Research on Thermal Neutron Scattering Data for Compounds

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ACE files applied by MCNP contain data only at several certain temperature points. It is necessary to process thermal ACE files at any interested temperature points including the high temperature for SCWR in order to make a more accurate calculation, especially for H2O and D2O which are very important in thermal neutron calculations. Based on the research on theory and process of thermal neutron scattering in compounds, ACE files for H2O, D2O, and some other important scattering kernels have been processed. We named this new ACE libaray SabDEP. Validation have been done by comparison of cross sections, neutron flux density spectrum, and the burnup calculation. Differences of D_2O data between ENDF/B-VI and VII have been found.

Keywords: ACE, Thermal Neutron Scattering, compounds.

1. Introduction

Thermal neutron scattering date in compound moderators such as H_2O,D_2O BeO and ZrH are very important for the design of nuclear reactors. In this energy, i.e. below 4.5eV, the binding of the scattering nucleus affects neutron cross sections and energy and angular distribution of secondary neutron a lot. In Evaluated Nuclear Data Files, these effects are described in the thermal sub-library (TSL) using File 7, which represents the underlying nuclear data from a physics viewpoint. But practical calculation requires special libraries for particle codes, for example ACE (A Compact ENDF) format data for MCNP. The majority of work on thermal neutron scattering was performed in the 1950s and 1960s. Subsequently (1970s), data libraries were generated mainly using the GASKET methodology[1], which was developed at General Atomic (GA). In early 1990s, new ENDF file[2] (ENDF/B-VI) that are accurate over a wider range of energy and momentum transfer than the existing files were calculated with the scattering law module LEAPR, together with the original GA physics models. Recently (2005) M. Mattes and J. Keiner[3] at IKE re-evaluated and reviewed the former used thermal scattering law data S(α,β) for H2O, D2O and ZrHx. This leaded to new version of TSL files- ENDF/B-VII thermal scattering sub library.

In China few researches on thermal neutron scattering was reported. Our work, generally, was processing ACE format thermal files from the original ENDF data with a translation code-NJOY. When the interested temperature not included in TSL files, we had to evaluate it by using the preliminary frequency spectra with LEAPR code. We called our thermal scattering ACE format data library SabDEP which was short for ACE formatting S(α,β) data generated in Department of Engineering Physics, including now six kinds of moderators, H in light water, D in heavy water, H in ZrH, Zr in ZrH, Graphic and BeO.

2. Thermal Neutron Scattering and Data Storage

2.1. Theory

The thermal neutron scattering cross section is usually divided into three different parts[4], inelastic, incoherent elastic, and coherent elastic. Inelastic scattering is important for all materials (both incoherent and coherent inelastic fall in this category) and described by the scattering law S(α,β). For elastic, the incoherent one is Important for hydrogenous solids like zirconium hydride and polyethylene or light water ice, while coherent should be considered for crystalline solids like graphite, beryllium or UO_2. Some basic theories about thermal scattering are included in documentation [2]. For H in H_2O and D in D_2O, only Inelastic Scattering is contained which describes the double differential scattering cross section as a function of S(α,β) as follows.

$$\frac{d^2}{d\Omega dE'}\sigma(\mathrm{E}\rightarrow\mathrm{E}',\mu,T)=\frac{\sigma_b}{4\pi\mathrm{kT}}(\frac{\mathrm{E}'}{\mathrm{E}})^{0.5}\exp(-\beta/2)\mathrm{S}(\alpha,\beta,T)$$

Generally, the scattering law S(α,β) is a complex function of α (momentum transfer) β (energy transfer), and ρ(ω) (frequency spectrum, a function of energy transfer ω=E/kT, where kT is the temperature in eV) which should be normalized as 1=∫ρ(ω)dω. The frequency spectra ρ(ω) is very important for it indicates the basic physical interactions. Lots of parameters are directly correlated to ρ(ω) such as: specific heat relation, effective scattering temperature, Debye-Waller integral, the average energy transfer, the average square of the energy transfer. This ρ(ω) can be decomposed into a sum of simple excitation spectra including translational spectrum, diffusion, discrete oscillator and solid-type spectrum. We can derive this spectra from measured double differential neutron scattering cross sections or theoretic results. Elastic, coherent or incoherent, then will be calculated from Debye-Waller integral γ(0) and effective scattering temperature.

