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Monte Carlo Modeling of a Time-of-Flight (TOF) Experiment for Determination of Fe Scattering Cross Sections

Michael T. Wenner[1*], Alireza Haghighat[1], James M. Adams[2], Allan D. Carlson[2], Steven M. Grimes[3], Thomas N. Massey[3]
[1]Department of Nuclear and Radiological Engineering, University of Florida, Gainesville, FL 32611
[2]National Institute of Standards and Technology, Gaithersburg, MD 20899
[3]Institute of Nuclear and Particle Physics, Department of Physics and Astronomy, Ohio University, Athens, OH 45701

This paper discusses the Monte Carlo modeling of a time-of-flight (TOF) experiment used to investigate the Fe-56 neutron scattering cross section. This involves utilizing experimental data to provide a Monte Carlo neutron source distribution for which experiments can be compared with simulation. Results indicate this can be an effective methodology for the generation of a source of this kind. Comparisons of calculation and experiment of the time of flight experiment have shown possible deficiencies in the Fe-56 scattering cross section.

KEYWORDS: Iron Cross Section, Fe-56, Scattering, Time of Flight, Monte Carlo

1. Introduction

Accurate determination of the fast-neutron fluence at a reactor pressure vessel has been accomplished by performing multidimensional transport calculations. Clearly, safe design and operation of nuclear systems are largely dependent on the nuclear data used. An important cross section for pressure vessel fluence estimation is the iron scattering cross section which has been suspected to have large uncertainties, especially for neutron energies between 1 and 8 MeV. In an attempt to improve the accuracy of these cross sections, neutron spherical-shell transmission experiments were performed with iron shells of different thicknesses using time-of-flight (TOF) spectroscopy of the scattered neutrons. The spectroscopy data were then utilized to devise a methodology for Monte Carlo analysis of the experiments to be compared with simulation. A Monte Carlo model was developed and a source modeling procedure that utilized experimental data to provide a detailed neutron source distribution was performed.

2. Experimental Background

Experimental data were obtained via a neutron spectroscopy technique, known as time-of-flight, using the spherical-shell transmission method. Iron shells are employed with different thicknesses, and neutron TOF spectra are obtained. Similar work was done in the past with a nearly monoenergetic 14 MeV neutron source at Lawrence Livermore National Laboratory (LLNL). (1) The present work was done with a number of different source reactions and a range of neutron energies though the source reactions were not monoenergetic.

* Corresponding author; Tel. 352-392-1401 Ext. 332, FAX 352-392-3380, E-mail: mtw125@ufl.edu

The experimental work was performed at the Ohio University accelerator laboratory. (2) A schematic of the experimental facilities is given in Fig. 1 which shows the beam swinger which allows angular distributions of the outgoing neutrons to be measured without moving the neutron detector.

