DE LA RECHERCHE À L'INDUSTRIE

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Reactivity temperature coefficient interpretation of Mistral benchmarks with different thermal scattering laws.

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OUTLINE

- **Objectives**
- **Introduction**
  - Thermal neutron scattering: inelastic scattering.
  - Model for light water molecule H into H2O
    - ✓ IKE model
    - ✓ CAB model
- **Mistral Program Benchmark (Mistral-1, Mistral-2, Mistral-3)**
- **Calculation scheme**
  - Crystal lattice effects in fuel
  - Materials thermal expansion
- **Results**
  - Interpolation of IKE model parameters for JEFF - 3.1.1
  - Interpolation of IKE model parameters for ENDF/B-VII.1
  - TSL files obtained with CAB model
  - Mistral-1
  - Mistral-2
  - Mistral-3
- **Conclusions**

CONTEXT

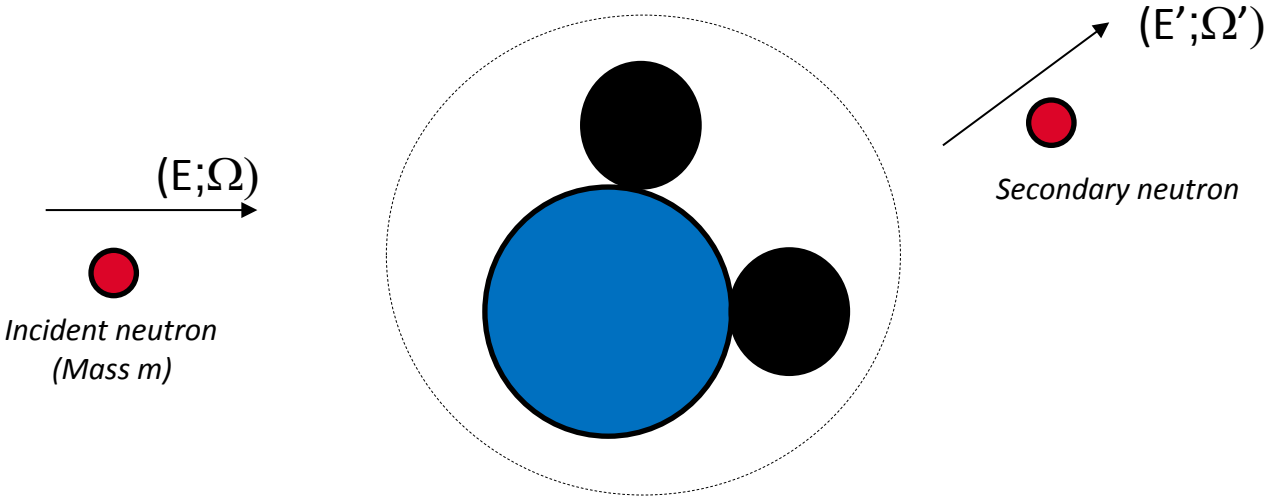
Objectives

- Perform Monte Carlo calculations taking into account chemical bindings of H1 in H2O molecule.
- Test of different thermal scattering law files for H(H2O).
- Interpretation of integral measurements carried out at EOLE reactor in CEA Cadarache.

THERMAL NEUTRON SCATTERING: Inelastic scattering

Double differential scattering cross section for thermal neutrons:

$$\frac{d^2\sigma}{d\Omega dE}(E \to E', \Omega \to \Omega') = \frac{\sigma_b}{4\pi kT}\sqrt{\frac{E'}{E}}e^{-\frac{\beta}{2}}S(\alpha,\beta)$$



H2O Molecule
σ_b: characteristic bound XS
T: temperature
M: mass

Thermal scattering law:

$$S(\alpha,\beta)$$

- *Contains dynamic and structural information about the target system.*
- *Determines energy and angular distribution of secondary neutrons.*

$\alpha = \frac{E'+E-2\sqrt{E'E}\cos\theta}{AkT}$ *momentum transfer; A=M/m*

$\beta = \frac{E'-E}{kT}$ *energy transfer*

THERMAL NEUTRON SCATTERING: Inelastic scattering

Approximations for evaluating the thermal scattering law:

-*Incoherence approximation*: $\sigma(H^1) = \sigma_{coh} + \sigma_{inc} \approx \sigma_{inc}$ We can neglect interference phenomena between waves reflected by close nuclei.

$$S_s(\alpha,\beta) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\beta t} I_s(\alpha,t)dt$$

- Using the *Gaussian approximation*, which consists of an approximation of the intermediate scattering function by a Gaussian:

$$S_s(\alpha,\beta) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\beta t} e^{-\gamma(t)} dt$$

$$P(\beta) = \frac{\rho(\beta)}{2\beta\sinh(\beta/2)}$$

ρ(β): frequency spectrum of material

$$\gamma(t) = \alpha\int_{-\infty}^{\infty} P(\beta)\left[1 - e^{-i\beta t}\right]e^{-\beta/2} d\beta$$

γ(t): width function

ρ(β)

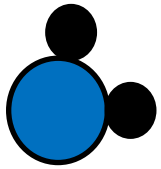
- ✓ Information about the excitation states of the scattering material.
- ✓ Obtained through experimental measures or molecular dynamic simulations.

