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Simulation of Photon Energy Spectra Using MISC, SOURCES, MCNP and GADRAS

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Abstract

The detector response functions included in the Gamma Detector Response and Analysis Software (GADRAS) are a valuable resource for simulating radioactive source emission spectra. Application of these response functions to the results of three-dimensional transport calculations is a useful modeling capability. Using a 26.2 kg shell of depleted uranium (DU) as a simple test problem, this work illustrates a method for manipulating current tally results from MCNP into the GAM file format necessary for a practical link to GADRAS detector response functions. MISC (MCNP Intrinsic Source Constructor) and SOURCES 4C were used to develop photon and neutron source terms for subsequent MCNP transport, and the resultant spectrum is shown to be in good agreement with that from GADRAS. A 1 kg DU sphere was also modeled with the method described here and showed similarly encouraging results.

1. Introduction

GADRAS (Gamma Detector Response and Analysis Software) is a one-dimensional, deterministic radiation transport program from Sandia National Laboratory (SNL) capable of calculating gamma-ray spectra augmented by neutron count rate information using physics-based detector response functions [1, 2]. GADRAS has been benchmarked against numerous photon sources [3, 4] and neutron sources [4].

MCNP is a three-dimensional Monte Carlo code from Los Alamos National Laboratory (LANL) capable of transporting neutrons, photons, and/or electrons based on a source specification and material specific cross section libraries [5]; this work used MCNP5 and the authors note MCNP6, the version of the code merged with MCNPX, contains additional particles and transport options. Use of MCNP requires knowledge or development of a source term. This work relied on MISC (MCNP Intrinsic Source Constructor) to calculate the photon source term [6] and SOURCES 4C to calculate the neutron source term [7]. MISC calculates the photon emission rate and spectrum for a material based on its composition and age – if decay libraries are available [6]. SOURCES 4C calculates the neutron emission rate and spectrum from (α,n) reactions, spontaneous fission, and delayed neutron emission based on material composition [7].

MCNP output can be manipulated into the format of an equivalent GADRAS output known as a *.gam* file. The detector response functions in GADRAS can then be used to produce a gamma-ray spectrum for a particular detector. This work focuses on the methodology of this process for a spherical shell of depleted uranium and compares the results of the hybrid MCNP/GADRAS simulation with those of a pure GADRAS simulation for the same materials and geometry. Similar work has been performed by Rawool-Sullivan [8, 9], however, that work used GADRAS to develop the MCNP source terms for photons, neutrons, and electrons.

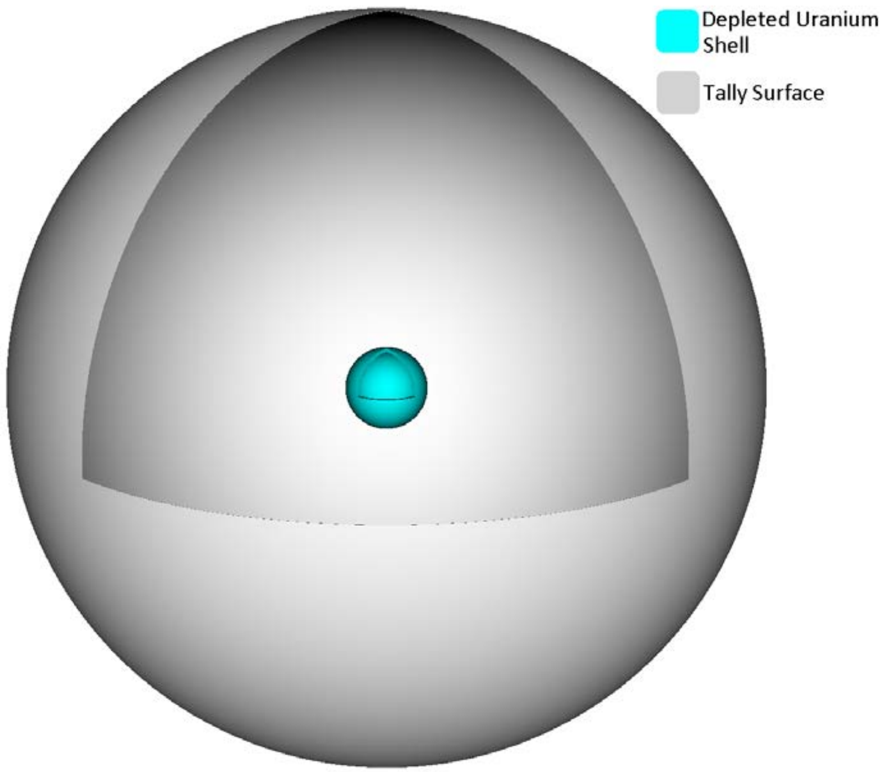

Fig. 1. Depleted uranium shell problem geometry generated with OsoLoco [11].

