DE LA RECHERCHE À L'INDUSTRIE

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H2O thermal scattering law uncertainties quantification and propagation to integral calculations

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OUTLINE OF THE PRESENTATION

- **Objectives**

- **Introduction**
  - Thermal neutron inelastic scattering
  - Studied models for producing the frequency spectrum of H in H2O: IKE and CAB models
  - Frequency spectrum of H in H2O of the models
  - H2O total cross section calculated with the models

- **Uncertainties of H(H2O) thermal scattering law of JEFF-3.1.1**
  - Thermal scattering law uncertainties quantification
  - Thermal scattering law uncertainties propagation to Mistral-1 experiment
  - Comparison with the impact of a new evaluation of U235 isotope (JEFF-3.3T1) on Mistral-1

- **Conclusions**

CONTEXT OF STUDY

Objectives

- Quantification and propagation of the thermal scattering law uncertainties of H in H2O to integral calculations (MISTRAL benchmark).

- Show that H in H2O has a similar impact on MISTRAL-1 reactivity temperature coefficient than the capture-to-fission cross section ratio of U235.

MODELS FOR FREQUENCY SPECTRUM OF H IN H2O

The processing of the TSL is done for both models with LEAPR module of NJOY code. S(α,β) is computed as a convolution of 3 components:

- *Molecular translation*: models the translation of the water molecule as free gas or diffusion.
- *Continuous spectrum* : model the intermolecular vibrations of the molecules
- *Discrete oscillators*: model the intramolecular vibrations of the molecule

IKE MODEL

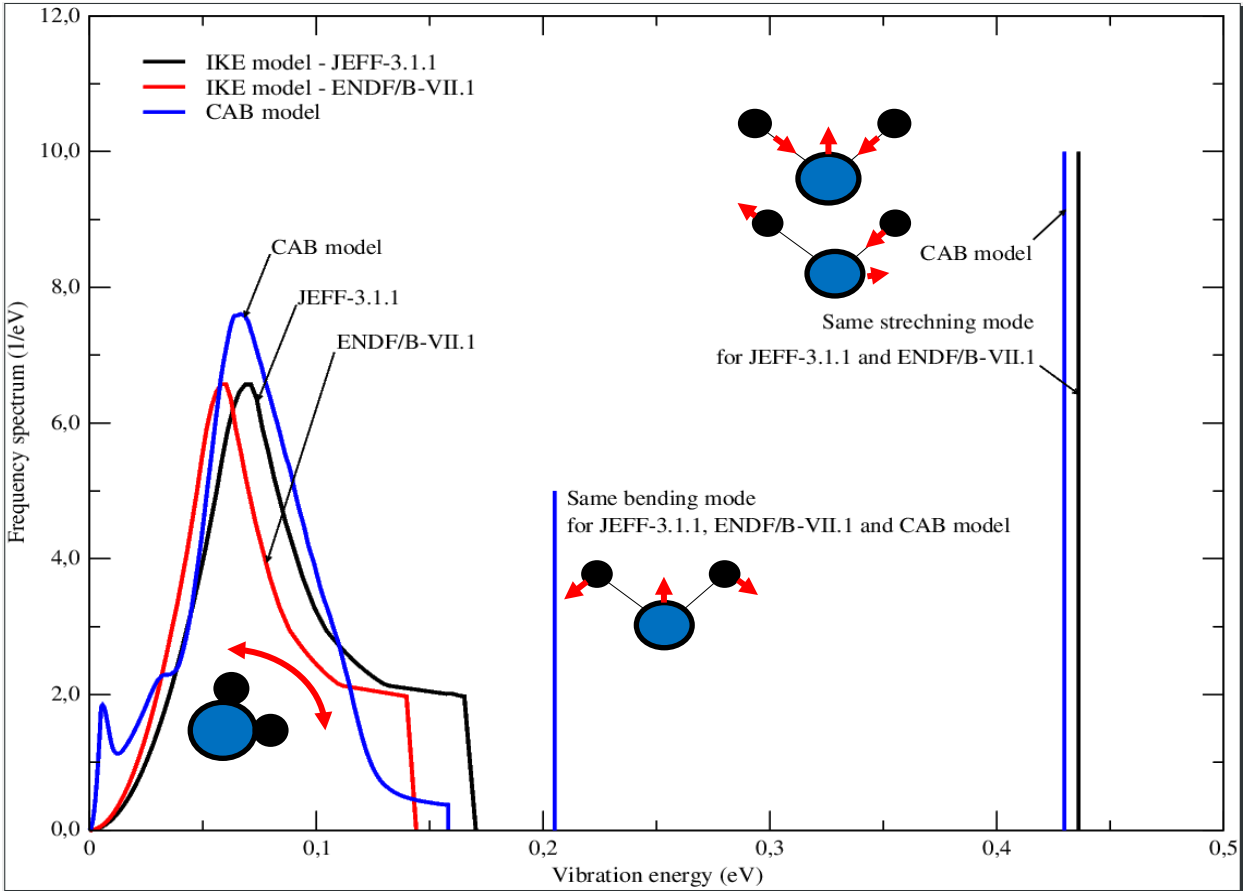
- *Keinert* & *Mattes* from KIT institute in Stuttgart (*1984*).
- The rotational mode is based on experimental measures between 294K and 550K.
- The translational mode is represented with the Free Gas Law.
- 2 discrete oscillators represent the intramolecular modes.
- The nuclear data libraries JEFF-3.1.1 and ENDF/B-VII.1 include this model.