MODEL FOR LIGHT WATER MOLECULE H INTO H2O

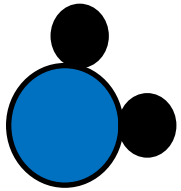
What are the possibilities of vibration of the molecule?

Intermolecular vibration

- Rotation

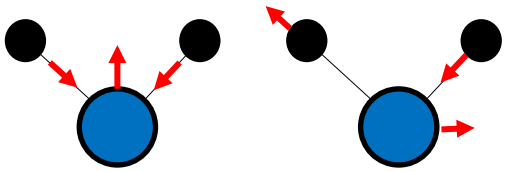


- Translation

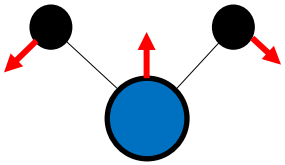


Intramolecular vibration

- Symmetric/Asymmetric stretching



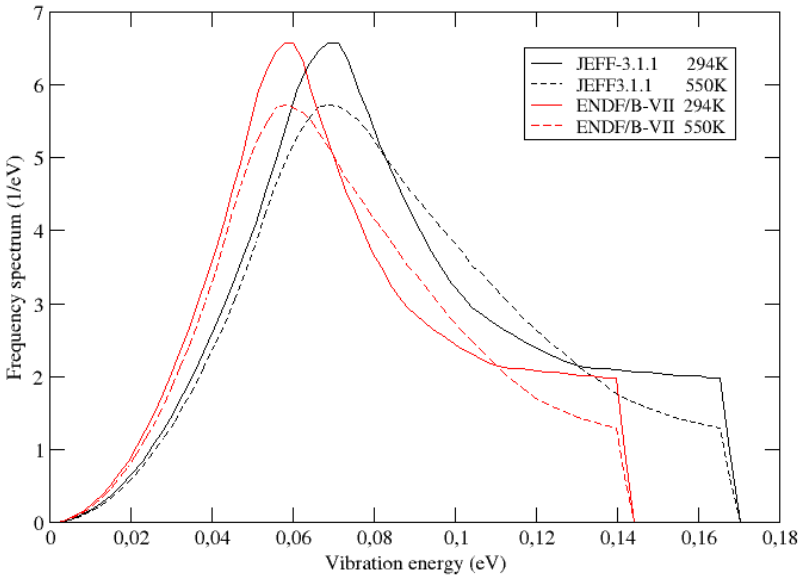
- Bending



MODEL FOR LIGHT WATER MOLECULE H INTO H2O

Frequency spectrum of IKE model for JEFF - 3.1.1 and ENDF/B-VII.1

Rotational mode (temperature dependent)
D. I. Page, B. C. Haywood (1968)



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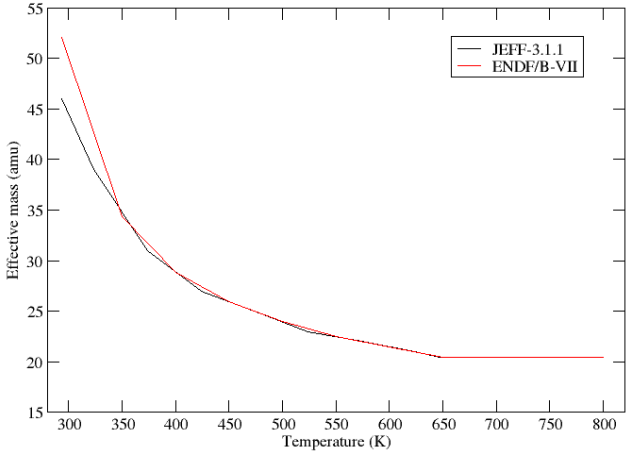
Translational mode (temperature dependent)
Eucken (1946)



Continuous frequency spectrum (low energy), with weight ω_R $\rho_j(\beta) = \rho_s(\beta)$

Intramolecular mode

+

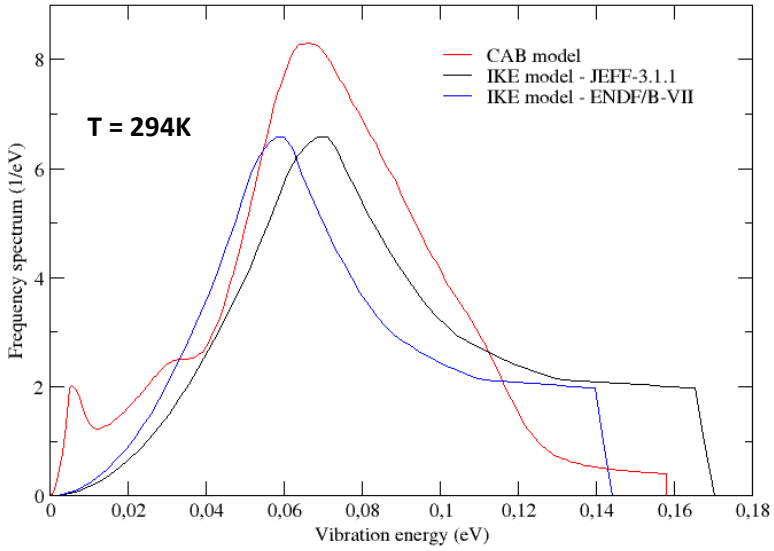
Effective temperature dependent masses, with weight ω_T $\rho_j(\beta) = \rho_t(\beta)$

2 discrete oscillators for bending (0.205 eV) and stretching modes (0.436 eV) $\rho_j(\beta) = w_j \delta(\beta_j)$

