

CAB ACTIVITY REPORT: THERMAL SCATTERING LIBRARIES FOR REACTOR APPLICATIONS

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WPEC SG-42 second meeting
May 9th-10th, 2016
OECD, Paris, France



WHO WE ARE: THERMAL SCATTERING NUCLEAR DATA GROUP AT CENTRO ATOMICO BARILOCHE



Rolando Granada
Scattering theory and
advanced neutron sources



Florencia Cantargi
Cold moderator materials
and neutron filters



Ignacio Marquez
Nuclear reactor
applications and
benchmarking

Past members: Monica Scaffoni (currently at IAEA), Victor Gillette (currently at University of Sharjah, U.A.E).

1. New light and heavy water TSL for ENDF/B-VIII.
2. TSL for H⁺ ions.
3. New TSL webpage at EXFOR.
4. An open source, standalone alternative to LEAPR/NJOY.
5. Other activities and collaborations.



- Available in the ENDF GForge server since Sept. 2015.
- Presented by D. Roubtsov at CSEWG meeting in Nov. 2015.
- Libraries for:
 - H-1 bound in H₂O (`tsl-HinH2O.endf`).
 - H-2 bound in D₂O (`tsl-DinD2O.endf`).
 - O-16 bound in H₂O (`tsl-OinD2O.endf`).
- Temperatures: 283 - 600 K.

- H⁺ ions present in acid solutions (particularly, HNO₃) have a different dynamics than H bound in H₂O. Assuming that H⁺ dissociate from the NO₃ and are free in the solution*, ions have:

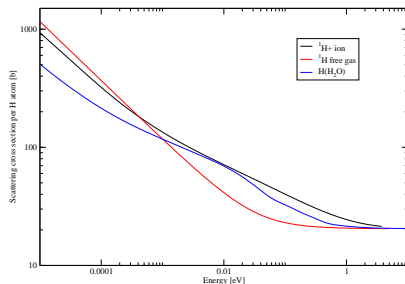
- No rotation,
 - No vibrations,
 - Only diffusion

- The concentration of H⁺ ions is sufficiently high in some fissile solution benchmarks to be ignored.

* this is not strictly true, and a more serious study should consider hydronium cations (H₃O⁺) and solvation water, but this gives an estimate of the impact of acids in critical systems

2) TSL FOR H+ IONS (CONT.)

- We developed a model for the scattering of thermal neutrons by free H+ ions.



Scattering cross section for different models of thermal neutron scattering in H atoms.

- We used this library applying the pseudo-material method in MCNP.
- The effect on case 1 of PU-SOL-THERM-018 (5.02 M acid molarity) is 28 ± 5 pcm.

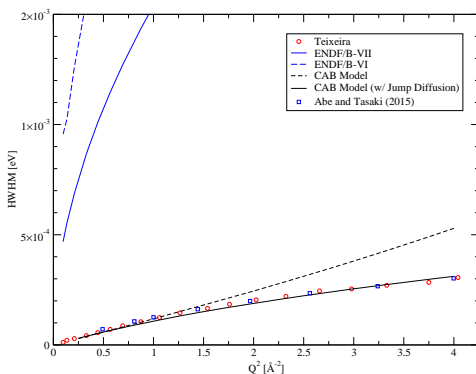
Conclusion: be aware that solution critical systems with high free acid concentrations may not be as reliable as benchmarks as we might think, if we do not take into account the free acid.

3) NON-GAUSSIAN DIFFUSION IN LEAPR

- LEAPR computes the thermal scattering law as the convolution of three terms:
 - Translation as diffusion or free gas
 - Solid-like phonons
 - Internal vibrations
- The free gas model in mode 7), modes 7) and 7) are inherently Gaussian.
- Diffusion in mode 7) is Gaussian because it uses the Egelstaff-Schofield model
- Diffusion in water is not Gaussian → replace the Egelstaff-Schofield diffusion model.

3) NON-GAUSSIAN DIFFUSION IN LEAPR (CONT)

- We implemented a random jump diffusion model in LEAPR (simplest non-Gaussian model).
- Results: we can reproduce the calculations performed by Abe and Tasaki using GAAQC.



Width of the quasielastic peak calculated with different models, compared with experimental data from Teixeira.

4) NEW TSL WEBPAGE AT EXFOR

- Nov. 2015 → EXFOR CM on thermal scattering data.
 - <https://www-nds.iaea.org/index-meeting-crp/CM-THSC-2015/>
 - Report INDC(NDS)-0697, "Compilation of Thermal Neutron Scattering Data for Experimental Nuclear Reaction Data Library (EXFOR)".
 - Recommendations on TSL data to be included in EXFOR.
 - Recommendation to create a separate database for derived data useful for evaluation.
- April-May 2016 → collaboration with EXFOR to implement the database.

