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Update of the ENDF/B-VIII.0 evaluation for thermal scattering in light water with extended temperature grid

Working Party on International Nuclear Data Evaluation Co-operation (WPEC) 33rd Meeting
Subgroup 48

PRESENTED BY J.I. MÁRQUEZ DAMIÁN

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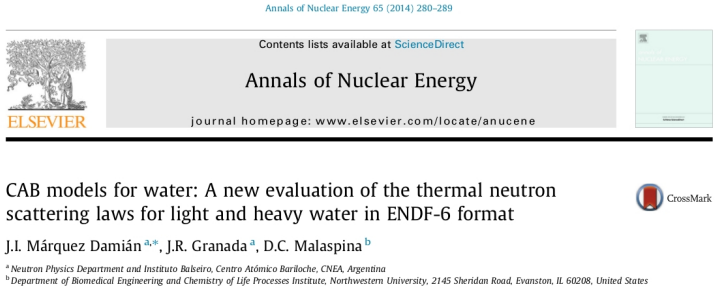

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CAB models for water: A new evaluation of the thermal neutron scattering laws for light and heavy water in ENDF-6 format

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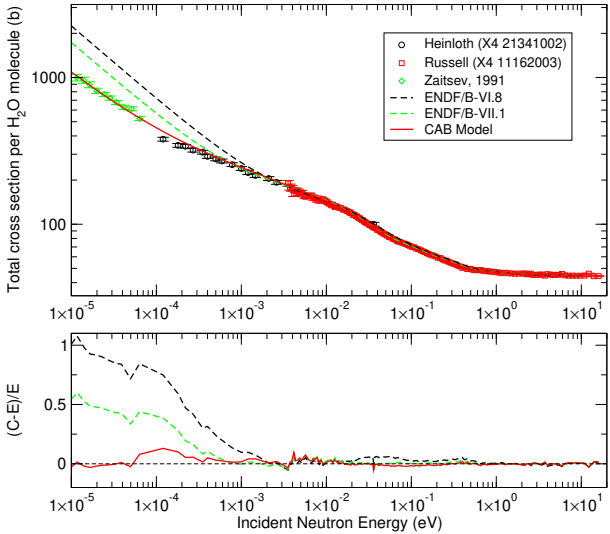
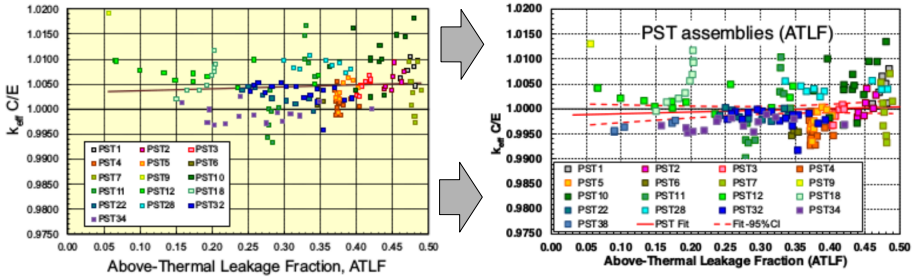
J.I. Marquez Damian, J. R. Granada, and D. C. Malaspina. "CAB models for water: a new evaluation of the thermal neutron scattering laws for light and heavy water in ENDF-6 format." Annals of Nuclear Energy 65 (2014): 280-289.

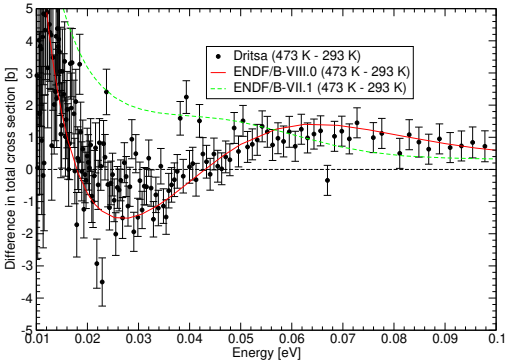

Total cross section per H_2O molecule (b)
1000
100
Heinloth (X4 21341002)
Russell (X4 11162003)
Zaitsev, 1991
ENDF/B-VI.8
ENDF/B-VII.1
CAB Model
1×10^-5
1×10^-4
1×10^-3
1×10^-2
1×10^-1
1×10^0
1×10^1
(C-E)/E
1
0.5
0
Incident Neutron Energy (eV)

