Verification of the ENDF7U Photonuclear Data Library for MCNP

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Introduction:

The ENDF7U Photonuclear Data Library at Los Alamos consists of 157 isotopes. Unlike photoatomic data which is elemental in nature (based on photon interactions with the electrons), photonuclear data is based on the isotopes (based on photon interactions with the nucleus). Furthermore, photonuclear data is generally only available above threshold energies, say a few MeV.

The predecessor library to ENDF7U was called LA150u(1) and consists of 13 isotopes. There are no changes between the 13 isotopes in LA150u and the same 13 isotopes in ENDF7U. So ENDF7U is a superset of LA150u.

A calculational benchmark based on experimental measurements is available for the re-verification of the ENDF7U library(2). An early version of the ENDF7U library was used in the MCNPX comparisons with the experimental measurements. Those verification calculations are repeated here with MCNP6 and the current version of ENDF7U.

The ENDF7u Library:

The data in the ENDF7U library is based on ENDF/B VII.0 data. The contents of the ENDF7U library are listed below. The energy threshold for photonuclear cross sections is also given.

Table 1 The isotopes in the ENDF7U photonuclear library:

Material	ZAID	Threshold	Comments
		(MeV)	
D	1002.70u	2.2246	late addition to LA150u
Be	4009.70u	0.999999	
C	6012.70u	7.366593	in LA150u, used in the experiment
	6013.70u	4.9463	used in the experiment
N	7014.70u	7.5506	
	7015.70u	10.95999	
O	8016.70u	12.49999	in LA150u
	8017.70u	4.499996	
	8018.70u	6.23	
Na	11023.70u	8.7941	
Mg	12024.70u	9.3106	
	12025.70u	7.3307	

	12026.70u	10.6118	
Al	13027.70u	8.499992	in LA150u, used in the experiment
Si	14028.70u	9.9843	in LA150u
	14029.70u	8.4739	
	14030.70u	10.6096	
S	16032.70u	6.9484	
	16033.70u	7.1161	
	16034.70u	7.923699	
	16036.70u	9.008099	
Cl	17035.70u	6.3704	
	17037.70u	7.8486	
Ar	18036.70u	6.6392	
	18038.70u	7.2076	
	18040.70u	6.7998	
Ca	20040.70u	7.0403	in LA150u
	20042.70u	6.2568	
	20043.70u	7.5925	
	20044.70u	8.855	
	20046.70u	10.3993	
	20048.70u	9.9399	
Ti	22046.70u	8.0033	
	22047.70u	8.8778	
	22048.70u	9.4428	
	22049.70u	8.1424	
	22050.70u	10.7102	
V	23051.70u	4.999999	
Cr	24050.70u	8.5568	
	24052.70u	9.3522	
	24053.70u	7.9395	
	24054.70u	7.929	
Mn	25055.70u	7.934199	
Fe	26054.70u	8.4179	
	26056.70u	7.6142	in LA150u
	26057.70u	7.3209	
	26058.70u	7.6466	
Co	27059.70u	6.9428	
Ni	28058.70u	6.3996	
	28060.70u	6.292	
	28061.70u	6.466	
	28062.70u	7.0186	
	28064.70u	8.1169	
Cu	29063.70u	5.7775	in LA150u, used in the experiment
	29065.70u	6.789899	used in the experiment
Zn	30064.70u	3.9563	
	30066.70u	4.5782	

	30067.70u	4.7917	
	30068.70u	5.3334	
	30070.70u	5.9569	
Ge	32070.70u	4.0879	
	32072.70u	5.002	
	32073.70u	5.3028	
	32074.70u	6.2875	
	32076.70u	7.5087	
Sr	38084.70u	5.1719	
	38086.70u	6.3517	
	38087.70u	7.3184	
	38088.70u	7.9117	
	38090.70u	5.1057	
Zr	40090.70u	6.676599	
	40091.70u	5.4431	
	40092.70u	2.9655	
	40093.70u	3.3341	
	40094.70u	3.7504	
	40096.70u	4.9439	
Nb	41093.70u	1.9326	
	41094.70u	2.3045	
Mo	42092.70u	5.6079	
	42094.70u	2.0677	
	42095.70u	2.2407	
	42096.70u	2.7599	
	42097.70u	2.8469	
	42098.70u	3.27	
	42100.70u	3.1689	
Pd	46102.70u	2.117899	
	46104.70u	2.5982	
	46105.70u	2.8905	
	46106.70u	3.2325	
	46107.70u	3.5385	
	46108.70u	3.8549	
	46110.70u	4.4439	
Ag	47107.70u	2.8076	
	47108.70u	3.0779	
	47109.70u	3.2969	
Cd	48106.70u	1.6419	
	48108.70u	2.2849	
	48110.70u	2.868899	
	48111.70u	3.3049	
	48112.70u	3.4831	
	48113.70u	3.8699	
	48114.70u	4.1017	