CAB MODEL

- *I. Marquez Damian* from Centro Atomico Bariloche (CAB), Argentina (2013).
- The rotational mode is based on molecular dynamic simulations with *GROMACS* code.
- The translational mode is represented by a Diffusion model established by Egelstaff and Schofield (Effective Width model).
- 2 discrete oscillators represent the intramolecular modes.

FREQUENCY SPECTRUM OF H IN H2O

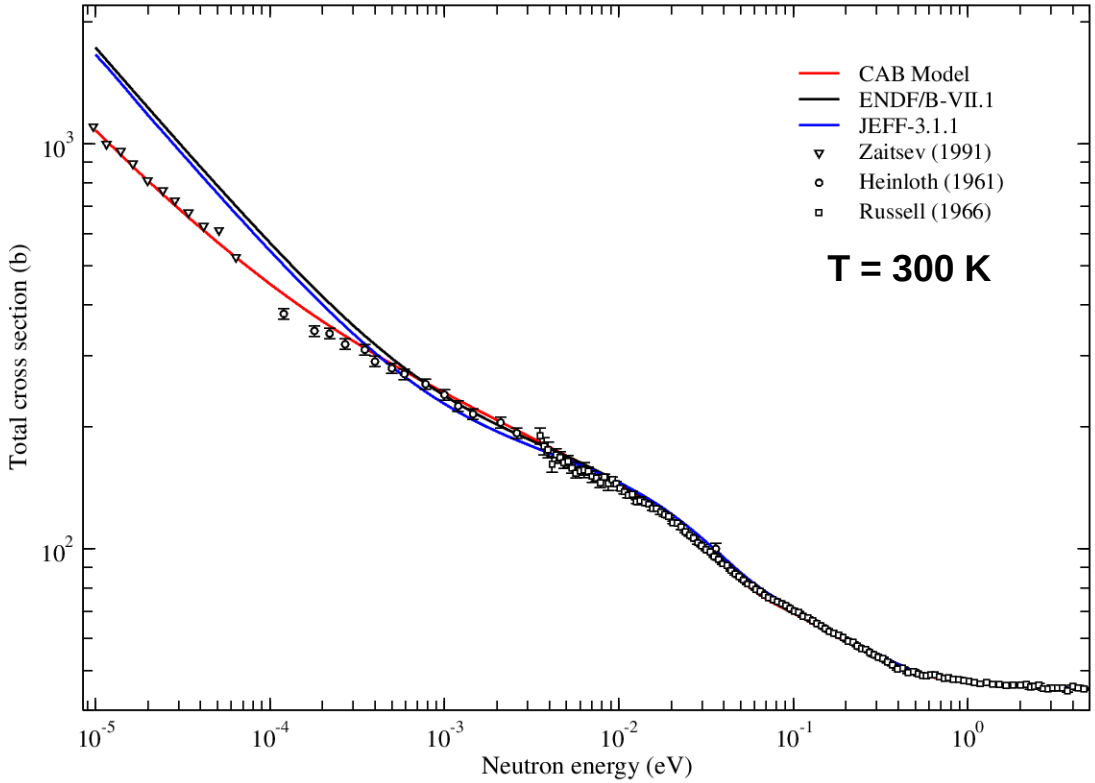
Phonon density of states of H(H2O) at T = 300K