MODEL FOR LIGHT WATER MOLECULE H INTO H2O

Frequency spectrum of CAB Model (Molecular dynamics simulation with GROMACS code - *Ignacio Marquez Damian*)

Rotational mode (temperature dependent)



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Molecular diffusion (temperature dependent)
(Egelstaff-Schofield model)

$$S_t(\alpha,\beta)=\frac{2cw_t\alpha}{\pi}e^{\left[2c^2w_t\alpha-\beta/2\right]}\frac{\sqrt{c^2+1/4}}{\sqrt{\beta^2+4c^2w_t^2\alpha^2}}K_1\left\{\sqrt{c^2+1/4}\sqrt{\beta^2+4c^2w_t^2\alpha^2}\right\}$$

$K_1(x)$ is the modified Bessel function of first kind

$c=\frac{M_H D}{w_t\hbar}$ is the dimensionless diffusion constant

D is the molecular diffusion constant

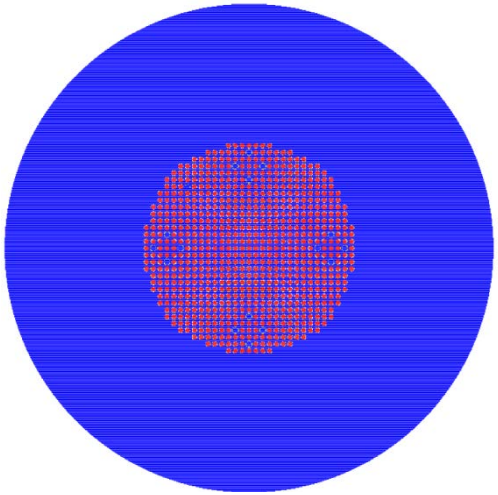
+

Intramolecular mode

2 discrete oscillators for bending (0.205 eV)
and stretching modes (0.430 eV)

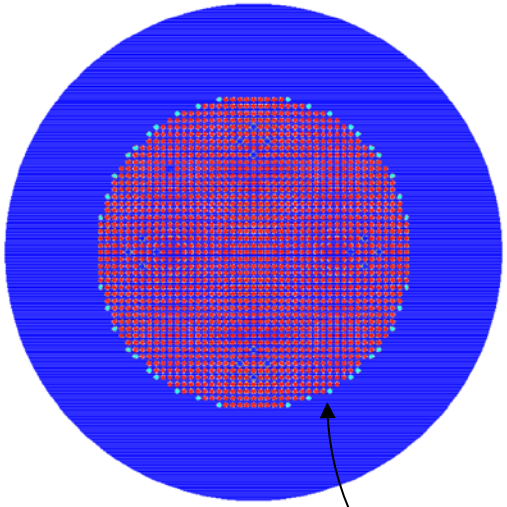
MISTRAL PROGRAM BENCHMARK

MISTRAL - 1



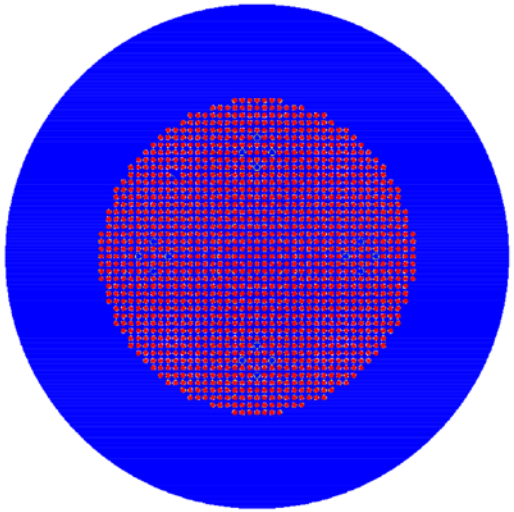
- 750 3.7% UOX cells
- 17 guide tubes
- Cell pitch 1.32 cm
- Moderation ratio 1.7
- Moderator: $H_2O+H_3BO_3$
- Reactivity control: $C_B=f(T)$

