OECD/NEA Meeting: WPEC SG42

"Thermal Scattering Kernel S(α,β): Measurement, Evaluation and Application" May 15 – 18, 2018 • Paris, France

SG42 Meeting Preliminaries

Gilles Noguere, CEA, France Ayman I. Hawari, NC State University, USA



Organisation for Economic Co-operation and Development Nuclear Energy Agency WPEC 2017 Meetings

Draft Agenda

Thermal Scattering Kernel S(α,β)

Measurement, Evaluation and Application

<u>SG-42</u>

OECD Headquarters Conference Center 2 Rue André Pascal, Paris 75016

Please note: Only registered participants with a valid ID card or passport will be allowed access to OECD premises.

Tuesday, May 15, 2018

10:00 - 12:00	SG42 meeting	Room CC 20
10:00 - 10:30	Welcome	Ayman I. HAWARI Gilles NOGUERE
10:30 - 11:00	NNL TSL evaluation work for ENDF/B-VIII.1	Michael L. ZERKLE
11:00 - 11:30	Thermal Scattering Physics Methods with Modeling Tools and Experiments	Jesse HOLMES
11:30 - 12:00	Contribution of Thermal Scattering Libraries from the Nuclear Data Group at Centro Atomico Bariloche	Florencia CANTARGI
12:00 - 12:30	GNDS-1.9 & future TSL format	David BROWN
12:30 - 14:00	Lunch Break	
14:00 - 18:00	Joint session SG44/SG42/GNDS	

Wednesday, May 16, 2018				
9:00 - 18:00	SG42 meeting			
9:00 - 9:30	Investigation of frequency spectrum of light water to generate thermal scattering law	Vaibhav JAISWAL		
9:30 - 10:00	The new thermal neutron scattering measurements and analysis	Emily LIU		
10:00 - 10:30	Recent Developments in Thermal Scattering Data and Methods at NCSU	Ayman I. HAWARI		
10:30 - 11:00	Coffee Break			
11:00 - 11:30	TSL activities in the frame of the NAUSICAA collaboration	Gilles NOGUERE		
11:30 - 12:30	Preparation of the final report	all		
12:30 - 14:00	Lunch Break			
14:00 - 16:00	Preparation of the final report	all		
16:00 - 16:30	Coffee Break			
16:30 - 18:00	Preparation of the final report	all		

SG42 Final Report

Draft version, SG42 report, 04/2018

SG42 Report Outline

1) Introduction/context

2) Theory: Development of evaluation methods and tools

Discussions of the different approaches, given that the major development over the past 20 years is the implementation of atomistic simulation methods to support TSL evaluation.

3) Experiments: Theory-Measurement connections

- Microscopic data ⇒ Transmission experiments, inelastic scattering experiments
- Semi-integral data ⇒ slowing down experiments
- Integral data ⇒ ICSBEP, IRPhE, non public benchmarks ...

4) Evaluation: progress on various materials and recent contributions to databases

- Reactor applications
- Criticality applications
- Neutron beam applications
- Cold neutron sources

5) Data format issues - GND format

- TSL library format
- TSL uncertainties

6) Summary and recommendations

APPENDIX if needed, such as LEAPR inputs and MCNP inputs of interest for this work.

Discussions : Development of evaluation methods and tools

\Rightarrow The major development over the past 20 years is the implementation of atomistic simulation methods to support TSL evaluation

