Thermal Scattering Libraries Processing (F4E, Task 6.2)

Emilio CASTRO and Oscar CABELLOS
Universidad Politécnica de Madrid (UPM)
Outline

1) Introduction
2) Types of Thermal Scattering
3) State of the Art
4) Processing TSLs in ACE format with NJOY
5) Graphics with NJOY
6) Technical Validation of the Generated Libraries
7) Conclusions
F4E is developing a Project for **Nuclear Data Improvements** and Development of Tools.

**Task 6.2** consists on Thermal Scattering Libraries Processing, that has the following objectives:

- Study the worldwide available TSL data libraries.
- Process TSL with NJOY to ACE format, to be used in MCNPX.
- Technically test the processed libraries into MCNPX

To fulfill these objectives the following work has been done:

- Study of the concept of Thermal Scattering
- Review of the State of the Art
- Processing with NJOY
- Some test cases have been run in MCNP
Low energy neutrons have high associated wavelengths, similar to the size of molecules of crystalline lattices.

It can exchange energy with materials by modifying:

- The speed of the molecule.
- The rotation
- The vibration

Types of Thermal Scattering

- **Inelastic**: Important for all materials and described by the scattering law $S(\alpha,\beta)$.
- **Incoherent elastic**: Important for hydrogenous solids such as HZr
- **Coherent elastic**: Important for crystalline solids like Graphite.
Inelastic scattering is present in all materials and it is given by the scattering law \( S(\alpha, \beta) \), where \( \alpha \) is the momentum transfer and \( \beta \) is the energy transfer.

\[
\frac{d^2 \sigma}{d \Omega dE'} = \sum_{n=0}^{N_S} \frac{M_n \sigma_{bn}}{4 \pi kT} \sqrt{\frac{E}{E'}} \exp\left(-\frac{\beta}{2}\right) S_n(\alpha, \beta, T)
\]

\[ \alpha = \frac{[E' + E - 2\mu \sqrt{EE'}]}{A_0 kT} \]

\[ \beta = \frac{(E' - E)}{kT} \]

\[ S^{SCT}(\alpha, \beta, T) = \frac{\exp\left(-\frac{(\alpha - |\beta|)^2}{4\alpha T_{\text{eff}}(T)} - \frac{|\beta|}{2}\right)}{\sqrt{4 \pi \alpha T_{\text{eff}}(T)}} \]
Elastic coherent scattering: Important in crystalline solids like: Be, BeO, UO2, Graphite, SiO2, Mg, Al, Fe. The information contained in the evaluated files is $S$.

\[
\frac{d^2 \sigma}{d \Omega \, dE'} = \frac{1}{E} \sum_{i=1}^{E_i < E} s_i(T) \delta(\mu - \mu_i) \delta(E - E')/2\pi
\]

Elastic incoherent scattering: Important in hydrogenous solids like: HZr, CaH2, TiH2, YH2, CeH2, solid CH4, CH2. The information contained in the evaluated files is $W'$

\[
\frac{d^2 \sigma}{d \Omega \, dE'} = \frac{\sigma_b}{4\pi} \exp^{-2E_W'(T)(1-\mu)} \delta(E - E')
\]
Thermal Scattering Information is available in **4 libraries:**

- ENDF/B-VI.8, ENDF/B-VII.0 and ENDF/B-VII.1
- INDL-TSL
- JEFF-3.1.X
- JENDL-4.0(u)

In total: **27 materials.**
The following information has been compiled:

- Identifiers
- Kind of elastic scattering: coherent or incoherent.
- Information of the secondary scatterer: Free gas, separated material, SCT.
- Source of information: experiments, models, evaluator, codes ...
- Temperatures
## State of the Art: Temperatures

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Compound</th>
<th>ENDF/B-VII.1</th>
<th>INDL-TSL</th>
<th>JEFF 3.1.X</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>H2O</td>
<td>293.6, 350, 400, 450, 500, 550, 600, 650, 800</td>
<td>293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, 623.6, 647.2, 800, 1000</td>
<td>293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, 623.6, 647.2, 800, 1000</td>
</tr>
<tr>
<td>H</td>
<td>Para-H</td>
<td>20</td>
<td>14, 16, 20.38</td>
<td>-</td>
</tr>
<tr>
<td>H</td>
<td>Ortho-H</td>
<td>20</td>
<td>14, 16, 20.38</td>
<td>-</td>
</tr>
<tr>
<td>H</td>
<td>HZr</td>
<td>296, 400, 500, 600, 700, 800, 1000, 1200</td>
<td>293.6, 400, 500, 600, 700, 800, 1000, 1200</td>
<td>293.6, 400, 500, 600, 700, 800, 1000, 1200</td>
</tr>
<tr>
<td>H</td>
<td>CaH2</td>
<td>-</td>
<td>-</td>
<td>296, 400, 500, 600, 700, 800, 1000, 1200</td>
</tr>
<tr>
<td>H</td>
<td>TiH2</td>
<td>-</td>
<td>293.6, 400, 500, 600, 700, 800, 1000, 1200</td>
<td>-</td>
</tr>
<tr>
<td>H</td>
<td>YH2</td>
<td>-</td>
<td>293.6, 400, 500, 600, 700, 800, 1000, 1200</td>
<td>-</td>
</tr>
<tr>
<td>H</td>
<td>CeH2</td>
<td>-</td>
<td>293.6, 400, 500, 600, 700, 800, 1000, 1200</td>
<td>-</td>
</tr>
<tr>
<td>H</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>D2O</td>
<td>293.6, 350, 400, 450, 500, 550, 600, 650</td>
<td>293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, 643.9,</td>
<td>293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, 643.9,</td>
</tr>
</tbody>
</table>
## State of the Art: Temperatures