MISTRAL - 2



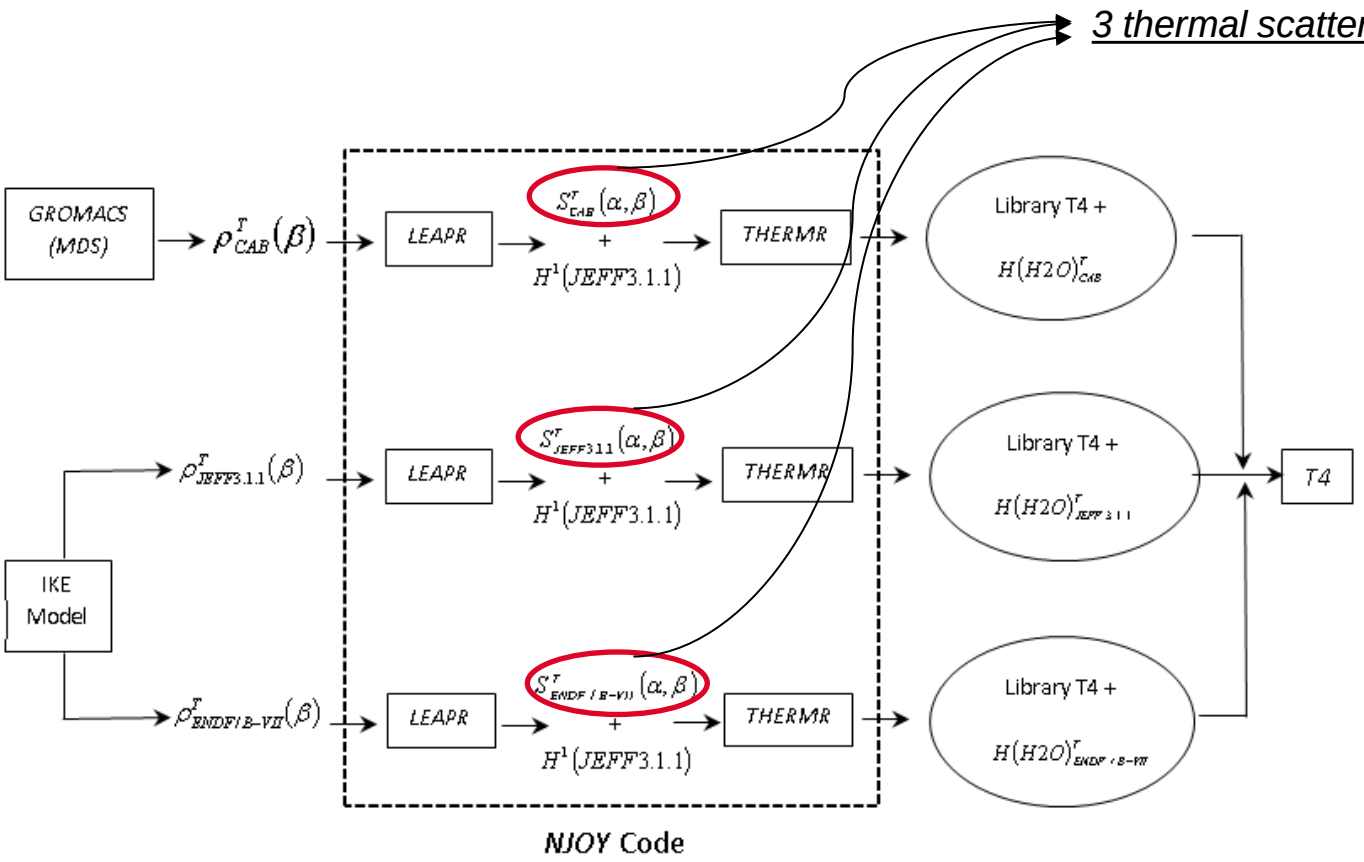
- 1600 7% MOX cells
- 17 guide tubes
- Cell pitch 1.32 cm
- Moderation ratio 1.7
- Moderator: H_2O
- Reactivity control: 8.7% MOX pins

MISTRAL - 3



- 1400 7% MOX cells
- 17 guide tubes
- Cell pitch 1.39 cm
- Moderation ratio 2.1
- Moderator: $H_2O+H_3BO_3$
- Reactivity control: $C_B=f(T)$

CALCULATION SCHEME



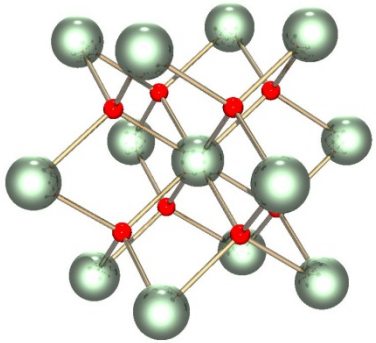
CRYSTAL LATTICE EFFECTS IN FUEL

Free Gaz Model

Incident neutron (m)

Target nucleus U238 (M)

Crystal Lattice Model (UO2 Matrix)



✓ Actual reactors physics codes are not prepared for crystal lattice calculations → *U238 Capture Reaction Rate Equivalency*

Total Capture reaction rate for Free Gas Model $I_\gamma^{FGM}(T_{eff}) = \int_g \sigma_\gamma^{FGM}(E,T_{eff})\phi(E)dE$

$$I_\gamma^{CLM}(T) = I_\gamma^{FGM}(T_{eff})$$

Total Capture reaction rate for Crystal Lattice Model $I_\gamma^{CLM}(T) = \int_g \sigma_\gamma^{CLM}(E,T)\phi(E)dE$

