1943 - 2003
Los Alamos
NATIONAL LABORATORY
Ideas That Change the World

To/MS: Distribution
From/MS: H. R. Trellue, X-1, MS F663
R. C. Little, X-1, MS F663
Phone: 5-9539/5-3487
Symbol: LA-UR-08-3628
Date: June 1, 2008

memorandum

Applied Physics Division
X-1 MS F699

SUBJECT: Release of New MCNP S(α,β) Library ENDF70SAB Based on ENDF/B-VII.0

Introduction

Neutron thermal scattering data (S(α,β)) exists for twenty different moderators in ENDF/B-VII.0.[1] All twenty moderator evaluations were processed using version 99.248 of NJOY[2] at all applicable temperatures (these vary for each evaluation – see Appendix A), and combined into the library ENDF70SAB for MCNP.[3] The final ENDF70SAB library contains a total of 111 tables for the twenty moderators.

Evaluated Data

ENDF/B-VII.0 includes thermal scattering data for twenty moderators. Eight of these are new evaluations: ^{27}Al, ^{56}Fe, beryllium (Be) and oxygen (O) in beryllium oxide (note Be and O are separately evaluated in this release), deuterium in heavy water, hydrogen in light water, and uranium and oxygen (separately) in uranium oxide. Twelve others are carried over from ENDF/B-VI.3: Be in beryllium metal, benzene, polyethylene (H in CH_2), graphite, hydrogen and zirconium (separately) in zirconium hydride, liquid and solid methane, ortho and para hydrogen, and ortho and para deuterium. The previous MCNP S(α,β) library, SAB2002,[4] is based on ENDF/B-VI.3.

Processing

The processing of the S(α,β) neutron thermal scattering data occurred using the NJOY processing system in two major steps: creating the PENDF files, and creating the ACE-formatted files. For S(α,β) processing, the key NJOY module executed in the PENDF processing sequence is THERMR. THERMR reads in both the pointwise output from BROADR and the applicable MF=7 thermal scattering ENDF/B-VII data. THERMR creates incoherent cross sections and scattering distributions from data in the evaluations for all moderators. Additionally, THERMR computes coherent elastic scattering cross sections and incoherent elastic scattering cross sections and angular distributions for the moderators for which such data are provided in the evaluations. Coherent elastic cross sections are included for ^{27}Al, ^{56}Fe, Be and O in BeO, Be metal, graphite, and O and U in UO_2. Incoherent elastic cross sections are included for polyethylene, H and Zr in ZrH, and solid methane. No elastic scattering data are provided for benzene, light water, heavy water, liquid methane, para and ortho hydrogen, and para and ortho deuterium.

The value 20 is used for the number of equally-likely discrete secondary cosines provided at each combination of incident and secondary energy for inelastic scattering, and at each incident energy for incoherent elastic scattering. This value is larger than the 16 provided for the previously library SAB2002, which was already greater than previous MCNP releases of thermal scattering data. The maximum neutron energy for the thermal treatment for most moderators was 10 eV. Exceptions were para and ortho H and para and ortho D, which all used 0.5 eV, and solid methane, which had a maximum energy value of 0.834 eV. Most tolerances in THERMR were set to 0.001, but for H in ZrH, it was 0.0015. Appendix B displays examples of the two different input files used for PENDF processing, one with which THERMR generates elastic scattering data and one where it does not (the difference is in the number of MT cards required).

ACE-formatted files for MCNP were created using the ACER module of NJOY. Both the PENDF file created in the previous step and the ENDF file for the S(α,β) moderator are required for the ACER processing, which must occur separately for each temperature. The number of secondary energies provided for each incident energy for inelastic scattering was 80, more than the 64 used in SAB2002. The new continuous tabulated option of providing data was NOT used for this processing because it would require additional modifications to MCNP. Sample ACER input files for NJOY are given in Appendix C. When elastic scattering data is produced in THERMR, two different MT input options are required, one for the incoherent cross sections and one for elastic cross sections. Otherwise, only the MT for inelastic cross sections is required in ACER.

