

DE LA RECHERCHE À L'INDUSTRIE



Thermal Scattering Law Data Files for JEFF

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NEEDS, NEA, Paris, 25 November 2014

Evaluation work on “thermal scattering data” for JEFF was mainly performed at the Karlsruhe Institute of Technology (KIT) by J. Keinert and M. Mattes

- 1981-2005 : this group produced Evaluated Nuclear Data Files (MF=7, MT=4) for H in H₂O, D in D₂O, H in ZrH, H in polyethylene, Graphite and Be metal
- 2003-2004: Three additional files were produced by CEA (H in CaH₂, Ca in CaH₂, Mg metal)

see also: “Thermal Scattering Law Data IAEA Nuclear Data Library”

<https://www-nds.iaea.org/indltsl/>

List of thermal scattering law data files

Material number	JEFF-3.1.1	ENDF/B-VII	JENDL-4.0
1	H(H ₂ O)	H(H ₂ O)	H(H ₂ O)
2		Para Hydrogen	Para Hydrogen
3		Ortho Hydrogen	Ortho Hydrogen
7	H(ZrH)	H(ZrH)	H(ZrH)
8	H(CaH ₂)		
11	D(D ₂ O)	D(D ₂ O)	D(D ₂ O)
12		Para Deuterium	Para Deuterium
13		Ortho Deuterium	Ortho Deuterium
26	Be metal	Be metal	Be metal
27		Be(BeO)	Be(BeO)
28		O(BeO)	
31	Graphite	Graphite	Graphite
33		Liquid Methane	Liquid Methane
34		Solid Methane	Solid Methane
37	H(CH ₂)	H(CH ₂)	
40		Benzine	Benzine
45		Al metal	
52	Mg metal		
56		Fe metal	
58		Zr(ZrH)	Zr(ZrH)
59	Ca(CaH ₂)		
75		O(UO ₂)	
76		U(UO ₂)	
Number of materials	9	20	14

List of thermal scattering law data files

⇒ Two different issues of the neutron scattering process as a function of the temperature

Material number	JEFF-3.1.1	ENDF/B-VII	JENDL-4.0
1	H(H2O)	H(H2O)	H(H2O)
2		Para Hydrogen	Para Hydrogen
3		Ortho Hydrogen	Ortho Hydrogen
	H(ZrH)	H(ZrH)	H(ZrH)
	H(CaH2)		
	D(D2O)	D(D2O)	D(D2O)
		Para Deuterium	Para Deuterium
		Ortho Deuterium	Ortho Deuterium
26	Be metal	Be metal	Be metal
27		Be(BeO)	Be(BeO)
28		O(BeO)	
31	Graphite	Graphite	Graphite
33		Liquid Methane	Liquid Methane
34		Solid Methane	Solid Methane
37	H(CH2)	H(CH2)	
40		Benzine	Benzine
45		Al metal	
52	Mg metal		
56		Fe metal	
58		Zr(ZrH)	Zr(ZrH)
59	Ca(CaH2)		
75		O(UO2)	
76		U(UO2)	
Number of materials	9	20	

