Title: Update of Continuous-Energy Data for Hydrogen and SiO2 Thermal Scattering

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memorandum

X-Computational Physics
Materials & Physical Data

Update of Continuous-Energy Data for Hydrogen and SiO$_2$ Thermal Scattering

The Nuclear Data Team has released updated continuous-energy neutron data files for: 1) hydrogen, and 2) $S(\alpha, \beta)$ (thermal scattering) on SiO$_2$. A list of new ZAIDs and the data that is updated (Old ZAID) is given in Table 1. The old data are still accessible, but are not the default.

I.   Hydrogen

Hydrogen was updated in response to a flaw in the ENDF71x data [1]. The original data originated from ENDF/B-VII.1 and was processed using NJOY99.396. This version of NJOY contained a bug that was first reported by Travis Trahan [4]. The NJOY bug creates incorrect photon production data for hydrogen when using ASCII evaluation files. The bug can be avoided by using binary files which retain additional precision that the ASCII files don't have.

The updated hydrogen data was processed with NJOY2012.50. This version of NJOY does not have the bug that caused the problem with the gamma data previously observed. The updated hydrogen files have been checked with `checkace` [3] which was modified to check for the problems that the original ENDF/B-VII.1-based ACE data contained and no issues were found.

II.   SiO$_2$

The original SiO$_2$ thermal scattering data originated from ENDF/B-VII.1. However, the evaluation file included in the final release ENDF/B-VII.1 was incorrect. Corrected files have been made available by Jesse Holmes [2] from Bettis Atomic Power Laboratory, the original evaluator for SiO$_2$.

The new (corrected) data contain two evaluation files for the solid alpha and beta phases of SiO$_2$. The alpha file was used for the data up to 800 K and the beta file was used for the two highest temperatures (e.g., 1000 K and 1100 K). NJOY2012.50 was used to process this data.

The SiO$_2$ data was checked by running MCNP on a "broomstick" problem. A broomstick problem consists of a very long, very thin cylinder. Source neutrons are located along the central axis of the cylinder and energy and angle tallies are created on planes perpendicular to the ends of the broomstick. In this way, we can determine the scattering angle and energy of the secondary neutrons. The secondary energy spectrum and secondary angular distribution can be seen in Figure 1. The energy spectrum compares the spectrum from the original data (green) as well as the new data (blue). The secondary angular distribution is shown for every temperature

There is a significant difference in the spectrum of scattered neutrons between the old and the new SiO_2 thermal scattering data. The difference is on the order of a factor of 2 and can have a significant effect on data using this thermal scattering treatment.

III. Availability

The data are available on the HPC machines at LANL in the standard location for Monte Carlo, type1 data: `/usr/projects/data/nuclear/mc/type1`. It is also available on the X-Division servers at: `/opt/local/codes/data/nuclear/mc/type1`.

References

[1] Jeremy Lloyd Conlin et al. *Continuous Energy Neutron Cross Section Data Tables Based upon ENDF/B-VII.1*. Tech. rep. LA-UR-13-20137. Los Alamos National Laboratory, Feb. 2013.

[2] Jesse C. Holmes. "Development of ENDF Thermal Neutron Scattering Libraries for Silicon Dioxide and MCNP Criticality Testing with an ISBEP Benchmark". MA thesis. North Carolina State University, 2011.

[3] D. Kent Parsons. *The Rules of CHECKACE – a Suite of Checking Codes for MCNP ACE Cross Section Files*. Memo XCP-5:15-032. Los Alamos National Laboratory, Apr. 2015.

[4] Travis Trahan. *Unexpected MCNP Photon Production Behavior in Hydrogen*. Memo XCP-4:15-021. Los Alamos National Laboratory, May 2015.