The plot shows the intermolecular (continuous part) and intramolecular (discrete oscillators) contributions (translational mode is not seen in the plot)

H2O TOTAL CROSS SECTION COMPARISON

Total cross section: $\sigma(E) = \int_0^{2\pi} d\varphi \int_0^{\pi} \sin(\theta) d\theta \int_0^{\infty} \frac{d^2\sigma}{d\hat{\Omega} dE} dE'$



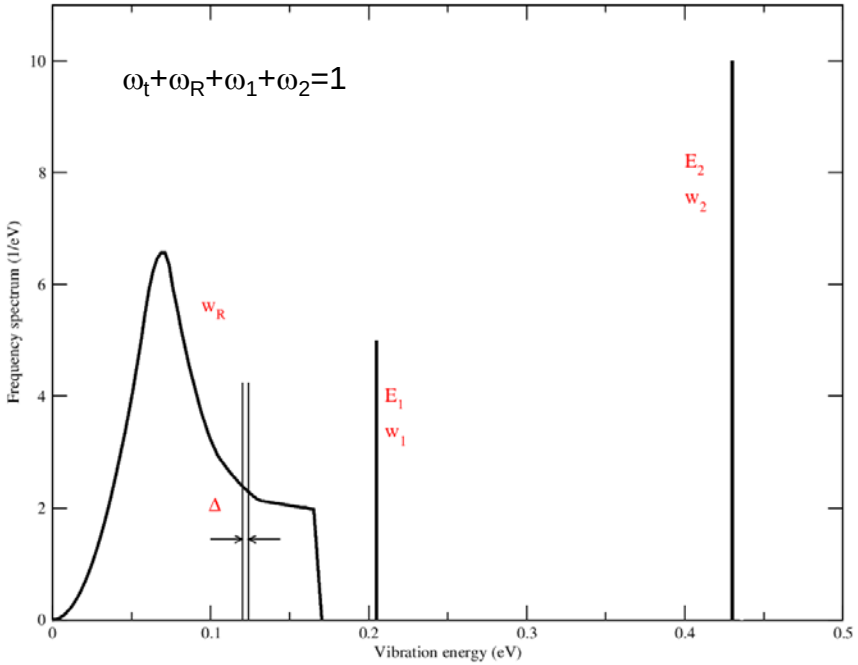
- Good agreement between the CAB model and the experimental data.
- Discrepancies between the CAB model, JEFF-3.1.1 and ENDF/B-VII.1 for the cold neutron energy range (E<0.2 meV).
- Large uncertainties on the parameters that describe low energy dynamics in JEFF-3.1.1 are expected.

TSL UNCERTAINTIES QUANTIFICATION

OBJECTIVE *: need for determining uncertainties associated to the TSL of* ***JEFF-3.1.1***

S(α,β) uncertainties ⟺ LEAPR module parameters uncertainties

Density of states of **H in H2O** at 293.6K **(JEFF-3.1.1)**



ω_t: translational mode weight

ω_R: rotational mode weight

Δ: energy binning of continuous spectrum

E_1: bending mode energy

E_2: stretching mode energy

ω_1: bending mode weight

ω_2: stretching mode weight

CONRAD code (*Code for Nuclear Reaction Analysis and Data Assimilation*, CEA Cadarache) uses the generalized least square method (GLS) to fit the LEAPR module parameters with light water total cross section.