4) NEW TSL WEBPAGE AT EXFOR (CONT.)

Currently hosted at CM page:

- CM presentations.
- TSL related data (phonon spectra, structure factors).
- EXFOR data related to TSL evaluation.
- TSL research groups with links.

This is a work in progress. Contributions and corrections are welcome.

- Submit new data to EXFOR.
- Propose new data for the TSL database.

Write to v.semkova@iaea.org.

(Discussions will continue at 17:30).

4) NEW TSL WEBPAGE AT EXFOR (CONT.)

EXFOR compilation of thermal neutron scattering data - Chromium

EXFOR compilation of the: x

https://www-nds.iaea.org/index-meeting-crp/CM-THSC-2015/

International Atomic Energy Agency
Nuclear Data Services
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Databases: EXFOR ENDF CTNDA IBANDL Medical PGAA NGASAS RIPL FENDL IRDP-2002 IRDFP

EXFOR compilation of thermal neutron scattering data
 (Consultants' Meeting, 2 to 4 November 2015, IAEA Headquarters, Vienna, Austria)

Thermal neutron scattering cross section data are important for calculations of reactor cores and spallation target design, safety and economy. At thermal energies, the scattering is affected by the binding of the scattering nucleus in a solid, liquid, or gas material. The purpose of the meeting is to discuss the key characteristic of the thermal neutron scattering measurement and evaluation techniques to provide guidelines for compilation of such data in the EXFOR data library.

Participants

- Li (Emily) Liu
- F. Cantargi
- D.V. Baxter
- E. Farhi
- Y. Kiyonagi
- J.I. Marquez Damian

Scientific Secretary
V. Semkova

NDS Staff Involved

- N. Otsuka
- S. Simakov
- V. Zerkov

Links

- Nuclear Data Services
- Nuclear Data Section
- NRDC Network
- IAEA
- EXFOR

Documentation

- "Neutron Scattering-A Primer" by Roger Pynn
- "Introduction to the Theory of Thermal Neutron Scattering" by G. L. Squires
- "Neutron Scattering Fundamentals" Edited by Felix Fernandez-Alonso and David L. Price
- LEXFOR

Codes

Templates

List of participants

Summary Report
The summary report will be published in INDC(NDS)-0697

Presentations

#	Author	Title	Link
1	Li (Emily) Liu	Thermal Neutron Scattering Measurements at Spallation Neutron Source	PDF
2	F. Cantargi	Total Neutron Cross Section Measurement for Thermal Scattering Library Evaluation	PDF
3	D.V. Baxter	Compact ADNS as tools for Nuclear Data	PDF
4	E. Farhi	Neutron Cross Sections: Experiments and MD	PDF
5	Y. Kiyonagi	Development of the Thermal Cross Section and its necessity for neutron applications	PDF
6	J.I. Marquez Damian	Experimental Data Needs for Thermal Scattering Library Evaluation	PDF
7	S.P. Simakov	Welcome address	PDF
8	N. Otsuka	Basic Questions on Compilation of Experimental Thermal Neutron Scattering Data	PDF
9	V. Semkova	Objectives of the Meeting	PDF

Data for Thermal Scattering Law Evaluation | TSL research groups

#	Reference	Material	Temp. [K]	Press. [Mpa]	Quantity	Data
1	S.N. Rapeanu et al., Rev. Roum. De Phys., 35, 185 (1990)	Heavy water	293		Angular cross section	Data
2	S.N. Rapeanu et al., Rev. Roum. De Phys., 35, 185 (1990)	Heavy water	348		Angular cross section	Data
3	S.N. Rapeanu et al., Rev. Roum. De Phys., 35, 185 (1990)	Heavy water	373		Angular cross section	Data

4) NEW TSL WEBPAGE AT EXFOR (CONT.)