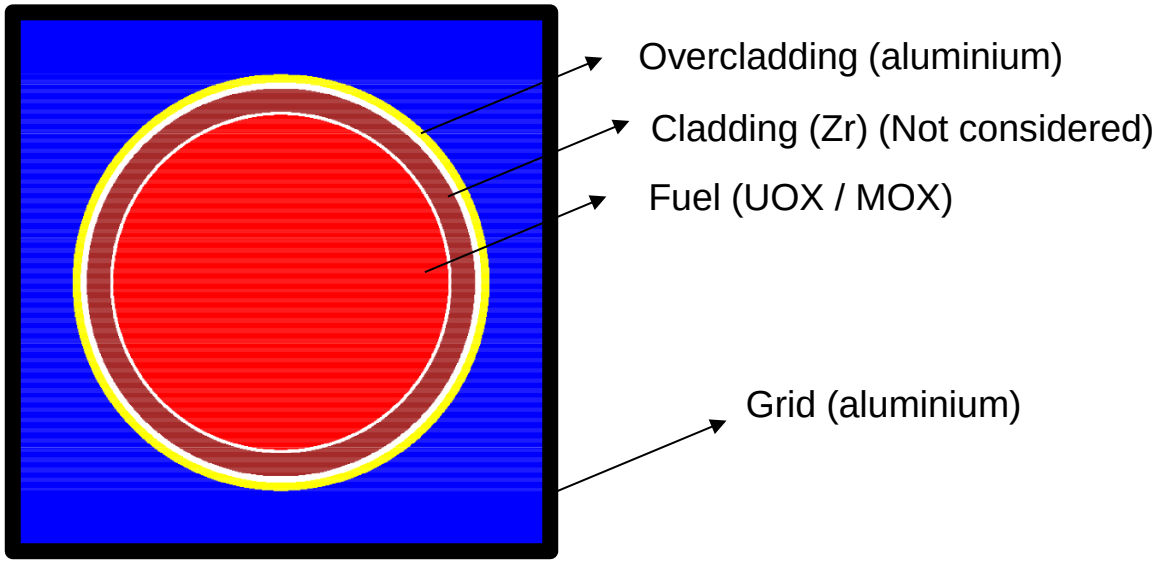
Effective fuel temperature recommended by Meister and Santamarina (1998)

$$\frac{T_{eff}^{MS}}{T} = 1 + \frac{8.6}{T} + \frac{3110}{T^2}$$

MATERIALS THERMAL EXPANSION

Temperature measurement range 5°C – 80°C

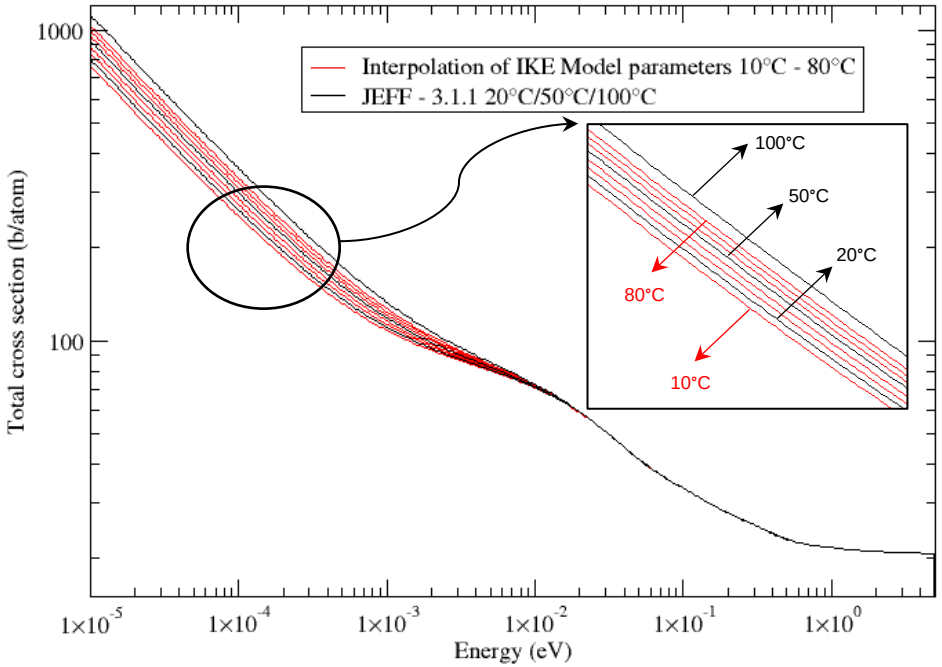
- ✓ Aluminium grid: increases the pitch, increases moderation ratio and decreases resonance absorption.
- ✓ Aluminium overcladding: opposite effect because its aim is to remove moderator and compensates the increase in the moderation ratio.
- ✓ Fuel: volume change of ~0.3%. Has impact on the resonance absorption.



RESULTS: interpolation of IKE model parameters for JEFF – 3.1.1

✓ Interpolation of IKE model parameters [10°C;80°C] ⟹ Interpolated XS [10°C;80°C]

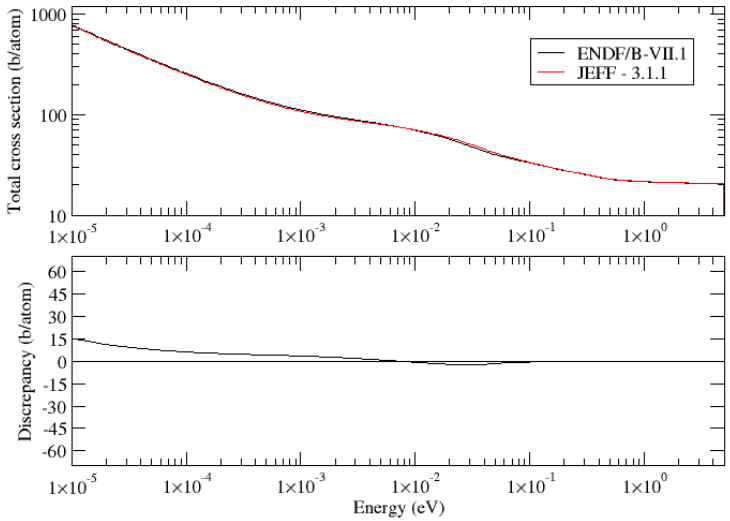
✓ Reference ⟹ XS JEFF-3.1.1 library @ 20°C, 50°C and 100°C