All processing occurred using the LINUX system Flash under: /usr/projects/data/nuclear/mc/endf7/sab. A directory was created for each moderator in which input files were generated and NJOY was run. The NJOY input file used for PENDF processing was named "inputP," and the output file was named "outputP." NJOY input files used for ACER processing at each temperature were called "inpa##," where ## is the identifier number for that temperature as given in Table 1 (such as inpa10 for .10t entries), and output files were named "outa##." Script files named "script*" were kept to track the output to the screen, and the final ACE-formatted files were named ***.%%% where *** is the same name as the directory moniker, and %%% is the temperature. Data for all moderators and temperatures was combined into one file and applicable XSDIR entries using MAKXSF.LINUX. The first entry for each moderator in the XSDIR was given at room temperature (if available) although it does not always have an identifier of ".10t".

MCNP Data Tables

S(α,β) data is valid for all isotopes listed in Appendix A for a given moderator but not always for all materials in a moderator. For example, lwtr.10t provides scattering data only for ^{1}H; O would still be represented by the default free-gas treatment. Benzene, however, includes scattering data appropriate for both ^{1}H and for C. One consequence of this is that users should never use benzene S(α,β) data to represent ^{1}H scattering in other moderators.

ENDF/B-VII provides S(α,β) data for both elements in 3 compounds: H and Zr in ZrH; O and U in UO_2; and Be and O in BeO. To utilize these data as intended, ZAID entries for both elements should be included on the same MCNP MT card. Note in particular, that the representation for BeO has been updated in ENDF/B-VII. Previous versions of ENDF/B provided on evaluation

that represented both Be and O in BeO; in ENDF/B-VII the two elements are evaluated separately.

Verification and Validation

Cross sections for each moderator have been plotted for each temperature and each reaction, and when applicable, compared to the previous thermal scattering data released in SAB2002. Average scattering energies and angles have been constructed and plotted. All data tables have been run in standard MCNP problems. Several data tables have been used to calculate various criticality benchmarks.

Summary

A new MCNP thermal S(α,β) library has been created, verified, and made available to users. The library is named ENDF70SAB and contains a total of 111 tables for 20 moderators based on ENDF/B-VII Release 0 evaluations. There are some substantial enhancements from previous evaluations and MCNP thermal data tables that warrant the data on ENDF70SAB being the new default for MCNP.

References

1. M. B. Chadwick et al., "Nuclear Data Sheets: Special Issue on Evaluation Nuclear Data File ENDF/B-VII.0," Elsevier Publishing, Volume 107, Number 12 (December 2006).

2. R. E. MacFarlane, and D. W. Muir, "The NJOY Nuclear Data Processing System Version 91," Los Alamos National Laboratory manual LA-12740-M (October 1994).

3. X-5 Monte Carlo Team, "MCNP – A General Monte Carlo N-Particle Transport Code, Version 5," Los Alamos National Laboratory report LA-UR-03-1987 (2003).

4. R. C. Little and R. E. MacFarlane, "SAB2002 – An S(α,β) Library for MCNP," Los Alamos National Laboratory memorandum X-5-03-21 (February 3, 2003).

Appendix A. Details on S(α,β) Tables Included on ENDF70SAB Library

The following table is modeled after Table G.1 from Appendix G of the MCNP manual. In this document, entries are provided only for the data tables included on the ENDF70SAB library. Entries in the table are described in the following:

Given in parenthesis are the nuclides for which the S(α,β) data are valid. For example, lwtr.10t provides scattering data only for ^{1}H; ^{16}O would still be represented by the default free-gas treatment.

The first column of the table contains the ZAID, which is the table identification to be specified on MCNP MTn cards. The portion of the ZAID before the decimal point provides a shorthand alphanumeric description of the material. The two digits after the decimal point differentiate among different tables for the same material. The final character in the ZAID is a "t" which indicates thermal S(α,β) table.