2.2. Data Storage

The thermal scattering data in ENDF format File 7 contains coherent or incoherent elastic (MT=2) information and tabulated S(α,β,T) for incoherent inelastic (MT=4), i.e. thermal neutron scattering law S(α,β,T) is given as a table of *S* versus α for various values of β in different Temperture [4]. File 7 can not be used directly by MCNP which need a particular kind of file called ACE [5]. In a certain temperature, cross sections for elastic and inelastic scattering are found on the tables (typically for neutron energies below 4 eV). A coupled energy/angle representation is used to describe the spectra of inelastically scattered neutrons. Angular distributions for elastic scattering are also provided the same as inelastic tables (that is for incoherent elastic) or $\mu = 1-2E_{Bi}/E$.

2.3. Processing of Thermal Neutron Scattering Data

The LEAPR model is used by employing a preliminary frequency spectra to prepare the scattering law S(α,β,T) in ENDF format which describe thermal neutron scattering from bounding moderators. This ENDF format data is then used by THERMR model and finally ACER by which ACE file is made. THERMR model is important when the α or β required is outside the range of the table in File 7 with Short-collision-time approximation (SCTA). RECONR and BROADR are necessary for the reason that “MCNP requires all the cross sections be given on a single union energy grid suitable for linear interpolation”[6]. Input files for LEAPR’s evaluation work can be founded in [3]or [2]. In fact, for most cases, we obtained the File 7 data from website http://t2.lanl.gov/njoy/theindex.html if the temperature needed is already included. When not, LEAPR was run for wanted temperature.

3. lwtr for H2O

3.1. Model Description

We employed IKE model[7] which improved over the one used at General Atomics in 1969 to produce the original ENDF/B-III evaluation. In this IKE model, the alpha and beta grids have been extended to allow for large incident energy. Frequency spectrum, ρ(ω), changed a lot that it was no longer harmonic approximation, i.e. not temperature dependence for ρ(ω) any longer. Hindered transition, indicating molecule translation in liquid, was treated with a free gas law by adopting temperature-dependent masses which could be thought to be clusters of single molecules as well as of two, four, and eight complexes of H2O molecules with varying fractions depending on temperature. Hindered rotations with a broad band of frequencies various from different temperature. For a specific temperature, interpolation was done between the two limiting curves at 294 and 624K. When above 624K, our treatment was the same as the high limit. For ice, which usually considered as a cold neutron moderator, not included in our SabDEP but in ColdDEP that we have designed for cold neutron scattering calculation, frequency was used as W.Bernnat mentioned in [8]. Fig 1 showed the frequency spectra we used, for liquid we got it from Matttes and ice from Bernnat. For vibration, two Einstein δ-oscillators were introduced to describe at 0.205 and 0.48eV in liquid, while ice at 0.409 and 0.203 eV, vapor at 0.460 and 0.198 eV. In table 1, we compared those frequency spectra used from original Nilkin model, to ENDF/B-VI's model found from Pro. MacFarlane's work, and now ENDF/B-VII light water's model-IKE model, the one we used in this issue.