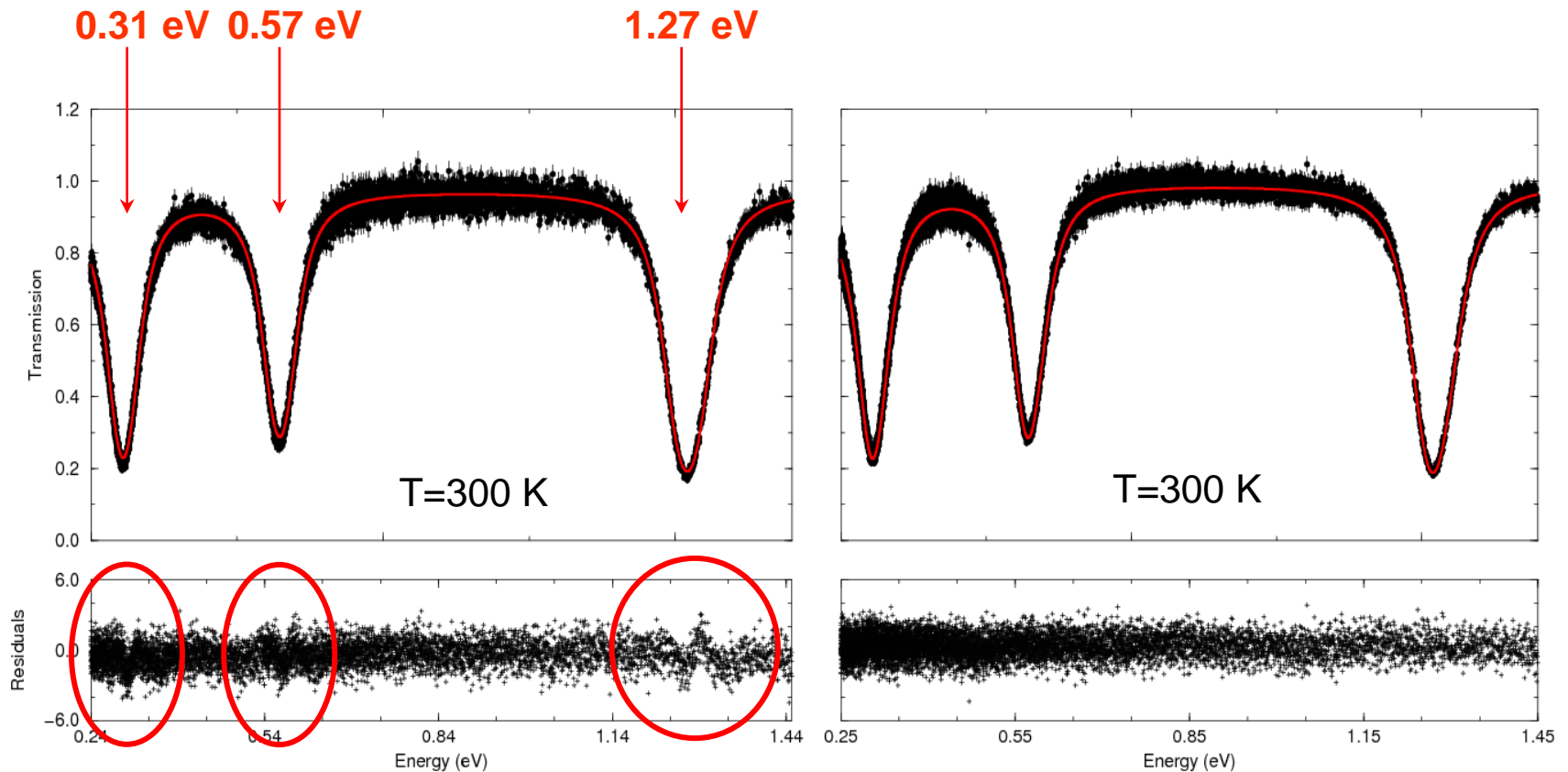
Moderator for light
and heavy water
reactors

