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Revisting the MCNP Shielding Validation Suite

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1 Introduction

The MCNP Shielding Validation Suite contains models of 18 benchmark experiments. The suite consists of 11 cases of the Livermore Pulsed Spheres[1], five cases of the Fusion Shielding experiments[1], and two photon experiments[2]. The Livermore Pulsed Sphere experiments had a 14 MeV neutron source inside a sphere of target material, and the leakage neutrons were measured at various distances from the source as a function of time. The Fusion Shielding experiments measured the spectra of leakage of neutrons and photons produced by neutrons collisions from different experimental configurations. The first photon experiment is the Skyshine experiment, which measured the flux of air scattered gammas as a function of distance. The second photon experiment is the "Co-60, air over ground experiment." This models a large Co-60 planar source and the kerma rate is calculated as a function of angle three feet ab

ove the ground. The errors (difference from experiment) for all of the benchmark experiments were calculated using an average relative error, and the reduced chi-squared, with the exception of the Co-60 air over ground experiment (the reduced chi-squared was not valid for this experiment because no experimental uncertainties are available).

2 Livermore Pulsed Spheres

In the Livermore Pulsed Sphere experiments, a sphere of target material was placed around a 14 MeV neutron source. The transmitted neutrons were detected as a function of time by instruments placed some distance away.

Eleven experiments are used from the Livermore Pulse Sphere experiments as benchmarks, which are shown in table I. All of the benchmark experiments are from Ref. 3, with the exception of U-235, U-238, and Pu-239 that are from Ref. 4.

Table I- LLNL Pulse Sphere Experiments Included in the suite

Material	Experiment Number	Flight Path (cm)	Angle (Degrees)
Lithium 6	4	765.2	30
Beryllium	9	765.2	30
Carbon	14	766.0	30
Nitrogen	18	765.2	30
Iron	31	766.0	30
Lead	37	766.0	30
Water	40	754.0	30
Concrete	52	975.4	120
U-235	55	766.0	30
U-238	59	765.2	30
Pu-239	62	766.0	30

The experimental data is in the mctal file so it is in the same format as the MCNP results. In the mctal file, the `tt` specifier is in the format:

```
tt (number of time bins + 1).
```

Following this, the time bins are specified in ascending order. Following the `tt` specifier, a `vals` specifier is present, followed by the experimental data in the same order as the time bins. The relative error follows its experimental value. An additional experimental data point of zero is the first experimental data point, so the experimental data can match the MCNP results since the first time bin on MCNP starts at negative infinity. To keep the same number of time bins as data points, another time bin is added. Examples can be found in Appendix B.

The data in the Livermore Pulsed Spheres report is in units of counts per nsec per total 14 MeV counts. The MCNP results are normalized to have the same units as the report, which is done by calculating the total number of 14 MeV source neutrons. To find this value, a copy of the MCNP input file is run with all of the materials in the cell cards set to air. The sum of the collided flux at the detector from the no sphere is used in the original MCNP input file as

$$\texttt{fm\#}\ \frac{1}{\text{sum of the collided flux at the detector for no sphere case}},$$

where # denotes the tally index. This `fm` card normalizes the MCNP results to the same units as the experimental results.

To account for MCNP's first time bin starting at negative infinity, a `tm` card is specified in the input files, which multiplies the value of the first time bin by zero and the rest by one. This makes the MCNP results match up with the experimental data. The detector response functions in the MCNP inputs files are normalized to one at 15 MeV. The measured data is not normalized so it will not match the MCNP data unless a factor is applied. To renormalize the MCNP input file, the area under the curve for both the MCNP data and the experimental data must be calculated. This is done by multiplying all the values in the mctal file by their time bin width and adding them up, which is the left endpoint integration method. These areas are used in the input file to normalize the MCNP results by changing the multiplier card:

$$\texttt{fm\#}\ \left(\frac{1}{\text{sum of the collided flux at the detector for no sphere case}}\right)\left(\frac{\text{area under the curve for measured data}}{\text{area under the curve for MCNP data}}\right).$$

The MCNP data is plotted against the experimental data using the MCNP plotter. The plot for the carbon sphere experiment is shown in Fig. 1.