The second column of the table is the evaluated source. For the ENDF70SAB library, all data are from ENDF/B-VI1 Release 0.

The third column is the library name; here, obviously, always ENDF70SAB.

The fourth column provides the date that the evaluated data was last modified.

The fifth column is the temperature of the data (in degrees Kelvin).

The sixth column contains the number of equally-likely discrete secondary cosines provided at each combination of incident and secondary energy for inelastic scattering, and for each incident energy for incoherent elastic scattering.

The seventh column gives the number of secondary energies provided for each incident energy for inelastic scattering.

There are three options for the elastic scattering entry in the eighth column:

none -- no elastic scattering data for this material.
coh -- coherent elastic scattering data provided for this material (Bragg scattering).
inco -- incoherent elastic scattering data provided for this material.

Appendix G - MCNP Data Libraries
S(α,β) DATA FOR USE WITH THE MTn CARD

Table G.1 - Thermal S(α,β) Cross-Section Libraries Maintained by X-1 NAD

ZAID	Library Name	Source	Eval Date	Temp (K)	Num of Angles	Num of Energies	Elastic Date
********** Aluminum-27 (13027) **********							
al27.10t	endf70sab	endf7.0	2005	20	20	80	coh
al27.11t	endf70sab	endf7.0	2005	80	20	80	coh
al27.12t	endf70sab	endf7.0	2005	293.6	20	80	coh
al27.13t	endf70sab	endf7.0	2005	400	20	80	coh
al27.14t	endf70sab	endf7.0	2005	600	20	80	coh
al27.15t	endf70sab	endf7.0	2005	800	20	80	coh
********** Beryllium Metal (4009) **********							
be.10t	endf70sab	endf7.0	1993	293.6	20	80	coh
be.11t	endf70sab	endf7.0	1993	400	20	80	coh
be.12t	endf70sab	endf7.0	1993	500	20	80	coh
be.13t	endf70sab	endf7.0	1993	600	20	80	coh
be.14t	endf70sab	endf7.0	1993	700	20	80	coh
be.15t	endf70sab	endf7.0	1993	800	20	80	coh
be.16t	endf70sab	endf7.0	1993	1000	20	80	coh
be.17t	endf70sab	endf7.0	1993	1200	20	80	coh
********** Beryllium in Beryllium Oxide (4009) **********							
be/o.10t	endf70sab	endf7.0	2005	293.6	20	80	coh
be/o.11t	endf70sab	endf7.0	2005	400	20	80	coh
be/o.12t	endf70sab	endf7.0	2005	500	20	80	coh
be/o.13t	endf70sab	endf7.0	2005	600	20	80	coh
be/o.14t	endf70sab	endf7.0	2005	700	20	80	coh
be/o.15t	endf70sab	endf7.0	2005	800	20	80	coh
be/o.16t	endf70sab	endf7.0	2005	1000	20	80	coh
be/o.17t	endf70sab	endf7.0	2005	1200	20	80	coh
********** Benzene (1001, 6000, 6012) **********							
benz.10t	endf70sab	endf7.0	1969	293.6	20	80	none
benz.11t	endf70sab	endf7.0	1969	350	20	80	none
benz.12t	endf70sab	endf7.0	1969	400	20	80	none
benz.13t	endf70sab	endf7.0	1969	450	20	80	none
benz.14t	endf70sab	endf7.0	1969	500	20	80	none
benz.15t	endf70sab	endf7.0	1969	600	20	80	none
benz.16t	endf70sab	endf7.0	1969	800	20	80	none
benz.17t	endf70sab	endf7.0	1969	1000	20	80	none
********** Ortho Deuterium (1002) **********							
dortho.10t	endf70sab	endf7.0	1993	19	20	80	none
********** Para Deuterium (1002) **********							
dpara.10t	endf70sab	endf7.0	1993	19	20	80	none
********** Iron-56 (26056) **********							
fe56.10t	endf70sab	endf7.0	2005	20	20	80	coh
fe56.11t	endf70sab	endf7.0	2005	80	20	80	coh
fe56.12t	endf70sab	endf7.0	2005	293.6	20	80	coh
fe56.13t	endf70sab	endf7.0	2005	400	20	80	coh
fe56.14t	endf70sab	endf7.0	2005	600	20	80	coh
fe56.15t	endf70sab	endf7.0	2005	800	20	80	coh
********** Graphite (6000, 6012) **********							