Cristal
lattice effect
in UOX fuel

Capture of neutrons by atoms in a crystal lattice

Am241 transmission measurements at the GELINA facility, IRMM, Geel

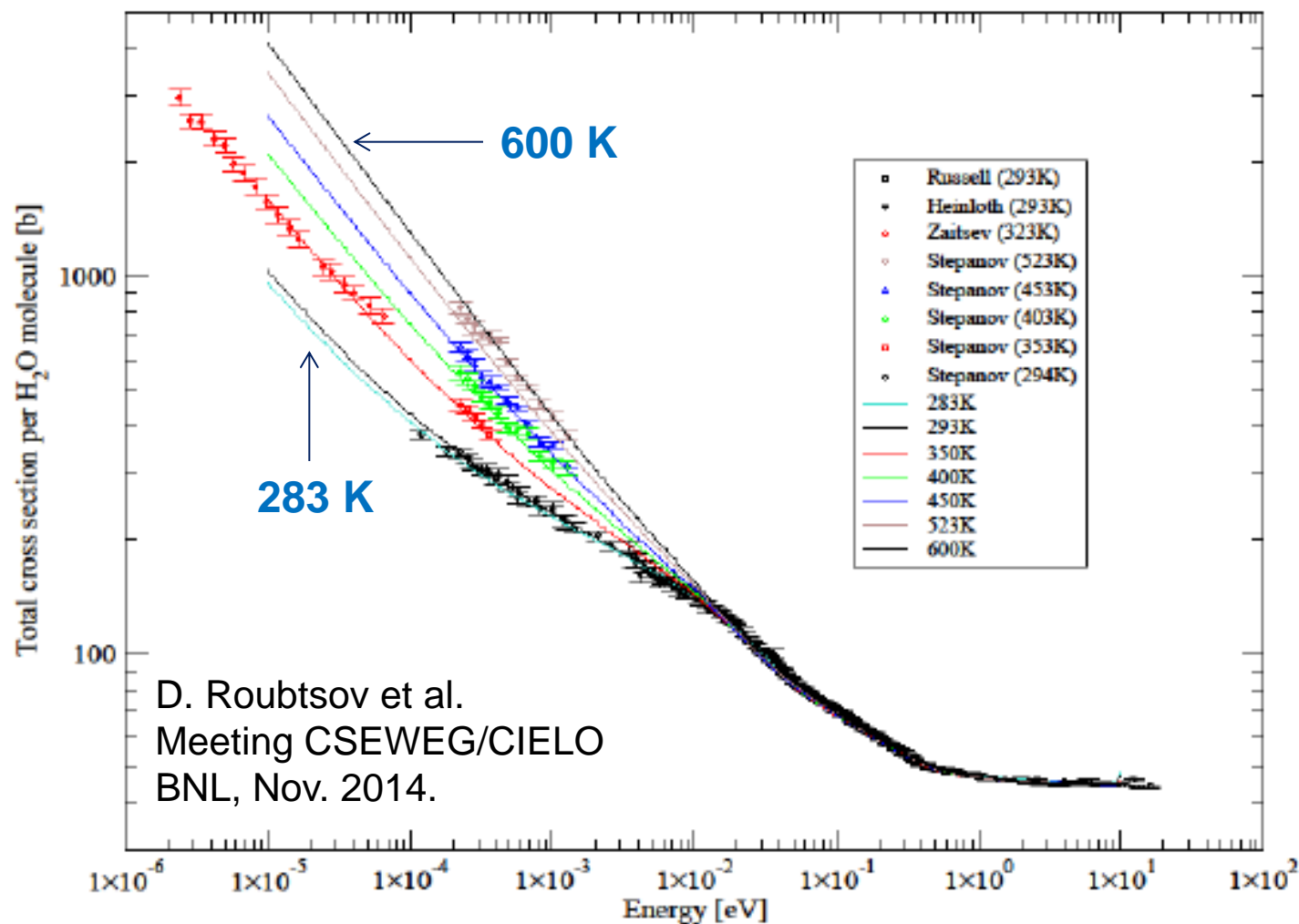
C. Lampoudis et al. Eur. Phys. J. Plus, 128, 86 (2013)



Free Gas Model (FGM)

Crystal Lattice Model (CLM)

Scattering of neutrons by Hydrogen bound in water



Scattering law of H in H₂O

One of the most important data for light water reactors is the scattering law of **H in H₂O**.

Since the release of JEFF-311, KIT evaluation is continuously used in many neutronic calculations to simulate experimental and power reactors.

Mat.	JEFF-3.1.1	Temp. (K)	Year	Authors	Institute	Code
1	H(H ₂ O)	293.6 323.6 373.6 423.6 473.6 523.6 573.6 623.6 647.2 800.0 1000.0	Jan. 2004	J. Keinert M. Mattes	Karlsruhe Institute of Technology	LEAPR NJOY-99.90++

