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Report

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NJOY Processing of ENDF/B VIII.0 Thermal Scattering Files

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"ENDF/B-VIII.0 provides a major update to the ENDF thermal scattering library. Indeed, it is nearly a completely new sub-library. Only the legacy evaluations for Al, Fe, liquid and solid methane, ortho- and para- hydrogen and deuterium and benzene and the ENDF/B-VII.1 evaluations for SiO2 are unchanged."[1,2]

Thirty four (34) materials are provided in ENDF/B-VIII.0 with a total of two hundred and forty-eight (248) temperatures. LEAPR input files are also included for each of the materials as well as "readme" files for most of the materials.

All of these 34 thermal scattering files have been processed with NJOY2016 version 9 or version 29 to produce 248 ACE files suitable for use in MCNP or other similar codes.

A few of the traditional material names have been changed from previous ACE libraries. Also notice that there are now three (3) different graphite evaluations. Crystalline graphite is the closest one to previous graphite TSL evaluations. Graphite with 10% porosity is typical for reactor usage, and graphite with 30% porosity is the most common form of graphite. These 3 forms of graphite have significantly different densities due to the porosity – say, about 2.2, 2.0, and 1.6 g/cc.

The procedure recommended by scientists at the Naval Nuclear Laboratory[3] was used to process the evaluation files into ACE format by NJOY. Specifically, the value of B(6) given in the MF = 7, MT = 4 section of the TSL evaluation file was used as the "natom" input of the second card of the THERMR input in NJOY. The MF = 7, MT = 4 section contains the incoherent inelastic scattering and is the only part of the overall $S(\alpha,\beta)$ scattering that exists at energies near Emax. In addition, the B(4) value (Emax) in the same section of the evaluation file was used for "emax" on card 4 of the THERMR input.

This procedure worked "correctly" for 27 of the 34 materials. "Correctly" means that the value of the $S(\alpha,\beta)$ scattering cross section at (or near) Emax was very close to the value of the MF = 3, MT = 2 elastic scattering cross section from the neutron sub-library evaluation file for the same material at the same temperature and at (or near) emax. This continuity is required for codes like MCNP to be able to substitute $S(\alpha,\beta)$ cross sections for the free gas cross sections when requested by the user (via a MCNP "mt_n" card).

The seven (7) evaluations which failed to produce a correct result were the new OinD2O evaluation and 6 older cold temperature evaluations, para- and ortho- H and D, and solid and liquid methane. For these evaluations, some adjustments were made in the TSL evaluation files and in the NJOY inputs to achieve continuity between the $S(\alpha,\beta)$ scattering and the free gas elastic scattering cross sections at Emax.

Table 1 lists the materials which are included in the ENDF/B-VIII.0 thermal scattering library.

	ENDF/B VIII.0 tsl files	number of temperatures	Emax (eV)	ACE ID
1	tsl-013_Al_027.endf	6	2.277	al-27
2	tsl-026_Fe_056.endf	6	2.277	fe-56
3	tsl-Be-metal.endf	8	5.000001	be-met
4	tsl-BeinBeO.endf	8	5.000001	be-beo
5	tsl-CinSiC.endf	8	5.000001	c-sic
6	tsl-DinD2O.endf	17	10.02133	d-d2o
7	tsl-HinC5O2H8.endf	1	5.000001	h-luci
8	tsl-HinCH2.endf	11	5.000001	h-poly
9	tsl-HinH2O.endf	18	10.00008	h-h2o
10	tsl-HinIceIh.endf	9	5	h-ice
11	tsl-HinYH2.endf	9	5	h-yh2
12	tsl-HinZrH.endf	8	1.9734	h-zrh
13	tsl-NinUN.endf	8	5.000001	n-un
14	tsl-OinBeO.endf	8	5.000001	o-beo
15	tsl-OinD2O.endf	17	10.02133	o-d2o
16	tsl-OinIceIh.endf	9	5	o-ice
17	tsl-OinUO2.endf	8	5.000001	o-uo2
18	tsl-SiO2-alpha.endf	5	2.46675	sio2
19	tsl-SiO2-beta.endf	2	2.46675	sio2
20	tsl-SiinSiC.endf	8	5.000001	si-sic
21	tsl-UinUN.endf	8	5.000001	u-un
22	tsl-UinUO2.endf	8	5.000001	u-uo2
23	tsl-YinYH2.endf	9	5	y-yh2
24	tsl-ZrinZrH.endf	8	1.00022	zr-zrh
25	tsl-benzene.endf	8	2	benz
26	tsl-crystalline-graphite.endf	9	5.000001	grph
27	tsl-l-CH4.endf	1	4.078125	lmeth
28	tsl-ortho-D.endf	1	7.59	orthoD
29	tsl-ortho-H.endf	1	7.59	orthoH
30	tsl-para-D.endf	1	7.59	paraD
31	tsl-para-H.endf	1	7.59	paraH
32	tsl-reactor-graphite-10P.endf	9	5.000001	grph10
33	tsl-reactor-graphite-30P.endf	9	5.000001	grph30
34	tsl-s-CH4.endf	1	11.385	smeth

Table 1: Listing of the TSL Materials in ENDF/B-VIII.0

Table 2 below lists all of the 248 ACE tables, the relevant atomic weight, and the temperatures which are available. Note, that if a room temperature version is available, it always has the ".80t" suffix.