2. Methodology

To compare GADRAS and MCNP, both programs were used to model a spherical shell of depleted uranium with an inner radius of 10 cm and an outer radius of 11 cm with void inside and outside the shell. The depleted uranium was composed of the following by weight: 0.001% ^{234}U, 0.196% ^{235}U, and 99.803% ^{238}U. Given a density of 18.9 g cm^{-3} for uranium metal [10], the shell contains about 26.2 kg of depleted uranium. There are two primary sources of photons for this problem: (n,γ) reactions and the radioactive decay of uranium and its daughter products. Figure 1 displays the problem geometry generated with OsoLoco [11]; the tally surface has a radius of 100 cm.

2.1 MISC

MISC was used to calculate the photon spectrum from the radioactive decay of uranium and its daughter products. The MISC input file is displayed in Figure 2. The pound symbol denotes a comment. The ZAID numbers of the three uranium isotopes in the problem are listed in the *matspec* card with negative numbers to indicate the given values as weight fractions. In this case, MISC will decay the depleted uranium mixture for 20 years (6.3072E+08 s), which is long enough to achieve secular equilibrium. Also notable is that MISC can calculate the photon production from bremsstrahlung; this feature has been activated here.

```
# ISCDATA path from environment
# output file
output = du-misc.out
# source file
srcout = du-misc.src
# radioactive decay data file
decayfile = endf7.dk
# natural abundance/mass data file
abundfile = nist.na
# default paricle emission library
pelib = endf7
# material specification
matspec = 92234 -0.00001
          92235 -0.00196
          92238 -0.99803
# mass density
density = -18.9
# output format
format = v
# source particle type
particle = 2
# age the material (seconds) 20 yr
age = 6.3072e8
# add bremsstrahlung to photon source
brems = y
# convert electrons to bremsstrahlung
estobrems = y
# bremsstrahlung multiplier
bremsmult = 1.0
biasing = uniform
```

Fig. 2. MISC input file

Running the program generates two files. The output file, in this case *du-misc.out*, summarizes the problem input and lists the amount of each nuclide produced by the parent isotope decay chains. It also provides the specific particle emission rate in cm^{-3} s^{-1} and g^{-1} s^{-1} for photons and alpha particles. The second file produced is the source distribution file which can be pasted directly into the SDEF card in an MCNP input file. For a complete description of the input file structure see the MISC user guide [6].

2.2 SOURCES

SOURCES4C was used to calculate the neutron source term to be used by MCNP. While SOURCES may consider neutrons from (α,n) reactions, spontaneous fission, and delayed neutron emission, only those from spontaneous fission were considered for this simple problem. A homogeneous mixture of the uranium nuclei was assumed and the neutron spectral data were arbitrarily divided into 750 linearly interpolated bins from 0 MeV to 10 MeV.

2.3 MCNP

Two MCNP input files were created to account for the total photon source emitted by the depleted uranium shell. Input P used the MISC-produced photon source term and tracked only the decay photons while Input NP used the SOURCES-produced neutron source term and tracked both neutrons and photons, the latter arising from (n,γ) reactions. Both input files used the geometry and material definitions described earlier. For Input P, a single photon current tally was made at 100 cm while two current tallies (one photon, one neutron) were made in Input NP. Photon current tallies were made in 1477 bins from 20 keV to 12 MeV as specified by GADRAS input structure and the neutron current tally was made in 79 bins from 0 MeV to 19.64 MeV. The neutron energy bin structure is one routinely used by SNL. Both MCNP input files tracked one billion histories. The photon tally in Input P has an average relative error of 3.43% with 125 empty bins (all above 4418.4 keV) and 70 bins with greater than 10% relative error, 20 of which have greater than 20% error. The photon tally in Input NP has an average relative error of 2.06% with 60 empty bins and 30 bins with greater than 10% error, 23 of which have greater than 20% error. The neutron tally in Input NP has an average relative error of 19.2% over all bins and 22.5% if the 12 empty bins are excluded. There are 26 bins with greater than 10% relative error, 21 of which have greater than 20% relative error. These tally results are plotted in Figure 3.