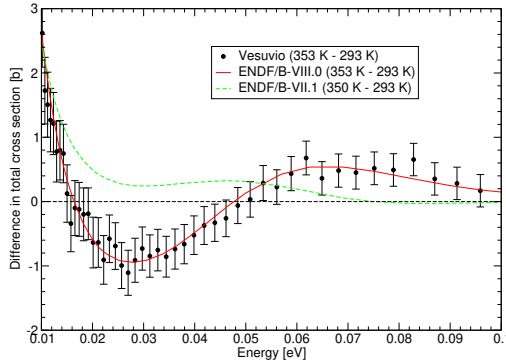
ENDF B-VII.1 (2011)

ENDF B-VIII.0 (2018)



D.A. Brown, et al. "ENDF/B-VIII. 0: The 8th major release of the nuclear reaction data library with CIELO-project cross sections, new standards and thermal scattering data." Nuclear Data Sheets 148, 1, (2018)





M. Dritsa and A. Kostikas. Total Cross Section of Water at Room Temperature and 200°C. Technical report EANDC (OR)-63L (1967).

J.I. Marquez Damian, et al. "Experimental validation of the temperature behavior of the ENDF/B-VIII. 0 thermal scattering kernel for light water." EPJ Web of Conferences, (239), 14001 (2020).

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REGULAR ARTICLE OPEN ACCESS

Impact of the thermal scattering law of H in H_2O on the isothermal temperature reactivity coefficients for UOX and MOX fuel lattices in cold operating conditions

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J.P. Scotta, G. Noguere, D. Bernard, J.I. Marquez Damian, and A. Santamarina. "Impact of the thermal scattering law of H in H 2 O on the isothermal temperature reactivity coefficients for UOX and MOX fuel lattices in cold operating conditions." (2016).

M&C 2017 - International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering, Jeju, Korea, April 16-20, 2017, on USB (2017)

The Impact of the New Nuclear Data Libraries on the Isothermal Reactivity Coefficient Determination

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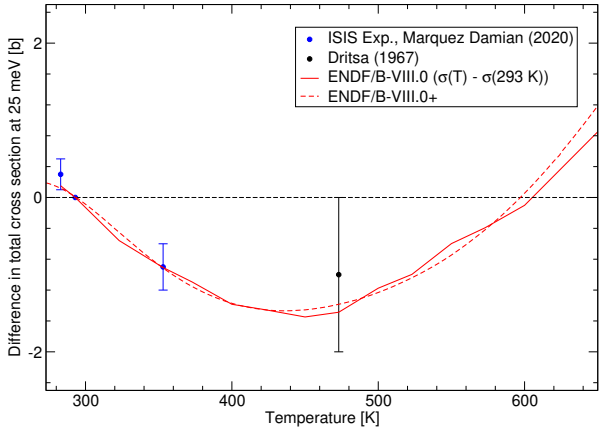
Abstract – *The impact of the new released evaluations for ^{235}U, ^{238}U, ^{16}O, and S(α,β) for hydrogen bound water, in the determination of the isothermal reactivity coefficient of thermal reactors fueled with slightly enriched uranium is addressed in this work. The experiment to serve as a benchmark for this kind of reactor response is the inversion point of the isothermal reactivity coefficient of the IPEN/MB-01 reactor recently approved to be included in the IRPhE handbook. The analysis reveal that the major impacts are due to new data of ^{235}U and to those of S(α,β) for hydrogen bound water. The (C-E)/E values for this case show an excellent progress in the theoretical determination of this very important reactor response. The new data for ^{238}U and ^{16}O show very little impact on the analysis.*

A. dos Santos, G. Simões de Andrade e Silva. "The Impact of the New Nuclear Data Libraries on the Isothermal Reactivity Coefficient Determination." MC 2017 (2017).

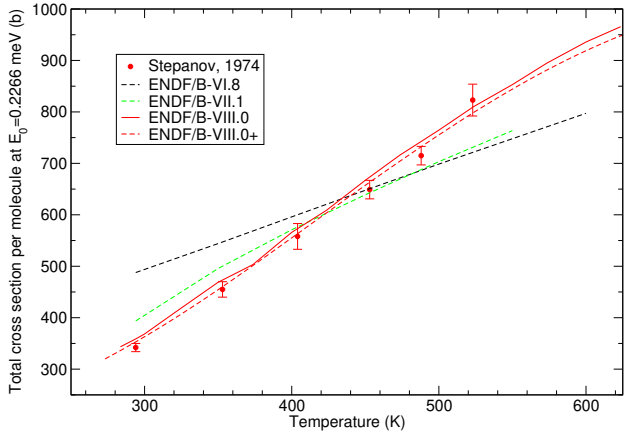
- Yet, the discrete nature of the molecular dynamics simulations made this library a collection of evaluations at different temperatures, instead of a single evaluation.
- To overcome this, we developed a new evaluation methodology in collaboration with Rolando Granada from Centro Atomico Bariloche, Argentina, and Danila Roubtsov from Canadian Nuclear Laboratories.