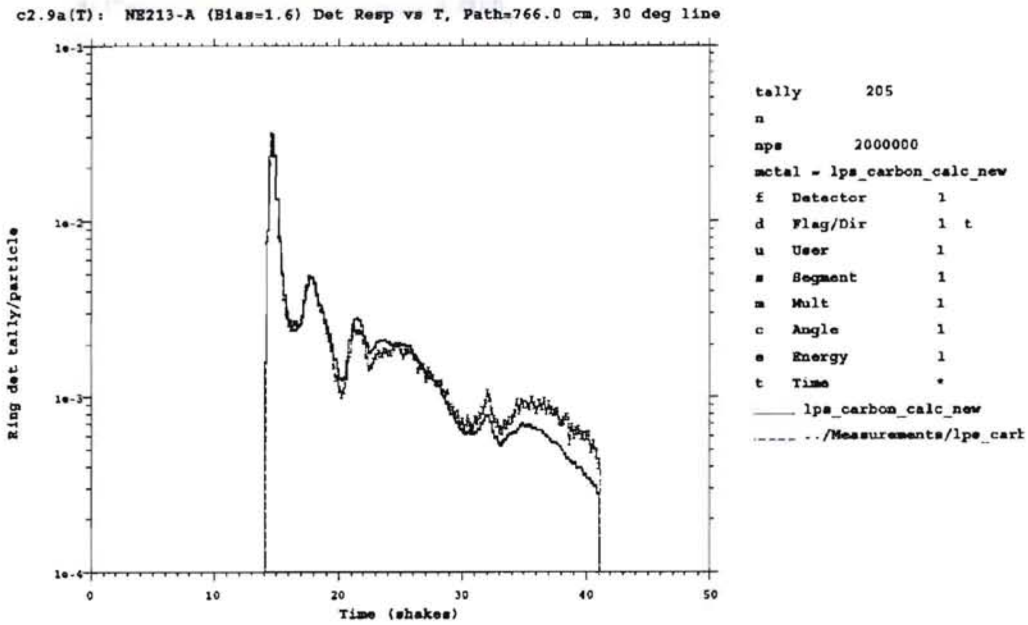

Fig. 1 - Carbon, Experimental and MCNP data

The validity of the MCNP results are shown by calculating the errors and the reduced chi-squared with respect to the experiments. The error is calculated as

$$E = \frac{\int (f_{exp}(t) - f_{calc}(t))^2 \, dt}{\int f_{exp}(t)^2 \, dt}, \qquad (1)$$

where f_{exp} is the experimental data, and f_{calc} is the MCNP calculated results. A rejection method for discarding outliers is used since a large amount of error is observed around the peaks for the Livermore Pulse Sphere benchmark experiments. The 90th percentile is multiplied by two and any error greater than that is discarded. The other metric to assess difference from experiment is the reduced chi-squared, which is

$$X^2_{red} = \frac{1}{N} \sum_{i=1}^{N} \frac{(f_{exp,i}(t) - f_{calc,i}(t))^2}{\sigma_i^2}. \qquad (2)$$

For this case, N is the number of points and σ is the relative uncertainties. The outliers that are removed for their error also have their chi-squared terms removed. Table II shows the errors and the reduced chi squares that are calculated for the benchmark experiments. The errors are lower for the scattered neutrons, and higher for the peak. Without rejecting errors, the errors around the peak dominate the error for the whole benchmark experiment, and the method for rejecting outliers show more of an overall error rather than just the error at the peak.