S(a,B)	AWR	Temp(MeV)	Temp K
al-27.80t	26.74975	2.530E-08	294
al-27.81t	26.74975	1.724E-09	20
al-27.82t	26.74975	6.894E-09	80
al-27.83t	26.74975	3.447E-08	400
al-27.84t	26.74975	5.170E-08	600
al-27.85t	26.74975	6.894E-08	800
be-beo.80t	8.93478	2.530E-08	294
be-beo.81t	8.93478	3.447E-08	400
be-beo.82t	8.93478	4.309E-08	500
be-beo.83t	8.93478	5.170E-08	600
be-beo.84t	8.93478	6.032E-08	700
be-beo.85t	8.93478	6.894E-08	800
be-beo.86t	8.93478	8.617E-08	1000
be-beo.87t	8.93478	1.034E-07	1200
be-met.80t	8.93478	2.551E-08	296
be-met.81t	8.93478	3.447E-08	400
be-met.82t	8.93478	4.309E-08	500
be-met.83t	8.93478	5.170E-08	600
be-met.84t	8.93478	6.032E-08	700
be-met.85t	8.93478	6.894E-08	800
be-met.86t	8.93478	8.617E-08	1000
be-met.87t	8.93478	1.034E-07	1200
benz.80t	0.999167	2.551E-08	296
benz.81t	0.999167	3.016E-08	350
benz.82t	0.999167	3.447E-08	400
benz.83t	0.999167	3.878E-08	450
benz.84t	0.999167	4.309E-08	500
benz.85t	0.999167	5.170E-08	600
benz.86t	0.999167	6.894E-08	800
benz.87t	0.999167	8.617E-08	1000
c-sic.80t	11.89365	2.585E-08	300
c-sic.81t	11.89365	3.447E-08	400
c-sic.82t	11.89365	4.309E-08	500
c-sic.83t	11.89365	5.170E-08	600
c-sic.84t	11.89365	6.032E-08	700
c-sic.85t	11.89365	6.894E-08	800
c-sic.86t	11.89365	8.617E-08	1000

c-sic.87t	11.89365	1.034E-07	1200
d-d2o.80t	1.9968	2.530E-08	294
d-d2o.81t	1.9968	2.444E-08	284
d-d2o.82t	1.9968	2.585E-08	300
d-d2o.83t	1.9968	2.789E-08	324
d-d2o.84t	1.9968	3.016E-08	350
d-d2o.85t	1.9968	3.220E-08	374
d-d2o.86t	1.9968	3.447E-08	400
d-d2o.87t	1.9968	3.650E-08	424
d-d2o.88t	1.9968	3.878E-08	450
d-d2o.89t	1.9968	4.081E-08	474
d-d2o.90t	1.9968	4.309E-08	500
d-d2o.91t	1.9968	4.512E-08	524
d-d2o.92t	1.9968	4.740E-08	550
d-d2o.93t	1.9968	4.943E-08	574
d-d2o.94t	1.9968	5.170E-08	600
d-d2o.95t	1.9968	5.374E-08	624
d-d2o.96t	1.9968	5.601E-08	650
fe-56.80t	55.45443	2.530E-08	294
fe-56.81t	55.45443	1.724E-09	20
fe-56.82t	55.45443	6.894E-09	80
fe-56.83t	55.45443	3.447E-08	400
fe-56.84t	55.45443	5.170E-08	600
fe-56.85t	55.45443	6.894E-08	800
grph.80t	11.89365	2.551E-08	296
grph.81t	11.89365	3.447E-08	400
grph.82t	11.89365	4.309E-08	500
grph.83t	11.89365	5.170E-08	600
grph.84t	11.89365	6.032E-08	700
grph.85t	11.89365	6.894E-08	800
grph.86t	11.89365	8.617E-08	1000
grph.87t	11.89365	1.034E-07	1200
grph.88t	11.89365	1.379E-07	1600
grph10.80t	11.89365	2.551E-08	296
grph10.81t	11.89365	3.447E-08	400
grph10.82t	11.89365	4.309E-08	500
grph10.83t	11.89365	5.170E-08	600
grph10.84t	11.89365	6.032E-08	700
grph10.85t	11.89365	6.894E-08	800
grph10.86t	11.89365	8.617E-08	1000
grph10.87t	11.89365	1.034E-07	1200
grph10.88t	11.89365	1.379E-07	1600
grph30.80t	11.89365	2.551E-08	296

