

Latest JEFF/EFF's Presentations on Neutron Thermal Scattering and Review of Recent International Activities

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- **Latest JEFF/EFF's Presentations**

- **EFFDOC-1205:** ***“Thermal Scattering Libraries Processing”***, E. Castro, O. Cabellos.
November 2013.

Deliverable: Task 6.2. Thermal Scattering Libraries Processing

Authors: E. Castro, O. Cabellos

F4E-GRT-168.01. “Nuclear Data Improvements and Development of Tools – Nuclear Data Evaluation”. 2012-13

- **JEF/DOC-1524:** ***“Propagation of U235-238, Pu239 and STL Nuclear Data Uncertainties for PWR core analysis”***, O. Cabellos. November 2013.

PROPAGATION OF NUCLEAR DATA UNCERTAINTIES FOR PWR CORE ANALYSIS

Authors: O. Cabellos, E. Castro, C. Ahnert, and C. Holgado


Published: <http://dx.doi.org/10.5516/NET.01.2014.709>

CSN, “Propagation of Uncertainties for Neutronic Calculations (P110530207) in Criticality Safety Analysis”

EFFDOC-1205: “Thermal Scattering Libraries Processing”, E. Castro, O. Cabellos. November 2013.

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NEA-1883 ZZ-TSL-ACE/2013.

last modified: 05-MAR-2014 | [catalog](#) | [categories](#) | [new](#) | [search](#) | [RSS](#)

ZZ TSL-ACE/2013, Thermal Scattering Libraries processed to ACE format

NAME OR DESIGNATION, COMPUTER, DESCRIPTION, METHODS, STATUS, REFERENCES, HARDWARE REQUIREMENTS, LANGUAGE, NAME AND ESTABLISHMENT OF AUTHORS, MATERIAL, CATEGORIES

1. NAME OR DESIGNATION: ZZ-TSL-ACE/2013 [\[top \]](#)

2. COMPUTERS [\[top \]](#)

To submit a request, click below on the link of the version you wish to order. Only liaison officers are authorised to submit online requests. Rules for requesters are available [here](#).

Program name	Package id	Status	Status date
ZZ-TSL-ACE/2013	NEA-1883/01	Arrived	05-MAR-2014

Machines used:

Package ID	Orig. computer	Test computer
NEA-1883/01	Linux-based PC	

3. DESCRIPTION [\[top \]](#)

Thermal neutron scattering cross section data libraries, processed in ACE format to be used with MCNP.

Format: ACE.

Number of groups: Continuous energy.

Processed Libraries: ENDF/B-VI.8, ENDF/B-VII.0, ENDF/B-VII.1, INDL-TSL, JEFF-3.1, JEFF-3.1.1, JEFF-3.1.2, JENDL-4.0, JENDL-4.0u

F4E-GRT-168.01: “Nuclear Data Improvements and Development of Tools – Nuclear Data Evaluation”. Task 6.2: Thermal Scattering Libraries Processing. 2012-13.



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State of the Art: Temperatures

Isotope	Compound	ENDF/B-VII.1	INDL-TSL	JEFF 3.1.X
H	H ₂ O	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	CaH ₂	-	-	296, 400, 500, 600, 700, 800, 1000, 1200
H	TiH ₂	-	293.6, 400, 500, 600, 700, 800, 1000, 1200	-
H	YH ₂	-	293.6, 400, 500, 600, 700, 800, 1000, 1200	-
H	CeH ₂	-	293.6, 400, 500, 600, 700, 800, 1000, 1200	-
D	D ₂ O	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,

EFFDOC-1205



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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	UO ₂	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	I-CH ₄	100	-	-
H	S-CH ₄	22	-	-
H	CH ₂	296, 350	-	293.6, 350



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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