TSL UNCERTAINTIES QUANTIFICATION (JEFF-3.1.1)

Sensibility of LEAPR module parameters to H2O total cross section at 293.6K

ω_t: translational mode weight

ω_R: rotational mode weight

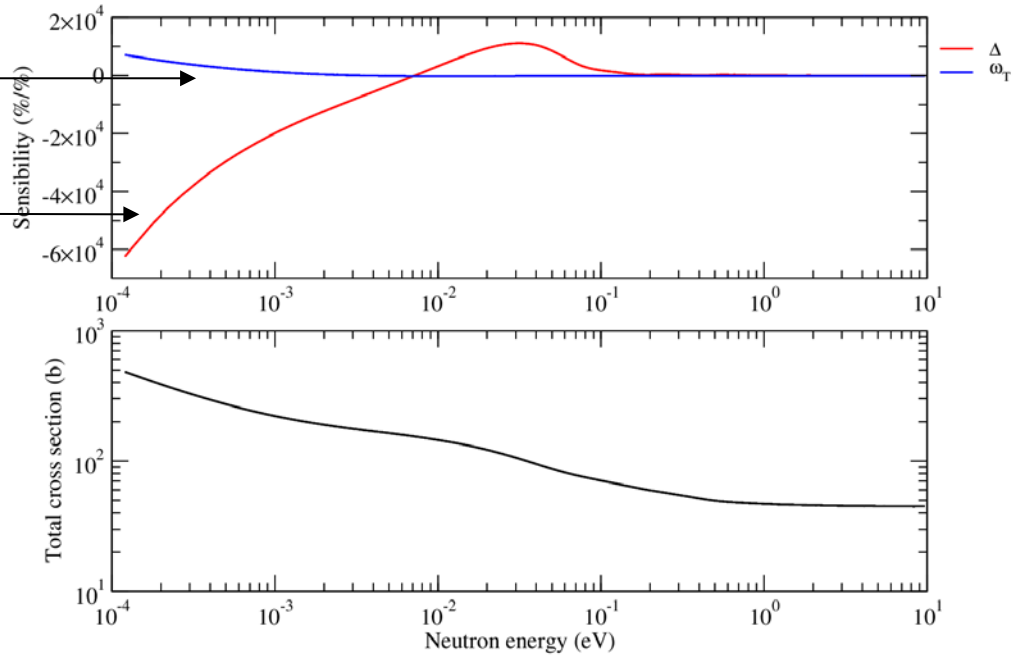
Δ: energy binning of continuous spectrum

E_1: bending mode energy

E_2: stretching mode energy

ω_1: bending mode weight

ω_2: stretching mode weight



The parameters Δ and ω_t are the most sensible to h2o total cross section. They will be used in the Marginalization technique with *CONRAD* (uncertainties of systematic origin like normalization and background).