grph30.81t	11.89365	3.447E-08	400
grph30.82t	11.89365	4.309E-08	500
grph30.83t	11.89365	5.170E-08	600
grph30.84t	11.89365	6.032E-08	700
grph30.85t	11.89365	6.894E-08	800
grph30.86t	11.89365	8.617E-08	1000
grph30.87t	11.89365	1.034E-07	1200
grph30.88t	11.89365	1.379E-07	1600
h-h2o.80t	0.999167	2.530E-08	294
h-h2o.81t	0.999167	2.444E-08	284
h-h2o.82t	0.999167	2.585E-08	300
h-h2o.83t	0.999167	2.789E-08	324
h-h2o.84t	0.999167	3.016E-08	350
h-h2o.85t	0.999167	3.220E-08	374
h-h2o.86t	0.999167	3.447E-08	400
h-h2o.87t	0.999167	3.650E-08	424
h-h2o.88t	0.999167	3.878E-08	450
h-h2o.89t	0.999167	4.081E-08	474
h-h2o.90t	0.999167	4.309E-08	500
h-h2o.91t	0.999167	4.512E-08	524
h-h2o.92t	0.999167	4.740E-08	550
h-h2o.93t	0.999167	4.943E-08	574
h-h2o.94t	0.999167	5.170E-08	600
h-h2o.95t	0.999167	5.374E-08	624
h-h2o.96t	0.999167	5.601E-08	650
h-h2o.97t	0.999167	6.894E-08	800
h-ice.80t	0.999167	9.910E-09	115
h-ice.81t	0.999167	1.621E-08	188
h-ice.82t	0.999167	1.794E-08	208
h-ice.83t	0.999167	1.966E-08	228
h-ice.84t	0.999167	2.009E-08	233
h-ice.85t	0.999167	2.138E-08	248
h-ice.86t	0.999167	2.182E-08	253
h-ice.87t	0.999167	2.311E-08	268
h-ice.88t	0.999167	2.354E-08	273
h-luci.80t	0.999167	2.585E-08	300
h-poly.80t	0.999167	2.530E-08	294
h-poly.81t	0.999167	6.635E-09	77
h-poly.82t	0.999167	1.689E-08	196
h-poly.83t	0.999167	2.008E-08	233
h-poly.84t	0.999167	2.585E-08	300
h-poly.85t	0.999167	2.611E-08	303
h-poly.86t	0.999167	2.697E-08	313

h-poly.87t	0.999167	2.783E-08	323
h-poly.88t	0.999167	2.870E-08	333
h-poly.89t	0.999167	2.783E-08	323
h-poly.90t	0.999167	2.870E-08	333
h-yh2.80t	0.999167	2.530E-08	294
h-yh2.81t	0.999167	3.447E-08	400
h-yh2.82t	0.999167	4.309E-08	500
h-yh2.83t	0.999167	5.170E-08	600
h-yh2.84t	0.999167	6.032E-08	700
h-yh2.85t	0.999167	6.894E-08	800
h-yh2.86t	0.999167	8.617E-08	1000
h-yh2.87t	0.999167	1.034E-07	1200
h-yh2.88t	0.999167	1.206E-07	1400
h-zrh.80t	0.999167	2.551E-08	296
h-zrh.81t	0.999167	3.447E-08	400
h-zrh.82t	0.999167	4.309E-08	500
h-zrh.83t	0.999167	5.170E-08	600
h-zrh.84t	0.999167	6.032E-08	700
h-zrh.85t	0.999167	6.894E-08	800
h-zrh.86t	0.999167	8.617E-08	1000
h-zrh.87t	0.999167	1.034E-07	1200
lmeth.80t	0.999167	8.617E-09	100
n-un.80t	13.88278	2.551E-08	296
n-un.81t	13.88278	3.447E-08	400
n-un.82t	13.88278	4.309E-08	500
n-un.83t	13.88278	5.170E-08	600
n-un.84t	13.88278	6.032E-08	700
n-un.85t	13.88278	6.894E-08	800
n-un.86t	13.88278	8.617E-08	1000
n-un.87t	13.88278	1.034E-07	1200
o-beo.80t	15.85751	2.530E-08	294
o-beo.81t	15.85751	3.447E-08	400
o-beo.82t	15.85751	4.309E-08	500
o-beo.83t	15.85751	5.170E-08	600
o-beo.84t	15.85751	6.032E-08	700
o-beo.85t	15.85751	6.894E-08	800
o-beo.86t	15.85751	8.617E-08	1000
o-beo.87t	15.85751	1.034E-07	1200
o-d2o.80t	15.85751	2.530E-08	294
o-d2o.81t	15.85751	2.444E-08	284
o-d2o.82t	15.85751	2.585E-08	300
o-d2o.83t	15.85751	2.789E-08	324
o-d2o.84t	15.85751	3.016E-08	350