Appendix G - MCNP Data Libraries
S(α,β) DATA FOR USE WITH THE MTn CARD

Table G.1 - Thermal S(α,β) Cross-Section Libraries Maintained by X-1 NAD

ZAID	Library Name	Source	Eval Date	Temp (K)	Num of Angles	Num of Energies	Elastic Date
********** Graphite (6000, 6012) **********							
grph.10t	endf70sab	endf7.0	1993	293.6	20	80	coh
grph.11t	endf70sab	endf7.0	1993	400	20	80	coh
grph.12t	endf70sab	endf7.0	1993	500	20	80	coh
grph.13t	endf70sab	endf7.0	1993	600	20	80	coh
grph.14t	endf70sab	endf7.0	1993	700	20	80	coh
grph.15t	endf70sab	endf7.0	1993	800	20	80	coh
grph.16t	endf70sab	endf7.0	1993	1000	20	80	coh
grph.17t	endf70sab	endf7.0	1993	1200	20	80	coh
grph.18t	endf70sab	endf7.0	1993	1600	20	80	coh
grph.19t	endf70sab	endf7.0	1993	2000	20	80	coh
********** Hydrogen in Zirconium Hydride (1001) **********							
h/zr.10t	endf70sab	endf7.0	1993	293.6	20	80	inco
h/zr.11t	endf70sab	endf7.0	1993	400	20	80	inco
h/zr.12t	endf70sab	endf7.0	1993	500	20	80	inco
h/zr.13t	endf70sab	endf7.0	1993	600	20	80	inco
h/zr.14t	endf70sab	endf7.0	1993	700	20	80	inco
h/zr.15t	endf70sab	endf7.0	1993	800	20	80	inco
h/zr.16t	endf70sab	endf7.0	1993	1000	20	80	inco
h/zr.17t	endf70sab	endf7.0	1993	1200	20	80	inco
********** Ortho Hydrogen (1001) **********							
hortho.10t	endf70sab	endf7.0	1993	20	20	80	none
********** Para Hydrogen (1001) **********							
hpara.10t	endf70sab	endf7.0	1993	20	20	80	none
********** Deuterium in Heavy Water (1002) **********							
hwtr.10t	endf70sab	endf7.0	2004	293.6	20	80	none
hwtr.11t	endf70sab	endf7.0	2004	350	20	80	none
hwtr.12t	endf70sab	endf7.0	2004	400	20	80	none
hwtr.13t	endf70sab	endf7.0	2004	450	20	80	none
hwtr.14t	endf70sab	endf7.0	2004	500	20	80	none
hwtr.15t	endf70sab	endf7.0	2004	550	20	80	none
hwtr.16t	endf70sab	endf7.0	2004	600	20	80	none
hwtr.17t	endf70sab	endf7.0	2004	650	20	80	none
********** Hydrogen in Liquid Methane (1001) **********							
lmeth.10t	endf70sab	endf7.0	1993	100	20	80	none
********** Hydrogen in Light Water (1001) **********							
lwtr.10t	endf70sab	endf7.0	2006	293.6	20	80	none
lwtr.11t	endf70sab	endf7.0	2006	350	20	80	none
lwtr.12t	endf70sab	endf7.0	2006	400	20	80	none
lwtr.13t	endf70sab	endf7.0	2006	450	20	80	none
lwtr.14t	endf70sab	endf7.0	2006	500	20	80	none
lwtr.15t	endf70sab	endf7.0	2006	550	20	80	none
lwtr.16t	endf70sab	endf7.0	2006	600	20	80	none
lwtr.17t	endf70sab	endf7.0	2006	650	20	80	none
lwtr.18t	endf70sab	endf7.0	2006	800	20	80	none
********** Oxygen in Beryllium Oxide (8016, 8017, 8018) **********							