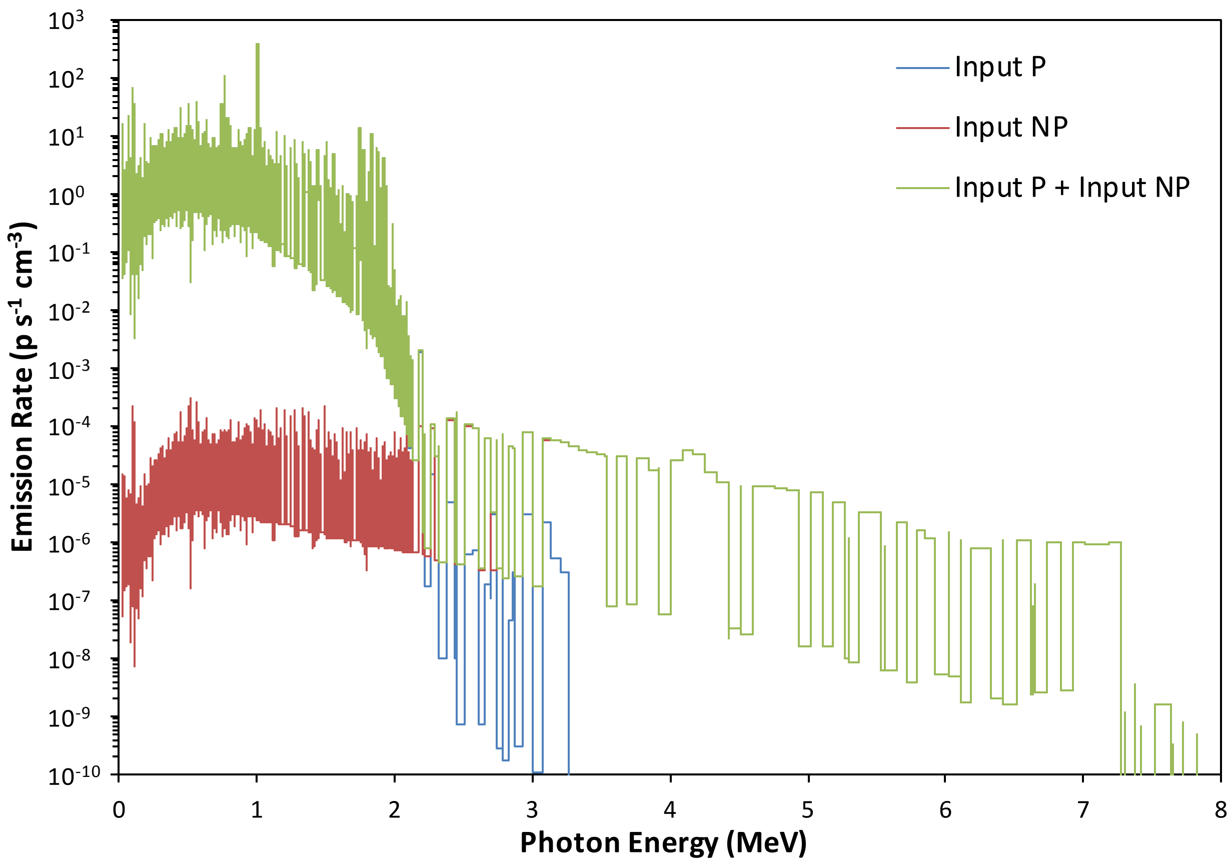

Fig. 3. Results of MCNP photon current tallies from Input P and Input NP and the combination of those tallies for input into GADRAS.

2.4 *GADRAS Input*

After running both MCNP input files, the photon tallies from each output were pasted into a spreadsheet for post-processing. Results from each problem were multiplied by their respective source terms (the MISC photon source term for Input P and the SOURCES neutron source term for Input NP) to convert from photons per source-particle to photons per second. The two tallies were then combined to form a single cumulative source term for input into GADRAS. The neutron tally from Input NP was also converted via spreadsheet from neutrons per source-particle to neutrons per second. Both conversions (photons/source-particle to photons/second and neutrons/source-particle to neutrons/second) could be performed within MCNP either by applying the appropriate weight to the SDEF entry or by applying a tally multiplier. However, the photon tallies from each output would still need to be combined. Figure 4 provides a flow chart describing the entire method for developing a GAM file to apply GADRAS detector response functions to MCNP transport calculations.