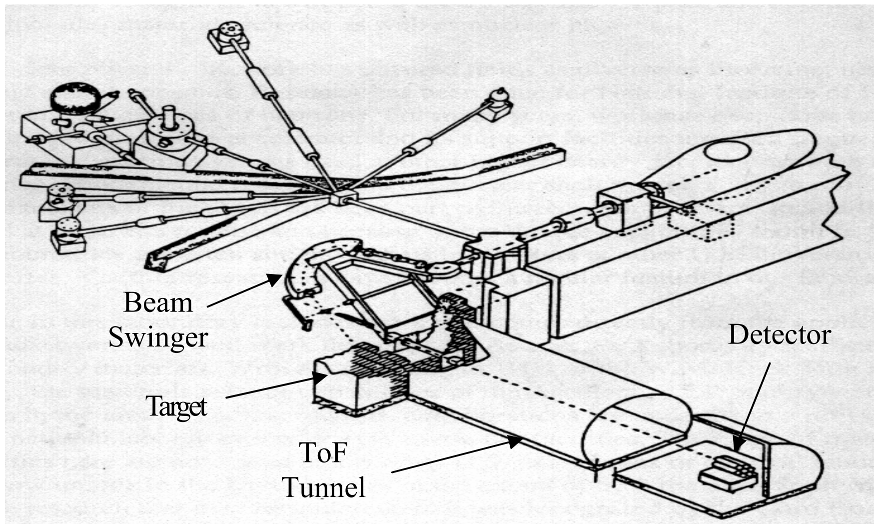

Fig. 1 Experimental Facilities Schematic

Neutron sources were generated based on incident deuteron energies of 3 MeV, 5 MeV and 7 MeV with the D(d,n) source reaction as well as with an incident proton energy of 5.1 MeV with the ^{15}N(p,n) reaction. For each incident particle energy and neutron source reaction, measurements were made at several different angles to provide data about the neutron angular source spectrum. Each of these measurements yields a spectrum which covers a range of neutron energies. For the NE-213 detector measurements, a spherical shell target of 8 cm thickness was used for all the sources. In addition, for that detector, measurements were made with a smaller spherical shell of ~3 cm thickness using the ^{15}N(p,n) source reaction. (3) These thicknesses were chosen to optimize the effect of neutron inelastic scattering. (4)

3. Monte Carlo Modeling

3.1 Monte Carlo Model

The simplified MCNP (5) model of the experiment is shown in 2-D slices in Figs. 2-6. It is simplified in that the source generation is not modeled, and represented by a source distribution. Fig. 2 shows a 2-D Y-Z view of the system, where the z axis is the axis of the accelerator tunnel. This effectively shows the whole system comprised of the source/iron sphere region, a void region up to the concrete wall, the concrete wall/collimator region, another void region, and a detector located at ~5.06 meters (detector midplane), from the source position. All materials were represented as accurately as possible.

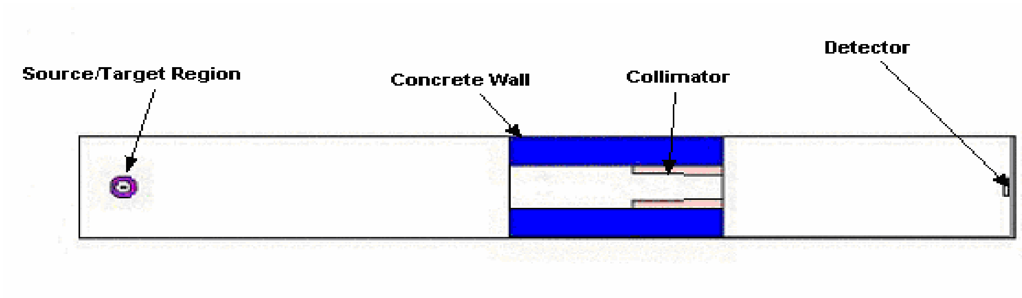

Fig. 2 Y-Z Schematic of MCNP Model Utilized

Figs. 3 - 5 show X-Y slices of the source/sphere region, the concrete wall region, concrete wall/collimator region, and the detector. These figures are effectively X-Y slices at different locations along the z-axis of Fig. 2. Fig. 3 shows the source region in which neutrons are born. Note that the hole in the iron sphere for the gas cell is not represented. Fig. 4 shows a slice of the concrete wall region before the collimator. Fig. 5 shows a similar slice where the collimator is present. Lastly, Fig. 6 shows the location of the problem boundaries with respect to the detector (tally) location. As can be seen the detector material itself is not represented.