Table II - Errors and Reduced Chi Squared Data for LLNL Pulsed Spheres

	X_{red}^2	E
Lithium	152.1	0.067
Beryllium	13.8	0.014
Carbon	51.2	0.045
Nitrogen	21.7	0.017
Iron	89.3	0.038
Lead	161.6	0.053
Water	10.5	0.018
Concrete	22.4	0.020
U235	1.6	0.024
U238	10.4	0.037
Pu239	1.6	0.025

3 Fusion Shielding

The Fusion Shielding experiments[4] are also in the suite. Five experiments were chosen from the Fusion Shielding experiments as benchmark experiments, which are shown in table III. The experiments measured neutrons and photons produced by neutron collisions with the detector on and off the axis of the deuteron beam.

Table III - Fusion Shielding Experiments in Suite

Configuration	Tally Type	Detector Geometry
1	Neutron	On-Axis
3	Neutron	Off-Axis
3	Gamma	On-Axis
7	Neutron	On-Axis
7	Gamma	Off-Axis

The experimental data is in the mctal files so it can be compared with the MCNP results. An `et` specifier indicates the following entries in the mctal file are energy binned, and has the following format:

```
et (number of energy bins + 1).
```

Following this, the energy bins are specified in ascending order. After the energy bins, a `vals` specifier is present, followed by pairs of the experimental data and the corresponding experimental uncertainty in the same order as the energy bins. An additional experimental data point of zero is the first experimental data point, so the experimental data can match the calculated MCNP results since the first energy bin in MCNP starts at zero MeV. To keep the same number of time bins as data points, another time bin is added.

The experimental data is given as an upper and lower confidence interval. The experimental values that are in the mctal file are an average of these two values. The relative uncertainties that are in the mctal file are the difference of the average value and one of the confidence bounds divided by the average value, which is

$$\text{relative uncertainty} = \frac{f_{avg}-f_{lower}}{f_{avg}}. \tag{3}$$

The experimental data is in units of $MeV^{-1}cm^{-2}$, which corresponds to the MCNP output so no normalizations are needed. The plot of the experimental data and the MCNP results for configuration 1, detecting neutrons, with the detector on the axis of the deuteron beam, is shown in Fig. 2.