o-d2o.85t	15.85751	3.220E-08	374
o-d2o.86t	15.85751	3.447E-08	400
o-d2o.87t	15.85751	3.650E-08	424
o-d2o.88t	15.85751	3.878E-08	450
o-d2o.89t	15.85751	4.081E-08	474
o-d2o.90t	15.85751	4.309E-08	500
o-d2o.91t	15.85751	4.512E-08	524
o-d2o.92t	15.85751	4.740E-08	550
o-d2o.93t	15.85751	4.943E-08	574
o-d2o.94t	15.85751	5.170E-08	600
o-d2o.95t	15.85751	5.374E-08	624
o-d2o.96t	15.85751	5.601E-08	650
o-ice.80t	15.85751	9.910E-09	115
o-ice.81t	15.85751	1.621E-08	188
o-ice.82t	15.85751	1.794E-08	208
o-ice.83t	15.85751	1.966E-08	228
o-ice.84t	15.85751	2.009E-08	233
o-ice.85t	15.85751	2.138E-08	248
o-ice.86t	15.85751	2.182E-08	253
o-ice.87t	15.85751	2.311E-08	268
o-ice.88t	15.85751	2.354E-08	273
o-uo2.80t	15.85751	2.551E-08	296
o-uo2.81t	15.85751	3.447E-08	400
o-uo2.82t	15.85751	4.309E-08	500
o-uo2.83t	15.85751	5.170E-08	600
o-uo2.84t	15.85751	6.032E-08	700
o-uo2.85t	15.85751	6.894E-08	800
o-uo2.86t	15.85751	8.617E-08	1000
o-uo2.87t	15.85751	1.034E-07	1200
orthoD.80t	1.9968	1.637E-09	19
orthoH.80t	0.999167	1.724E-09	20
paraD.80t	1.9968	1.637E-09	19
paraH.80t	0.999167	1.724E-09	20
si-sic.80t	27.737	2.585E-08	300
si-sic.81t	27.737	3.447E-08	400
si-sic.82t	27.737	4.309E-08	500
si-sic.83t	27.737	5.170E-08	600
si-sic.84t	27.737	6.032E-08	700
si-sic.85t	27.737	6.894E-08	800
si-sic.86t	27.737	8.617E-08	1000
si-sic.87t	27.737	1.034E-07	1200
sio2.80t	15.85751	2.530E-08	294
sio2.81t	15.85751	3.016E-08	350

sio2.82t	15.85751	3.447E-08	400
sio2.83t	15.85751	4.309E-08	500
sio2.84t	15.85751	6.894E-08	800
sio2.85t	15.85751	8.617E-08	1000
sio2.86t	15.85751	9.479E-08	1100
smeth.80t	0.999167	1.896E-09	22
u-un.80t	236.0058	2.551E-08	296
u-un.81t	236.0058	3.447E-08	400
u-un.82t	236.0058	4.309E-08	500
u-un.83t	236.0058	5.170E-08	600
u-un.84t	236.0058	6.032E-08	700
u-un.85t	236.0058	6.894E-08	800
u-un.86t	236.0058	8.617E-08	1000
u-un.87t	236.0058	1.034E-07	1200
u-uo2.80t	236.0058	2.551E-08	296
u-uo2.81t	236.0058	3.447E-08	400
u-uo2.82t	236.0058	4.309E-08	500
u-uo2.83t	236.0058	5.170E-08	600
u-uo2.84t	236.0058	6.032E-08	700
u-uo2.85t	236.0058	6.894E-08	800
u-uo2.86t	236.0058	8.617E-08	1000
u-uo2.87t	236.0058	1.034E-07	1200
y-yh2.80t	88.1421	2.530E-08	294
y-yh2.81t	88.1421	3.447E-08	400
y-yh2.82t	88.1421	4.309E-08	500
y-yh2.83t	88.1421	5.170E-08	600
y-yh2.84t	88.1421	6.032E-08	700
y-yh2.85t	88.1421	6.894E-08	800
y-yh2.86t	88.1421	8.617E-08	1000
y-yh2.87t	88.1421	1.034E-07	1200
y-yh2.88t	88.1421	1.206E-07	1400
zr-zrh.80t	89.1324	2.551E-08	296
zr-zrh.81t	89.1324	3.447E-08	400
zr-zrh.82t	89.1324	4.309E-08	500
zr-zrh.83t	89.1324	5.170E-08	600
zr-zrh.84t	89.1324	6.032E-08	700
zr-zrh.85t	89.1324	6.894E-08	800
zr-zrh.86t	89.1324	8.617E-08	1000
zr-zrh.87t	89.1324	1.034E-07	1200

Table 2: Listing of all 248 ACE File ZAID's and their Temperature Parameters

Table 3 lists the modified parameters used in the processing of the 7 evaluations which did not process correctly with the standard procedure. The values highlighted in red were changed from the original tsl values or procedures recommended by the Naval Nuclear Laboratories.

ENDF/B VIII.0 tsl files	B(1) total xs	B(6) Mo	THERMR natom
tsl-OinD2O.endf	7.5878	2	2
tsl-para-D.endf	13.58	4	4
tsl-ortho-D.endf	13.58	4	4
tsl-ortho-H.endf	40.87268	4	4
tsl-para-H.endf	40.87268	4	4
tsl-l-CH4.endf	81.74536	8	4
tsl-s-CH4.endf	81.74536	8	4

Table 3: Modified Processing parameters for the 7 evaluations which did not originally have continuity

Inputs for a MCNP xsdir directory file were also generated for each of the 248 ACE files. In the installation of these tables, some of the relative file addresses may need to be modified to match the local computer file system.

Verification and Validation of the ACE files produced by NJOY Processing of the TSL Files

Initial verification of the processed ACE files was the continuity check already referred to. In addition to this test, a mechanical check of the files was performed using a sample MCNP deck which calls at least 1 temperature set from each TSL material evaluation. Not surprisingly, this mechanical check uncovered a few typos in the initial data and directory files.