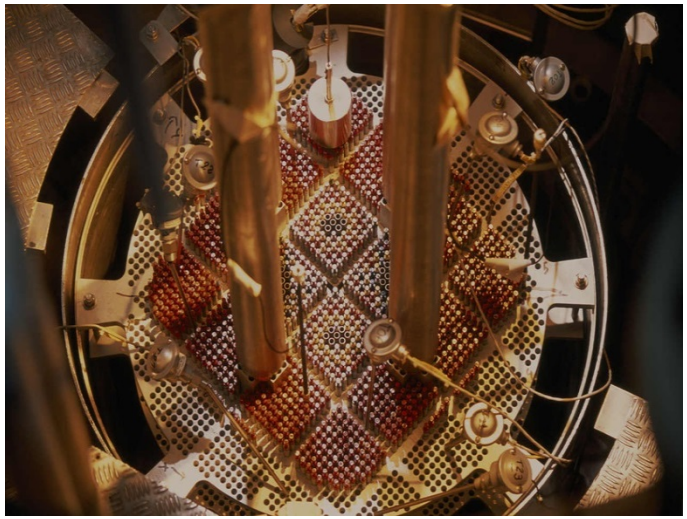
ω_t = 0.0214 ± 0.0183

Δ = 0.00254 ± 0.00036

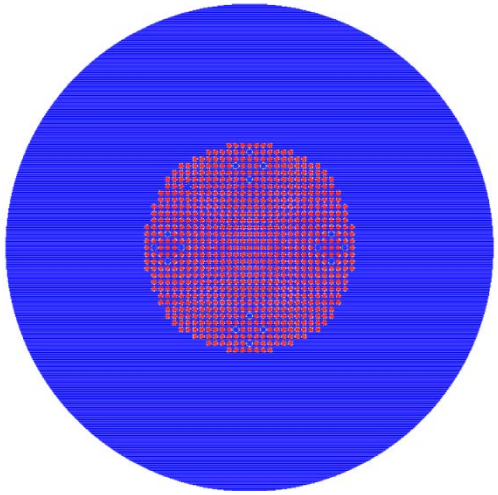
Large uncertainties on ω_t due to the poor description of the total cross section in the cold neutron energy range (as seen before).

TSL UNCERTAINTY PROPAGATION FOR MISTRAL-1 (JEFF-3.1.1)

- MISTRAL program was carried out in EOLE research reactor at CEA Cadarache (France).
- The main safety neutronic parameters were measured from 10°C to 80°C in three core configurations.
- This study is focused on the *isothermal reactivity temperature coefficient* on **Mistral-1** (UOX core).



Photograph of **Mistral-1 core**



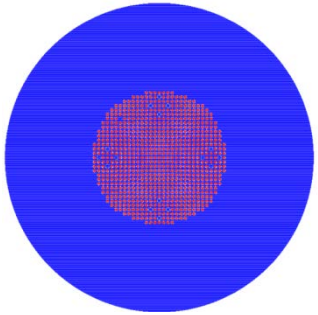
Model of **Mistral-1 core** done with Monte Carlo code TRIPOLI4

- 750 3.7% **UOX** cells
- 17 guide tubes
- Cell pitch 1.32 cm
- Moderation ratio 1.7
- Moderator: $H_2O+H_3BO_3$
- Reactivity control: $C_B=f(T)$

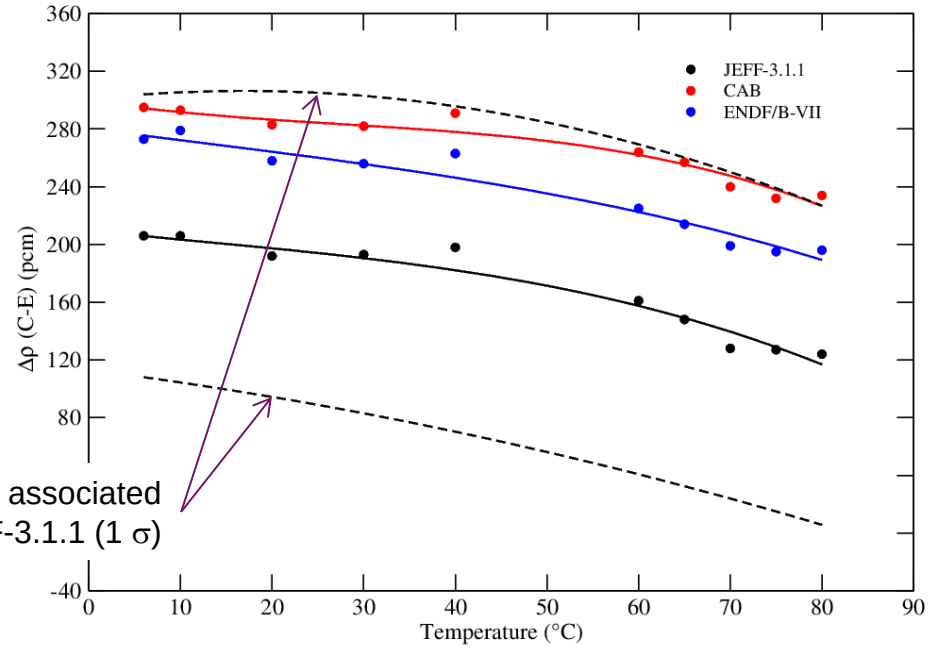
The calculated reactivity was obtained with the Monte Carlo code ***TRIPOLI4***, the processing tool ***NJOY*** and ***JEFF-3.1.1*** nuclear data library.

TSL UNCERTAINTY PROPAGATION FOR MISTRAL-1 (JEFF-3.1.1)

Direct propagation of LEAPR module parameters uncertainties



Estimation of the contribution of the
TSL uncertainties in all the temperature range.



