Thermal Scattering Libraries Processing (F4E, Task 6.2)

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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) Processed TSL: Validation
7) Conclusions

Introduction

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

Types of Thermal Scattering

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.

Types of Thermal Scattering

Inelastic scattering is present in all materials and it is given by the scattering law **S(α,β)**, where α is the momentum transfer and β is the energy transfer

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

```
[MAT, 7, 4 / ZA, AWR, 0, LAT, LASYM, 0]HEAD
[MAT, 7, 4 / 0.0, 0.0, LLN, 0, NI, NS/B(N) ] LIST
[MAT, 7, 4 / 0.0, 0.0, 0, 0, NR, NB/βint] TAB2
[MAT, 7, 4 / T0, β1, LT, 0, NR, NP/ αint / S(α, β1,T0) ] TAB1
[MAT, 7, 4 / T1, β1, LI, 0, NP, 0/ S(α, β1, T1) ] LIST
------------------------------
<continue with LIST records for T2,T3,...TLT+1>
------------------------------
[MAT, 7, 4 / T0, β2, LT, 0, NR, NP/ αint / S(α,β2,T0) ] TAB1
------------------------------
<continue with TAB1 and LIST records for remaining of β and T
------------------------------
[MAT, 7, 4 / 0.0, 0.0, 0, 0, NR, NT/ Tint / Teff0(T) ] TAB1
------------------------------
[MAT, 7, 0 / 0.0, 0.0, 0, 0, 0, 0] SEND
```

$$\alpha = \left[E' + E - 2\mu\sqrt{EE'}\right] / A_0 kT$$

$$\beta = (E' - E)/kT$$

$$S^{SCT}(\alpha,\beta,T) = \frac{\exp\left(\frac{-(\alpha-|\beta|)^2}{4\alpha T_{eff}(T)} - \frac{|\beta|}{2}\right)}{\sqrt{4\pi\alpha \frac{T_{eff}(T)}{T}}}$$

Types of Thermal Scattering

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.

```
[MAT, 7, 2/ ZA, AWR, LTHR, 0, 0, 0] HEAD LTHR=1
[MAT, 7, 2/ T0, 0.0, LT, 0, NR, NP/ Eint / S(E,T0) ] TAB1
[MAT, 7, 2/ T1, 0.0, LI, 0, NP, 0/ S(Ei,T1) ] LIST
---------------------------
<repeat LIST for T2, T3, ...TLT>
--------------------------
[MAT, 7, 0/0.0, 0.0, 0, 0, 0, 0] SEND
```

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

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'

```
[MAT, 7, 2/ ZA, AWR, LTHR, 0, 0, 0]HEAD (LTHR=2)
[MAT, 7, 2/ SB, 0.0, 0, 0, NR, NP/ Tint / W'(T) ]TAB1
[MAT, 7, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND
```

$$\frac{d^2\sigma}{d\Omega\, dE'} = \frac{\sigma_b}{4\pi}\exp^{-2EW'(T)(1-\mu)}\,\delta(E-E')$$

State of the Art

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

Isotope	Compound	ENDF/B-VII.1	INDL-TSL	JEFF 3.1.X
H	H2O	293.6, 350, 400, 450, 500, 550, 600, 650, 800	293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, 623.6, 647.2, 800, 1000	293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, 623.6, 647.2, 800, 1000
H	Para-H	20	14, 16, 20.38	-
H	Ortho-H	20	14, 16, 20.38	-
H	HZr	296, 400, 500, 600, 700, 800, 1000, 1200	293.6, 400, 500, 600, 700, 800, 1000, 1200	293.6, 400, 500, 600, 700, 800, 1000, 1200
H	CaH2	-	-	296, 400, 500, 600, 700, 800, 1000, 1200
H	TiH2	-	293.6, 400, 500, 600, 700, 800, 1000, 1200	-
H	YH2	-	293.6, 400, 500, 600, 700, 800, 1000, 1200	-
H	CeH2	-	293.6, 400, 500, 600, 700, 800, 1000, 1200	-
D	D2O	293.6, 350, 400, 450, 500, 550, 600, 650	293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, 643.9,	293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, 643.9,