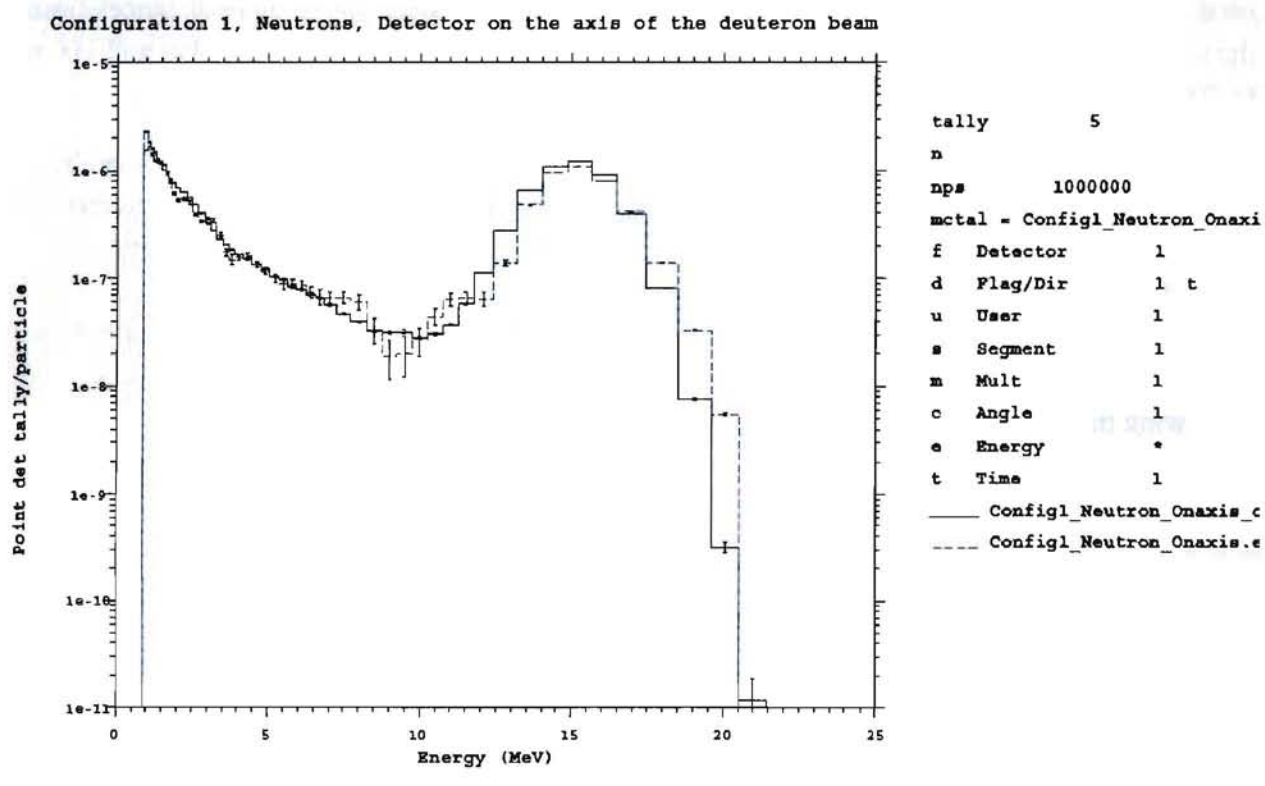

Fig. 2 – Fusion Shielding for Configuration 1, detecting neutrons, on the axis of the deuteron beam

To validate the MCNP results for the Fusion Shielding experiments, the errors are calculated using Eq. (1), and the reduced chi-squared is calculated using Eq. (2). The same rejection method for discarding outliers is also used. The errors for the benchmark experiments are shown in Table IV. Similar to the Livermore Pulse Sphere experiments, the errors are lower for the scattered neutrons and higher around the peak. The reduced chi-squared terms are much larger for the experiments detecting neutrons.

Table IV - Errors for Fusion Shielding experiments

	X_{red}^2	E
Config1_Neutrons_Onaxis	288.0	0.082
Config3_Gamma_Onaxis	57.9	0.094
Config3_Neutrons_Offaxis	253.2	0.031
Config7_Gamma_Offaxis	29.8	0.175
Config7_Neutrons_Onaxis	86.6	0.040

4 Photon Benchmarks

4.1 Skyshine

The Skyshine experiment[5] is also in the suite. In this experiment, a Co-60 source was used and the radiation was collimated upward. Detectors were placed at different distances from the source and measured the air-reflected gammas. The detectors were placed at 50 m and 100 m to 700 m in increments of 100 m.

The experimental data are given in units of m^2*mircrorad/hr/Ci. The data is divided by πr^2, where r is the corresponding distance from the source. The experimental data is corrected for the detector efficiency[5]. For the experimental results to be comparable to the MCNP data, the detector efficiencies are divided out of the experimental data in the mctal file. In the experimental data, multiple data points are shown for each distance; the values are averaged into one data point so they can be entered into a mctal file. A `vals` specifier is in the mctal file. Following the `vals` specifier, the data is given in pairs of the collided flux and then the uncollided flux for each distance. The data that is given in the experiment is the collided flux. The values of the uncollided flux are zero in the mctal file, since those values are meaningless.