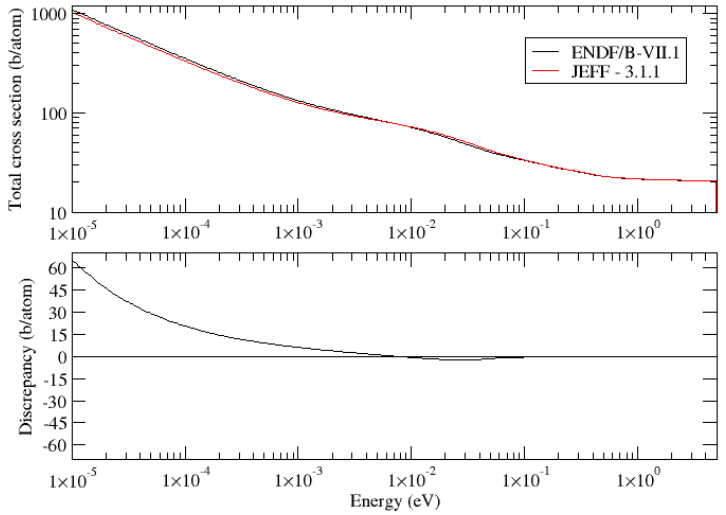
Taking as reference the total cross section of JEFF - 3.1.1, it was verified that the calculated cross sections were correctly obtained and in coherence with the official library.

RESULTS: interpolation of IKE model parameters for ENDF/B-VII.1

Comparison between Total XS obtained with TSL from JEFF-3.1.1 and ENDF/B-VII.1



T=10°C

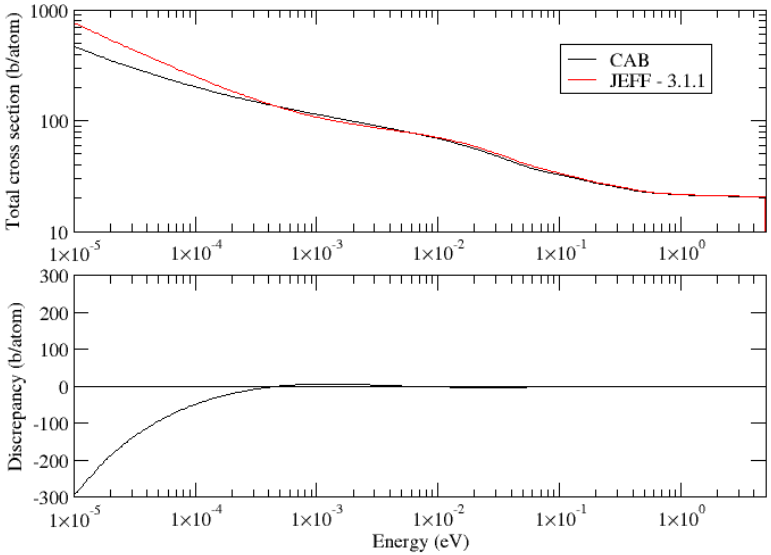


T=80°C

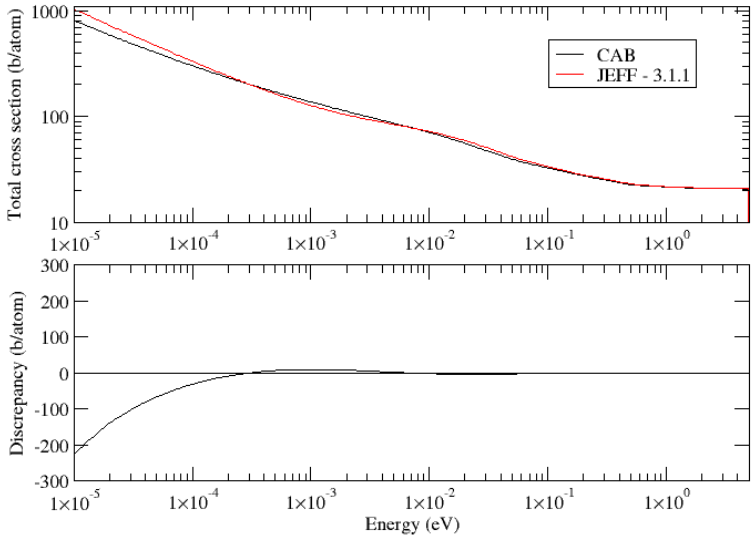
- ✓ Minor discrepancies for E<25meV
- ✓ σ(ENDF/B-VII.1)> σ(JEFF-3.1.1) ∀Energy
- ✓ Possible trend: difference increases with T

RESULTS: thermal scattering files obtained with CAB model

Comparison between Total XS obtained with TSL from JEFF-3.1.1 and CAB model



T=10°C



T=80°C

- ✓ Important discrepancies for E<10^{-4}eV.
- ✓ σ(JEFF-3.1.1)> σ(CAB) ∀Energy
- ✓ Possible trend: difference decreases with T