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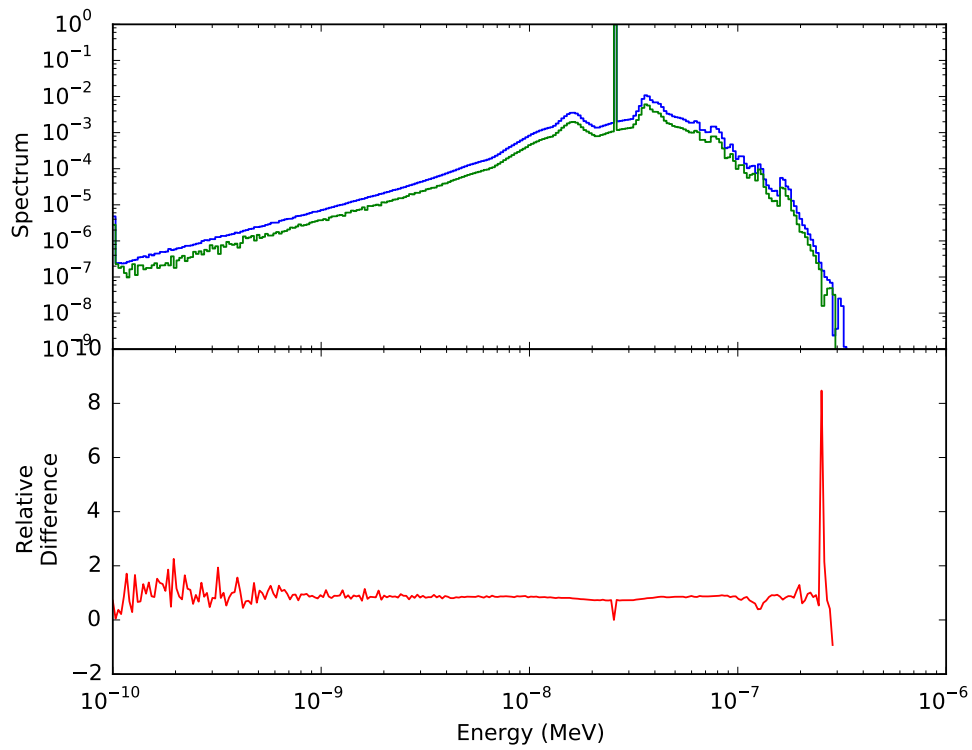
(a) Secondary Energy
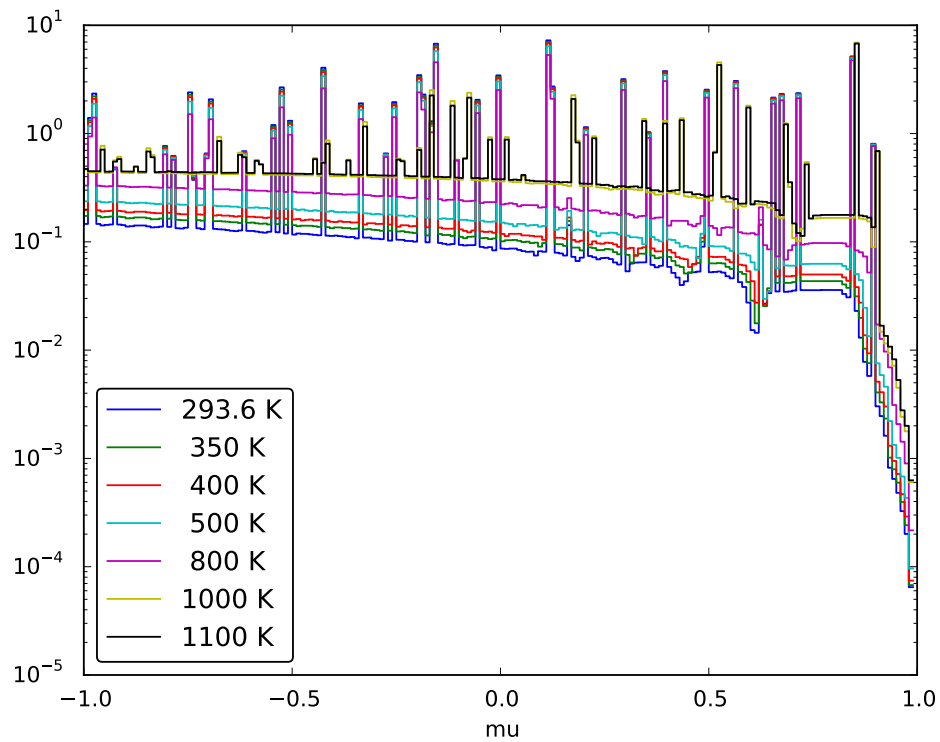
(b) Secondary Angle

Figure 1: Secondary energy and angle distributions for scattering off of SiO$_2$

New ZAID	Old ZAID	Temperature (K)
1001.90c	1001.80c	293.6
1001.91c	1001.81c	600
1001.92c	1001.82c	900
1001.93c	1001.83c	1200
1001.94c	1001.84c	2500
1001.95c	1001.85c	0.1
1001.96c	1001.86c	250
sio2.10t	sio2.30t	293.6
sio2.11t	sio2.31t	350
sio2.12t	sio2.32t	400
sio2.13t	sio2.33t	500
sio2.14t	sio2.34t	800
sio2.15t	sio2.35t	1000
sio2.16t	sio2.36t	1100*

Table 1: List of new and old ZAIDs for updated data along with the associated temperature for that ZAID.