In the MCNP input file, all of the detectors are specified on one tally card allowing them to be plotted together. An `fm` card is in the input file,

```
fm# rho m -5 -6,
```

where `rho` is the number density of the absorbing material and `m` is the material number. The reaction number of `-5` gives the total photon cross section, and the `-6` gives the photon heating number. The number density of the absorbing material in the detector is 4.541E-5/cm/barn. Adding the number density and the reaction numbers to the `fm` card will give the MCNP tally in units of MeV/cm^3. The experimental results are in units of microrad/hr/Ci. The tally is changed into units of microrad/hr/Ci by multiplying the MCNP input file by 1.94E15 cm^3*microrad/MeV/Ci/hr, or

$$\frac{1.602\text{E-6 erg}}{\text{MeV}} \times \frac{1 \text{ rad}}{100 \text{ erg/g}} \times \frac{\text{cm}^3}{.0011\text{g}} \times \frac{3.7\text{E10}}{\text{sec*Ci}} \times \frac{3600 \text{ sec}}{\text{hr}} \times \frac{1\text{E6 microrad}}{\text{rad}} = 1.94\text{E15} \ \frac{\text{cm}^3\text{microrad}}{\text{MeV Ci hr}} \tag{4}$$

The number density is multiplied by this factor to get 8.80954E+10, which is on the `fm` card as

```
fm# 8.80954E+10 m -5 -6,
```

and gives the MCNP tally in units of microrad/hr/Ci. The plot of the MCNP and experimental results are shown in Fig. 3.

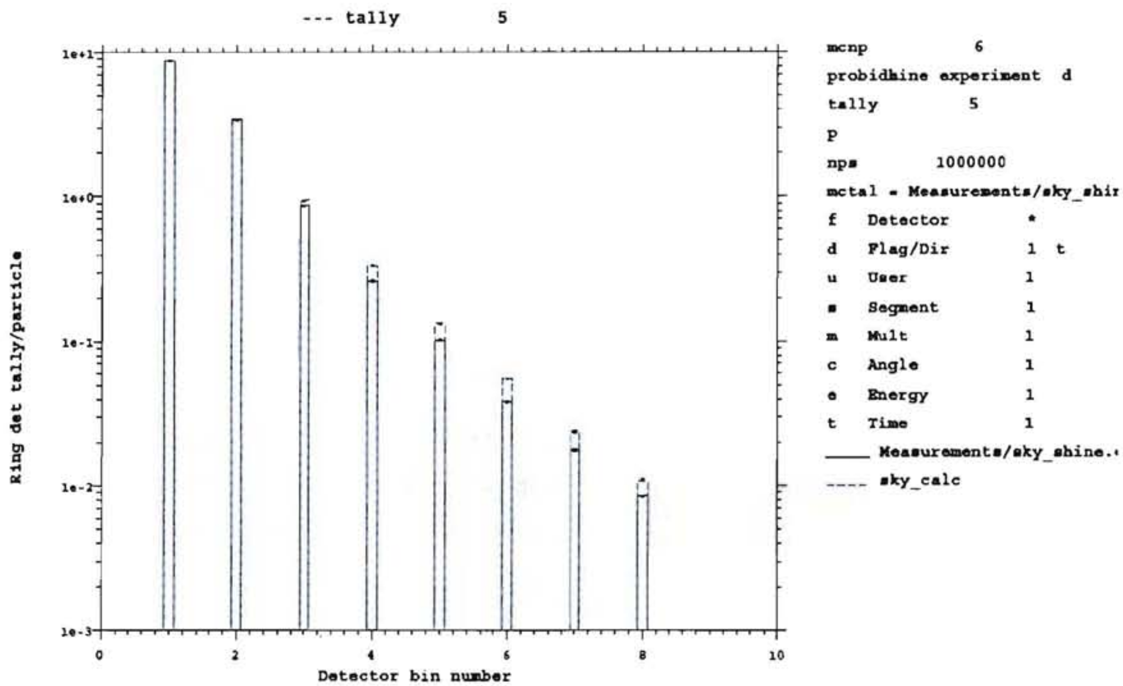

Fig. 3 - Skyshine, experimental data and MCNP results at various distances.

To validate the MCNP results for the Skyshine experiment, the error is calculated using Eq. (1), and the reduced chi-squared is calculated using Eq. (2). The error for the benchmark experiment is shown in Table V. The error relative to each detector increases with distance from the source. The same rejection method for discarding outliers is also used, but none of the points are discarded. The error at every detector location is used to find E.