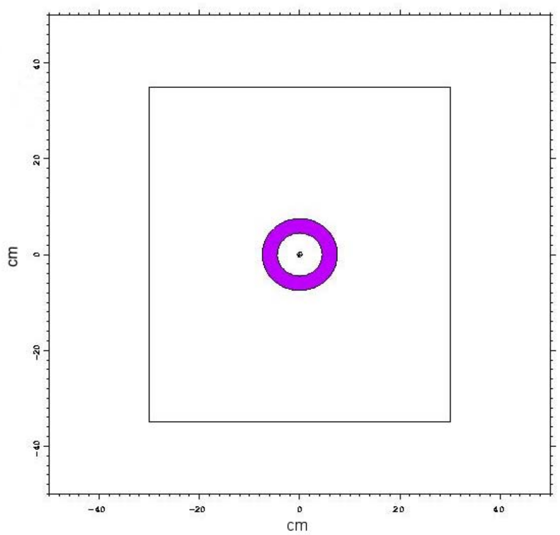

Fig. 3 X-Y Slice of Source/Sphere Region

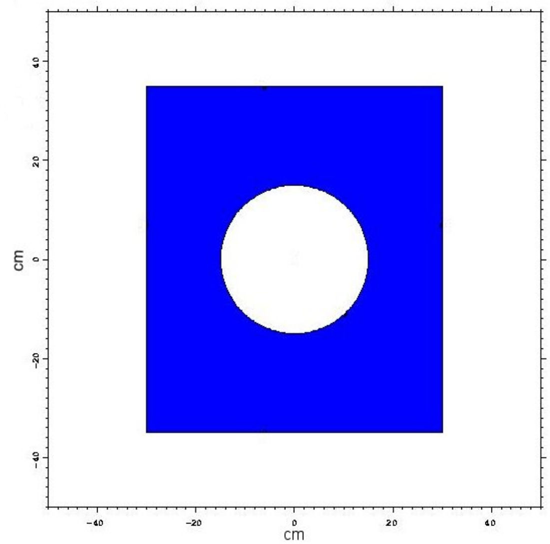

Fig. 4 X-Y Slice of the Concrete Region

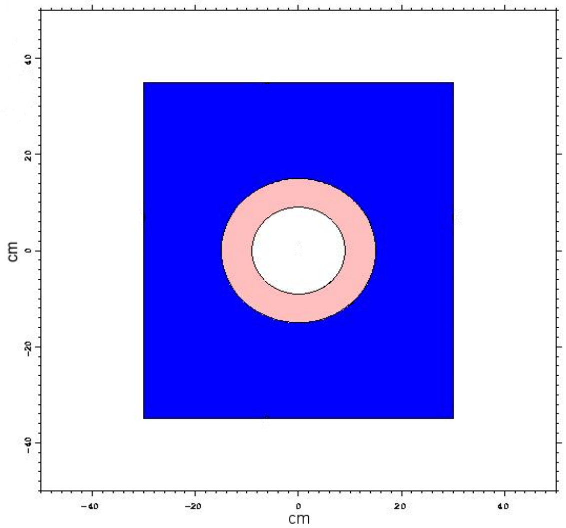

Fig. 5 MCNP X-Y Slice of the Concrete/Collimator Region

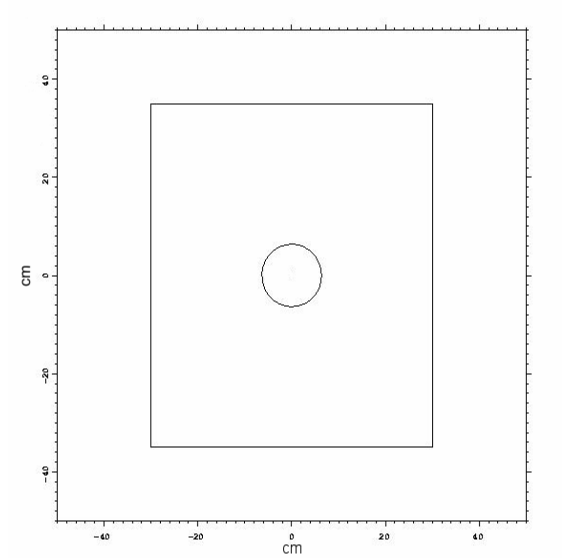

Fig. 6 X-Y Slice of the Detector Region

3.2 Monte Carlo Source Generation

To simulate the location of the experimental source, a cylindrical volume source was set up inside the gas cylinder volume, where source particles are born. Fig. 7 shows the 8 cm thick iron shell unassembled, revealing the hole in which the gas cylinder is inserted.