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

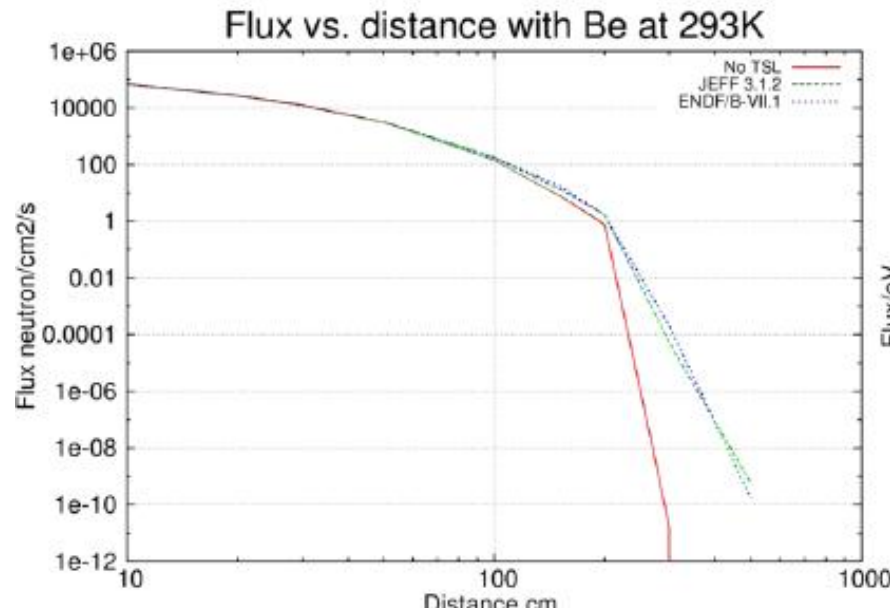
Material in JEFF-3.1.2	MCNP Identifier	Library	Suffix
H(H ₂ O)	lw00.32t	ENDF/B-VI.8	.68t
H(HZr)	h zr00.32t	ENDF/B-VII.0	.70t
D(D ₂ O)	hw00.32t	ENDF/B-VII.1	.71t
Be	be00.32t	INDL-TSL	.20t
Graphite	gra00.32t	JEFF-3.1	.30t
CH ₂	poly00.32t	JEFF-3.1.1	.31t
Mg	mg00.32t	JEFF-3.1.2	.32t
H(CaH ₂)	hca00.32t	JENDL-4.0	.40t
Ca(CaH ₂)	cah00.32t	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.

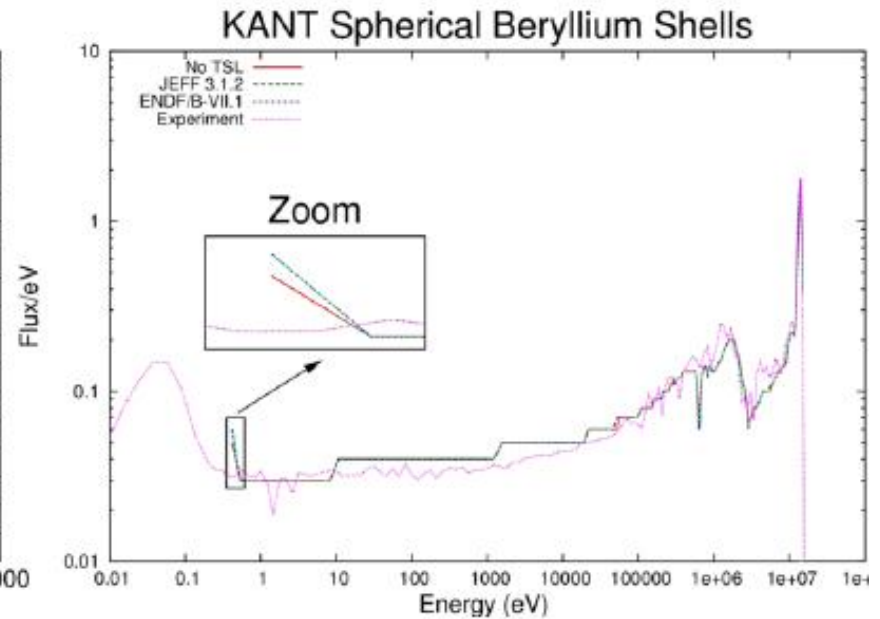


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Processed TSL: Validation



Simulating an **Am-Be neutron source** surrounded with materials at several temperatures.



Using test cases from **SINBAD** |

JEF/DOC-1524: “Propagation of U235-238, Pu239 and STL Nuclear Data Uncertainties for PWR core analysis”, O. Cabellos. November 2013.