- In this new methodology the computed vibrational spectra for all temperatures is decomposed as a sum of Gaussian distributions, following the work by Esch [1], Lisichkin [2] and Maul [3]. The parameters for these Gaussians are fitted with quadratic functions in temperature, under the assumption that no discontinuities are expected in the liquid phase.
- These fitted functions allow to reconstruct the parameters for the evaluation at any temperature.

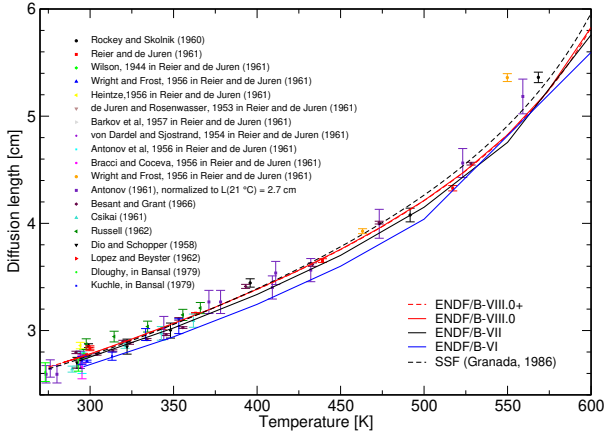
[1] Esch, L. J. "Temperature Dependence of the Neutron Transport Cross Section in Polyethylene and Paraffin." Nucl. Sci. and Eng, 16, 196 (1963).
[2] Lisichkin, Y., et al. "Temperature Dependence of the Generalized Frequency Distribution of Water Molecules: Comparison of Experiments and Molecular Dynamics Simulations." Molecular Simulation, 31, 1019 (2005).
[3] Maul, L., J.I. Márquez Damián, G. Braoudakis, M. Ho, and G. H. Yeoh. "Perturbation Scheme for Estimating Uncertainties in Thermal Scattering Cross Sections of Water." Ann. of Nucl. Energy, 121, 232 (2018).



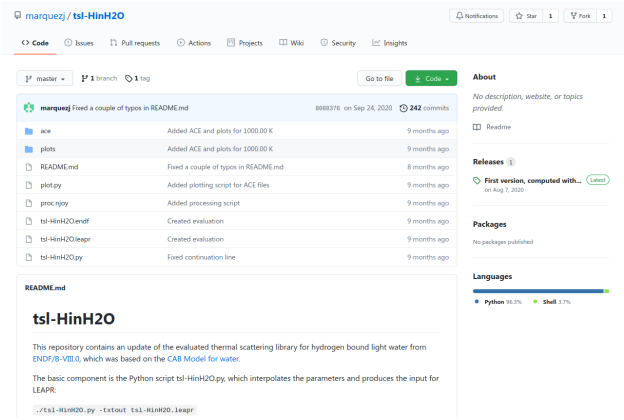
Difference in total cross section of light water at 25 meV compared to the experiments reported in the ND2019 paper



Total cross section at 0.2266 meV compared with measurements by Stepanov.



Calculation of the diffusion length as a function of temperature with the new model, compared with experimental data from various authors, calculations performed with the ENDF/B libraries versions VI, VII, VIII.0 and the Synthetic Scattering Function.



`https://github.com/marquezj/tsl-HinH2O`
+ randomized files from D. Rochman:
`https://tendl.web.psi.ch/tendl_2021/randomTSL.html`.

Conclusions

- An update of the ENDF/B-VIII.0 evaluation of the thermal scattering kernel for light water is currently available.
- This evaluation is based on a parameterization of the CAB Model designed to preserve the good agreement found at room temperature, and to ensure smooth derivatives.
- Calculated results compare well with experimental data.
- This evaluation is presented as a set of files with a 5 K grid, plus a Python script to generate the cross sections at any arbitrary temperature.
- Randomized files based on this model are available in the TENDL website for Total Monte Carlo.

Thanks for your time.
Questions?