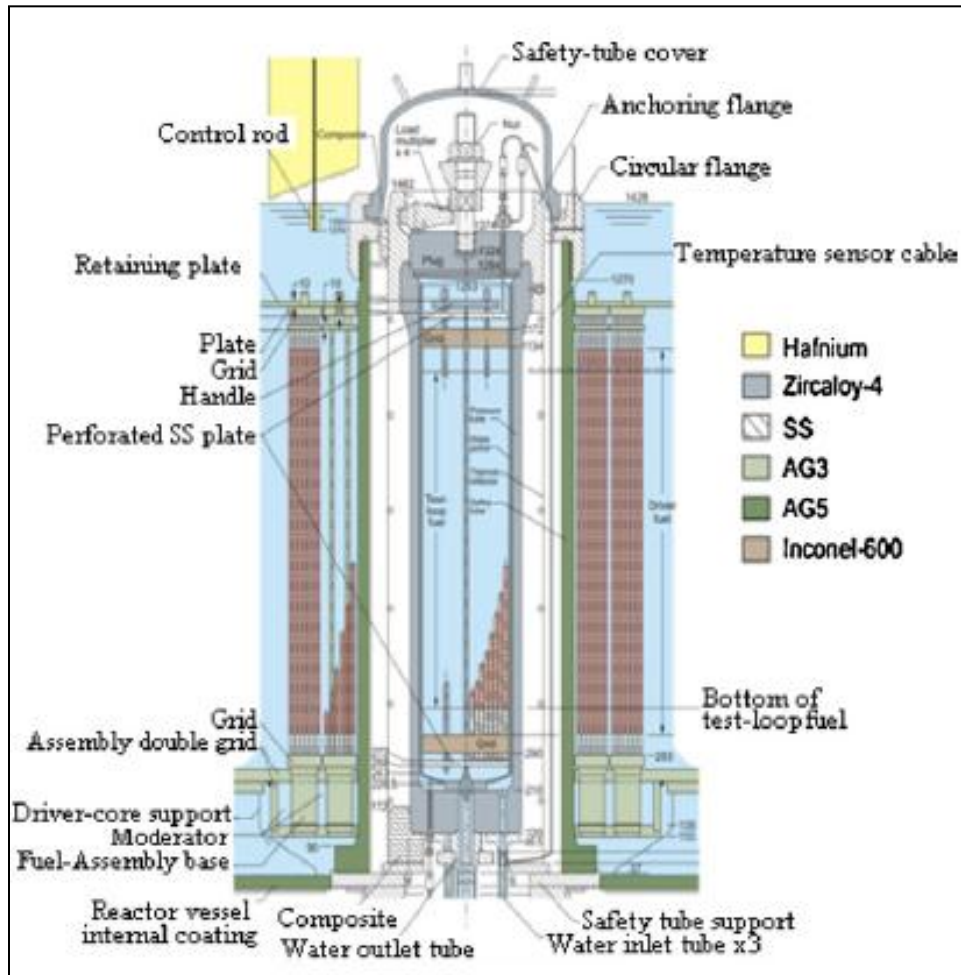
Reactivity Temperature Coefficient (RTC)

Contributions of different physical phenomena to the **Reactivity Temperature Coefficient (RTC)** in typical light water moderated lattices have been investigated using the **APOLLO2** code with a multi-group cross-section library based on JEFF data

For **UOX fuel**, two integral experiments were performed in the **EOLE facility** of CEA Cadarache:

- **CREOLE experiment**
⇒ 20°C to 289°C (P=120 bar)
- **MISTRAL-1 experiment**
⇒ 10°C to 80°C



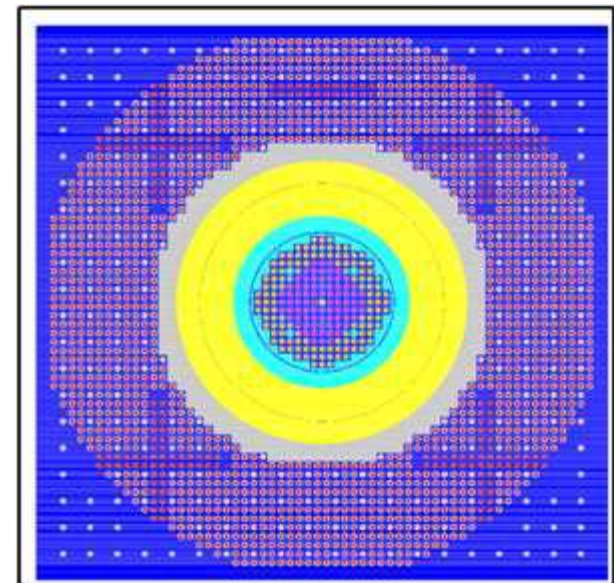


Vertical cross section of the CREOLE facility showing the safety-tube vacuum gap and driver assemblies.