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State of the Art: Temperatures

Isotope	Compound	ENDF/B-VII.1	INDL-TSL	JEFF 3.1.X
D	Para-D	19	19, 23.65	-
D	Ortho-D	19	19, 23.65	-
Be	Be metal	293.6, 350, 400, 450, 500, 550, 600, 650	-	293.6, 400, 500, 600, 700, 800, 1000, 1200
Be	BeO	293.6, 400, 500, 600, 700, 800, 1000, 1200	-	-
U	UO2	296, 400, 500, 600, 700, 800, 1000, 1200	-	-
C	Graphite	296, 400, 500, 600, 700, 800, 1000, 1200, 1600, 2000	293.6, 400, 500, 600, 700, 800, 1000, 1200, 1600, 2000, 3000	293.6, 400, 500, 600, 700, 800, 1000, 1200, 1600, 2000, 3000
H	l-CH4	100	-	-
H	S-CH4	22	-	-
H	CH2	296, 350	-	293.6, 350

State of the Art: Temperatures

Isotope	Compound	ENDF/B-VII.1	INDL-TSL	JEFF 3.1.X
H	C6H6	296, 350, 400, 450, 500, 600, 800, 1000	-	-
O	BeO	293.6, 400, 500, 600, 700, 800, 1000, 1200	-	-
Si	SiO2	293.6, 350, 400, 500, 800, 1000, 1200	-	-
Mg	Mg	-	-	20, 100, 296, 773
Al	Al	20, 80, 293.6, 400, 600, 800	-	-
Fe	Fe	20, 80, 293.6, 400, 600, 800	-	-
Zr	HZr	296, 400, 500, 600, 700, 800, 1000, 1200	-	-
Ca	CaH2	-	-	296, 400, 500, 600, 700, 800, 1000, 1200
O	UO2	296, 400, 500, 600, 700, 800, 1000, 1200	-	-

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Processing with NJOY

Using NJOY, the libraries have been processed to ACE format to be use in MCNPX

MODER → RECONR → BROADR → THERMR → ACER

Options used in the example of water:

- THERMR
  - Linc=4: process S(α,β)
  - Lcoh=0: water has no elastic scattering
  - Natom=2. Number of H atoms
  - Tempr=293.6K
- ACER
  - Iopt=2: process thermal data
  - Suffix=.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/
0.001 0. 0.001/ err tempr 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/ errthn 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
```

Processing with NJOY

Sctructure of MCNP identifiers: **MatTemp.Libt**, where

Material in JEFF-3.1.2	MCNP Identifier
H(H2O)	lw00.32t
H(HZr)	hzr00.32t
D(D2O)	hw00.32t
Be	be00.32t
Graphite	gra00.32t
CH2	poly00.32t
Mg	mg00.32t
H(CaH2)	hca00.32t
Ca(CaH2)	cah00.32t

Library	Suffix
ENDF/B-VI.8	.68t
ENDF/B-VII.0	.70t
ENDF/B-VII.1	.71t
INDL-TSL	.20t
JEFF-3.1	.30t
JEFF-3.1.1	.31t
JEFF-3.1.2	.32t
JENDL-4.0	.40t
JENDL-4.0u	.41t

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 xsdir file.

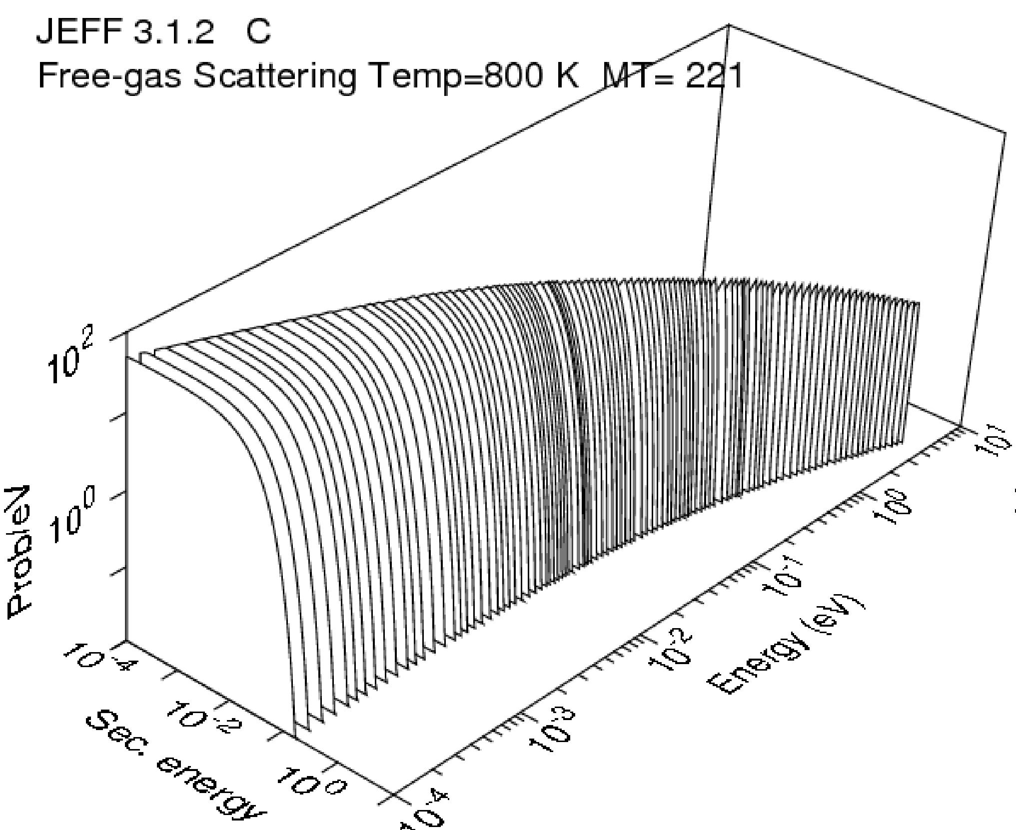
Processing with NJOY

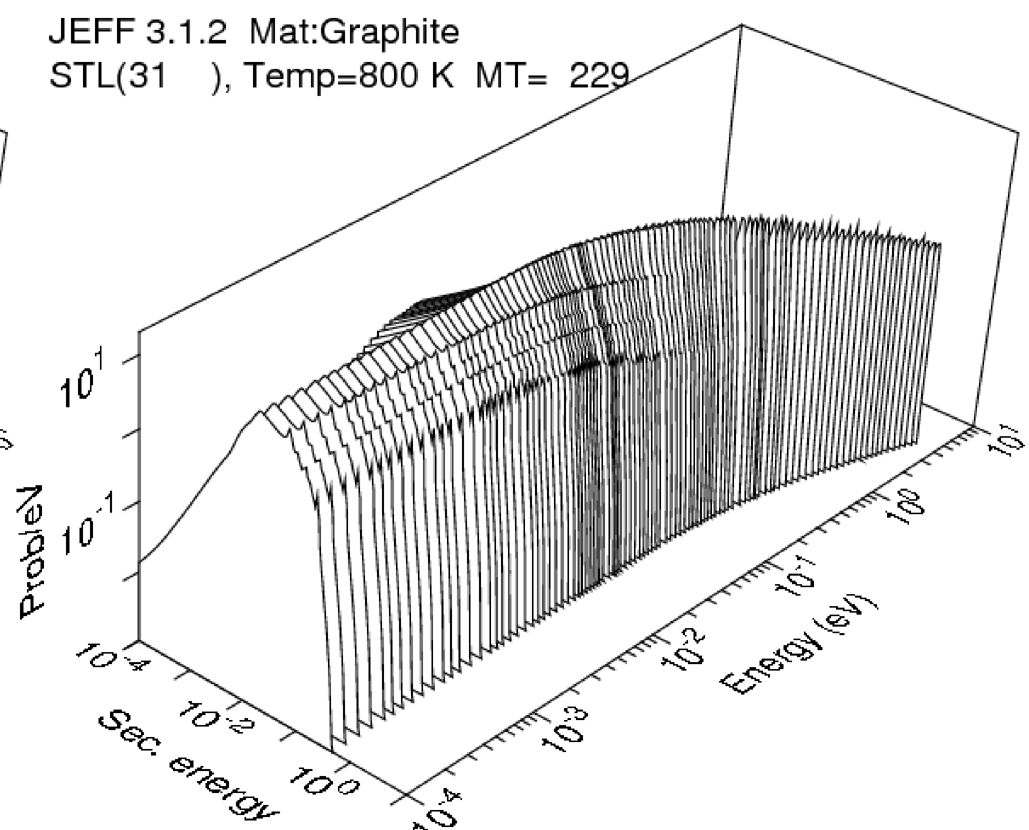
Structure of Filenames: **Isotope_Material-Temp.Lib**, where:

Temperature	Filename	MCNP identifier