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Compound</th>
<th>ENDF/B-VII.1</th>
<th>INDL-TSL</th>
<th>JEFF 3.1.X</th>
</tr>
</thead>
<tbody>
<tr>
<td>D</td>
<td>Para-D</td>
<td>19</td>
<td>19, 23.65</td>
<td>-</td>
</tr>
<tr>
<td>D</td>
<td>Ortho-D</td>
<td>19</td>
<td>19, 23.65</td>
<td>-</td>
</tr>
<tr>
<td>Be</td>
<td>Be metal</td>
<td>293.6, 350, 400, 450, 500, 550, 600, 650</td>
<td>-</td>
<td>293.6, 400, 500, 600, 700, 800, 1000, 1200</td>
</tr>
<tr>
<td>Be</td>
<td>BeO</td>
<td>293.6, 400, 500, 600, 700, 800, 1000, 1200</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>U</td>
<td>UO2</td>
<td>296, 400, 500, 600, 700, 800, 1000, 1200</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>C</td>
<td>Graphite</td>
<td>296, 400, 500, 600, 700, 800, 1000, 1200, 1600, 2000</td>
<td>293.6, 400, 500, 600, 700, 800, 1000, 1200, 1600, 2000, 3000</td>
<td>293.6, 400, 500, 600, 700, 800, 1000, 1200, 1600, 2000, 3000</td>
</tr>
<tr>
<td>H</td>
<td>I-CH4</td>
<td>100</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>H</td>
<td>S-CH4</td>
<td>22</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>H</td>
<td>CH2</td>
<td>296, 350</td>
<td>-</td>
<td>293.6, 350</td>
</tr>
</tbody>
</table>
## State of the Art: Temperatures

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Compound</th>
<th>ENDF/B-VII.1</th>
<th>INDL-TSL</th>
<th>JEFF 3.1.X</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>C6H6</td>
<td>296, 350, 400, 450, 500, 600, 800, 1000</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>O</td>
<td>BeO</td>
<td>293.6, 400, 500, 600, 700, 800, 1000, 1200</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Si</td>
<td>SiO2</td>
<td>293.6, 350, 400, 500, 800, 1000, 1200</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Mg</td>
<td>Mg</td>
<td>-</td>
<td>-</td>
<td>20, 100, 296, 773</td>
</tr>
<tr>
<td>Al</td>
<td>Al</td>
<td>20, 80, 293.6, 400, 600, 800</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Fe</td>
<td>Fe</td>
<td>20, 80, 293.6, 400, 600, 800</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Zr</td>
<td>HZr</td>
<td>296, 400, 500, 600, 700, 800, 1000, 1200</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Ca</td>
<td>CaH2</td>
<td>-</td>
<td>-</td>
<td>296, 400, 500, 600, 700, 800, 1000, 1200</td>
</tr>
<tr>
<td>O</td>
<td>UO2</td>
<td>296, 400, 500, 600, 700, 800, 1000, 1200</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
Using NJOY, the libraries have been processed to ACE format to be used in MCNPX.

**Options used in the example of water:**

- **THERMR**
  - Linc=4: process $S(\alpha,\beta)$
  - Lcoh=0: water has no elastic scattering
  - Natom=2. Number of H atoms
  - Tempr=293.6K

- **ACER**
  - lopt=2: process thermal data
  - Suffix=0.32, for JEFF-3.1.2
  - Tname=lw00

**MCNP identifier is:** lw00.32t

---

```
reconr / Reconstruct XS for neutrons
21 22
'JEFF3.1.2 PENDF for 1-H-1'/
125 2/
0.00 0. 0.001/ err temp errmax
'JEFF3.1: 1-H-1 from JEFF-3.1.2'/
'Processed by NJOY99.364,NEA_Dec2011'/
0/
broadr / Doppler broaden XS
21 22 23
125 1 0 0 0./
0.001 -2.0e+6 0.001/ errthm thnmax errmax
293.6
0/
thermr / Add thermal scattering data (free gas)
0 23 62
0 125 12 1 1 0 1 221 1/ 
293.6
0.001 4.0
thermr / Add thermal scattering data (bound)
61 62 27
1 125 16 1 4 0 2 222 1/ 
293.6
0.001 4.0
acer / Prepare ACE files
21 27 0 28 29
2 0 1 32/
'H-H2O 293.6 K from (JEFF-3.1.2) NJOY99.364, NEA_Dec2011'/
125 293.6 'lw00' /
1001 0 0 /
222 64 0 0 1 4.0 0/
acer / Check ACE files
0 28 0 71 81
7 1 1 -1/
stop
```
Sctructure of MCNP identifiers: **MatTemp.Libt**, where