Fig.7 8cm Thick Iron Shell, Unassembled

The azimuthal angles are always sampled uniformly from 0 to 360 degrees, however, a source distribution is set up for the angular dependence in μ (which is the cosine of the angle between the source reference vector and the particle direction (Ω)). These distributions were obtained from experimental data.

It was assumed that the neutron TOF spectra obtained from the 'sphere off' cases represent the uncollided neutrons. Considering the distance to the detector a known quantity, the TOF spectra obtained for the sphere off cases can be converted directly to energy spectra using the relativistic kinetic energy equation given by

$$KE = \frac{m_o c^2}{\sqrt{1 - v^2 / c^2}} - m_o c^2, \tag{1}$$

where m_o is rest mass, v is neutron velocity, and c is the speed of light.

Now, let v=d/t where d is distance from the source to the detector, and t is the time of flight, then Eq. 1 reduces to

$$KE = \frac{m_o c^3}{\sqrt{c^2 - d^2 / t^2}} - m_o c^2 . \tag{2}$$

This procedure was repeated once for each beam angle, incoming particle energy and source reaction to characterize the source, yielding eight energy spectra. This procedure was used for each charged-particle source. Experimental data were recorded for several different experimental setups as presented in Table 1.

Table 1 Experimental Source Reactions & Beam Angles

5.0 MeV 15N(p,n)			3.0 MeV D(d,n)		5.0 MeV D(d,n)		7.0 MeV D(d,n)	
Sphere Off	*Small Sphere*	*Large Sphere*	*Sphere Off*	*Large Sphere*	*Sphere Off*	*Large Sphere*	*Sphere Off*	*Large Sphere*
0	0	0	0	0	0	0	0	0
15	45	45	15	45	15	45	15	45
45	90	90	45	90	45	90	45	90
60	120	120	60	120	60	120	60	120
90	135	135	90	135	90	135	90	135
100			100		100		100	
120			120		120		120	
135			135		135		135	

To obtain a more reliable estimate of the actual angular and energy dependant source distribution, an interpolation routine was developed to provide data between each of the measured angular spectra. This interpolation is performed in both time and energy.

To automate the interpolation procedure, the NERISRC code was developed. Not only is it necessary to interpolate over the experimental data, but since experimental data are only available in the range from 0 to 135 degrees, an extrapolation routine is incorporated to provide as complete a source distribution as possible.

Because of the limited amount of data for each source (eight point angular distributions), we have designed an interpolation formulation which preserves the peak behavior by using the shape of the known distributions and a bilinear technique. For example, Fig. 8 shows the available data for the D(d,n) experiment for 5 MeV incident deuterons. Note that each experiment yields one distribution per angle.