Appendix G - MCNP Data Libraries
S(α,β) DATA FOR USE WITH THE MTn CARD

Table G.1 - Thermal S(α,β) Cross-Section Libraries Maintained by X-1 NAD

ZAID	Library Name	Source	Eval Date	Temp (K)	Num of Angles	Num of Energies	Elastic Date
********** Oxygen in Beryllium Oxide (8016, 8017, 8018) **********							
o/be.10t	endf70sab	endf7.0	2005	293.6	20	80	coh
o/be.11t	endf70sab	endf7.0	2005	400	20	80	coh
o/be.12t	endf70sab	endf7.0	2005	500	20	80	coh
o/be.13t	endf70sab	endf7.0	2005	600	20	80	coh
o/be.14t	endf70sab	endf7.0	2005	700	20	80	coh
o/be.15t	endf70sab	endf7.0	2005	800	20	80	coh
o/be.16t	endf70sab	endf7.0	2005	1000	20	80	coh
o/be.17t	endf70sab	endf7.0	2005	1200	20	80	coh
********** Oxygen in UO2 (8016, 8017, 8018) **********							
o2/u.10t	endf70sab	endf7.0	2005	293.6	20	80	coh
o2/u.11t	endf70sab	endf7.0	2005	400	20	80	coh
o2/u.12t	endf70sab	endf7.0	2005	500	20	80	coh
o2/u.13t	endf70sab	endf7.0	2005	600	20	80	coh
o2/u.14t	endf70sab	endf7.0	2005	700	20	80	coh
o2/u.15t	endf70sab	endf7.0	2005	800	20	80	coh
o2/u.16t	endf70sab	endf7.0	2005	1000	20	80	coh
o2/u.17t	endf70sab	endf7.0	2005	1200	20	80	coh
********** Hydrogen in Polyethylene (1001) **********							
poly.10t	endf70sab	endf7.0	1969	293.6	20	80	inco
poly.11t	endf70sab	endf7.0	1969	350	20	80	inco
********** Hydrogen in Solid Methane (1001) **********							
smeth.10t	endf70sab	endf7.0	1993	22	20	80	inco
********** Uranium-238 in UO2 (92238) **********							
u/o2.10t	endf70sab	endf7.0	2005	293.6	20	80	coh
u/o2.11t	endf70sab	endf7.0	2005	400	20	80	coh
u/o2.12t	endf70sab	endf7.0	2005	500	20	80	coh
u/o2.13t	endf70sab	endf7.0	2005	600	20	80	coh
u/o2.14t	endf70sab	endf7.0	2005	700	20	80	coh
u/o2.15t	endf70sab	endf7.0	2005	800	20	80	coh
u/o2.16t	endf70sab	endf7.0	2005	1000	20	80	coh
u/o2.17t	endf70sab	endf7.0	2005	1200	20	80	coh
********** Zirconium in Zirconium Hydride (40000, 40090, 40091, 40092, 40094, 40096) **********							
zr/h.10t	endf70sab	endf7.0	1993	293.6	20	80	inco
zr/h.11t	endf70sab	endf7.0	1993	400	20	80	inco
zr/h.12t	endf70sab	endf7.0	1993	500	20	80	inco
zr/h.13t	endf70sab	endf7.0	1993	600	20	80	inco
zr/h.14t	endf70sab	endf7.0	1993	700	20	80	inco
zr/h.15t	endf70sab	endf7.0	1993	800	20	80	inco
zr/h.16t	endf70sab	endf7.0	1993	1000	20	80	inco
zr/h.17t	endf70sab	endf7.0	1993	1200	20	80	inco