1.1.2 Random Inelastic Cross-Section: H in H₂O

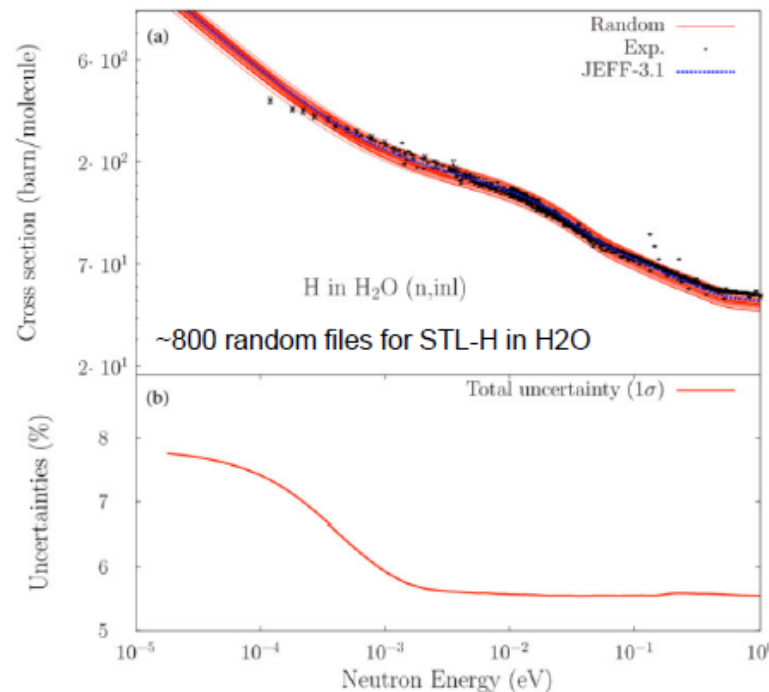


Figure: Incoherent random inelastic scattering cross section of H in H₂O compared to experimental data and the inelastic cross section from the JEFF-3.1 library. Inelastic scattering is described by the scattering law $S(\alpha, \beta)$,

Figure: Uncertainties in the inelastic cross section calculated from 1330 random inelastic cross sections

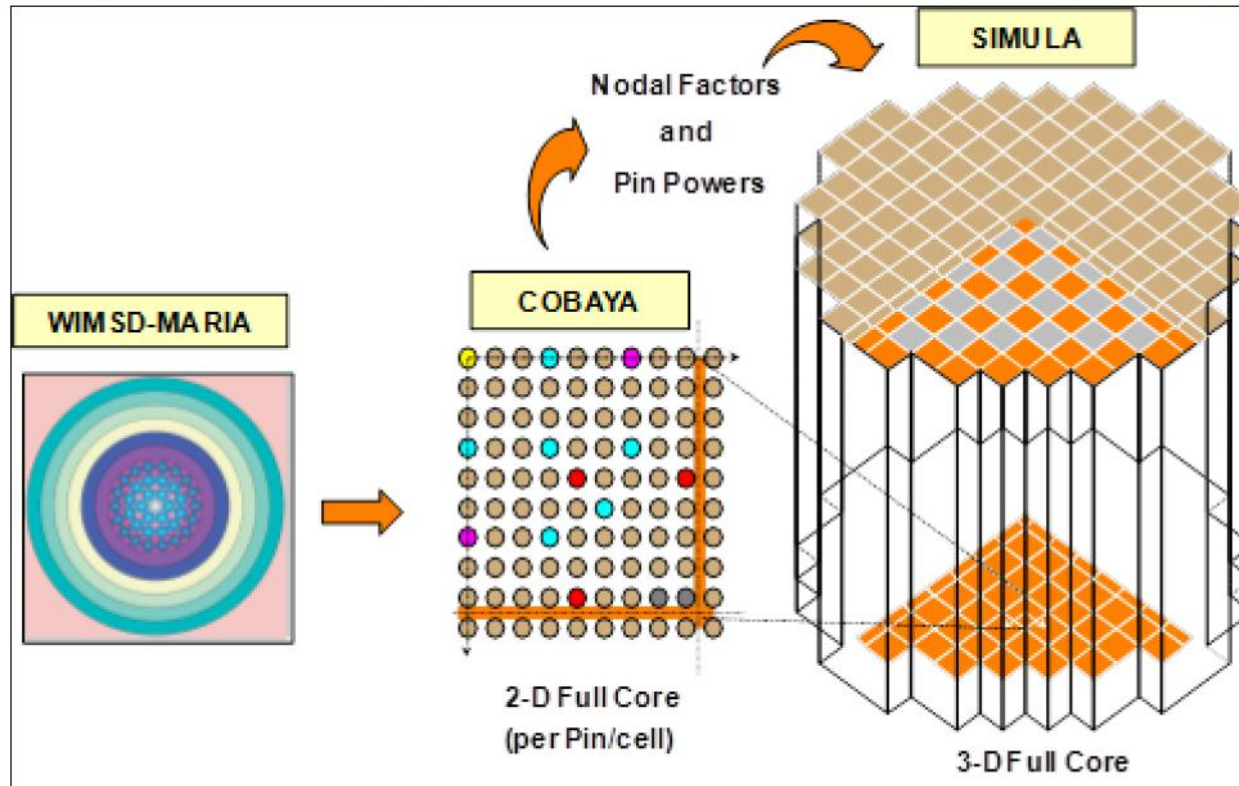
- A NEARLY full correlated energy-energy correlation matrix for the incoherent inelastic scattering for H in H₂O is found

