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42-Group Photon Library for DANTSYS

The purpose of this memo is to announce the availability of a 42-group photon interaction library for DANTSYS.[1] The library is based on work done by Bob MacFarlane in Group T-2 to create a DTF-format file starting with the Livermore EPDL evaluation.[2] MacFarlane processed the EPDL library into DTF format using the NJOY nuclear data processing code system.[3]

Cross sections are available for 99 materials (Z=1 through Z=99). The 42 groups are those of the VITAMIN-J structure, and extend from 1 keV up to 50 MeV. The boundaries are provided in Table 1. The weight function used to collapse the cross sections is built-in to NJOY as IWT=3. It consists of a 1/E region at intermediate energies with roll-offs at lower energies (below 100 keV) to account for photoelectric absorption, and at higher energies (above 10 MeV) to account for a shoulder in photon spectra corresponding to the maximum Q-value for capture (see Attachment 1, which is page B-6 of Ref. 3 for more details). Six Legendre scattering tables are provided (i.e., P5). In preparing these tables, NJOY includes bound electron effects via coherent form factors and incoherent scattering functions. In addition to the standard edits (particle-balance absorption cross section, nubar*fission cross section [obviously zero for this set], and total cross section; all in barns), a heating edit is also available for calculating energy deposition. The units of the heating edit are ev-barns.

To make this data conveniently available to DANTSYS users, an input file has been created that accomplishes two things: 1) it converts the DTF-formatted file, which is in machine-independent ASCII format, into the more efficient (but platform-dependent) BXSLIB binary format, and 2) it assigns auxiliary information to the BXSLIB file that the user may need for subsequent calculations, such as edit names, isotope names and atomic weights, and group chis, velocities, and energy boundaries. This information is not available to DANTSYS from the original DTF file. The input file that accomplishes these tasks is gam42.inp, and is included in the tar file described next.

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1. DANTSYS and MCNP are trademarks of the Regents of the University of California, Los Alamos National Laboratory.

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Table 1: Energy Boundaries (eV) of the 42 Groups

Group	Upper Boundary	Group	Upper Boundary	Group	Upper Boundary
1	5.0e+07	15	4.0e+06	29	5.1e+05
2	3.0e+07	16	3.5e+06	30	4.5e+05
3	2.0e+07	17	3.0e+06	31	4.0e+05
4	1.4e+07	18	2.5e+06	32	3.0e+05
5	1.2e+07	19	2.0e+06	33	2.0e+05
6	1.0e+07	20	1.66e+06	34	1.5e+05
7	8.0e+06	21	1.5e+06	35	1.0e+05
8	7.5e+06	22	1.34e+06	36	7.5e+04
9	7.0e+06	23	1.33e+06	37	7.0e+04
10	6.5e+06	24	1.0e+06	38	6.0e+04
11	6.0e+06	25	8.0e+05	39	4.5e+04
12	5.5e+06	26	7.0e+05	40	3.0e+04
13	5.0e+06	27	6.0e+05	41	2.0e+04
14	4.5e+06	28	5.12e+05	42	1.0e+04
				lower boundary	1.0e+03

All necessary files are stored on CFS in tar format as /t1green/xslibrary/gam42.tar (open partition) and /t1red/xslibrary/gam42.tar (closed partition). Six files are included in gam42.tar. They are listed in Table 2. The full contents of the README file are attached to this memo as Attachment 2.

Table 2: Files Included in gam42.tar

File	Description
README	description of contents; reproduced here as Attachment 2
dtf	cross-section file in DTF format
gam42.inp	DANTSYS input file used to convert dtf to BXSLIB format

Table 2: Files Included in gam42.tar

File	Description
flxwgt	flux weighting spectrum
test.inp	simple spherical test problem
test.outp	output from test.inp

To test this library, a simple problem was constructed and calculated in DANTSYS and MCNP.[4] The geometry consisted of nested spheres of aluminum (outer radius = 7.5 cm), lead (outer radius = 12.5 cm), and water (outer radius = 25 cm). The source was isotropic, uniformly distributed over the inner 1 cm of the aluminum, and had an energy distribution consisting of equal probabilities in each of the 16 groups between 0.1 and 2.0 MeV. Total leakage from the outer sphere was calculated. The MCNP continuous-energy results are from photon cross sections based on ENDF/B-IV.[5] MCNP's default thick-target bremsstrahlung model was turned off for this calculation, since such contributions are not accounted for by the photon-only multigroup library. MCNP multigroup results are from a version of gam42 processed through the CRSRD code.[6] Results are given in Table 3.

Table 3: Test Problem Results

Code	Leakage
DANTSYS	0.0151
MCNP - multigroup	0.0152 (0.32%)
MCNP - continuous energy	0.0163 (0.27%)

Note that the DANTSYS and multigroup MCNP calculations are in very good agreement, while the continuous energy MCNP results differ somewhat. We believe that this is likely due to the significant amount of lead in the test problem. Lead has a large photoelectric absorption cross section with an edge at about 500 keV. The presence of a strong absorber in the intermediate energy regime results in a flux spectrum having a non-1/E shape, which conflicts with the weighting function assumed for this library. Thus, we feel that the library is most reliable at these energies for lower-Z materials. Other possible sources of discrepancies between multigroup and continuous energy are that the source itself for this problem is not 1/E, and that the continuous-energy cross sections are based on a different evaluation than are the multigroup cross sections.

In summary, a 42-group photon library based on EPDL has been made available for DANTSYS. In the future, a version of this library will also be made available for MCNP. Additional future work might also involve generating new multigroup photon libraries,

with energy boundaries and weight functions designed specifically for problems of interest.

References

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3. R.E.MacFarlane and D.W.Muir, "The NJOY Nuclear Data Processing System Version 91," LA-12740-M (Oct. 1994).

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6. J.C.Wagner, E.L.Redmond II, S.P.Palmtag, and J.S.Hendricks, "MCNP: Multigroup / Adjoint Capabilities," LA-12704 (April 1994).