	48116.70u	4.8119	
Sn	50112.70u	1.829899	
	50114.70u	2.6339	
	50115.70u	3.205	
	50116.70u	3.3698	
	50117.70u	3.7742	
	50118.70u	4.0573	
	50119.70u	4.4018	
	50120.70u	4.808699	
	50122.70u	5.6619	
	50124.70u	6.6892	
Sb	51121.70u	3.0715	
	51123.70u	3.9157	
Te	52120.70u	2.848	
	52122.70u	1.0779	
	52123.70u	1.528	
	52124.70u	1.8462	
	52125.70u	2.2458	
	52126.70u	2.546	
	52128.70u	3.1796	
	52130.70u	3.7519	
I	53127.70u	2.1831	
	53129.70u	2.6739	
Cs	55133.70u	2.0039	
	55135.70u	2.6299	
	55137.70u	3.0929	
Pr	59141.70u	2.999997	
Sm	62144.70u	8	
	62147.70u	6	
	62148.70u	8	
	62149.70u	5.5	
	62150.70u	7.5	
	62151.70u	5.5	
	62152.70u	8	
	62154.70u	1.1969	
Tb	65158.70u	0.1569	
	65159.70u	0.1379	
Ho	67165.70u	4	
Ta	73181.70u	7.5	in LA150u, used in the experiment
W	74180.70u	4.999999	
	74182.70u	4.999999	
	74183.70u	3.999999	
	74184.70u	7.499999	in LA150u
	74186.70u	4.999999	
Au	79197.70u	8	

Pb	82206.70u	8	in LA150u, used in the experiment
	82207.70u	6.5	in LA150u, used in the experiment
	82208.70u	7.499999	in LA150u, used in the experiment
Bi	83209.70u	7	
U	92235.70u	3.25	used in the measured experiment
	92238.70u	3.419999	used in the measured experiment
Np	93237.70u	0.999999	
Pu	94239.70u	3.5	
	94240.70u	3.999999	
Am	95241.70u	0.999999	

Verification and Consistency Checks:

Using the published experimental results(2) and previous MCNPX calculations with LA150u and ENDF7U, 62 MCNP6 calculations were carried out using ENDF7U. The experiment has 15% uncertainties, so it is not a benchmark, per se. The experiment involves an electron beam impinging on various targets. The electrons produce photons which then produce the neutrons of interest.

The MCNP6 with ENDF7U results were consistently off from previous MCNPX and ENDF7U calculations by ~2.2%. The problem was not in the Doppler Broadening of the photonuclear cross sections – for which MCNP6 and MCNPX indeed do different things.

It turns out that MCNP6 handles electron transport differently than MCNPX. MCNP6 can be made to run electron transport like MCNPX by setting certain parameters in the DBCN array. From a Michael R. James memo(3):

Other Important DBCN entries.

DBCN(18). This entry controls the energy indexing algorithm for electron transport related to bin interpolation. MCNPX used dbcn(18)=0 by default which was the "bin-centered" treatment. MCNP6 has implemented a better Landau treatment, dbcn(18)=2, which is superior. All electron transport problems will show differences due to this change.

DBCN(27). Antiparticle promotion. Use DBCN(27)=1 to lump particle and antiparticle pairs under one particle type (MCNPX behavior).

DBCN(38). Set = 1 to use older barpol.dat. By default, MCNP6 will use the newer barpol2001.dat data file.

DBCN(39). This entry controls the default S(a,b) smoothing behavior which was present in MCNPX but not in MCNP5. In MCNP6, the option is OFF by default. Use dbcn(39)=1 to turnthis on.

DBCN(43). Interpolation of Form Factors. Set = 0 to use the linear interpolation from MCNPX. The default treatment is now logarithmic inversion or log-log.

DBCN(52).Set = 1 to use MCNPX functionality in emission of Auger electrons.

In summary, the line

DBCN 17j 0 8j 1 10j 1 1 3j 0 8j 1

will maximize similarity to MCNPX when using MCNP6.

With these DBCN settings, MCNP6 with ENDF7U was re-run on all 62 problems and the differences between these new results and the previous published results fell to ~0.1 %.

Other verification efforts included:

(1) Sn calculations using the NDI gamma libraries on selected problems, but Sn gamma calculations do not include photonuclear (no gamma up-scatter to neutron) and Sn gamma calculations do not include electrons turning into photons. Thus, the verification by Sn is only good for lower photon energies without bremsstrahlung or photonuclear reactions. However, coupled neutron-photon deterministic calculations can include both neutron and photon sources in the same calculation[(4)].
(2) photon pencil beam calculations in MCNP6 – using a photon source (instead of electron) If the forced collision routine in MCNP included photonuclear reactions (in addition to the photoatomic reactions which are included), then a consistency check between hand calculations and MCNP results would be feasible – using a ridiculously small spherical photon source cell and neutron leakage tallies.
(3) I have verified that protons and neutrons are produced for selected test problems

References:

(1) Morgan C. White, "Release of the LA150u Photonuclear Library", Memo X-5:MCW-00-87(U), Los Alamos National Laboratory, (2000). Note that deuterium was added somewhat later to the original 12 isotopes in LA150u.
(2) Matthias Frankl & Rafael Macián-Juan (2016) Photonuclear Benchmarks of C, Al, Cu, Ta, Pb, and U from the ENDF/B-VII Cross-Section Library ENDF7U Using MCNPX, **Nuclear Science and Engineering**, 183:1, 135-142, DOI: 10.13182/NSE15-47
(3) Michael R. James, "MCNPX to MCNP6 Migration Notes", LA-UR-13-22694. Los Alamos National Laboratory, (2013).
(4) John C. Wagner, "Coupled Neutron-Photon Multigroup versus Continuous Energy MCNP", Memo X-6:JCW-94-412, Los Alamos National Laboratory, (1994).