- Recommendations to correctly use these methods
- Limits/advantages
- Others

	-					
	File name	Main source	Last mod.	Lab.	Year	Note
	tsl-ortho-D.endf	ENDF/B-VII.0	2016	LANL	1993	
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	tsl-para-D.endf	ENDF/B-VII.0	2016	LANL	1993	
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	tsl-ortho-H.endf	ENDF/B-VII.0	2016	LANL	1993	
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	tsl-para-H.endf	ENDF/B-VII.0	2016	LANL	1993	
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	tsl-013_Al_027.endf	ENDF/B-VII.0	2016	LANL	2005	
	tsl-026_Fe_056.endf	ENDF/B-VII.0	2016	LANL	2005	
	tsl-Be-metal.endf	ENDF/B-VIII.0	2016	NCSU	2016	DFT/AILD
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	tsl-BeinBeO.endf	ENDF/B-VIII.0	2016	NCSU	2016	DETUND
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	tsl-OinBeO.endf	ENDF/B-VIII.0	2016	NCSU	2016	DETIAILD
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	tsl-HinH2O.endf	ENDF/B-VIII.0	2016	CAB (Argentina)	2016	MD
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	tsl-HinIceIh.endf	ENDF/B-VIII.0	2016	BAPL	2016	DETAILD
$ \begin{array}{c cccc} tsl-DinD2O.endf & ENDF/B-VIII.0 & 2016 & CAB (Argentina) 2016 & MC \\ tsl-DinD2O.endf & ENDF/B-VIII.0 & 2016 & CAB (Argentina) 2016 & MC \\ tsl-benzene.endf & ENDF/B-VIII.0 & 2017 & GA & 1969 Corrected spelling; No LEAPR inputs available \\ \hline tsl-HinC5O2H8.endf & ENDF/B-VIII.0 & 2016 & NCSU & 2015 & MC \\ tsl-B-CH4.endf & ENDF/B-VIII.0 & 2016 & LANL & 1993 \\ tsl-s-CH4.endf & ENDF/B-VIII.0 & 2016 & LANL & 1993 \\ tsl-scH4.endf & ENDF/B-VIII.0 & 2016 & NCSU & 2016 & LANL & 1993 \\ tsl-scH4.endf & ENDF/B-VIII.0 & 2016 & NCSU & 2016 & LANL & 1993 \\ tsl-scH4.endf & ENDF/B-VIII.0 & 2016 & NCSU & 2016 & LANL & 1993 \\ tsl-scH4.endf & ENDF/B-VIII.0 & 2016 & NCSU & 2016 & LANL & 1993 \\ tsl-sch4.endf & ENDF/B-VIII.0 & 2016 & NCSU & 2016 & LANL & 1993 \\ tsl-sch4.endf & ENDF/B-VIII.0 & 2016 & NCSU & 2016 & LANL & 1993 \\ tsl-sch4.endf & ENDF/B-VIII.0 & 2016 & NCSU & 2016 & LANL & 1993 \\ tsl-sch4.endf & ENDF/B-VIII.0 & 2016 & NCSU & 2016 & LANL & 1993 \\ tsl-sch4.endf & ENDF/B-VIII.0 & 2016 & NCSU & 2016 & LANL & 1993 \\ tsl-sch4.endf & ENDF/B-VIII.0 & 2016 & NCSU & 2016 & LANL & 1993 \\ tsl-sch4.endf & ENDF/B-VIII.0 & 2016 & NCSU & 2016 & LANL & 1993 \\ tsl-sch4.endf & ENDF/B-VIII.0 & 2016 & NCSU & 2016 & LANL & 1993 \\ tsl-sch4.endf & ENDF/B-VIII.0 & 2016 & NCSU & 2014 & DFT/ALD & LANL & 1993 \\ tsl-sch4.endf & ENDF/B-VIII.0 & 2016 & NCSU & 2014 & DFT/ALD & LANL & 1993 & LANL & LANL & 1993 & LANL &$	tsl-OinIceIh.endf	ENDF/B-VIII.0	2016	BAPL	2016	DETAILD
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	tsl-DinD2O.endf	ENDF/B-VIII.0	2016	CAB (Argentina)	2016	ND
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	tsl-OinD2O.endf	ENDF/B-VIII.0	2016	CAB (Argentina)	2016	MD
