the effect of target thickness on the fraction of inelastic neutrons reaching the detector region. In this effort, the previously described model is modified to simulate different source energies and target thicknesses. The (initial) source energies utilized are 2.5, 3.0, 3.5, 3.8, 4.0, 4.2, 4.5, 5.0, 6.0, 7.0 and 8.0 MeV. The target thicknesses utilized are 1.0, 2.5, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0, 10.0, 12.0, 16.0 and 20.0 cm. The total number of inelastic neutrons tallied is normalized by the total histories to determine the fraction of source neutrons contributing to the detector. Figure 2 compares the fraction of neutrons that have undergone at least one inelastic scattering event within the target and then traverse the detector region for different combinations of source energy and target thickness.

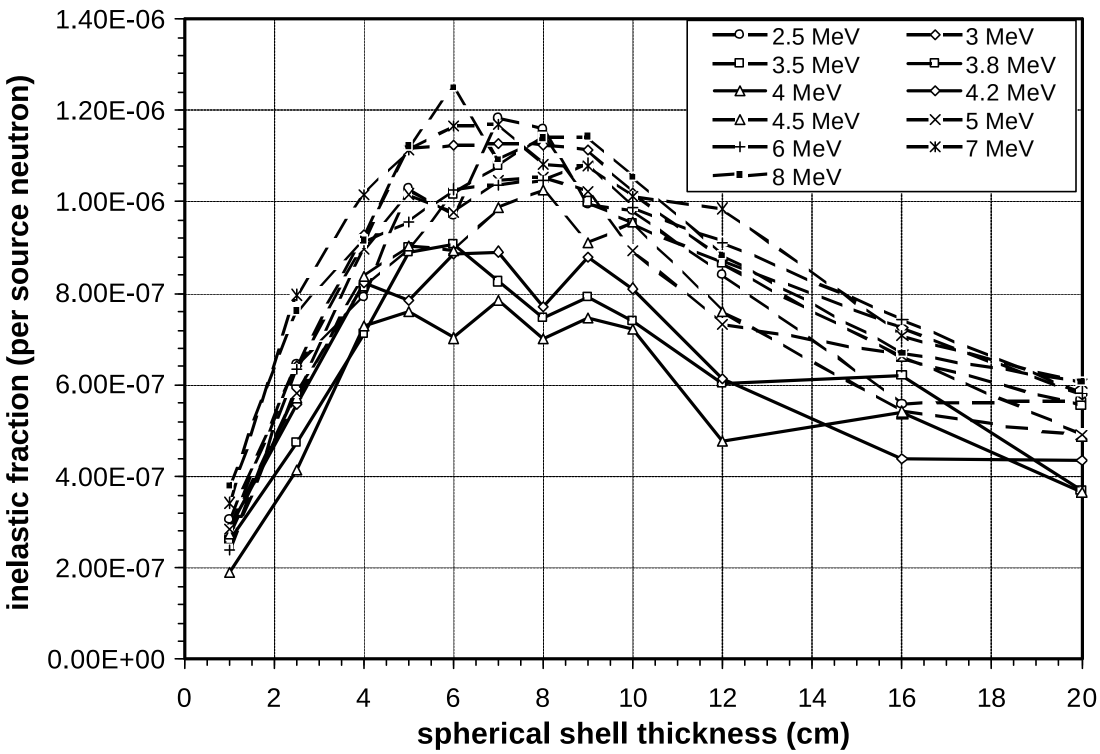


Fig. 2 Inelastic fraction as a function of target thickness

This analysis shows clearly that, for most source energies tested, there is a range of ~4 to ~9 cm target thickness where the fraction of inelastically scattered neutrons is relatively large. It also indicates that for source energies of about 4 MeV, there is a significant decrease in this fraction. This can be attributed to the fact that at about 4 MeV there is a significant decrease in the forward and backward scattering, while there is a significant increase in scattering about 90 degrees which in turn results in higher leakage. Because of this leakage, the number of inelastic neutrons that propagate to the detector drops as depicted in Fig. 2.

It is important to note that these results were obtained based on the currently available ENDF/B-VI iron cross-section library. As part of our continuing effort, we are extending this study by examining other cross section libraries and performing supporting experiments for a few selected combinations of source energy and target thickness.

5. CONCLUSION

A new and versatile tallying methodology, for tallying a group of particles that are scattered (elastically and inelastically) in a particular region of interest has been developed. This methodology has been implemented in the MCNP code system and verified with the conventional F4 tally option. This approach has been applied to a real physical system, namely, the optimization of the detector response in a SST experiment. For the ENDF/B-VI cross-section library, we have shown that there is a range of target thickness from ~4 cm to ~9 cm, where the fraction of inelastically scattered neutrons at the detector region is relatively large. To further optimize the experiment, we are currently performing simulations to estimate the fraction of neutrons scattered from the concrete in the SST experiment. This can be minimized by proper placement of the target and detector. Furthermore, since with the new tally methodology we can distinguish between different types of interactions that particles have gone through, we will be able to reduce the existing uncertainty in the TOF correlation procedure, and therefore the non-elastic cross-section. In addition, as a part of our future work to reduce the high computational cost of these simulations, we are investigating a new problem-specific variance reduction technique based on this new tallying algorithm. In a continuing effort, we will examine other cross section libraries and perform a few selected experiments.

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