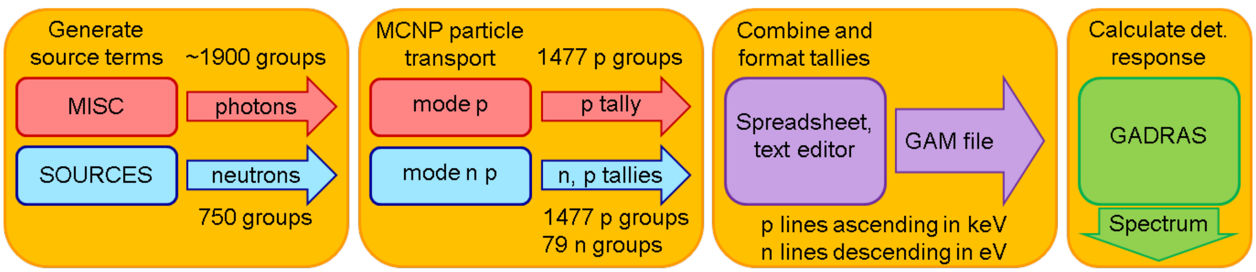

Fig 4. Flow chart of method for applying GADRAS detector response functions to MCNP transport calculations

```
0             0             0
0             1477          79
1.00000E+00   2.26240E+04      ! photon lines
2.00000E+01   2.59252E+03
2.93500E+01   4.93000E+01
    ...           ...
    ...           ...
    ...           ...
1.16500E+04   0.00000E+00
1.17900E+04   0.00000E+00
1.20000E+04   0.00000E+00
1.96400E+07   1.04252E-08      ! neutron groups
1.73320E+07   1.41930E-07
1.41910E+07   5.83927E-07
    ...           ...
    ...           ...
    ...           ...
5.00000E-04   0.00000E+00
1.00000E-05   0.00000E+00
0.00000E+00   0.00000E+00
```

Fig. 5. Truncated GADRAS input file

A truncated GADRAS file is shown in Figure 5. Comments are indicated by exclamation points. The first line contains three numbers and describes the problem; the first 0 indicates spherical geometry (the other two zeros, not considered here, are for future cylindrical and rectilinear options). The second line also contains three numbers: the first number, 0 for MCNP calculations, represents the number of ray-traced photon lines while the second and third entries represent the number of photon and neutron groups, respectively. The photon source definition begins on the third line with the energy bins (keV) in ascending order in the left column and the intensity of each bin (photons/second) in the right column. The neutron source definition begins directly below the photon source definition. Neutron energy bins (eV) are listed in descending order in the left column while the intensity of each bin (neutrons/second) follows in the right column. A complete description of GADRAS input is found in the GADRAS User Manual [1].

3. Results

Results of the MCNP simulation compared favorably with those of the GADRAS simulation after applying GADRAS detector response functions for an Ortec Detective-EX [12]. Figure 6 shows a co-plot of the results from the simulations. The largest visible discrepancy between the two spectra occurs at the low energy end of the plot in the Bremsstrahlung energy range. This is likely due to the use of a thick target Bremsstrahlung approximation when generating the photon source term with MISC [13]. Table 1 compares the simulation results for four important ^{238}U photopeaks as defined by the PANDA Manual [14]. For the peaks at 1001.0 keV, 786.3 keV, and 766.4 keV, the results from the MCNP transport calculation match those from the GADRAS transport calculation with less than 10% relative error. However, the 742.8 keV photopeak results are much poorer, with 25.2% relative error. This discrepancy is likely caused by a difference in the branching ratios used by GADRAS and MISC for the decay of ^{234m}Pa. As seen in Table 2 the greatest difference between ratios is for the 742.8 keV peak.

Table 1. Comparison of photon intensity results for ^{238}U photopeaks [14] from GADRAS and MCNP transport calculations after applying GADRAS detector response functions.