inputs available inputs available inputs available tsl-HinC502H8.endf ENDF/B-VIII.0 2016 NCSU 2015 Mo tsl-bCH4.endf ENDF/B-VIII.0 2016 LANL 1993 tsl-sCH4.endf ENDF/B-VIII.0 2016 NCSU 2016 tsl-scH4.endf ENDF/B-VIII.0 2016 NCSU 2016 tsl-scH4.endf ENDF/B-VIII.0 2016 NCSU 2016 tsl-cmaft ENDF/B-VIII.0 2016 NCSU 2014 tsl-cmaft ENDF/B-VIII.0 2016 NCSU 2014 tsl-cmaft ENDF/B-VIII.0 2016 NCSU 2014 tsl-cmaft ENDF/B-VIII.0 2016 NCSU <	tsl-benzene.endf	ENDF-269	2017	GÁ	1969	Corrected spelling; No LEAPR
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$						inputs available
tsl-FlinCH2.endf ENDF/B-VIII.0 2016 NCSU 2015 MD tsl-ICH4.endf ENDF/B-VII.0 2016 LANL 1993 tsl-scH4.endf ENDF/B-VII.0 2016 LANL 1993 tsl-scH4.endf ENDF/B-VII.0 2016 NCSU 2016 tsl-scH4.endf ENDF/B-VIII.0 2016 NCSU 2016 tsl-scH4.endf ENDF/B-VIII.0 2016 NCSU 2016 tsl-scH4.endf ENDF/B-VIII.0 2016 NCSU 2016 <td>tsl-HinC5O2H8.endf</td> <td>ENDF/B-VIII.0</td> <td>2016</td> <td>NCSU</td> <td>2015</td> <td>MD</td>	tsl-HinC5O2H8.endf	ENDF/B-VIII.0	2016	NCSU	2015	MD
tsl-s-CH4.endf ENDF/B-VII.0 2016 LANL 1993 tsl-s-CH4.endf ENDF/B-VII.0 2016 LANL 1993 tsl-s-CH4.endf ENDF/B-VII.0 2016 NCSU 2016 tsl-graphite.endf ENDF/B-VIII.0 2016 NCSU 2016 tsl-graphite.endf ENDF/B-VIII.0 2016 NCSU 2016 tsl-cractor-graphite.endf ENDF/B-VIII.0 2016 NCSU 2014 tsl-CinSiC.endf ENDF/B-VIII.0 2016 NCSU 2014 tsl-SinSiC.endf ENDF/B-VIII.0 2016 NCSU 2014	tsl-HinCH2.endf	ENDF/B-VIII.0	2016	NCSU	2015	MD
tsl-s-CH4.endf ENDF/B-VII.0 2016 LANL 1993 tsl-graphite.endf ENDF/B-VIII.0 2016 NCSU 2016 tsl-reactor-graphite.endf ENDF/B-VIII.0 2016 NCSU 2016 tsl-cinsiC.endf ENDF/B-VIII.0 2016 NCSU 2014 tsl-SinsiC.endf ENDF/B-VIII.0 2016 NCSU 2014	tsl-l-CH4.endf	ENDF/B-VII.0	2016	LANL	1993	
tsl-graphite.endf ENDF/B-VIII.0 2016 NCSU 2016 DFT/AILD tsl-reactor-graphite.endf ENDF/B-VIII.0 2016 NCSU 2016 DFT/AILD tsl-CinSiC.endf ENDF/B-VIII.0 2016 NCSU 2014 DFT/AILD tsl-SinSiC.endf ENDF/B-VIII.0 2016 NCSU 2014 DFT/AILD tsl-SinSiC.endf ENDF/B-VIII.0 2016 NCSU 2014 DFT/AILD	tsl-s-CH4.endf	ENDF/B-VII.0	2016	LANL	1993	
tsl-reactor-graphite.endf ENDF/B-VIII.0 2016 NCSU 2016 DF1/ALD tsl-CinSiC.endf ENDF/B-VIII.0 2016 NCSU 2014 DF1/ALD tsl-SiinSiC.endf ENDF/B-VIII.0 2016 NCSU 2014 DF1/ALD	tsl-graphite.endf	ENDF/B-VIII.0	2016	NCSU	2016	
tsl-CinSiC.endf ENDF/B-VIII.0 2016 NCSU 2014 tsl-SiinSiC.endf ENDF/B-VIII.0 2016 NCSU 2014 DFT/AILD 2016 NCSU 2014	tsl-reactor-graphite.endf	ENDF/B-VIII.0	2016	NCSU	2016	DF1/AILD
tsl-SlinSiC-endf ENDF/B-VIII.0 2016 NCSU 2014	tsl-CinSiC.endf	ENDF/B-VIII.0	2016	NCSU	2014	DETAUD
LOUGA LE LE ENDE DUILLA AGAA NOCH AGAA	tsl-SiinSiC.endf	ENDF/B-VIII.0	2016	NCSU	2014	UF TAILU
tsl-SiO2-alpha.endf ENDF/B-VIII.0 2016 NCSU 2011 DETAILD	tsl-SiO2-alpha.endf	ENDF/B-VIII.0	2016	NCSU	2011	DET/All D
tsl-SiO2-beta.endf ENDF/B-VIII.0 2016 NCSU 2011	tsl-SiO2-beta.endf	ENDF/B-VIII.0	2016	NCSU	2011	