Ref. “Random Adjustment of the H in H₂O Neutron Thermal Scattering Data”, D. Rochman and A. J. Koning, NUCLEAR SCIENCE AND ENGINEERING: **172**, 287–299 (2012)



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II.2 Scheme of the PWR Core Analysis SEANAP System



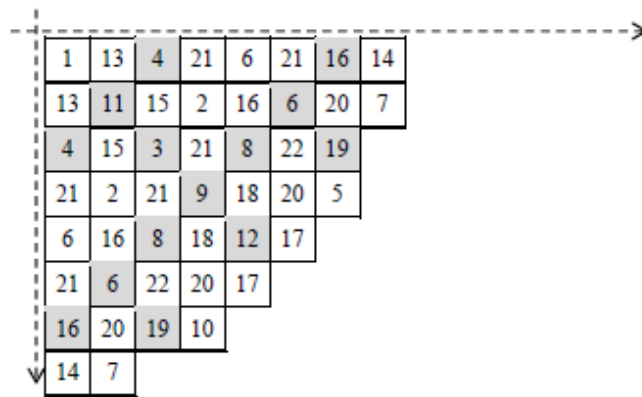
SEANAP: WIMS-D4+COBAYA+SIMULA



III.1 PWR description

PWR (WESTINGHOUSE), 3 loops , 157 FA, power 2775. MWth

¼ CORE



AVE. BURNUP PER FUEL ASSEMBLY

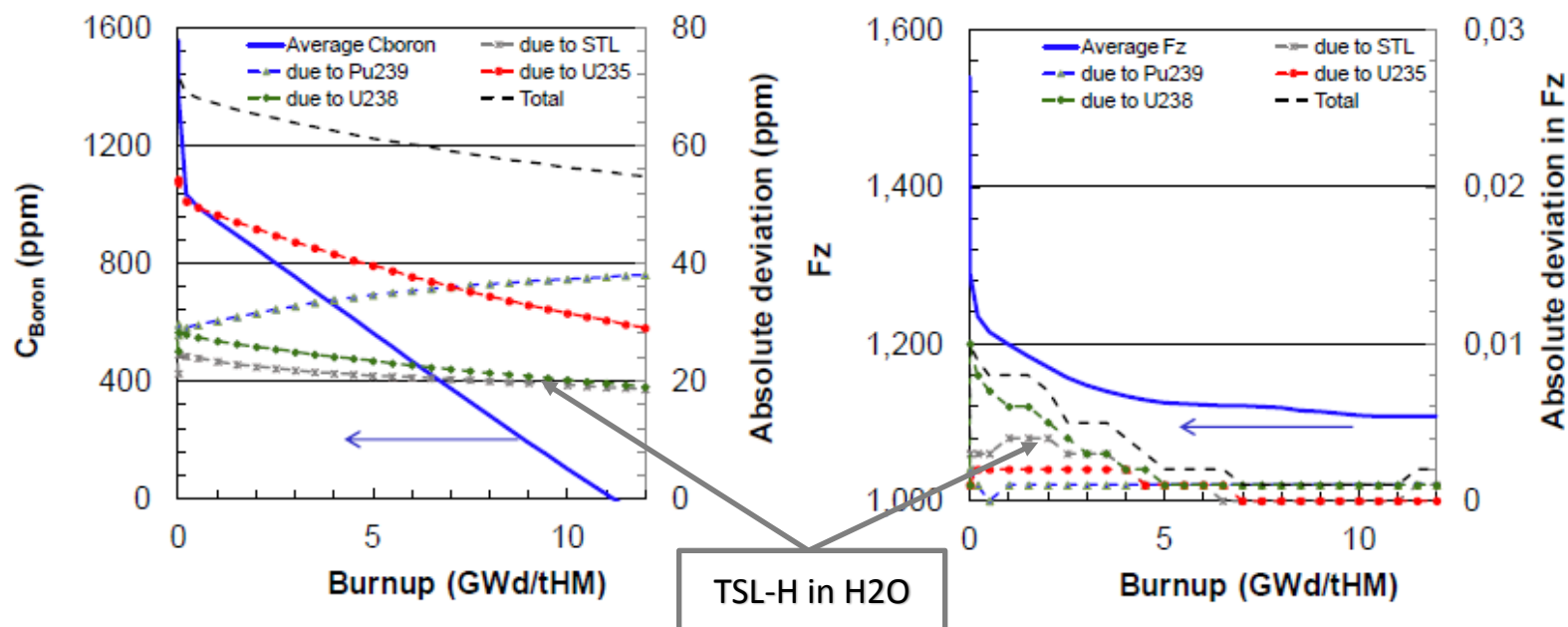
	1	2	3	4	5	6	7	8
1	18.137	11.662	27.397	0.000	30.867	0.000	14.984	11.662
2	11.662	16.188	13.130	28.902	12.155	28.866	0.000	30.191
3	27.397	13.130	27.572	0.000	22.778	0.000	0.000	
4	0.000	28.902	0.000	30.755	15.236	0.000	30.124	
5	30.867	12.155	22.778	15.236	13.123	14.882		
6	0.000	28.866	0.000	0.000	14.882			
7	14.984	0.000	0.000	30.503				
8	11.662	30.191						

FUEL	TYPE	w/o (%)	WABAS
1	OFA	2.10	0
2	OFA	3.10	0
3	OFA	3.24	0
4	OFA	3.24	0
5	OFA	3.24	0
6	OFA	3.24	0
7	OFA	3.24	0
8	OFA	3.24	0
9	OFA	3.24	0
10	OFA	3.24	0
11	OFA	3.24	0
12	AEF	3.60	0
13	AEF	3.60	0
14	AEF	3.60	0
15	AEF	3.60	0
16	AEF	3.60	0
17	AEF	3.60	0
18	AEF	3.60	0
19	AEF	3.60	0
20	AEF	3.60	4
21	AEF	3.60	8
22	AEF	3.60	12



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III.3 U&Q for Core Analysis: Average value and absolute deviation as a function of the burnup: C_{boron} and F_z