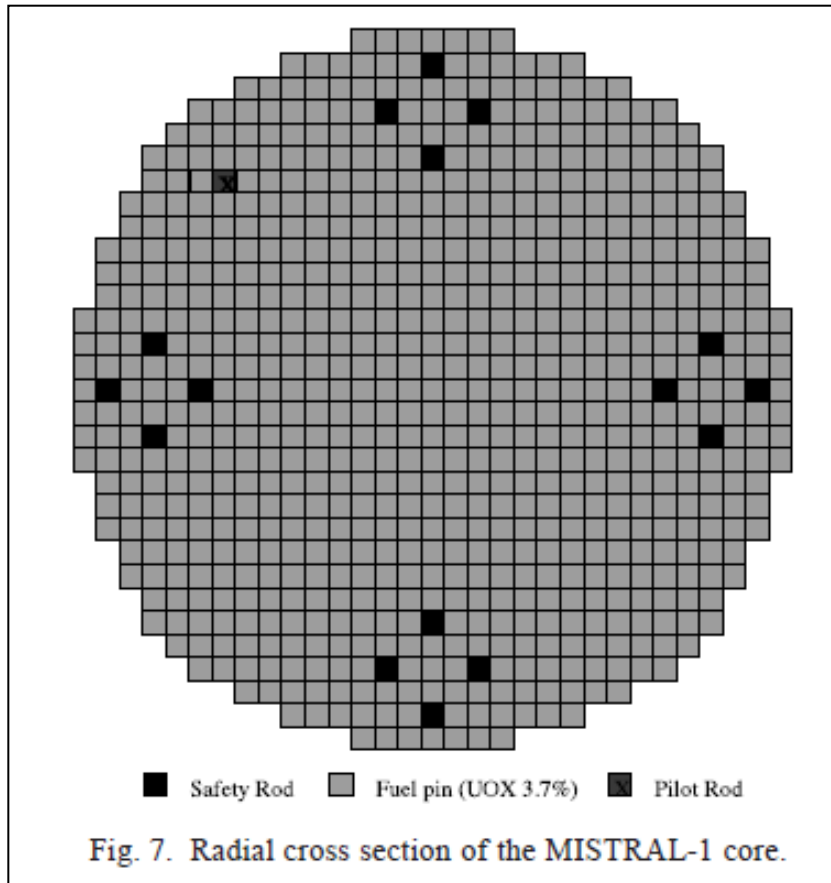
CREOLE experiment

The experimental facility consists of a pressurized central test loop in which it was possible to achieve operating conditions of a large PWR power reactor in terms of pressure and moderator temperature

⇒ 20°C to 289°C (P=120 bar)



Horizontal cut-off



MISTRAL-1 experiment

The MISTRAL program was carried out in the EOLE facility from 1996 to 2000 in the framework of a collaboration between the CEA and the Japan organization NUPEC.

MISTRAL-1 is a regular enriched UO₂ (~3.7% of ²³⁵U) core with about 750 fuel pins in a square pitch of 1.32 cm. The criticality was obtained by adjusting the soluble boron concentration.

The reactivity measurements were carried out in atmospheric conditions with temperatures ranging from **10°C to 80°C by steps of 5°C.**

Summary of the results expressed in terme of « total RTC error » (C-E) in pcm/°C

Hot Zero Power (HZP) condition

CREOLE experiment				
Code	20-111°C	111-186°C	186-242°C	242-289°C
TRIPOLI4	+ 0.01±0.13	+ 0.12±0.15	+ 0.08±0.17	0.00±0.20
APOLLO2	+ 0.10±0.12	+ 0.17±0.14	+ 0.17±0.16	+ 0.20±0.18

MISTRAL-1 experiment			
Code	10-40°C	40-80°C	10-80°C
APOLLO2	0.0±0.3	- 0.1±0.4	0.0±0.3

« Cold » conditions in atmospheric pressure



Excellent results with JEFF in « cold » and HZP conditions (UOX fuel)

Ten years after the release of the latest “scattering data” files, **R&D activities on this topic are no longer discussed within the JEFF project.**

Mat.	JEFF-3.1.1	Temp. (K)	Year	Authors	Institute	Code
1	H(H ₂ O)	293.6 323.6 373.6 423.6 473.6 523.6 573.6 623.6 647.2 800.0 1000.0	Jan. 2004	J. Keinert M. Mattes	Karlsruhe Institute of Technology	LEAPR NJOY-99.90++

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New measurements of the scattering laws + total cross section of H(H2O) in « cold » and HZP conditions are needed (steps of 5°C + as a function of pH) ⇒ **production of covariance matrices**