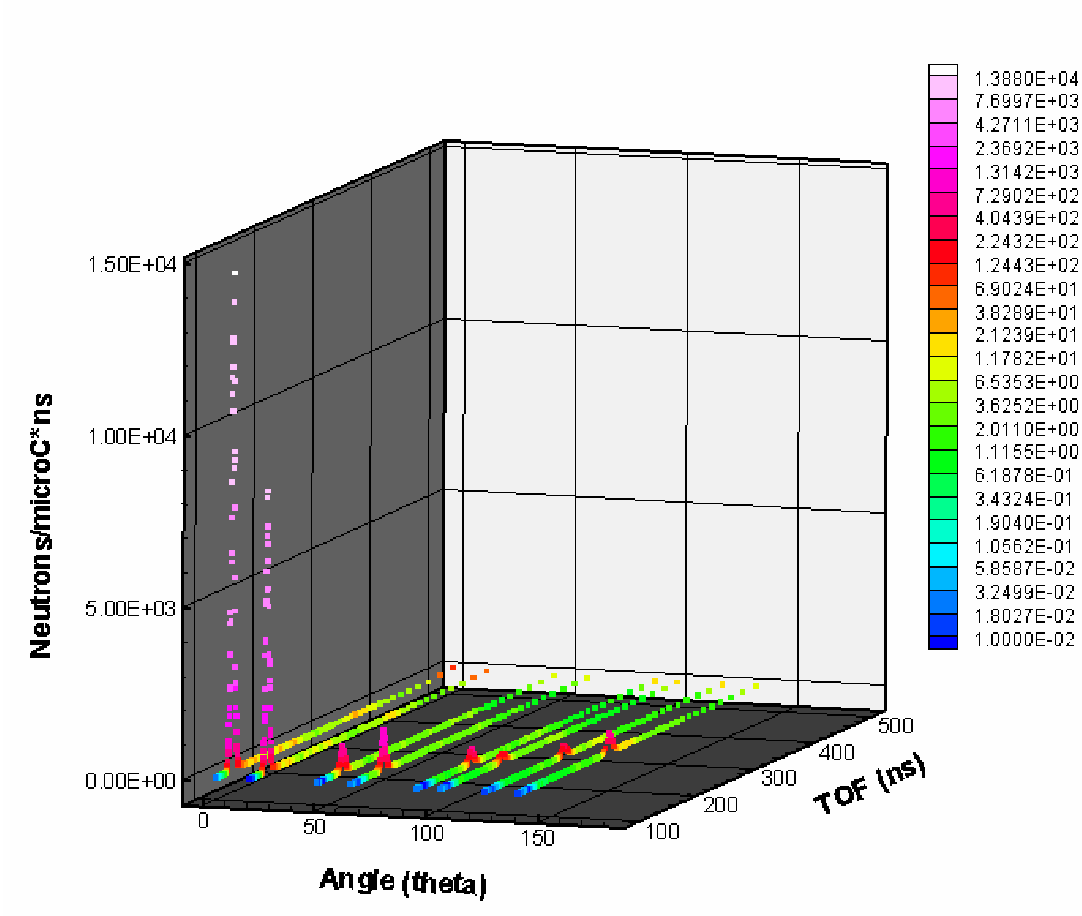

Fig.8 Experimental Source Distribution for 5 MeV incoming deuterons with the D(d,n) Reaction

The source distribution resulting from the interpolation procedure utilized is shown in Fig. 9. The eight experimental data sets are interpolated over the complete angular range.