Appendix B. Sample PENDF Input Files for S(α,β) Processing of (1) Hydrogen in Light Water (H_2O) and (2) Uranium in UO_2

1. Hydrogen in Light Water at 9 temperatures [no elastic scattering]

```
 moder
 20 -21
 reconr
 -21 -22
 'pendf tape for ENDF/B-VII 1-H-1'/
 125 14 0/
 .001/
 '1-H-1 from ENDF/B-VII'/
 'processed with njoy at 0.1%'/
 'the following reaction types are added'/
 '     mt20x   gas production'/
 '     mt221   free thermal scattering'/
 '     mt222   h in h2o thermal scattering'/
 '     mt223   h in poly inelastic thermal scattering'/
 '     mt224   h in poly elastic thermal scattering'/
 '     mt225   h in zrh inelastic thermal scattering'/
 '     mt226   h in zrh elastic thermal scattering'/
 '     mt227   h in benzine thermal scattering'/
 '     mt301   total heating kerma factor'/
 '     mt443   kinematic kerma'/
 '     mt444   total damage energy production'/
 0/
 broadr
 -21 -22 -23
 125 9/
 .001/
 293.6  350  400  450  500  550  600  650  800 /
 0/
 heatr
 -21 -23 -24/
 125 4/
 302 402 443 444 /
 thermr
 30 -24 -25
 1 125 20 9 4 0 2 222 0/
 293.6  350  400  450  500  550  600  650  800
 .001 10./
 gaspr
 -21 -25 -27
 moder
 -27 28
 stop
```

2. Uranium in UO_2 at 8 temperatures [with elastic scattering]

```
moder
 20 -21
 reconr
 -21 -22
 'pendf tape for ENDF/B-VII 92-U-238 '/
 9237 13/
```

```
.001/
'92-U-238 from ENDF/B-VII'/
'processed with njoy at 0.1%'/
't= 293.6 400 500 600 700 800 1000 1200'/
'the following reaction types are added'/
'     mt20x   gas production'/
'     mt221   free thermal scattering'/
'     mt231   be metal inelastic thermal scattering'/
'     mt232   be metal elastic thermal scattering'/
'     mt233   bebeo inelastic thermal scattering'/
'     mt234   bebeo elastic thermal scattering'/
'     mt301   total heating kerma factor'/
'     mt443   kinematic kerma'/
'     mt444   total damage energy production'/
0/
broadr
-21 -22 -23
9237 8/
.001/
293.6 400 500 600 700 800 1000 1200/
0/
heatr
-21 -23 -24/
9237 4/
302 402 443 444/
thermr
30 -25 -24
76 9237 20 8 4 0 1 245 0/
293.6 400 500 600 700 800 1000 1200/
.001 10./
gaspr
-21 -24 -27
moder
-27 28
stop
```

Appendix C. Sample ACER Input Files for S(α,β) Processing of (1) Hydrogen in Light Water (H_2O) at 293.6 K and (2) Uranium in UO_2 at 293.6 K

1. Hydrogen in Light Water at 293.6 K [no elastic scattering]

```
 acer
 30 28 0 31 32
 2 0 1 .10/
 'H in h2o at 293.6k from ENDF/B-VII'/
 125 293.6 'lwtr'/
 1001/
 222 80 0 0 1 10 0/
 acer
 0 31 35 33 34/
 7 1/
 'H in h2o at 293.6k from ENDF/B-VII'/
 stop
```

2. Uranium in UO_2 at 293.6 K [with elastic scattering]

```
 acer
 30 28 0 31 32
 2 0 1 .10/
 'u(uo2) at 293.6K from ENDF/B-VII'/
 9237 293.6 'u/o2'/
 92232 92233 92234 92235 92236 92237 92238 92239 92240 92241/
 245 80 246 0 1 10 0/
 acer
 0 31 35 33 34/
 7 1/
 'u(uo2) at 293.6K from ENDF/B-VII'/
 stop
```