EXFOR compilation of thermal neutron scattering data - Chromium

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V. Semkova Objectives of the Meeting PDF

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3	S.N. Rapeanu et al., Rev. Roum. De Phys., 35, 185 (1990)	Heavy water	373		Angular cross section	Data
4	S.N. Rapeanu et al., Rev. Roum. De Phys., 35, 185 (1990)	Heavy water	423		Angular cross section	Data
5	S.N. Rapeanu et al., Rev. Roum. De Phys., 35, 185 (1990)	Heavy water	473		Angular cross section	Data
6	S.N. Rapeanu et al., Rev. Roum. De Phys., 35, 185 (1990)	Heavy water	498		Angular cross section	Data
7	S.N. Rapeanu et al., Rev. Roum. De Phys., 35, 185 (1990)	Light water	293		Molecular structure factor	Data
8	S.N. Rapeanu et al., Rev. Roum. De Phys., 35, 185 (1990)	Light water	348		Molecular structure factor	Data
9	S.N. Rapeanu et al., Rev. Roum. De Phys., 35, 185 (1990)	Light water	373		Molecular structure factor	Data
10	S.N. Rapeanu et al., Rev. Roum. De Phys., 35, 185 (1990)	Light water	423		Molecular structure factor	Data
11	S.N. Rapeanu et al., Rev. Roum. De Phys., 35, 185 (1990)	Light water	473		Molecular structure factor	Data
12	S.N. Rapeanu et al., Rev. Roum. De Phys., 35, 185 (1990)	Light water	498		Molecular structure factor	Data
13	A.G. Novikov et al., Jour. Of Struct. Chem., 31, 77 (1990)	Light water	300		Frequency spectrum	Data
14	A.G. Novikov et al., Jour. Of Struct. Chem., 31, 77 (1990)	Light water	400		Frequency spectrum	Data
15	A.G. Novikov et al., Jour. Of Struct. Chem., 31, 77 (1990)	Light water	500		Frequency spectrum	Data
16	A.G. Novikov et al., Jour. Of Struct. Chem., 31, 77 (1990)	Light water	600		Frequency spectrum	Data
17	A.K.Soper, Chem. Phys., 258, 121, (2000)	Light water	268	27	HH Radial distribution function	Data
18	A.K.Soper, Chem. Phys., 258, 121, (2000)	Light water	268	27	OH Radial distribution	Data

4) NEW TSL WEBPAGE AT EXFOR (CONT.)

EXFOR compilation of thermal neutron scattering data - Chromium

EXFOR compilation of th: x

https://www-nds.iaea.org/index-meeting-crp/CM-THSC-2015/

U235U4 (2013)					Spectrum	
107	M. Utsuro, Jour. Of Nuclear Science and Technology, Vol.18, Issue 9, p.739 (1981), Japan	Heavy water	15		Total cross section	X4:21751
108	M. Utsuro, Jour. Of Nuclear Science and Technology, Vol.18, Issue 9, p.739 (1981), Japan	Heavy water	77		Total cross section	X4:21751
109	F. Kropff, Internal Report	Heavy water	293		Total cross section	X4:30283
110	L.J. Rainwater, Physical Review, Vol.73, p.733 (1948), USA	Heavy water			Total cross section	X4:11145
111	V.W. Meyers, Priv.Comm: Meyers (1953)	Heavy water			Total cross section	X4:11019
112	S. Dritsa, Priv.Comm: Dritsa (1971)	Heavy water	295		Total cross section	X4:20038
113	S. Dritsa, Priv.Comm: Dritsa (1971)	Heavy water	473		Total cross section	X4:20038
114	S.B. Herdade, Brazilian report to the I.N.D.C., No.3, p.4 (1971), Austria	Polyethylene	296		Total cross section	X4:30229
115	J.R. Granada, Nucl. Instrum. Methods in Physics Res., Sect.A, Vol.261, p.573 (1987), Netherlands	Polyethylene	293		Total cross section	X4:30229
116	V. Tarina, J.Chemical Physics, Vol.46, p.3273 (1967), USA	Benzene	77		Double Diff. Cross section	X4:30228
117	J.V. Lolich, Atomkernenergie, Vol.35, Issue.1, p.23 (1980), Germany	Benzene	296		Total cross section	X4:30551
118	K. Heinloth, Zeitschrift fuer Physik, Vol.163, p.218 (1961), Germany	Benzene	291		Total cross section	X4:21341
119	L. Torres, Nucl. Instrum. Methods in Physics Res., Sect.B, Vol.251, p.304 (2006), Netherlands	Benzene	90		Total cross section	X4:31588
120	J.R. Beyster, Nuclear Science and Engineering, Vol.31, p.254 (1968), USA	Light water			Ang. Diff. Cross section	X4:11029
121	L. Torres, Nucl. Instrum. Methods in Physics Res., Sect.B, Vol.251, p.304 (2006), Netherlands	Light water	115		Total cross section	X4:31588
122	S. Dritsa, Report from misc. OECD Countries to EANDC, No.63L (1967), France	Light water	473		Total cross section	X4:22613
123	J.L. Russell, General Atomic Div. Reports, No.7581 (1966), USA	Light water			Total cross section	X4:11162
124	S.B. Herdade, Brazilian report to the I.N.D.C., No.2, p.22 (1969), Austria	Light water	296		Total cross section	X4:22613
125	R.B. Walton, Priv.Comm: Walton (1960)	Light water			Total cross section	X4:22613
126	V.T. Springer, Nukleonik, Vol.3, p.110 (1961), Germany	Light water			Total cross section	X4:21078

4) NEW TSL WEBPAGE AT EXFOR (CONT.)