➤ C_{boron} vs Burnup

- Max unc.: 50-70 ppm
- Most important contrib.: ^{235}U and ^{239}Pu

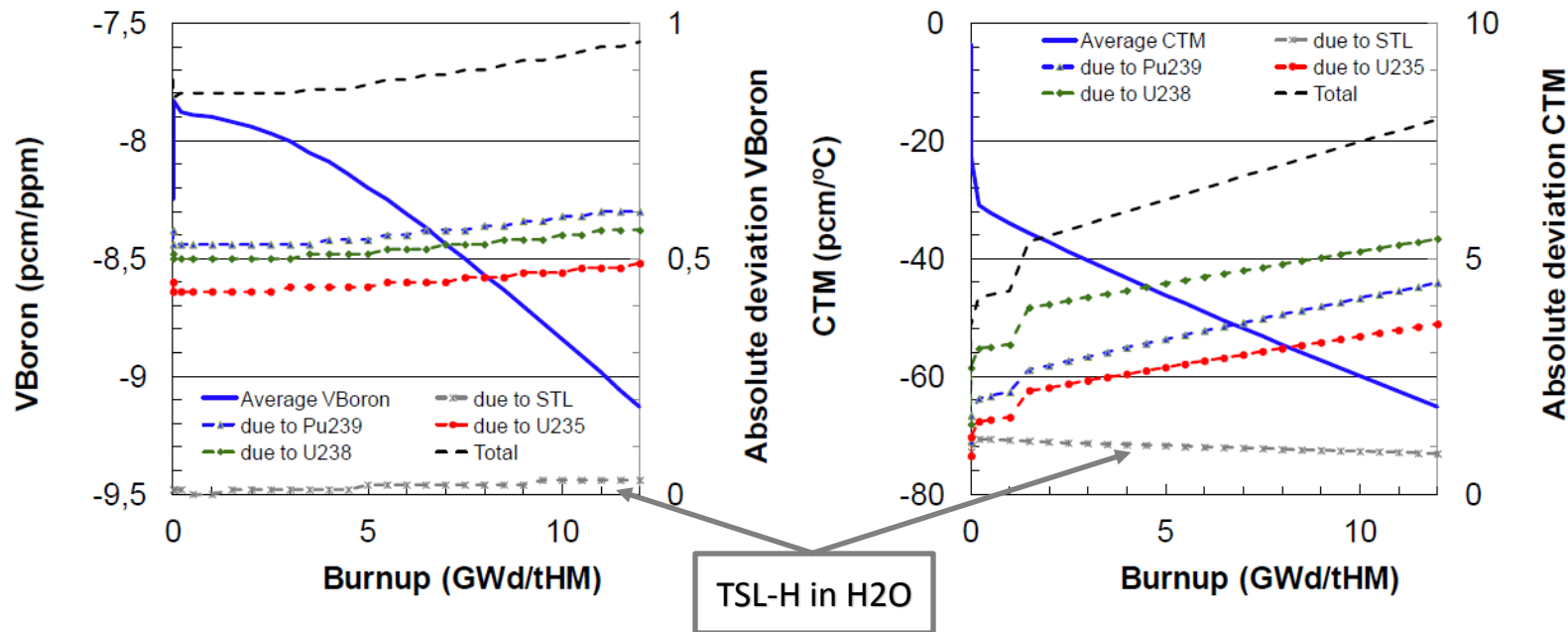
➤ F_z vs Burnup

- Max unc.: 0.01-0.02 (~1-2%)
- Most important contrib.: ^{238}U



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III.3 U&Q for Core Analysis: Average value and absolute deviation as a function of the burnup: V_{Boron} and CTM



➤ Boron Worth vs Burnup

- Max unc.: 1 pcm/ppm (~12%)
- Most important contrib.: $^{235,238}\text{U}$ & ^{239}Pu

➤ CTM vs Burnup

- Max unc.: 5-7 pcm/°C (~10%)
- Most important contrib.: $^{235,238}\text{U}$ & ^{239}Pu



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III.3 U&Q for Core Measurements: Relative percentage assembly power calculated as: $(M-C)/C \cdot 100$

➤ Relative percentage assembly power core distribution between measured (M) and calculated (C) at **BOC-HFP and Xenon equilibrium**

