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