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Data for Thermal Scattering Law Evaluation | TSL research groups

Research groups related to TSL development, and examples of their work.

Argentina

Centro Atómico Bariloche
F. Cantargi
V.H. Gillette (currently at Sharjah University)
J.R. Granada
J.I. Marquez Damian

#	Materials	Reference
1	Ethanol, deuterated ethanol	http://dx.doi.org/10.1016/S0168-583X(00)00006-9
2	Teflon	http://dx.doi.org/10.1016/0168-9002(94)01535-X
3	Liquid hydrogen, liquid deuterium	http://dx.doi.org/10.1080/1023816031000100888
4	Dyphenil, dowtherm-A	http://dx.doi.org/10.1016/0022-3115(91)90370-M
5	PMMA	http://dx.doi.org/10.1016/0306-4549(89)90130-8
6	PMMA	http://dx.doi.org/10.1016/0306-4549(91)90042-V
7	Polyethylene	http://dx.doi.org/10.1016/0168-9002%2887%2990370-6
8	Mesitylene, toluene	http://www.sciencedirect.com/science/article/pii/S0168583X08013177
9	Sapphire, Silicon	http://dx.doi.org/10.1016/j.anucene.2015.01.020
10	Mesitylene	http://dx.doi.org/10.1016/j.nimb.2006.04.161
11	Methane, Solid deuterium	http://dx.crossref.org/10.3938/jkps.59.1076
12	Solice Benzene, water ice	http://dx.doi.org/10.1016/j.nimb.2006.05.027
13	Aromatic hydrocarbons	http://dx.doi.org/10.1016/j.nimb.2010.04.030
14	H2O, D2O, Benzene	http://dx.doi.org/10.1103/PhysRevA.36.5594
15	H2O, D2O	http://dx.doi.org/10.1016/j.anucene.2013.11.014
16	H2O, D2O	http://link.aps.org/link/doi/10.1063/1.4812828

Centro Atómico Ezeiza
R.L. Ramos

#	Materials	Reference
1	Biological materials	http://dx.doi.org/10.1016/j.apradiso.2015.06.019

China

Northwest Institute of Nuclear Technology
L. Wang

#	Materials	Reference
1	LiH	http://dx.doi.org/10.1016/j.nucengdes.2013.05.010

France

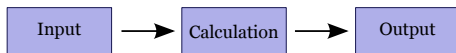
CEA Cadarache
G. Noguere
J.P. Scotta

5) AN OPEN SOURCE, STANDALONE ALTERNATIVE TO LEAPR/NJOY

- Using LEAPR/NJOY for TSL evaluation has some limitations:
 - NJOY is export controlled software → we cannot give thermal scattering workshops and classes using it.
 - Current trends on TSL evaluation use models that are not implemented in LEAPR (or no models at all).
- TANGO: and open source, standalone alternative to LEAPR.

5) AN OPEN SOURCE, STANDALONE ALTERNATIVE TO LEAPR/NJOY

- Programmed from scratch in C to reproduce LEAPR results (first stage).
- Modular:



Input

- Currently focused on what LEAPR can calculate

- GFD, VACF, $G(r, t)$.

- Educational use could be improved with a GUI.

Calculation

- Models currently implemented in LEAPR

- Time integration of GA, GASKET-like decomposition.

- Direct Fourier transform in time and space, GAAQC.

- GAAQC.

Output

- ENDF-6 library.

- Calculation of XS, DXS, DDXS.

- Adaptable to new formats in the future (GND)

- Currently at early stages of development. There will be a developer release soon.

6) OTHER ACTIVITIES AND COLLABORATIONS

- Collaboration with CEA Cadarache:
 - Analysis of new experimental DDXS data from ILL and ISIS (see J.P. Scotta talk Wed 10:00).
 - Coupling GROMACS with CONRAD for covariance evaluation (see G. Noguere talk Wed 16:00).
- Collaboration with UC Berkeley: generation of perturbed TSL's for GPT calculations in Serpent.
- Participation on the IAEA CRP "Advanced Moderators for Intense Cold Neutron Beams in Materials Research" (common interest on water, collaboration with IU. See next talk by F. Cantargi).

THANKS FOR YOUR TIME.



SANTA ANA WATERFALL
BARILOCHE, ARGENTINA