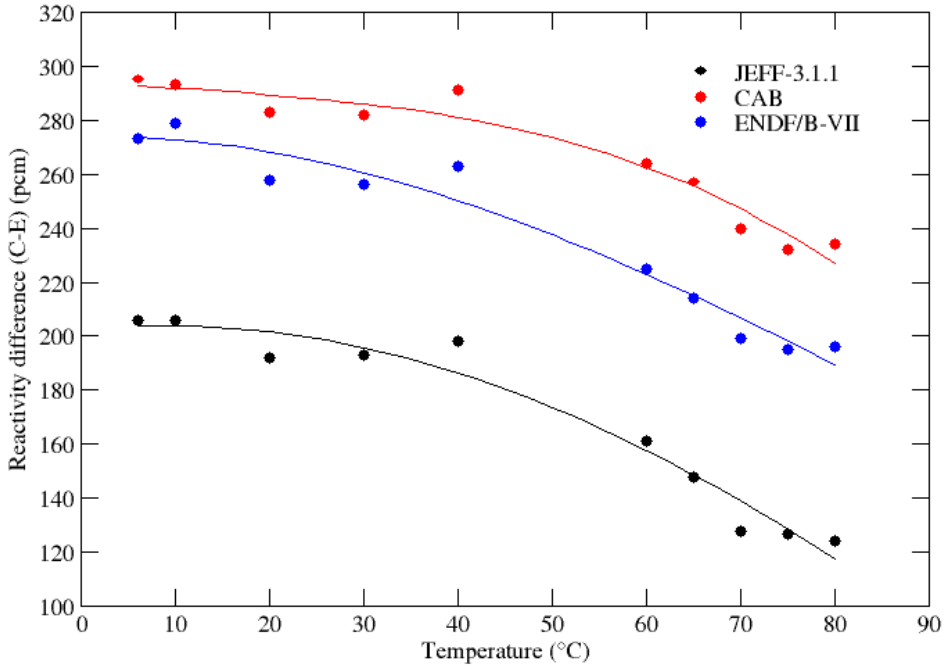
RESULTS: MISTRAL-1

Mistral-1 reactivity difference C-E $\Delta\rho$(pcm)

- TRIPOLI4 code + JEFF-3.1.1
- TRIPOLI4 code + CAB
- TRIPOLI4 code + ENDF/B-VII.1

Third order polynomial fitting

$$\Delta\rho = AT^3 + BT^2 + CT + D$$



Being JEFF-3.1.1 the reference library, CAB and ENDF/B-VII TSL overestimate calculated reactivity in all temperature range.

✓ Mean difference between CAB and JEFF-3.1.1 = +100 pcm.

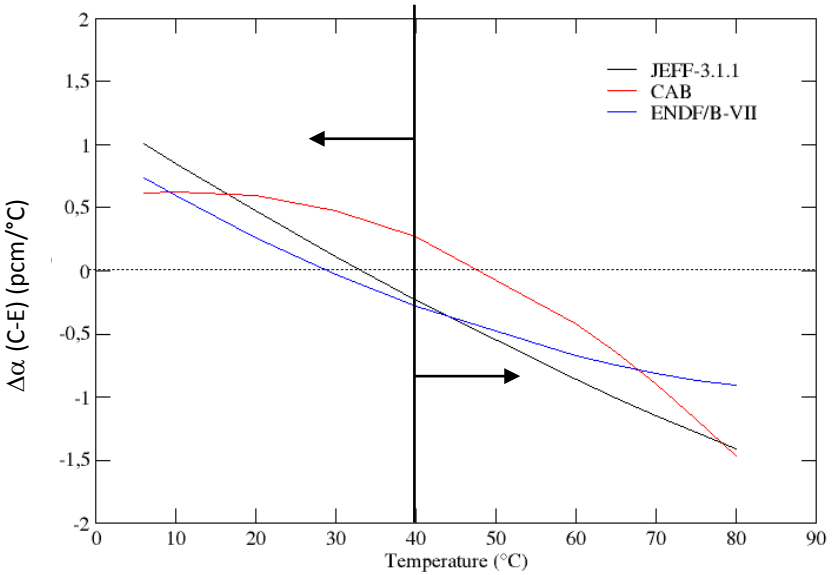
✓ Mean difference between ENDF/B-VII and JEFF-3.1.1 = +65 pcm.

RESULTS: MISTRAL-1

Mistral-1 reactivity temperature coefficient error $\Delta\alpha$(pcm/°C)

- TRIPOLI4 code + JEFF-3.1.1
- TRIPOLI4 code + CAB
- TRIPOLI4 code + ENDF/B-VII.1
- APOLLO2 code + JEFF-3.1.1

$$\Delta\alpha = \frac{d(\Delta\rho)}{dT}$$



Mistral - 1 RTC error (C-E) pcm/°C			
	6°C to 40°C	40°C to 80°C	6°C to 80°C
Uncertainty	*±0.4*	*±0.4*	*±0.3*
JEFF - 3.1.1	+0.4	-0.8	-0.3
CAB	+0.5	-0.5	+0.0
ENDF/B-VII.1	+0.2	-0.6	-0.3

✓ Same tendency for all TSL.

✓ T<40°C ⇒ spectral component of the error in RTC correctly accounted → $\sigma_\gamma/\sigma_f(U^{235})$ *ok*

✓ T>60°C ⇒ underestimation of RTC (water density change effect).