TSL uncertainties associated to JEFF-3.1.1 (1 σ)

The obtained uncertainties range from 98 pcm to 112 pcm

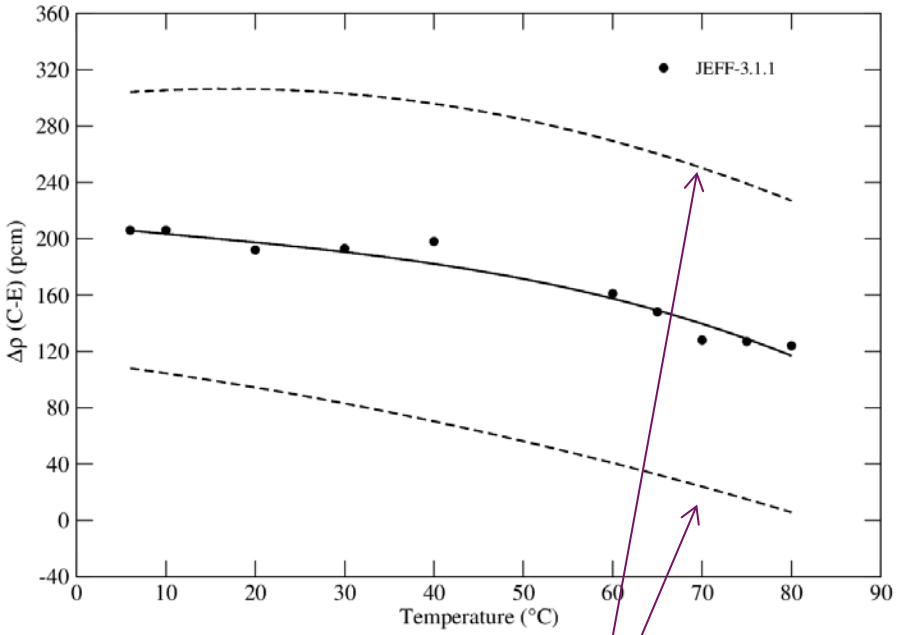
Temperature (°C)	Δρ (pcm)
6.0	206 ± **98**
30.0	193 ± **110**
75.0	127 ± **112**

- For UOX configuration, the uncertainty on the reactivity associated to JEFF-3.1.1 is close to 100 pcm.
- The uncertainty band associated to JEFF-3.1.1 overlaps the C-E values calculated with the CAB model.

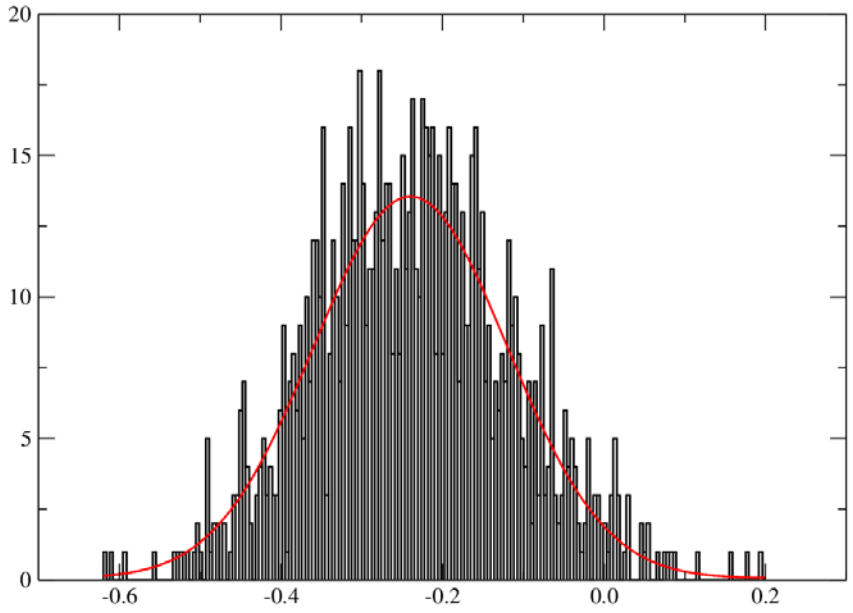
TSL UNCERTAINTY PROPAGATION FOR MISTRAL-1 (JEFF-3.1.1)