Table V – Errors for the Skyshine experiments

Reduced Chi-Squared	E
135.5	0.073

4.2 Co-60, Air over Ground

The Co-60 air over ground experiment[7] is also in the suite. In this experiment, Co-60 was spread out as an infinite plane source. The kerma rate in air was measured three feet above the ground as a function of the cosine of the angle.

The experimental data used for this benchmark is from a plot in Ref. 8. The plot is missing its x-axis, although it is clear that the x-axis is the cosine of the angle from -1 to 1. The relative uncertainty used for the experimental data is the uncertainty of reading the values off of the plot. This data is in the mctal file. The `c` specifier is given in the mctal in the format:

```
c (number of cosine bins + 1).
```

The values of the cosine bins are specified after this card. These values represent the separations in between bins, with the first bin starting at negative one. Following the `c` specifier, a `vals` specifier is present, with the values of the total flux given after the `vals` specifier.

In the MCNP input file, the first multiplier card originally was

```
fmβ rho m -5 -6,
```

where β is the tally index, `rho` is 5.20704e-5, and `m` is the material number. The reaction number of `-5` gives the total photon cross section, and the `-6` gives the photon heating number. This gave the total flux and uncollided flux at the detector. The multiplier card now looks like

```
fmβ rho/(uncollided flux) m -5 -6,
```

where the final value in the multiplier card is 1.75668E+10. The uncollided flux is calculated using the original multiplier card. The multiplier card now gives the buildup rate for the total flux, and the uncollided flux should be about 1.

The experimental data is given in units of a kerma rate (ergs/g/sec). The MCNP results are changed into a kerma rate using a second multiplier card in the form

```
fm# C m -5 -6,
```

where # is the tally index, `m` is the material number, and `C` is the conversion factor to get the results into a kerma rate. The conversion factor C is

$$\mathrm{C} = \alpha(1.602\mathrm{E}\text{-}6\,\frac{\mathrm{erg}}{\mathrm{MeV}})(\frac{1}{\rho})(\frac{2}{\text{area of tally sphere}})(\pi r^2), \tag{5}$$

where α is the atomic density of air which is 5.3736×10^{-5} atoms/cm/barn, ρ is the density air that is .00129 g/cm^3, and r is the radius of the circle plane of Co-60 that is 10^5 cm. The conversion factor C is 1317.25.

A c# card is specified in the MCNP input file to give the MCNP results in the same cosine bins as the experimental data. The tally number # on the c# card is the same as the tally number on the second multiplier card. The inputs on the c# card have the same values as the c specifier in the mctal file. The kerma rate of each angle bin is normalized to be per steradian with

$$\frac{1}{2\pi(\cos(\theta)_{i+1}-\cos(\theta)_i)}, \tag{6}$$

where θ is the angle. The values for each angle bin are in the cm# card, corresponding to the same order as the cosine bins in the c# card. The tally number on the cm# card also corresponds to the tally number on the second multiplier card.

The plot of the MCNP and experimental results are shown in Fig. 4.