The first step of data validation was to calculate the thermal diffusion time ("t_d") in MCNP6 for an infinite mass of each material with and without S(α,β) cross sections. The initial source of neutrons can be assumed to be a Maxwellian shape available as a built-in source function in MCNP6. The average neutron lifetime given in the MCNP balance table was then compared with old published reactor physics data[4] for common moderators. While these old data (based on theory and some measurements) are not very precise, and the presence of impurities in the moderators (e.g., H in D2O, and B in Graphite) can also affect the results, it is still the case that the thermal diffusion times should be approximately consistent between the MCNP6 calculation and the published data. Furthermore, the theory predicts that the diffusion time will be independent of the scattering cross section. It is only dependent on the inverse macroscopic absorption cross section and the average neutron velocity. Therefore, the S(α,β) results should be the same as the free gas results for the thermal diffusion time.

Furthermore, the average number of collisions per source particle, the neutron mean free path (mfp), the averaged neutron velocity, and the neutron flux spectrum in energy were calculated as well. The calculated thermal flux spectra are not exactly Maxwellian in energy, -- though they are close -- because the 1/v absorption in the moderator preferentially absorbs the lower energy neutrons.

A sample MCNP6 input deck is given below for H_2O at 600 K:

```
test deck for ENDF/B VIII S(a,B) in MCNP
1     1       -1.00           -1    imp:n=1
2     0                   1         imp:n=0

1     so    10000.0

sdef  pos=0 0 0 erg=d1 nrm=1.0
sp1   -2   5.17e-8
nps   1000000
print
tmp     5.17e-8  5.17e-8
m1      1001.01    2.0     8016.01   1.0
mt1     h-lwtr.94t
f4:n      1
e4   1.0e-10 2298i 2.3e-7  100   T
f14:n  1
fm14   1 -2
phys:n  20 20
```

Figure 1: A Sample MCNP6 Input Deck

Notice that implicit capture is turned off by the phys:n card. Otherwise, MCNP will count all the collisions by reduced weight particle histories as full collisions. The lifetime and the number of collisions are taken from the balance table in the MCNP output. The mfp edit is given in the neutron activity by cell table. The average neutron velocity is deduced from the ratio of the F4 tally divided by the F14 tally (which has a 1/v multiplier on it – see the fm14 card). Also notice that the energy spectrum of the F4 tally must include all possible neutron energies to be consistent with the F14 tally. The detailed energy tally from the E4 card can be used to plot the resultant neutron spectrum as a function of energy.

The starting neutron source has a Maxwellian shape in energy as specified by the SDEF and the SP1 card inputs. This shape is not exactly the same as the final shape, but it is a good guess. The free gas nuclear data files accessed by the M1 card entries are adjusted to the material temperatures given in the TMP card.

Tables 4 and 5 present some of room temperature (and near room temperature) calculational results and comparisons. The calculations were carried out with one million source particles to suppress statistical fluctuations. Unfortunately, MCNP6 does not give uncertainties on the quantities used here, except for the flux tallies. In all cases, the flux tallies had relative errors of 0.001, or 0.1%. The other MCNP quantities are believed to have similar uncertainties.

moderator	density (g/cc)	published td (sec)	S(α,β)	average lifetime (sec)	average no. of collisions	mfp (cm)
H_2O	1.00	2.10E-04	h	2.05E-04	163	0.33
D_2O	1.10	1.40E-01	d, o	1.16E-01	13313	2.20
D_2O	1.10	1.40E-01	d	1.16E-01	13288	2.20
D_2O	1.10	1.40E-01	o	1.16E-01	11726	2.51
Be	1.85	3.00E-03	be	3.67E-03	682	1.64
BeO	2.96	6.70E-03	be, o	6.25E-03	1078	1.70
BeO	2.96	6.70E-03	be	6.24E-03	982	1.59
BeO	2.96	6.70E-03	o	6.25E-03	1247	1.25
Graphite	1.60	1.70E-02	gr30	1.47E-02	1413	2.64
Graphite	2.00		gr10	1.18E-02	1405	2.13
Graphite	2.20		grph	1.07E-02	1414	1.95

moderator	density (g/cc)	published td (sec)	neutron file	average lifetime (sec)	average no. of collisions	mfp (cm)
H_2O	1.00	2.10E-04	free gas	2.04E-04	106	0.50
D_2O	1.10	1.40E-01	free gas	1.16E-01	11659	2.51
Be	1.85	3.00E-03	free gas	3.67E-03	731	1.25
BeO	2.96	6.70E-03	free gas	6.25E-03	1152	1.35
Graphite	1.60	1.70E-02	free gas	1.46E-02	1444	2.52
Graphite	2.00		free gas	1.17E-02	1441	2.02
Graphite	2.20		free gas	1.06E-02	1441	1.84

Tables 4 and 5: S(α,β) and free gas calculations of the thermal diffusion time (“t_d”)

Informative comparisons can also be made between older and newer S(α,β) data, between different temperatures of the same material, and even between the 3 graphite evaluations.