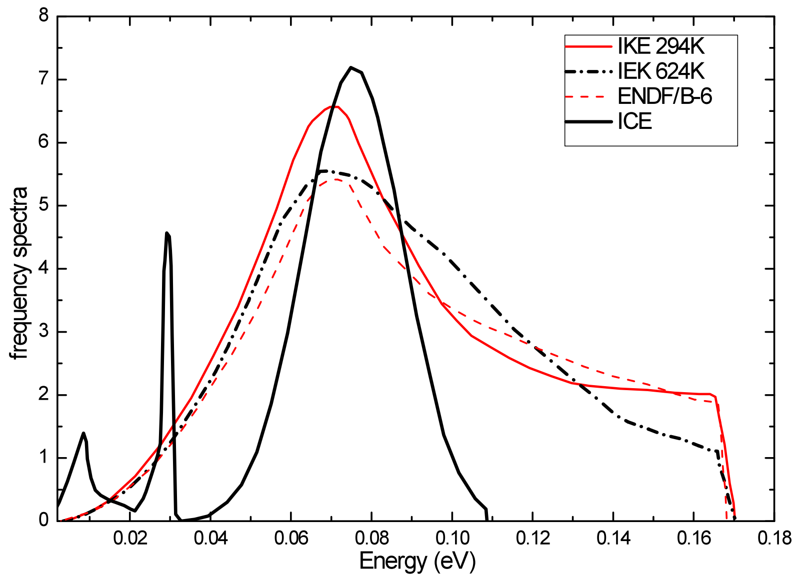

Fig 1 Frequency spectra for light water and ice

Table 1 discrete frequency spectrum function

	Nelkin Model		ENDF/B-VI		ENDF/B-VII(293.6K)	
	ω_i (eV)	$\rho_i(\omega_i)$	ω_i (eV)	$\rho_i(\omega_i)$	ω_i (eV)	$\rho_i(\omega_i)$
Hindered transition	/	0.0556	/	0.0556	/	0.0217
hindered rotation	0.065	0.4310	0.165	0.4444	0.165	0.4891
bending vibration	0.205	0.1709	0.205	0.1667	0.205	0.1630
Stretching vibration	0.481	0.3413	0.480	0.3333	0.436	0.3261
Diffusion	Free gas		Free gas		Free gas	

3.2. Neutron Cross Section and Validation

For convenience, we only represented result at 293.6K, our data lwtrDE.01t, which corresponded to lwtr.60t from Sab2002(based on ENDF/B-VI.3). In Fig2, we compared cross section and average cosine of the neutron scattering angle (mubar) for H2O at 293.6K as a primary validation, where H2O LA was down loaded from website http://t2.lanl.gov/data/thermal7.html. Neutron flux spectrum in H2O were calculated by MCNP-4C for a simple example. This example[9] was a bare (unreflected) UO_2F_2 solution cylinder (LA-10860 p.32).The weight percent of 235U in the uranium was 4.89 %. The solution had a radius of 20.12cm and a height of 100.0 cm. An aluminum tank with a thickness of 0.1587 cm on the sides and bottom, and a height of 110.0 cm contains the solution. No lid on the tank was taken and the region from the top of the solution to the top of the aluminum tank was void. Moreover, burnup for a AFA3G assembly is Calculated with different data. Fuel is UO2 with radius 0.49cm and clad Zr 0.5588cm. 39 rods is contained in calculation including 12 half-rods.

Good agreement could be found for cross section from our lwtrDE.01t and LANL light water data, while we can see a slightly difference to the old ENDF/B-VI.3 based lwtr.60t. Neutron flux spectra and burnup calculation, shown in Fig3, also indicated the correction of our data, though some differences to the old data could be found, which we thought was reasonable.