Estimation by Monte-Carlo of the uncertainties on $\Delta\alpha_{iso}$ due to the TSL uncertainties associated to JEFF-3.1.1

$\Rightarrow$ Realistic uncertainties on $\Delta\alpha_{iso}$ are obtained



Uncertainties on the calculated reactivity due to the TSL uncertainties associated to JEFF-3.1.1



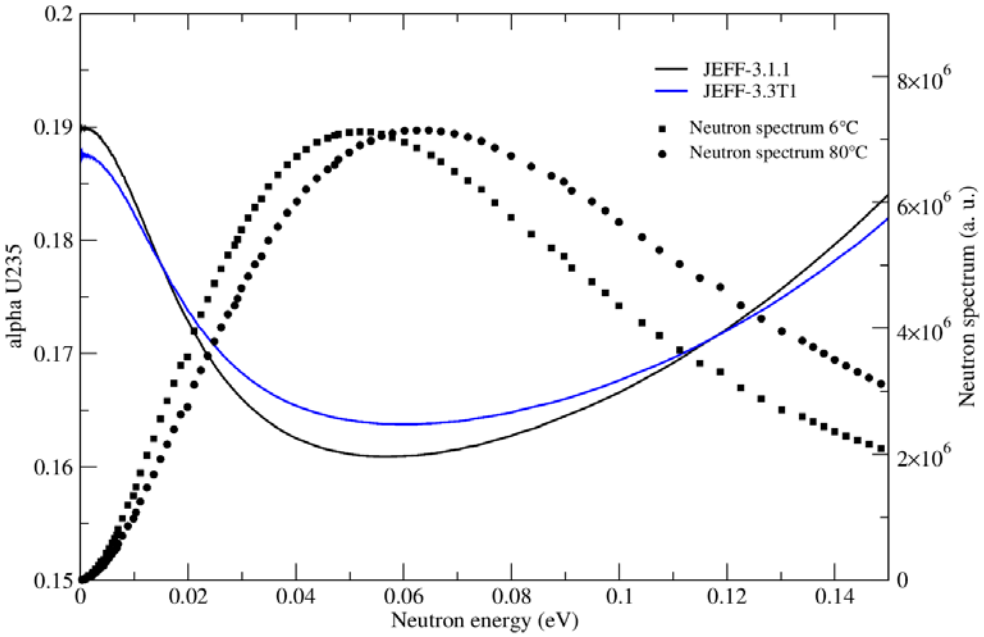
$$\overline{\Delta\alpha_{iso}} = -0.24 \pm 0.12\ pcm/°C$$

Uncertainty on the calculated reactivity temperature coefficient (between 6°C and 80°C) due to the TSL uncertainties associated to JEFF-3.1.1

NEW U235 EVALUATION (JEFF-3.3T1)