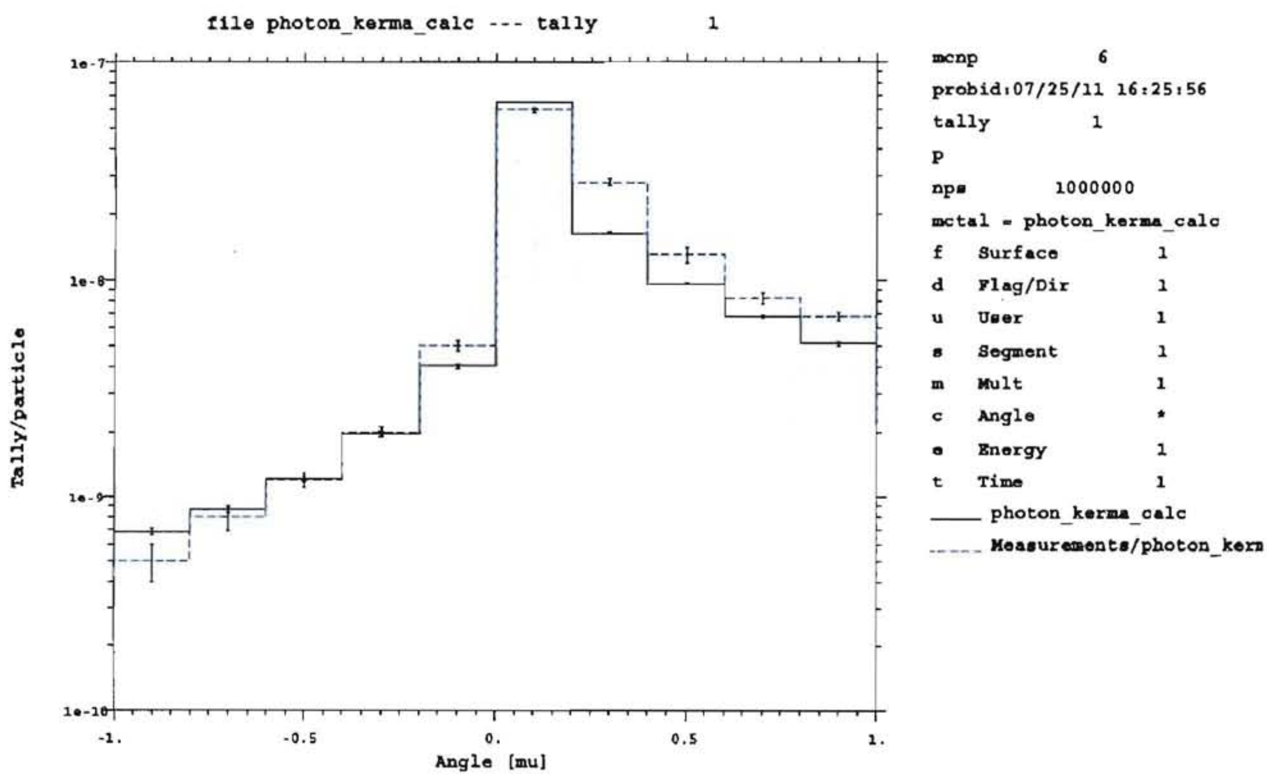

Fig. 4- Co-60 Air over Ground, MCNP results and experimental data.

The error for the Co-60 air over ground experiment is calculated using Eq. 1. The reduced chi squared is not meaningful since the only uncertainties that are available for this benchmark experiment are obtained from reading the values off of the plot in Ref. 8. The errors for this benchmark experiment are shown in table VI.

Table VI

Reduced Chi-Squared	E
NA	0.052

5 Conclusion

These benchmark experiments are chosen as a way to validate neutrons and photons transport capabilities of MCNP and the associated ENDF/B-VII.0. The first benchmark experiment is the Livermore Pulsed Sphere experiments, which measured neutrons as a function of time. Comparing the experimental data to the MCNP results, the errors are lower for the scattered neutrons and higher for the peak.

The second benchmark experiment is the Fusion Shielding experiments, which measured neutrons and photons as a function of energy. Just like the Livermore Pulsed Spheres experiments, the errors are lower for the scattered neutrons and photons, and higher for the peak. The reduced chi-squared is found to be much larger in the neutron experiments than it is in the photon experiments.

The last benchmarks are the photon experiments, which consist of the Skyshine experiment and Co-60 air over ground experiment. In the Skyshine experiment, air scattered photons were measured as a function of distance. The error relative to each detector increases with distance from the source. In the Co-60 air over ground, the kerma rate was measured as a function of angle. This experiment is probably not as useful for validating MCNP as the other benchmark experiments since the only uncertainty associated with the experimental data is reading the values off the plot.

6 References

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