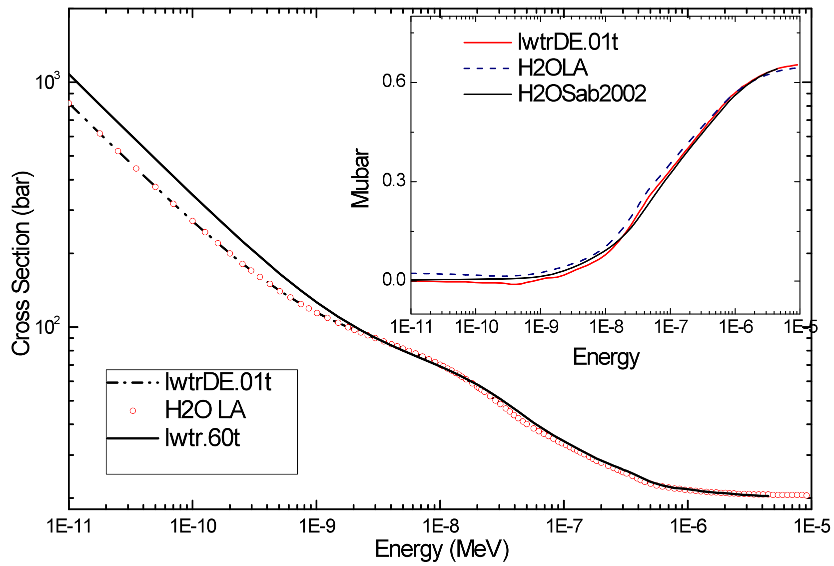

Fig 2 Cross section and average cosine of the neutron scattering angle for H2O

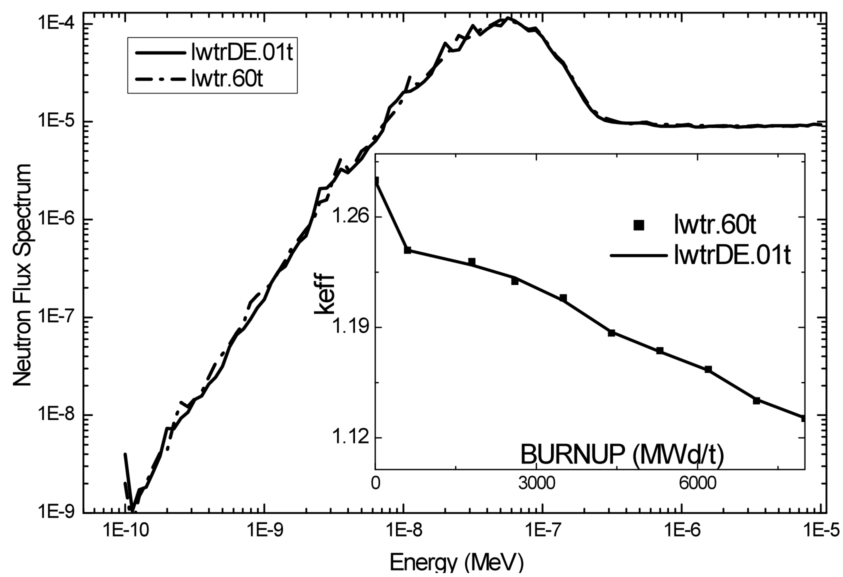

Fig 3 neutron flux density spectra for simple example and Burnup for AFA3G assembly

4. D in heavy water

4.1. Model Description

Still we took IKE model for D in D2O. The weight of the hindered translational mode was taken to be 0.05, corresponding to an effective translational mass of 20. For the three rotational degrees of freedom, a broad band of frequencies was assumed according to the results of Haywood and Page being dependent on temperature. The three vibrational degrees of freedom were represented by two discrete Einstein δ-oscillators at 145 and 338 meV with weights of .16666667 and .33333333. Above was only the incoherent treatment. From Mattes, as deuterium was a dominant **coherent** neutron scatterer, an improvement of the scattering law data for D in D2O ought to be considered by the intermolecular D-D interference. With a static structure factor S(κ), a correction of the incoherent data file according to the Sköld approximation was done. This coherent correction was the most important improvement of ENDF/B-VII to the former version. Cross section bellow will show this improvement which is totally different from the old data.

4.2. Neutron Cross Section

We only presented cross section of D in heavy water. As above, our result was named hwtrDE.01t, downloaded cross section from LA (based on ENDF/B-VII) was named LA D2O, and hwtr.60t from sab2002 (ENDF/B-VII based). We can notice these big difference of our and LA's data to the old one.

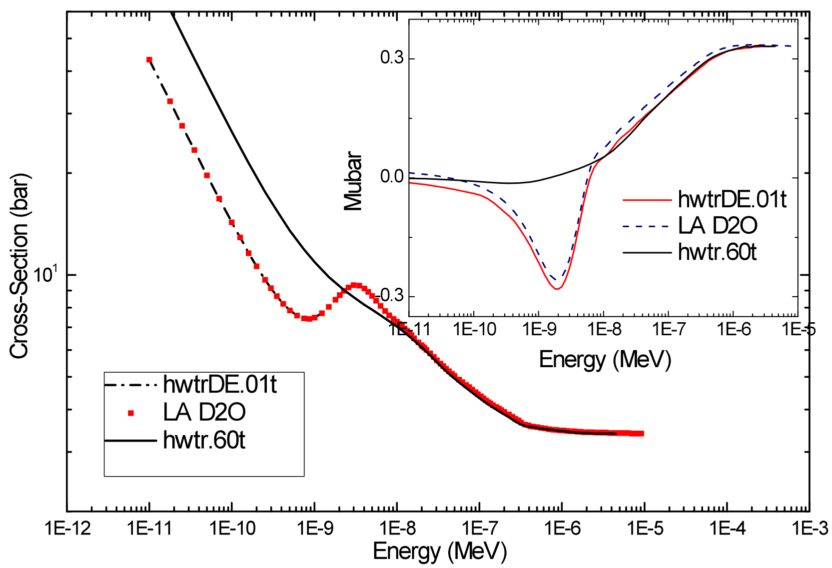

Fig 4 Cross section and average cosine of the neutron scattering angle for D2O

5. Conclusion

Some other moderators were also included in our SabDEP library. For ZrH, either H in ZrH or Zr in ZrH, BeO, and graphite no changes were made for ENDF/B-VII. We should notice that, first elastic scattering ought to be considered for these materials, and translational weight was set to zero because they were crystals.

As a conclusion, we have generated our ACE format S(α,β) library based on the latest ENDF/B-VII thermal scattering sub-library and the latest evaluation method was used for some specific temperatures. Improvement was made for H in light water as we saw above. While this improvement was revolutionary for D in heavy water adding the consideration of coherent effects between D-D.

6. Acknowledgment

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