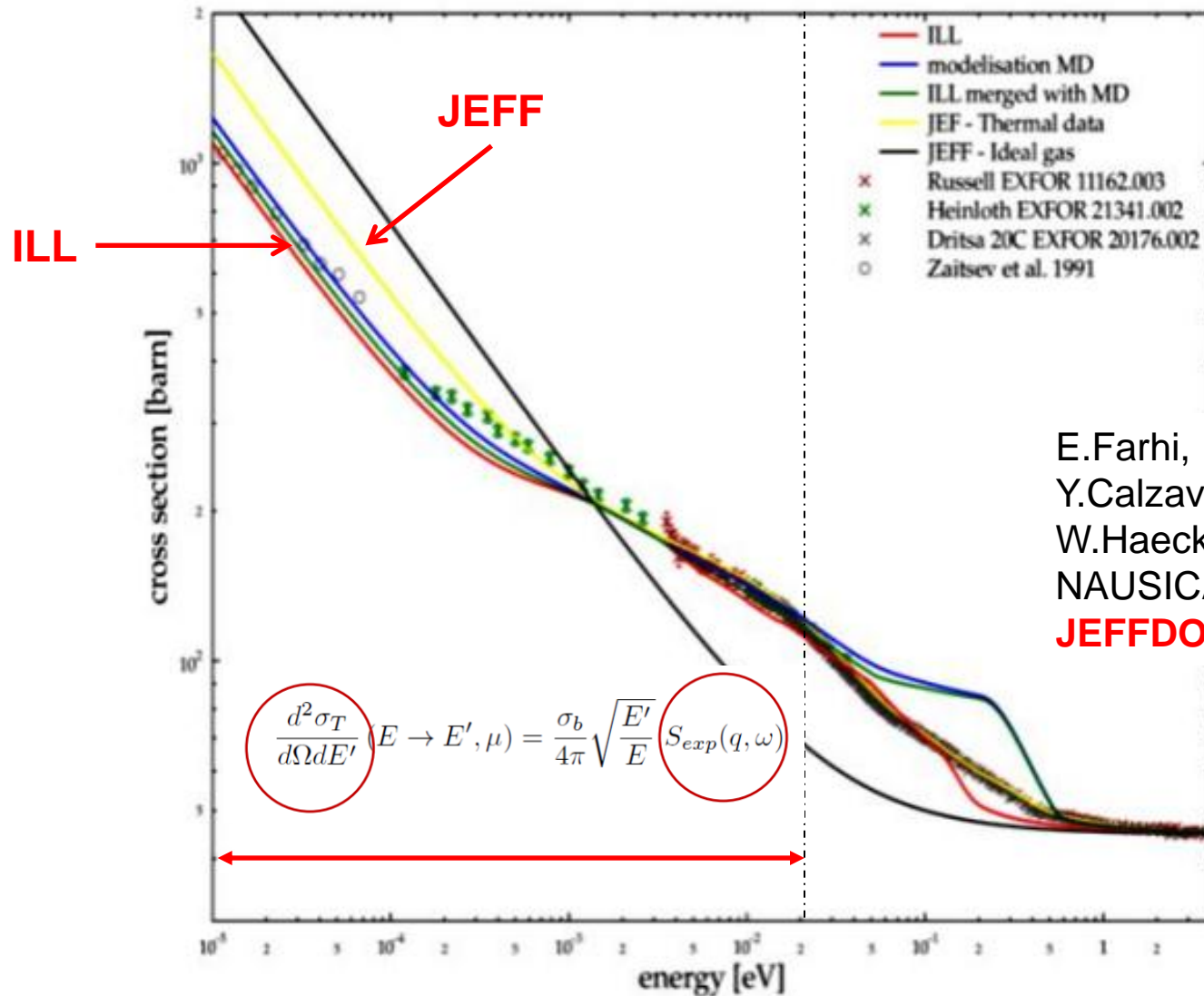
⇒ See presentation of Oscar Cabellos about the propagation of nuclear data uncertainties for PWR core analysis

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Replace LEAPR by recent experimental results, obtained using ILL neutron inelastic scattering instruments + Molecular Dynamic calculations ⇒ **see JEFFDOC-1578**

Ex: H2O cross section



E.Farhi, E.Pellegrini,
Y.Calzavara, G.Ferran,
W.Haack, E.Guarini,
NAUSICAA project,
JEFFDOC-1578

- **NAUSICAA collaboration** \Rightarrow First workshop in **July 2014** was the kick-off meeting of a collaborative project aiming to increase the accuracy of thermal neutron cross section data thanks to a new way to evaluate these data (ILL initiative).
- **Proposal for a JEFF working group on “thermal scattering data”** \Rightarrow kick off meeting at the NEA during the JEFF meeting of **April 2015**
- **Proposal for a new working group of the WPEC (Working Party on International Nuclear Data Evaluation Co-operation)** \Rightarrow kick off meeting at the NEA in **May 2015** before the WPEC meeting

+ new PhD thesis (Juan Pablo Scotta, CEA Cadarache) started in October 2014