Energy (keV)	GADRAS (cps)	MCNP (cps)	ε
742.8	1121	1403	-25.2%
766.4	2691	2951	-9.7%
786.3	924	999	-8.1%
1001.0	7261	7667	-5.6%

Table 2. Select ^{234m}Pa branching ratios used by GADRAS and MISC.

Energy (keV)	742.8	766.4	786.3	1001.0
GADRAS	9.46E-04	3.22E-03	5.54E-04	8.39E-03
MISC	1.06553E-03	3.17302E-03	5.43707E-04	8.41651E-03
ε	-12.6%	1.5%	1.9%	-0.3%

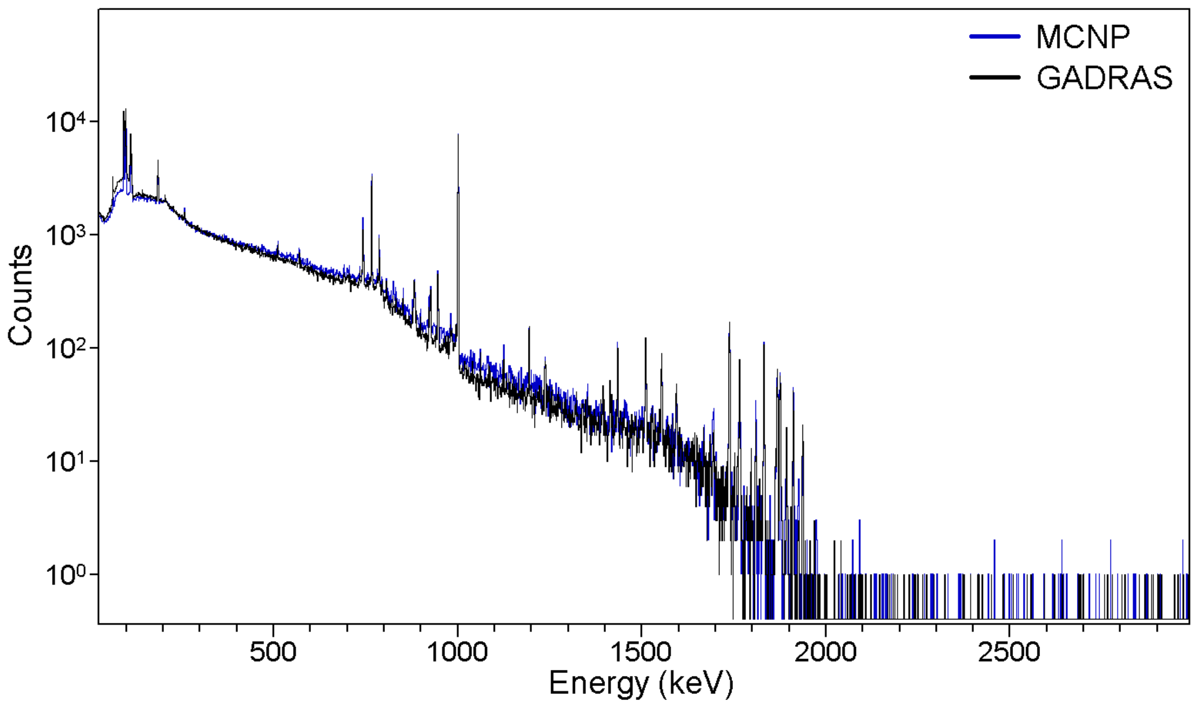

Fig. 6. MCNP and GADRAS simulation results from 0 to 3000 keV for a 26.2 kg DU shell after applying GADRAS HPGe detector response functions plotted with PeakEasy.