293.6	H_H2O-00.J32	lw00.32t
323.6	H_H2O-01.J32	lw01.32t
373.6	H_H2O-02.J32	lw02.32t
423.6	H_H2O-03.J32	lw03.32t
473.6	H_H2O-04.J32	lw04.32t
523.6	H_H2O-05.J32	lw05.32t
573.6	H_H2O-06.J32	lw06.32t
623.6	H_H2O-07.J32	lw07.32t
647.2	H_H2O-08.J32	lw08.32t
800	H_H2O-09.J32	lw09.32t
1000	H_H2O-10.J32	lw10.32t

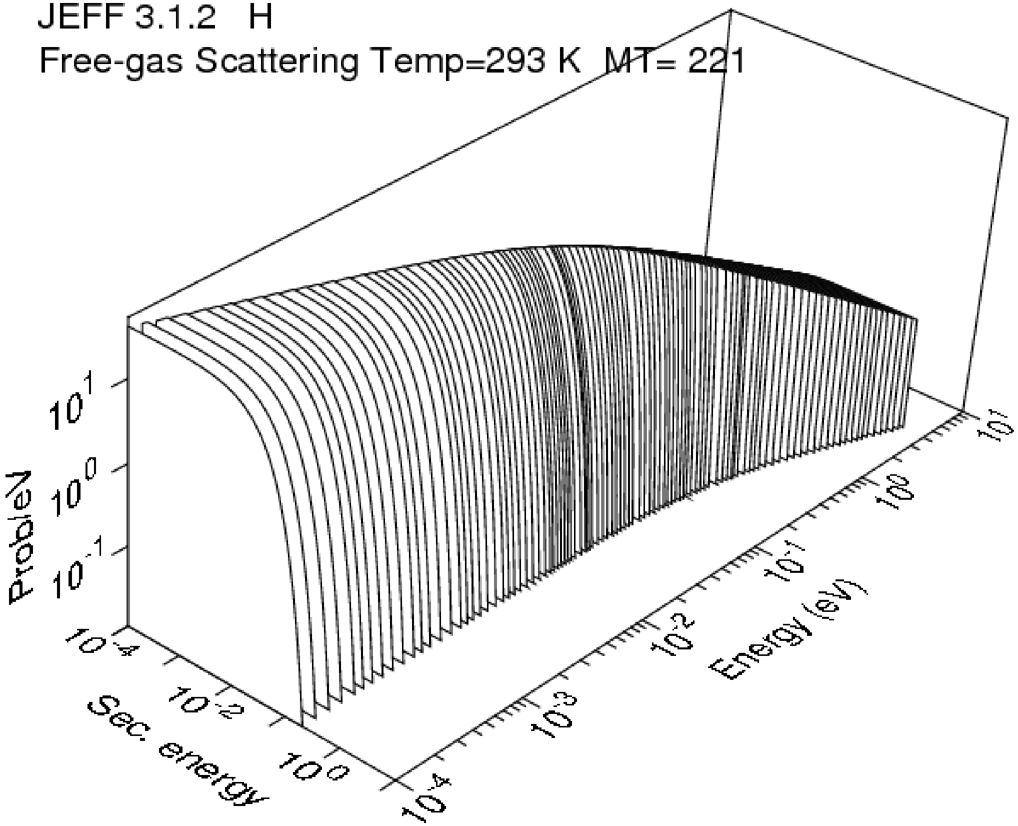
Graphics

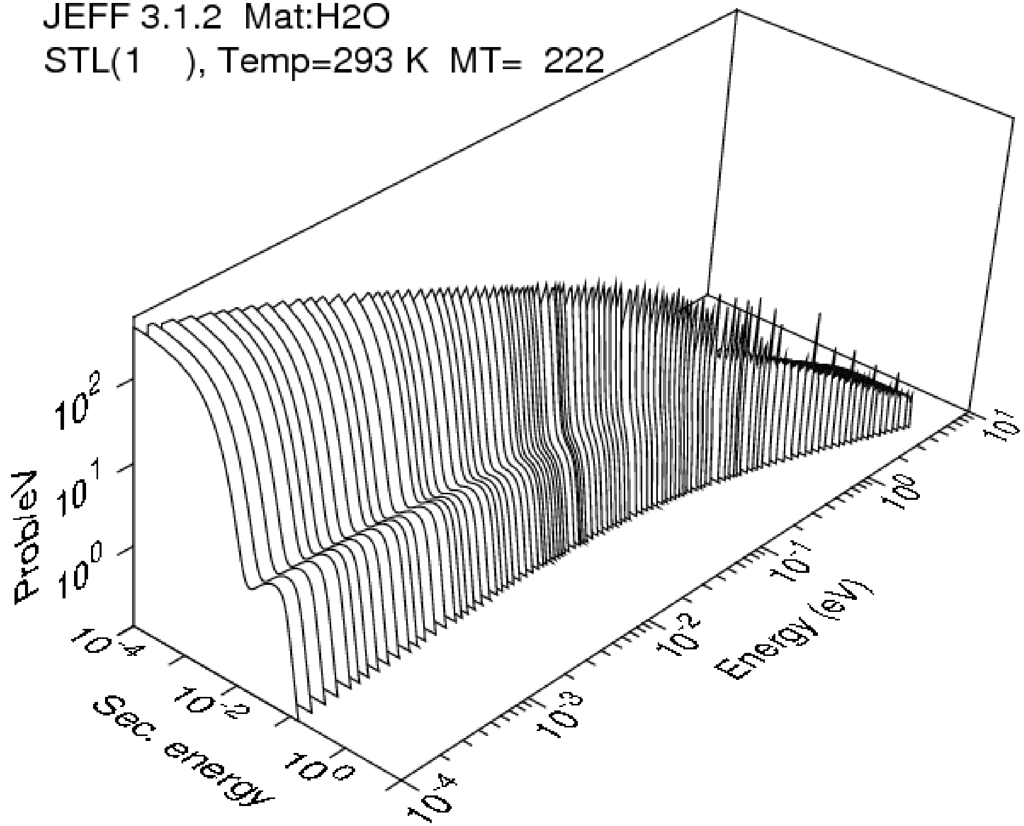
While processing, graphics for all materials have been generated for all available temperatures using the modules plotr and viewr of NJOY.