Temperature effects for some common moderators are shown in the following Tables. A constant density was assumed for all temperatures – to make the verification comparisons a little more clear. Also note that the average neutron velocity is somewhat larger than the more commonly referenced most probable velocity. For a Maxwellian velocity distribution, the averaged velocity is 2/sqrt(π) times larger than the most probable velocity. (The commonly referenced 2200 km/sec value at room temperature is a most probable velocity value.)

Flux Spectrum plots are also given for room temperature H_2O and D_2O in Figures 2 and 3. Notice that the calculated spectra are not quite Maxwellian, but they are pretty close.

H_2O S(α,β)	temp (MeV)	temp (K)	avg. no. collisions	lifetime (sh)	mfp (cm)	avg n vel (km/sec)
	2.44E-08	284	161.82	2.05E+04	0.329	2441
	2.53E-08	294	162.99	2.05E+04	0.333	2483
	2.59E-08	300	163.69	2.05E+04	0.335	2510
	2.79E-08	324	166.20	2.05E+04	0.343	2607
	3.02E-08	350	169.03	2.05E+04	0.350	2711
	3.22E-08	374	171.43	2.05E+04	0.357	2801
	3.45E-08	400	174.03	2.05E+04	0.364	2899
	3.65E-08	424	176.35	2.05E+04	0.369	2983
	3.88E-08	450	178.93	2.05E+04	0.375	3074
	4.08E-08	474	181.31	2.05E+04	0.379	3154
	4.31E-08	500	183.97	2.05E+04	0.384	3241
	4.51E-08	524	186.20	2.05E+04	0.388	3316
	4.74E-08	550	188.73	2.05E+04	0.392	3399
	4.94E-08	574	190.93	2.05E+04	0.396	3471
	5.17E-08	600	193.26	2.05E+04	0.400	3550
	5.37E-08	624	195.44	2.05E+04	0.403	3619
	5.60E-08	650	197.66	2.05E+04	0.407	3695
	6.89E-08	800	211.36	2.05E+04	0.423	4099

Table 6: Temperature Effects due to the S(α,β) Cross Sections for light water (constant density)

