Proposal for a JEFF working group on “thermal scattering data”

Context

Evaluation work on “thermal scattering data” for JEFF was mainly performed at the Karlsruhe Institute of Technology (KIT) by J. Keinert and M. Mattes (see Table 1). This group produced Evaluated Nuclear Data Files (MF=7, MT=4) for H in H20, D in D20, H in ZrH, H in polyethylene, Graphite and Be metal over a long period from 1981 to 2005 [1-4]. Two additional files were produced by CEA (H in CaH2, Ca in CaH2, Mg metal) between 2003 and 2004 [5,6]. One of the most important data for light water reactors is the scattering law of H in H20. Since the release of JEFF-311, KIT evaluation is continuously used in many neutronic calculations to simulate experimental and power reactors. However, ten years after the release of the latest “scattering data” files, R&D activities on this topic are no longer discussed within the JEFF project.

Recent experimental results, obtained using ILL neutron inelastic scattering instruments and coupled with Molecular Dynamic calculations, may lead to the production of improved “scattering data” files. The creation of a long term expert group is now needed to maintain and develop knowledge, skills and competences within the JEFF project.

Compilation of existing evaluated nuclear data files

Table 2 list the materials available in the international libraries. Only 9 materials are present in the JEFF libraries. One of a task could be the selection and compilation in JEFF of existing evaluated nuclear data files. The JEFF “thermal data” group will provide advices on the quality of the selected files and recommendations for improving their content.

Propose new evaluated nuclear data files

Experimental and theoretical studies have to be encouraged in order to propose new evaluated nuclear data files over a large range of temperatures with a refined mesh. Four starter files were already identified for light water, heavy water and cryogenic liquids (liquid hydrogen and deuterium). These files still need to be improved.

Decisions will be taken by the group before replacing older evaluations by new ones. Such a decision may depend on the results of integral benchmarks. Suggestions for inclusion of new materials will be considered as part of this project.

“Benchmarking” activity

The validation and the qualification of the “thermal data” are essential parts of the evaluation work. These steps are crucial for improving the “thermal scattering” libraries of JEFF. Related work could be presented during the “JEFF measurement, evaluation, processing and benchmarking” session.

Promote new experimental and theoretical approaches

The JEFF "thermal group" will promote new experimental approaches and improved theoretical calculations in the Molecular Dynamic field in connection with short term working groups (Cf. WPEC) and long term collaborative projects, such as NAUSICAA [9]. The latter project aims to increase the accuracy of thermal neutron cross section data thanks to a new way to evaluate these data without using the LEAPR module of NJOY.

Organisation of the JEFF "thermal data" group

The "thermal data" group will meet once a year in a dedicated session during the JEFF spring meeting (April). Results will be share with the NEEDS and JEFF communities during the nuclear data week in autumn (NEEDS meeting, "JEFF joint session" or "JEFF measurement, evaluation, processing and benchmarking" session). Specific issues on covariances will be share with the JEFF covariance group.

Chairman of the JEFF "thermal data" group

TBD

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Table 1: General information on the materials available in the JEFF library.

Mat.	JEFF-3.1.1	Temp. (K)	Year	Authors	Institute	Code
1	H(H20)	293.6 323.6 373.6 423.6 473.6 523.6 573.6 623.6 647.2 800.0 1000.0	Jan. 2004	J. Keinert M. Mattes	Karlsruhe Institute of Technology	LEAPR NJOY-99.90++
7	H(ZrH)	293.6 400.0 500.0 600.0 700.0 800.0 1000.0 1200.0	Jan. 2005	J. Keinert	Karlsruhe Institute of Technology	LEAPR NJOY-99.90++
8	H(CaH2)	296.0 400.0 500.0 600.0 700.0 800.0 1000.0 1200.0	Oct. 2004	O. Serot	CEA Cadarache	LEAPR NJOY
11	D(D2O)	293.6 323.6 373.6 423.6 473.6 523.6 573.6 643.9	Feb. 2004	J. Keinert M. Mattes	Karlsruhe Institute of Technology	LEAPR NJOY-99.90++
26	Be metal	293.6 400.0 500.0 600.0 700.0 800.0 1000.0 1200.0	Dec. 1989	J. Keinert M. Mattes	Karlsruhe Institute of Technology	GASKET
31	Graphite	293.6 400.0 500.0 600.0 700.0 800.0 1000.0 1200.0 1600.0 2000.0 3000.0	Jan. 2005	J. Keinert M. Mattes	Karlsruhe Institute of Technology	LEAPR NJOY-99.90++
37	H(CH2)	293.6 350.0	Sept. 1981	J. Keinert M. Mattes	Karlsruhe Institute of Technology	GASKET
52	Mg metal	20.0 100.0 296.0 773.0	Sept. 2003	C. Mounier	CEA Saclay	LEAPR NJOY
59	Ca(CaH2)	296.0 400.0 500.0 600.0 700.0 800.0 1000.0 1200.0	Oct. 2004	O. Serot	CEA Cadarache	LEAPR NJOY

Table 2: List of materials in the JEFF, ENDF/B and JENDL libraries

Material number	JEFF-3.1.1	ENDF/B-VII	JENDL-4.0
1	H(H20)	H(H2O)	H(H2O)
2		Para Hydrogen	Para Hydrogen
3		Ortho Hydrogen	Ortho Hydrogen
7	H(ZrH)	H(ZrH)	H(ZrH)
8	H(CaH2)		
11	D(D2O)	D(D20)	D(D2O)
12		Para Deuterium	Para Deuterium
13		Ortho Deuterium	Ortho Deuterium
26	Be metal	Be metal	Be metal
27		Be(BeO)	Be(BeO)
28		O(BeO)	
31	Graphite	Graphite	Graphite
33		Liquid Methane	Liquid Methane
34		Solid Methane	Solid Methane
37	H(CH2)	H(CH2)	
40		Benzine	Benzine
45		Al metal	
52	Mg metal		
56		Fe metal	
58		Zr(ZrH)	Zr(ZrH)
59	Ca(CaH2)		
75		O(UO2)	
76		U(UO2)	
Number of materials	**9**	**20**	**14**

REFERENCES

[1] JEF Report 2, JEF-1 Scattering Law Data, J. Keinert, M. Mattes, 1984.

[2] JEFDOC-41, JEF-1 Scattering Law Data, J. Keinert, M. Mattes, 1984.

[3] JEFDOC-1021, Thermal neutron scattering data, M. Mattes, J. Keinert, 2004.

[4] JEFDOC-1124, Thermal neutron scattering data at low temperatures, M. Mattes, 2005.

[5] JEFDOC-1006, Mg thermal neutron scattering cross sections, C. Mounier, 2004.

[6] JEFDOC-1005, CaHx Thermal neutron scattering cross sections, O. Serot, 2004.

[7] EFFDOC-1205, Thermal Scattering Libraries Processing (F4E, Task 6.2), E. Castro, 2013.

[8] EFFDOC-1146, Thermal scattering He-4 data at cryogenic temperature for ITER, J. Izquierd, 2011.

[9] NAUSICAA (Neutron AUgmented Sαβ In Cross sections Alternative Assessment) <https://www.ill.eu/?id=15488> (2014-)