➤ Relative error in % for random cases (STL and ^{239}Pu) is provided

- Low unc. due to STLs < 0.3%
- Max. unc. due to ^{239}Pu < 1.8%

5.3 5.9±0.1 4.8±1.8	3.7 4.1±0.2 3.3±1.4	4.9 5.6±0.2 4.5±1.3	-0.6 0.0±0.2 -0.7±0.4	1.9 2.2±0.0 1.8±0.4	-1.8 -1.8±0.0 -1.6±0.6	-0.3 -0.9±0.1 -0.2±0.6	1.9 1.6±0.0 2.1±0.7	WIMS-D4 Random STL Random ^{239}Pu
3.4 3.8±0.2 3.0±1.4	2.2 2.6±0.1 1.7±1.4	2.8 3.3±0.2 2.5±1.1	4.6 5.2±0.2 4.3±0.8	1.0 1.1±0.1 1.0±0.2	0.5 0.4±0.0 0.6±0.2	-1.3 -1.6±0.1 -0.9±1.1	3.4 3.1±0.0 3.4±0.6	
4.0 4.7±0.2 3.6±1.3	2.2 2.6±0.2 1.8±1.1	4.6 5.2±0.1 4.4±1.0	-1.6 -1.2±0.1 -1.6±0.2	0.0 -0.1±0.1 -0.1±0.2	-1.6 -1.9±0.1 -1.3±0.8	-0.4 -0.7±0.1 0.0±1.3		
-1.7 -1.1±0.2 -1.8±0.4	3.5 4.1±0.2 3.2±0.8	-1.9 -1.6±0.1 -1.9±0.2	0.0 0.0±0.1 -0.2±0.5	-1.4 -1.9±0.2 -1.5±0.1	-2.0 -2.3±0.2 -1.7±0.8	2.5 2.0±0.0 2.5±0.7		
0.4 0.8±0.0 0.3±0.4	-0.4 -0.3±0.1 -0.5±0.2	-1.0 -1.0±0.1 -1.1±0.2	-2.3 -2.7±0.2 -2.4±0.1	-1.8 -2.4±0.3 -1.9±0.1	-0.7 -1.2±0.2 -0.7±0.2			
-3.1 -3.1±0.0 -2.9±0.6	-1.0 -1.2±0.0 -1.0±0.2	-2.9 -3.2±0.1 -2.6±0.8	-2.6 -2.9±0.2 -2.3±0.8	-1.0 -1.5±0.3 -1.0±0.2				
-0.8 -1.4±0.1 -0.7±0.6	-2.0 -2.2±0.1 -1.6±1.1	-1.5 -1.6±0.1 -1.0±1.3	0.5 0.2±0.0 0.7±0.7					
1.6 1.2±0.0 1.9±0.7	3.1 3.1±0.0 3.4±0.6							

C = Calculated M = Measured

Higher unc.
value <0.3%
TSL-H in H2O



Fresh Fuel



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III.3 U&Q for Core Analysis: Average value and absolute deviation as a function of the burnup for control bank worth

	Average (ppm)	Absolute standard deviation (ppm)				
		STL	²³⁹ Pu	²³⁵ U	²³⁸ U	Total
D-IN	120.3	1.3	0.5	0.7	0.7	1.7
C-IN	92.2	0.8	2.6	1.4	1.1	3.2
B-IN	138.1	0.9	0.5	1.6	0.8	2.0
A-IN	92.3	0.5	3.5	3.9	0.7	5.3
SB-IN	88.9	1.1	3.3	2.4	1.4	4.5
SA-IN	120.3	0.8	2.3	3.2	0.6	4.0
D+C-IN	237.8	2.1	2.9	0.7	1.6	4.0
D+C+B-IN	419.2	3.5	4.5	1.0	2.4	6.2
D+C+B+A-IN	565.2	4.1	1.6	6.5	1.7	8.0
D+C+B+A+SB-IN	701.8	5.6	2.8	3.9	2.9	7.9
ARI	917.5	7.8	2.6	5.4	3.2	10.3

- Uncertainty for each of the nuclear data varied (STL-H in H₂O, ^{235,238}U and ²³⁹Pu) and the sum of the different contributions < ~2%

- Review of Recent International Activities

- Journals

- Models:

- “*Evaluation of the neutron scattering cross-section for light water by molecular dynamics*”. Y. Abe et al., NIMA, 735(2014)568–573
- “*CAB models for water: A new evaluation of the thermal neutron scattering laws for light and heavy water in ENDF-6 format*”, J.I. Marquez Damian et al., ANE, 65 (2014) 280–289

- Uncertainties/Covariances:

- “*Generation of an $S(\alpha, \beta)$ Covariance Matrix by Monte Carlo Sampling of the Phonon Frequency Spectrum*”, J.C. Holmes and A.I. Hawari, NDS 118 (2014) 392–395
- “*Random Adjustment of the H in H_2O Neutron Thermal Scattering Data*”, D. Rochman and A. J. Koning, NSE, 172, 287–299 (2012)

- Interpolation

- “*Comparison of thermal scattering processing options for $S(a,b)$ cards in MCNP*”, Štefan Čerba et al., ANE, 55 (2013) 18–22
- “*On-the-fly sampling of temperature-dependent thermal neutron scattering data for Monte Carlo simulations*”, Andrew T. Pavlou, Wei Ji. ANE, 71 (2014) 411–426

- Meetings

- SG38, October 2014: “*Thermal Scattering Law Data*”, D. Brown, W. W. Haack
- SG40, November 2014: “*On Improvement of Thermal Neutron Scattering Libraries ($S(\alpha, \beta)$ data) for H_2O and D_2O* ”, D. Roubtsov et al.