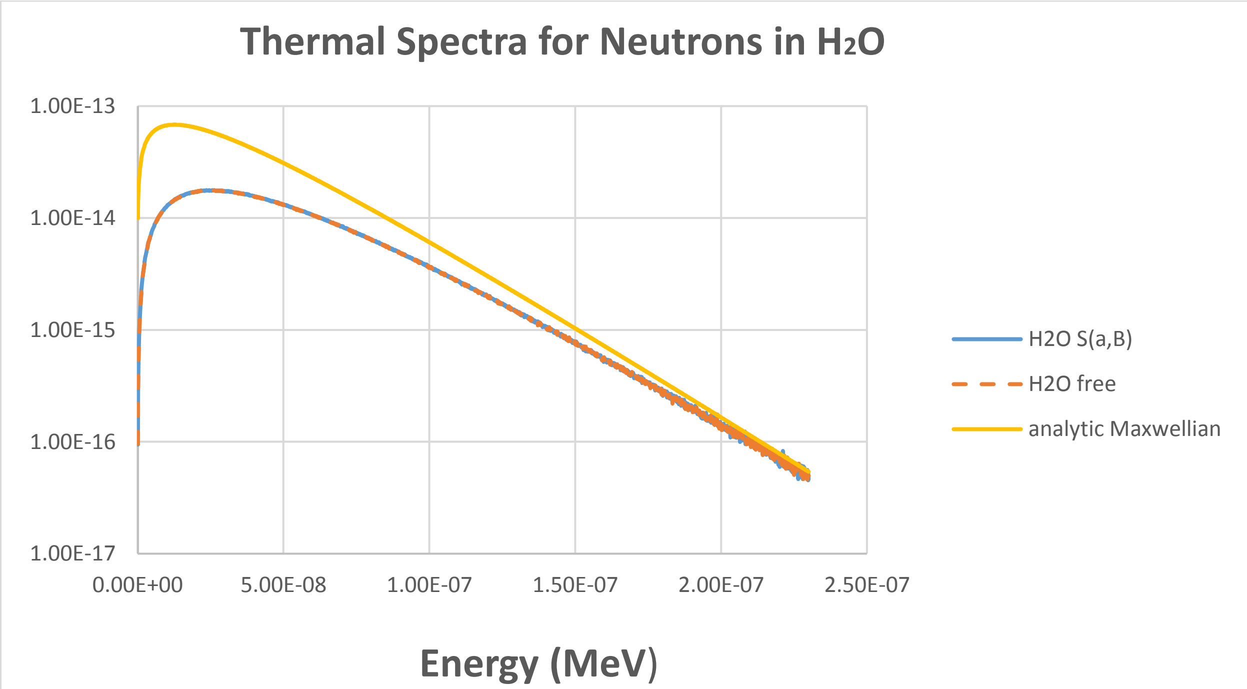

Figure 2: Thermal Neutron Spectra in Room Temperature Light Water

D_2O S(α,β)	temp (MeV)	temp (K)	avg. no. collisions	lifetime (sh)	mfp (cm)	avg n vel (km/sec)
	2.44E-08	284	13112	1.16E+07	2.1982	2441
	2.53E-08	294	13313	1.16E+07	2.2036	2483
	2.59E-08	300	13428	1.16E+07	2.2082	2510
	2.79E-08	324	13847	1.16E+07	2.2241	2607
	3.11E-08	360	14322	1.16E+07	2.2376	2711
	3.22E-08	374	14717	1.16E+07	2.2511	2801
	3.45E-08	400	15159	1.16E+07	2.2626	2899
	3.65E-08	424	15539	1.16E+07	2.271	2983
	3.88E-08	450	15947	1.16E+07	2.281	3074
	4.08E-08	474	16290	1.16E+07	2.2905	3154
	4.31E-08	500	16714	1.16E+07	2.2957	3241
	4.51E-08	524	17087	1.16E+07	2.2995	3316
	4.74E-08	550	17490	1.16E+07	2.3041	3399
	4.94E-08	574	17882	1.16E+07	2.3044	3471
	5.17E-08	600	18327	1.16E+07	2.3029	3550
	5.37E-08	624	18714	1.16E+07	2.3014	3619
	5.60E-08	650	19135	1.16E+07	2.3012	3695

Table 7: Temperature Effects due to the S(α,β) Cross Sections for heavy water (constant density)

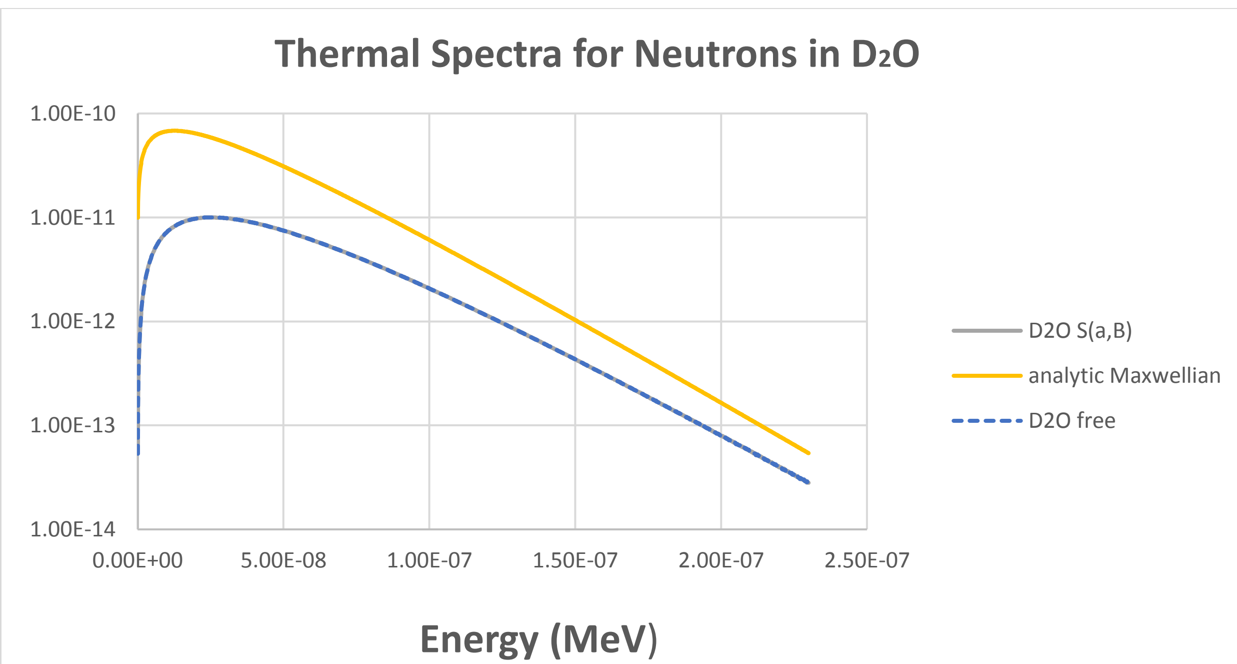

Figure 3: Thermal Neutron Spectra in Room Temperature Heavy Water

grph S(α,β)	temp (MeV)	temp (K)	avg. no. collisions	lifetime (sh)	mfp (cm)	avg n vel (km/sec)
	2.55E-08	296	1413.8	1.07E+06	1.955	2494
	3.45E-08	400	1654.3	1.07E+06	1.892	2899
	4.31E-08	500	1856.4	1.07E+06	1.873	3242
	5.17E-08	600	2037.1	1.07E+06	1.865	3551
	6.03E-08	700	2200.8	1.07E+06	1.861	3835
	6.89E-08	800	2352.7	1.07E+06	1.859	4100
	8.62E-08	1000	2633.5	1.07E+06	1.856	4584
	1.03E-07	1200	2889.4	1.07E+06	1.855	5022
	1.38E-07	1600	3340.2	1.07E+06	1.853	5798