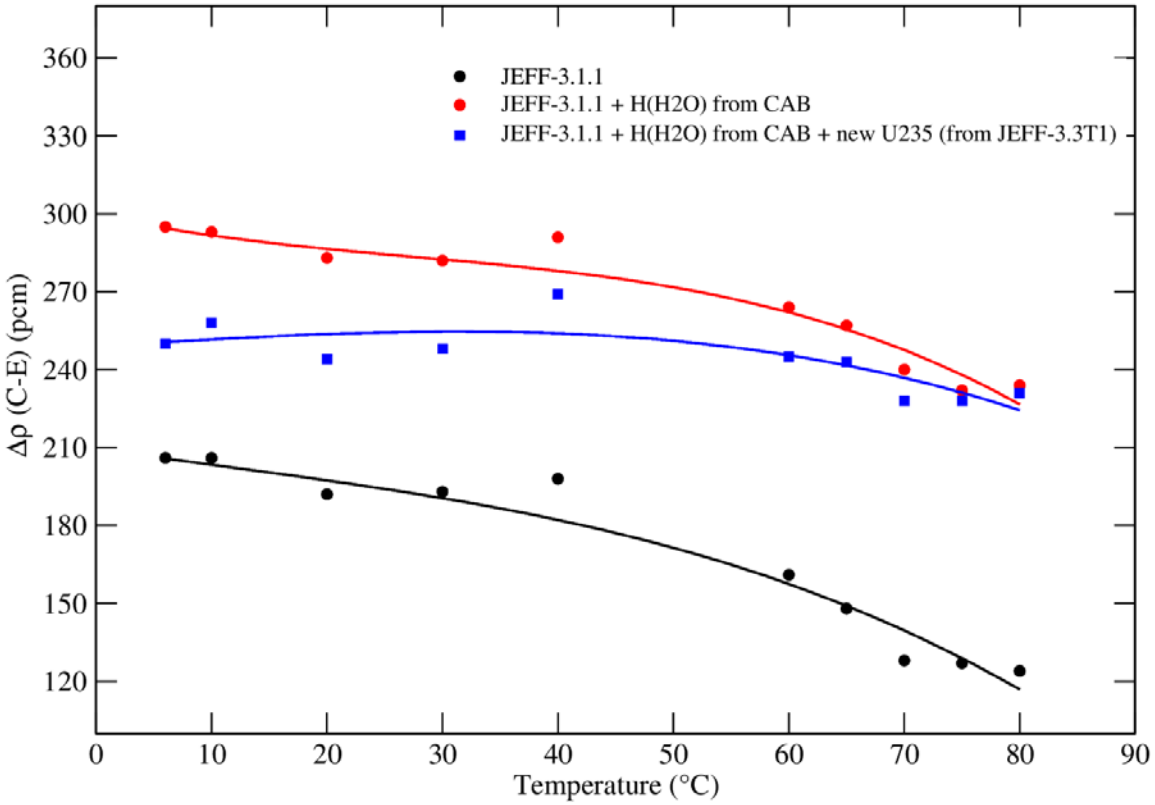
***OBJECTIVE**: show that H in H2O has similar impact on the calculated reactivity temperature coefficient of MISTRAL-1 than the capture-to-fission cross section ratio of U235*

- New U235 evaluation by L. Leal (JEFF-3.3T1)
- Modification of the capture to fission cross section ratio of U235 isotope $\Rightarrow \alpha_{U5} = \frac{\sigma_\gamma(E)}{\sigma_f(E)}$



⇒ Due to spectral shift effects, a sizeable impact on the calculated RTC is expected at low temperatures (T < 40°C).

IMPACT OF THE NEW U235 ON MISTRAL-1



$\overline{\Delta\alpha_{iso}} = -0.02\,pcm/°C$

$\overline{\Delta\alpha_{iso}} = +0.52\,pcm/°C$

$\overline{\Delta\alpha_{iso}} = -0.29\,pcm/°C$

The change in U235 capture-to-fission cross section ratio has an impact on the $\Delta\alpha_{iso}$ comparable to a change in the thermal scattering data (from JEFF-3.1.1 to CAB model).

- *Impact on the $\Delta\alpha_{iso}$ in changing the α(U235) = +0.5 pcm/°C*
- *Impact on the $\Delta\alpha_{iso}$ in changing the TSL of H in H20 = +0.3 pcm/°C*

CONCLUSIONS

1. Propagation of the uncertainties associated to H(H20) of JEFF-3.1.1 on the calculated reactivity and RTC. Results obtained for the MISTRAL-1 configuration (from 6°C to 80°C) :

   - The uncertainties on the calculated reactivity is close to $\pm$ 100pcm.
   - The uncertainty on the calculated $\Delta\alpha_{iso}$ is close to $\pm$ 0.12 pcm/°C.

2. The impact of the capture-to-fission cross section ratio of U235 (from JEFF-3.3T1) was estimated on Mistral-1. We found that TSL and α(U235) have similar impact on $\Delta\alpha_{iso}$:

   - α(U235) : from JEFF-3.1.1 to JEFF-3.3T1 $\Rightarrow$ + 0.5 pcm/°C
   - H(H2O) : from JEFF-3.1.1 to CAB model $\Rightarrow$ + 0.3 pcm/°C