Graphics


JEFF 3.1.2 H
Free-gas Scattering Temp=293 K MT= 221
ProbleV
Sec. energy
Energy (eV)

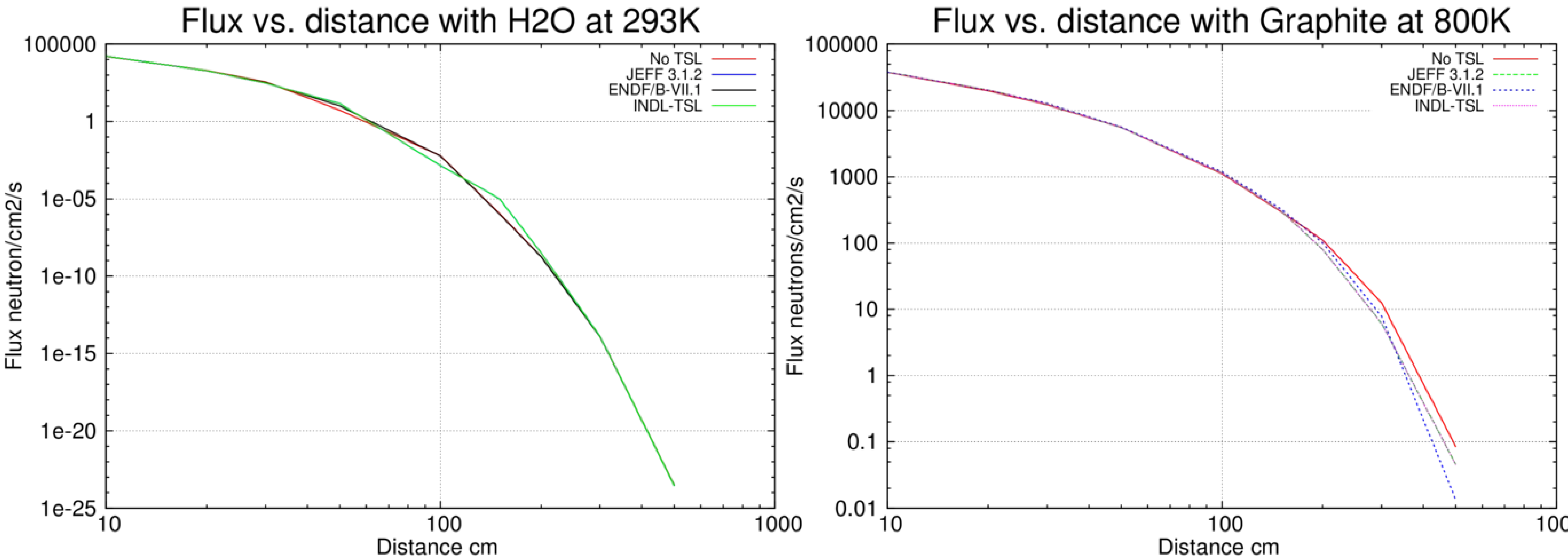

JEFF 3.1.2 Mat:H2O
STL(1), Temp=293 K MT= 222
ProbleV
Sec. energy
Energy (eV)

Processed TSL: Validation

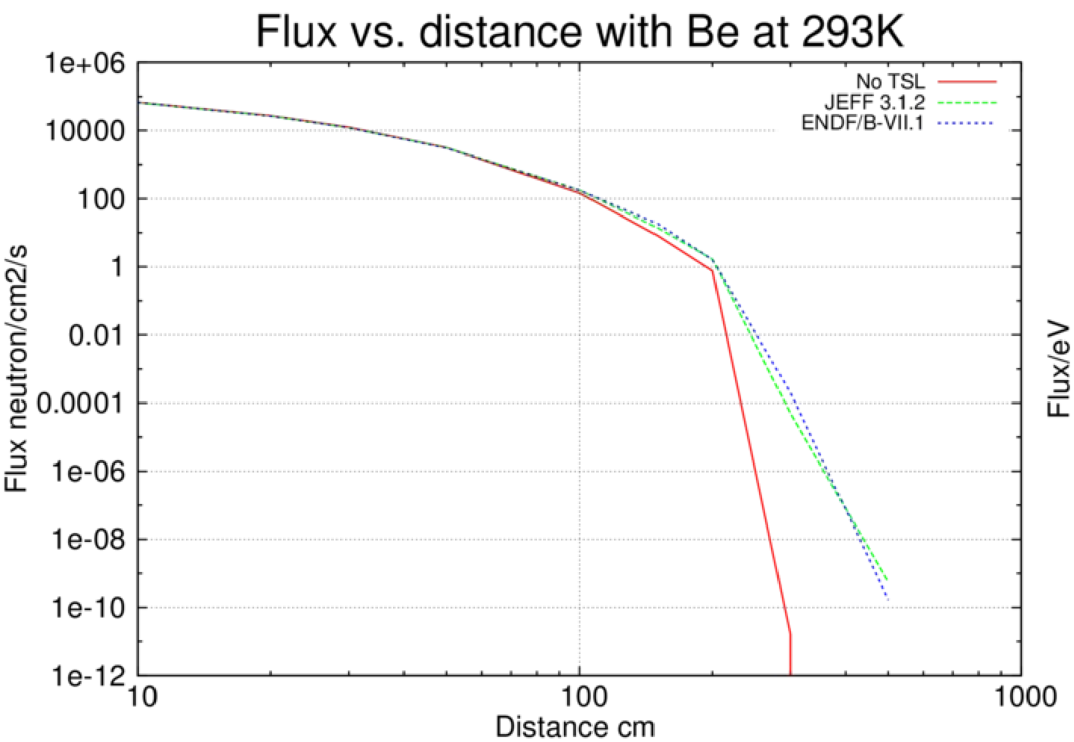
The generated files have been tested in MCNP using two different methodologies:

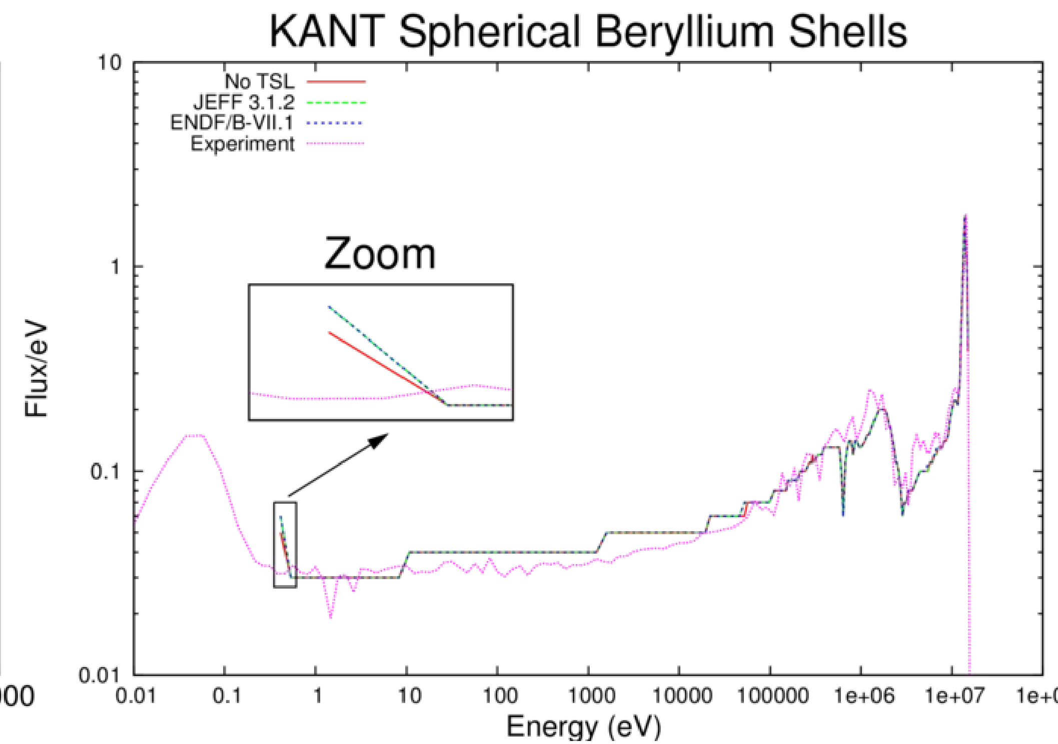
- Simulating an **Am-Be neutron source** surrounded with materials at several temperatures.
  - The neutron source is pointwise
  - The result is Flux versus Distance
  - This procedure allows to test all materials and temperatures
- Using test cases from **SINBAD** repository.
  - KANT Beryllium Shells
  - Neutron Leakage from Water Spheres (NIST Experiment)

Processed TSL: Validation



Processed TSL: Validation





Conclusions

Work done:

- Thermal Scattering concepts have been studied.
- The State of the Art of Thermal Scattering Libraries has been analized.
- 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.