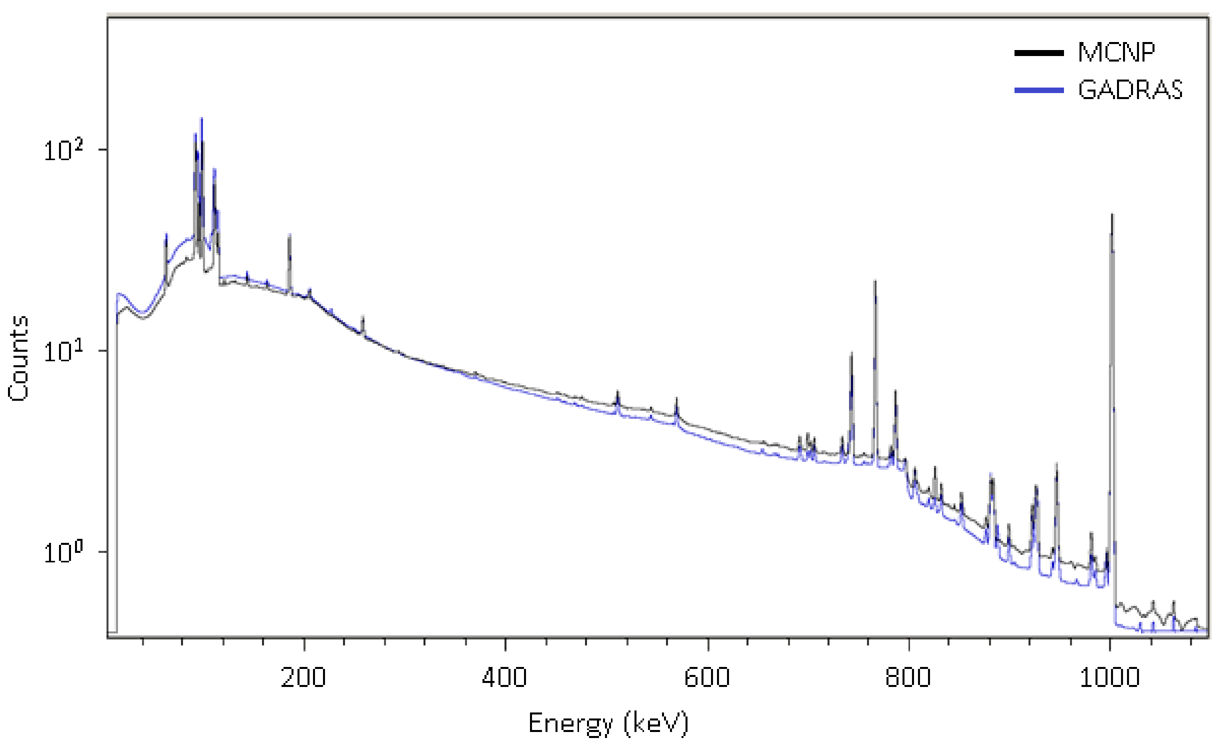

Fig. 7. MCNP and GADRAS simulation results from 0 to 1100 keV for a 1 kg DU sphere after applying GADRAS HPGe detector response functions plotted with PeakEasy.