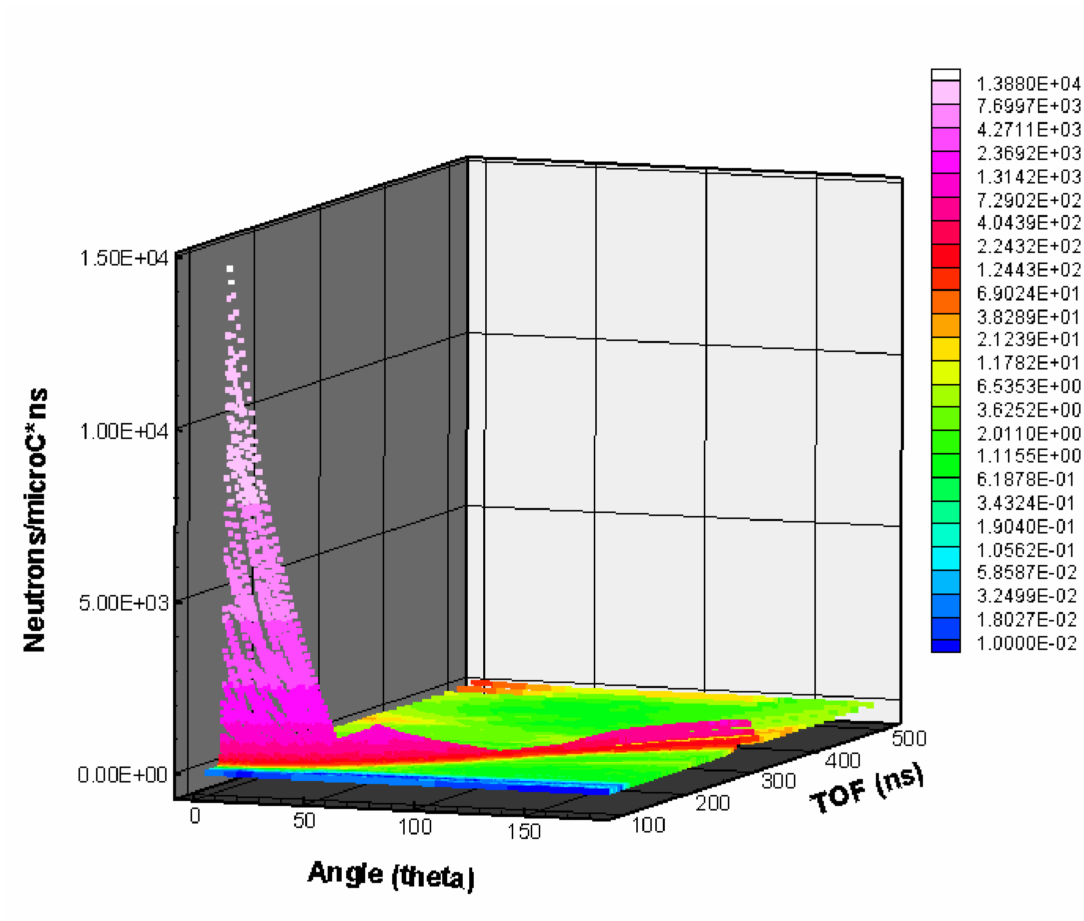

Fig.9 Complete Corrected D(d,n) Source Distribution for incoming 5 MeV deuterons

A total of four source distributions are generated: The source distribution for the 15N(p,n) reaction with an incident proton energy of 5.1 MeV and the other three for the D(d,n) reaction with incident deuteron energies of 3 MeV, 5 MeV, and 7 MeV. For a closer look at a particular angle, Fig. 10 shows a comparison of the 3 MeV D(d,n) Monte Carlo source prediction and experimental Data for 0 degrees.

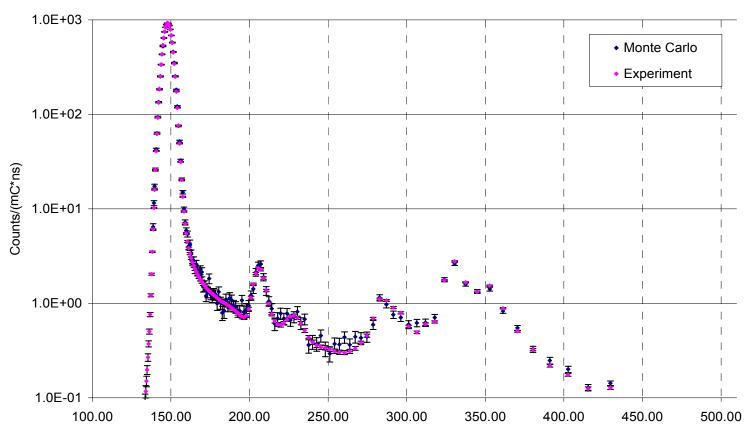

Fig.10 Comparison of the D(d,n) Monte Carlo Source Calculations for incident deuterons of 3 MeV and Experimental Data for the 0 Degree Angle

These results indicate a relative difference of ~1.5% in the peak region of the spectra, and a maximum relative difference of ~48% in the remainder of spectra. The differences can be attributed to the statistical uncertainties of Monte Carlo simulations and the inaccuracy of the interpolated source which was based on preserving the peak behavior. For this comparison, the statistical uncertainty is ~< 1% in the peak region, while it can be greater than 10% in off-peak regions. A summary of the source distribution analysis is provided in Table 2.

Table 2 Experiment and Calculation Differences for Selected Beam Sources

Beam Energy	Angle (Degrees)	Peak (%)	Max. Relative Difference (%)
3 MeV D(d,n)	0	1.5	48
	45	16	52
	90	4.6	85
5 MeV D(d,n)	0	0.22	41
7 MeV D(d,n)	0	1.0	30
	45	14	45
	90	2.6	54
5.1 MeV 15N(p,n)	0	-	2.1
	45	-	3.4
	90	-	3.5

From these results, we see that the peak behavior is well represented, however outside of the peak regions, larger differences exist. The $^{15}N(p,n)$ data for an incident proton energy of 5.1 MeV shows good agreement throughout the entire spectrum since there is less variation with angle in the source distribution and the time of flight bin structure used has a better energy resolution for this reaction.