Table 8: Temperature Effects due to the S(α,β) Cross Section for Crystalline Graphite

grph10 S(α,β)	temp (MeV)	temp (K)	avg. no. collisions	lifetime (sh)	mfp (cm)	avg n vel (km/sec)
	2.55E-08	296	1401.4	1.17E+06	2.1252	2494
	3.45E-08	400	1642.5	1.17E+06	2.0826	2899
	4.31E-08	500	1844.9	1.17E+06	2.0665	3241
	5.17E-08	600	2026.7	1.17E+06	2.0581	3550
	6.03E-08	700	2193	1.17E+06	2.0528	3835
	6.89E-08	800	2345.9	1.17E+06	2.0492	4099
	8.62E-08	1000	2629.2	1.17E+06	2.0443	4583
	1.03E-07	1200	2887.2	1.17E+06	2.0409	5021
	1.38E-07	1600	3344.7	1.17E+06	2.0365	5797

Table 9: Temperature Effects due to the S(α,β) Cross Sections for 10% Porosity Graphite

grph30 S(α,β)	temp (MeV)	temp (K)	avg. no. collisions	lifetime (sh)	mfp (cm)	avg n vel (km/sec)
	2.55E-08	296	1412.6	1.47E+06	2.6438	2494
	3.45E-08	400	1655.7	1.47E+06	2.5872	2899
	4.31E-08	500	1854.6	1.46E+06	2.5678	3241
	5.17E-08	600	2039.7	1.47E+06	2.559	3551
	6.03E-08	700	2202.8	1.47E+06	2.5541	3835
	6.89E-08	800	2355.6	1.46E+06	2.5511	4099
	8.62E-08	1000	2637.2	1.46E+06	2.5473	4583
	1.03E-07	1200	2893.1	1.46E+06	2.545	5021
	1.38E-07	1600	3345.7	1.46E+06	2.5417	5797

Table 10: Temperature Effects due to the S(α,β) Cross Sections for 30% Porosity Graphite

h-poly S(α,β)	temp (MeV)	temp (K)	avg. no. collisions	lifetime (sh)	mfp (cm)	avg n vel (km/sec)
	6.64E-09	77	119.97	1.72E+04	0.185	1272
	1.69E-08	196	161.21	1.72E+04	0.226	2029
	2.01E-08	233	168.47	1.72E+04	0.237	2213
	2.53E-08	294	177.47	1.72E+04	0.255	2483
	2.59E-08	300	178.29	1.72E+04	0.257	2510
	2.61E-08	303	178.69	1.72E+04	0.258	2522
	2.70E-08	313	180.03	1.72E+04	0.261	2564
	2.78E-08	323	181.28	1.72E+04	0.263	2604
	2.87E-08	333	182.4	1.72E+04	0.266	2645
	2.96E-08	343	183.45	1.72E+04	0.269	2684
	3.02E-08	350	184.24	1.72E+04	0.270	2711

Table 11: Temperature Effects due to the S(α,β) Cross Sections for H in Polyethylene

Be S(α,β)	temp (MeV)	temp (K)	avg. no. collisions	lifetime (sh)	mfp (cm)	avg n vel (km/sec)
	2.55E-08	296	682.52	3.67E+05	1.6403	2494
	3.45E-08	400	806.18	3.67E+05	1.404	2899
	4.31E-08	500	909.44	3.67E+05	1.3409	3241
	5.17E-08	600	1002.4	3.67E+05	1.3148	3551
	6.03E-08	700	1088.3	3.67E+05	1.3012	3835
	6.89E-08	800	1167.4	3.67E+05	1.293	4100
	8.62E-08	1000	1311.5	3.66E+05	1.2833	4584
	1.03E-07	1200	1442.8	3.66E+05	1.2777	5021

Table 12: Temperature Effects due to the S(α,β) Cross Sections for Be metal

BeO S(α,β)	temp (MeV)	temp (K)	avg. no. collisions	lifetime (sh)	mfp (cm)	avg n vel (km/sec)
	2.53E-08	294	1078.2	6.25E+05	1.7041	2483
	3.45E-08	400	1279.2	6.25E+05	1.489	2898
	4.31E-08	500	1437.5	6.24E+05	1.436	3240
	5.17E-08	600	1585	6.25E+05	1.4145	3550
	6.03E-08	700	1716.9	6.25E+05	1.4032	3834
	6.89E-08	800	1839.5	6.24E+05	1.3961	4099
	8.62E-08	1000	2067.4	6.24E+05	1.387	4584
	1.03E-07	1200	2271.1	6.24E+05	1.3808	5021

Table 13: Temperature Effects due to the S(α,β) Cross Sections for BeO

References:

1. Excerpted from David A. Brown, “README.txt” documentation file supplied with the thermal scattering data of ENDF/B-VIII.0, National Nuclear Data Center, Feb 2018.
2. David A. Brown, et al. "ENDF/B-VIII.0: The 8th Major Release of the Nuclear Reaction Data Library with CIELO-project Cross Sections, New Standards and Thermal Scattering Data," Nuclear Data Sheets 148, 1 (2018).
3. Jesse Holmes and Michael Zerkle, personal e-mail communications, 2017.
4. See Table 8-4 and Equation (8-82) on p. 263 of John R. Lamarsh, *Introduction to Nuclear Reactor Theory*, Addison Wesley Publishing Company, Second Printing, September 1972.