TABLE XLVII: Summary of the origins of and recent changes to the thermal neutron scattering (thermal_scatt) sublibrary. Evaluations modified for ENDF/B-VIII.0 are given in bold. Note all files were modified to correct the MAT numbering of the sublibrary.

TABLE XLVII: Summary of the origins of and recent changes to the thermal neutron scattering (thermal.scatt) sublibrary. Evaluations modified for ENDF/B-VIII.0 are given in bold. Note all files were modified to correct the MAT numbering of the sublibrary.

File name	Main source	Last mod.	Lab.	Year	Note
tsl-HinYH2.endf	ENDF/B-VIII.0	2016	BAPL	2016	DET/AILD
tsl-YinYH2.endf	ENDF/B-VIII.0	2016	BAPL	2016	
tsl-HinZrH.endf	ENDF/B-VII.0	2016	LANL	1993	
tsl-ZrinZrH.endf	ENDF/B-VII.0	2016	LANL	1993	
tsl-OinUO2.endf	ENDF/B-VIII.0	2016	NCSU	2016	DETIAN D
tsl-UinUO2.endf	ENDF/B-VIII.0	2016	NCSU	2016	DETAILD
tsl-NinUN.endf	ENDF/B-VIII.0	2017	NCSU	2017	057/4110
tsl-UinUN.endf	ENDF/B-VIII.0	2017	NCSU	2017	UF I/AILU

\Rightarrow However, final results are still accommodated to LEAPR formalism

- How to improve this approach
 - New evaluation tools
 - Improved theoretical treatment
- Accuracy of the results (VVUQ)
- Others ...

Discussions : Theory-Measurements Connections

- \Rightarrow Experimental validation of the calculated DOS (vDOS vs. gDOS)
- To be discussed
- \Rightarrow Experimental validation of the double-differential neutron cross sections using TOF chopper spectrometers (inelastic measurements)
- Difficult to achieve good agreement between calculated and experimental results
- Origin of the discrepancies are difficult to identify (Simulation or LEAPR ?)
- Others ...
- ⇒ Experimental validation of the neutron total cross section using transmission technique
- Easy to perform
- Limited number of facilities
- Difficult to get experimental results below 1 meV
- Others
- \Rightarrow Experimental validation using slowing down experiments
- To be discussed
- \Rightarrow Experimental validation using integral benchmarks
- They only give trends
- Sensitivity studies are needed to identify the various contributions
- Others ...

Discussions : Data Format Issues

\Rightarrow Data format requirements for LEAPR parameters

- Make clear the LEAPR input parameter files
- Others
- \Rightarrow Data format requirements for MF=7
- To be discussed
- \Rightarrow Data format requirements for covariance matrix
- LEPAR parameter covariance
- Covariance matrix for MTs in MF=7