4. Results of Experiments With Iron Shells

Experiments were performed at beam source angles of 0, 45, 90, 120 and 135 degrees with the iron shell surrounding the target. The measured spectra were then compared to Monte Carlo simulations for several cases. A representative example shown in Fig. 11 compares the experimental and Monte-Carlo results for the 0 degree case with the D(d,n) source for an incident deuteron energy of 3 MeV. Reasonable agreement is achieved between experiment and calculation distributions, however, a difference of approximately 8% is observed in the peak region.

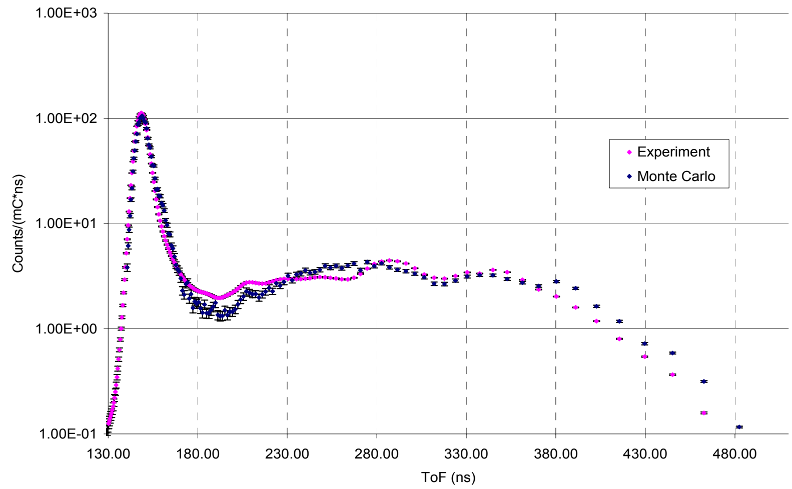

Fig. 11 Comparison of the D(d,n) Monte Carlo Calculations for 3 MeV incident deuterons and Experimental Data for the 0 Degree Angle

Due to the interpolation and extrapolation techniques used with a limited amount of data, we determined that the generated source distributions are most accurate for the 0 degree cases in the peak regions. This is because the bilinear interpolation is based on fitting the peak data in which the 0 degree data dominate, especially in the D(d,n) reactions. Consequently, the 3 MeV, 5 MeV and 7 MeV D(d,n) cases were processed for the 0 degree angle only. However, since the source generated for the $^{15}N(p,n)$ reaction was in close agreement for all angles of experimental data, results were obtained at 0, 45 and 90 degrees. Another source of error comes from the experimental time resolution coupled with the source interpolation procedure. Detector resolution is not adequate in some areas of the TOF spectrum, causing an inability to distinguish neutrons in neighboring bins. Problems arise from this since the detector efficiency is not a smooth function causing non-physical behavior in the measured neutron spectra in these areas. Interpolation utilizing these areas further compounds this non-physical behavior.

The calculated spectra differed from the experimental values by 20%, 21% and 11% for the $^{15}N(p,n)$ small sphere cases of 0, 45 and 90 degrees respectively. For the larger sphere $^{15}N(p,n)$ source, differences of 7%, 21% and 12% were obtained for angles of 0, 45 and 90 degrees respectively. Lastly, for the 3 MeV, 5 MeV and 7 MeV cases at 0 degrees, differences of ~8%, ~13%, and ~18% were obtained. These results were all for peak regions only. Outside of the main peak region, larger differences may exist.

5. Conclusion

We have developed a methodology which can be utilized to model a TOF experiment utilizing the MCNP code. A source distribution generation method was developed to utilize experimental data to provide a detailed angular and energy dependant source distribution to provide the source in MCNP. Results indicate this method can be adequate provided enough accurate experimental data is acquired. Utilizing this methodology, we have shown deficiencies may exist in the Fe-56 cross section data.

Acknowledgements

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