<table>
<thead>
<tr>
<th>Material in JEFF-3.1.2</th>
<th>MCNP Identifier</th>
<th>Library</th>
<th>Suffix</th>
</tr>
</thead>
<tbody>
<tr>
<td>H(H2O)</td>
<td>lw00.32t</td>
<td>ENDF/B-VI.8</td>
<td>.68t</td>
</tr>
<tr>
<td>H(HZr)</td>
<td>hzr00.32t</td>
<td>ENDF/B-VII.0</td>
<td>.70t</td>
</tr>
<tr>
<td>D(D2O)</td>
<td>hw00.32t</td>
<td>ENDF/B-VII.1</td>
<td>.71t</td>
</tr>
<tr>
<td>Be</td>
<td>be00.32t</td>
<td>INDL-TSL</td>
<td>.20t</td>
</tr>
<tr>
<td>Graphite</td>
<td>gra00.32t</td>
<td>JEFF-3.1</td>
<td>.30t</td>
</tr>
<tr>
<td>CH2</td>
<td>poly00.32t</td>
<td>JEFF-3.1.1</td>
<td>.31t</td>
</tr>
<tr>
<td>Mg</td>
<td>mg00.32t</td>
<td>JEFF-3.1.2</td>
<td>.32t</td>
</tr>
<tr>
<td>H(CaH2)</td>
<td>hca00.32t</td>
<td>JENDL-4.0</td>
<td>.40t</td>
</tr>
<tr>
<td>Ca(CaH2)</td>
<td>cah00.32t</td>
<td>JENDL-4.0u</td>
<td>.41t</td>
</tr>
</tbody>
</table>

As a result, one ACE file containing the cross section is generated for all materials at all available temperatures. Also, one dir file is generated per ACE file, with information for the xsdirt file.
Structure of Filenames: **Isotope_Material-Temp.Lib**, where:

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Filename</th>
<th>MCNP identifier</th>
</tr>
</thead>
<tbody>
<tr>
<td>293.6</td>
<td>H_H2O-00.J32</td>
<td>lw00.32t</td>
</tr>
<tr>
<td>323.6</td>
<td>H_H2O-01.J32</td>
<td>lw01.32t</td>
</tr>
<tr>
<td>373.6</td>
<td>H_H2O-02.J32</td>
<td>lw02.32t</td>
</tr>
<tr>
<td>423.6</td>
<td>H_H2O-03.J32</td>
<td>lw03.32t</td>
</tr>
<tr>
<td>473.6</td>
<td>H_H2O-04.J32</td>
<td>lw04.32t</td>
</tr>
<tr>
<td>523.6</td>
<td>H_H2O-05.J32</td>
<td>lw05.32t</td>
</tr>
<tr>
<td>573.6</td>
<td>H_H2O-06.J32</td>
<td>lw06.32t</td>
</tr>
<tr>
<td>623.6</td>
<td>H_H2O-07.J32</td>
<td>lw07.32t</td>
</tr>
<tr>
<td>647.2</td>
<td>H_H2O-08.J32</td>
<td>lw08.32t</td>
</tr>
<tr>
<td>800</td>
<td>H_H2O-09.J32</td>
<td>lw09.32t</td>
</tr>
<tr>
<td>1000</td>
<td>H_H2O-10.J32</td>
<td>lw10.32t</td>
</tr>
</tbody>
</table>
While processing, graphics for all materials have been generated for all available temperatures using the modules plotr and viewr of NJOY.

JEFF 3.1.2  C
Free-gas Scattering Temp=800 K, MT= 221

JEFF 3.1.2  Mat:Graphite
STL(31 ), Temp=800 K, MT= 229
JEFF 3.1.2  H
Free-gas Scattering Temp=293 K  MT= 221

JEFF 3.1.2  Mat:H2O
STL(1), Temp=293 K  MT= 222
The generated files have been tested in MCNP using two different methodologies:

- Simulating an **Am-Be neutron source** surrounded with materials at several temperatures.
  - The neutron source is pointwise
  - The result is Flux versus Distance
  - This procedure allows to test all materials and temperatures

- Using test cases from **SINBAD** repository.
  - KANT Beryllium Shells
  - Neutron Leakage from Water Spheres (NIST Experiment)
Flux vs. distance with H2O at 293K

Flux vs. distance with Graphite at 800K
Flux vs. distance with Be at 293K

KANT Spherical Beryllium Shells

Zoom
Conclusions

Work done:

- Thermal Scattering concepts have been studied.
- The State of the Art of Thermal Scattering Libraries has been analyzed.
- TSL have been processed with NJOY to ACE format.
- The produced libraries have been technically tested into MCNPX

As a result, the following files have been produced:

- 727 files with the processed cross section in ACE format.
- 727 dir files, with the information for xsdir.
- 727 input files for NJOY.
- 33 figures, as the result of technically testing the processed files

This information will be used in the following steps of the project.