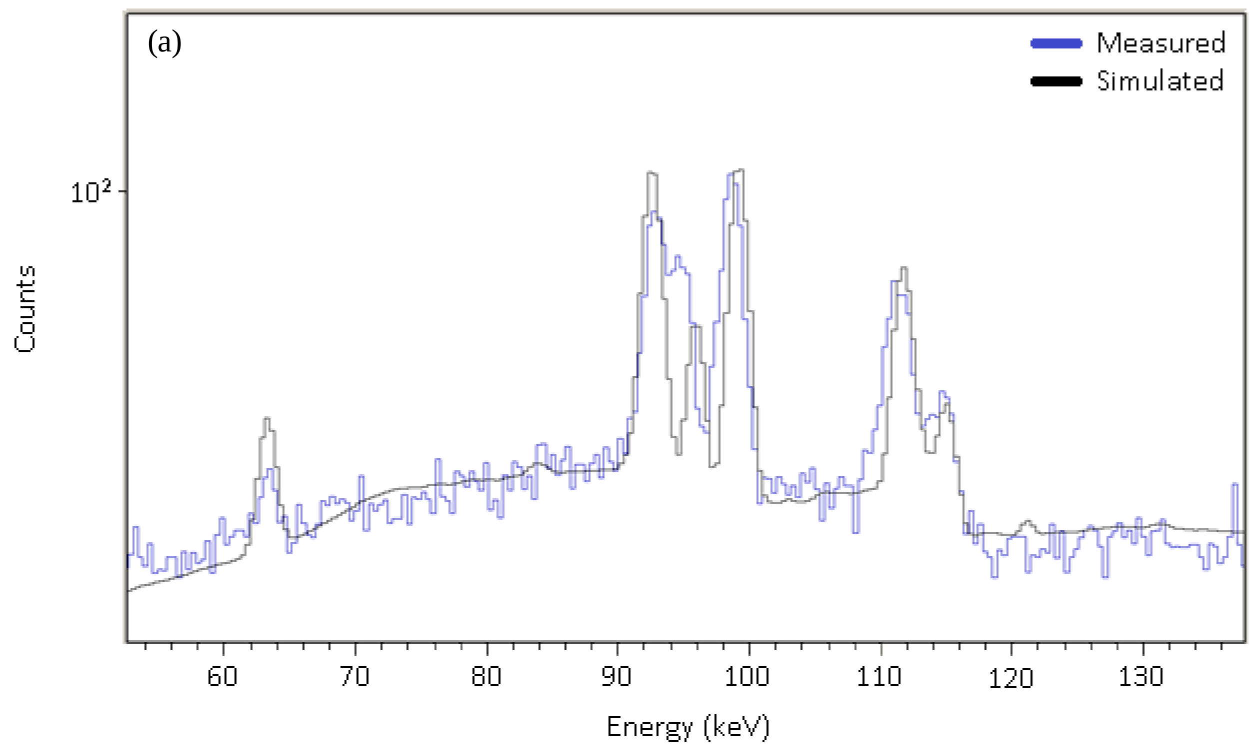

Fig. 8. Spectral data generated with GADRAS detector response functions for a 1 kg DU sphere co-plotted with measured data using PeakEasy. (a) From an MCNP-generated GAM file. (b) From a GADRAS generated GAM file

Table 3. Comparison of count rate results for important uranium photopeaks [14] from GADRAS and MCNP transport calculations after applying GADRAS detector response functions.

Photopeak keV	MCNP counts	GADRAS counts	ε
185.7	90.2 ± 20.7	88.5 ± 20.8	1.9%
742.8	40.7 ± 10.5	29.3 ± 9.6	38.9%
766.3	115.5 ± 13.4	105.6 ± 12.8	9.4%
786.3	20.2 ± 9.1	17.9 ± 8.7	12.8%
1000.1	299.3 ± 17.8	296.6 ± 17.6	0.9%

The process summarized in Section 2 was also applied to a 1 kg depleted uranium solid sphere. The sphere's composition in weight percent was 0.0015% ^{234}U, 0.2% ^{235}U, and 99.7985% ^{238}U with a density of 18.95 g cm^{-3}. It was aged twenty years to ensure secular equilibrium was achieved. These specifications are identical to those used by Rawool-Sullivan [9]. And like Rawool-Sullivan's work, this simulation also provided a favorable comparison between MCNP, GADRAS, and measured data. Figure 7 is a co-plot of the MCNP and GADRAS simulation results. As with the results for the 26.2 kg DU shell, the largest discrepancy exits around 100 keV, indicating a difference in how bremsstrahlung radiation is treated by the codes. Figure 8 shows spectral data generated by the detector response functions in GADRAS compared with measured data in the 50 to 140 keV region. In Figure 8(a) the measured spectrum is compared to simulated data based on an MCNP generated GAM file, while in Figure 8(b) the simulated data is based on a GAM file generated with the 1D transport calculator native to GADRAS. The results of the simulations for several important uranium photopeaks are listed in Table 3. As expected, the results agree well except for the 742.8 keV peak, which also exhibits the largest difference in ^{234m}Pa branching ratios.

4. Summary and Conclusions

After using MISC and SOURCES to develop photon and neutron source definitions (SDEF), MCNP was used to calculate the leakage from a depleted uranium sphere. The results of photon and neutron current tallies with particular energy bins were exported to a spreadsheet for manipulation into GAM file format. Another GAM file representing the same problem was produced directly by GADRAS. Detector response functions for an HPGe detector were applied to the 3D transport calculations from MCNP as well as 1D calculations from GADRAS. In general, the two spectra compared favorably, though some discrepancies exist in the Bremsstrahlung energy range perhaps due to the thick-target Bremsstrahlung model in MISC. There was also notable disagreement at 742.8 keV due to a difference in the branching ratios used by GADRAS and MISC. Overall, however, this method has been demonstrated to be an effective means of predicting the spectra produced by a one cm thick 26.2 kg shell of depleted uranium and a 1 kg sphere of depleted uranium. This conclusion corroborates that of Rawool-Sullivan [8, 9] and expands the number of tested cases for combining MCNP and GADRAS.

5. References

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