✓ Target accuracy of 1 pcm/°C for RTC error is achieved

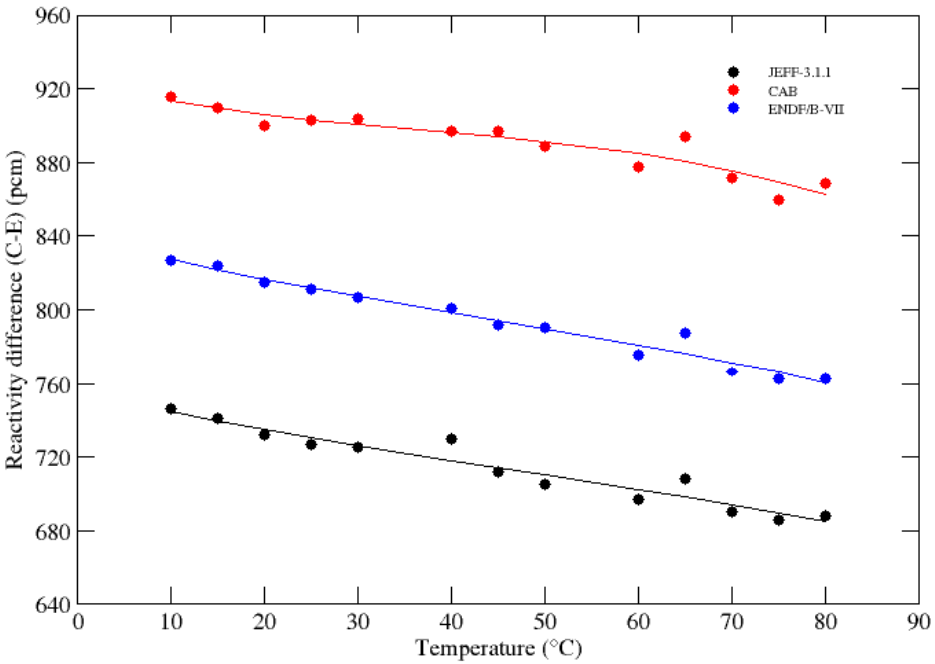
RESULTS: MISTRAL-2

Mistral-2 reactivity difference C-E $\Delta\rho$(pcm)

- TRIPOLI4 code + JEFF-3.1.1
- TRIPOLI4 code + CAB
- TRIPOLI4 code + ENDF/B-VII.1

Third order polynomial fitting

$$\Delta\rho = AT^3 + BT^2 + CT + D$$



Still same tendency as Mistral-1: overestimation of calculated reactivity for CAB and ENDF/B-VII TSL.

✓ Mean difference between CAB and JEFF-3.1.1 = +180 pcm (more accentuated for MOX??)

✓ Mean difference between ENDF/B-VII and JEFF-3.1.1 = +80 pcm (equivalent to Mistral-1).

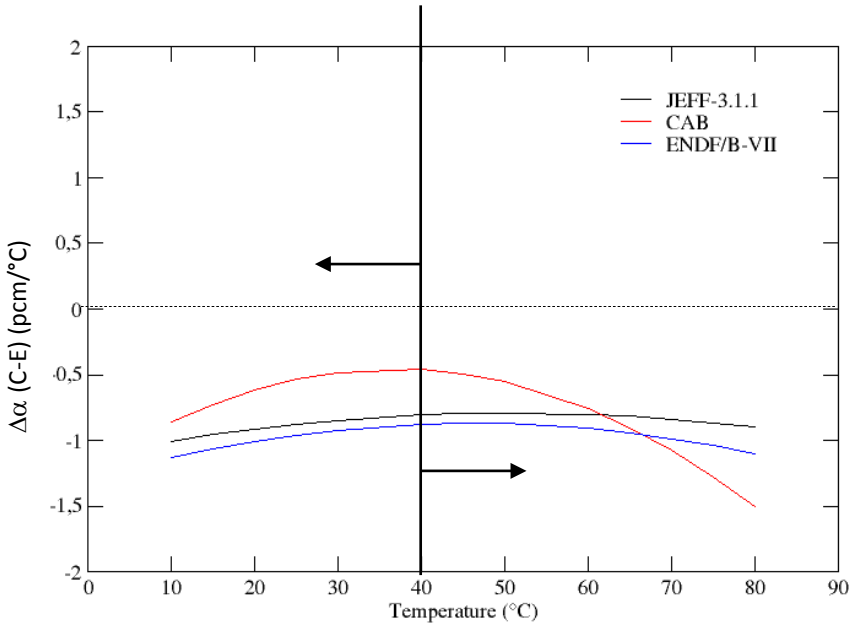
RESULTS: MISTRAL-2

Mistral-2 reactivity temperature coefficient error $\Delta\alpha$(pcm/°C)

- TRIPOLI4 code + JEFF-3.1.1
- TRIPOLI4 code + CAB
- TRIPOLI4 code + ENDF/B-VII.1
- APOLLO2 code+JEFF-3.1.1

$$\Delta\alpha = \frac{d(\Delta\rho)}{dT}$$

Mistral - 2 RTC error (C-E) pcm/°C			
	10°C to 40°C	40°C to 80°C	10°C to 80°C
Uncertainties	*±0.4*	*±0.4*	*±0.3*
JEFF - 3.1.1	-0.9	-0.8	-0.8
CAB	-0.6	-0.8	-0.7
ENDF/B-VII.1	-1.0	-0.9	-1.0



✓ Still the same tendency for all TSL.

✓ Underestimation of RTC throughout all temperature range, for all cases.

✓ No appreciable difference in behavior at low and high temperature.

✓ Mean error in RTC from 10°C to 80°C still below 1 pcm/°C.

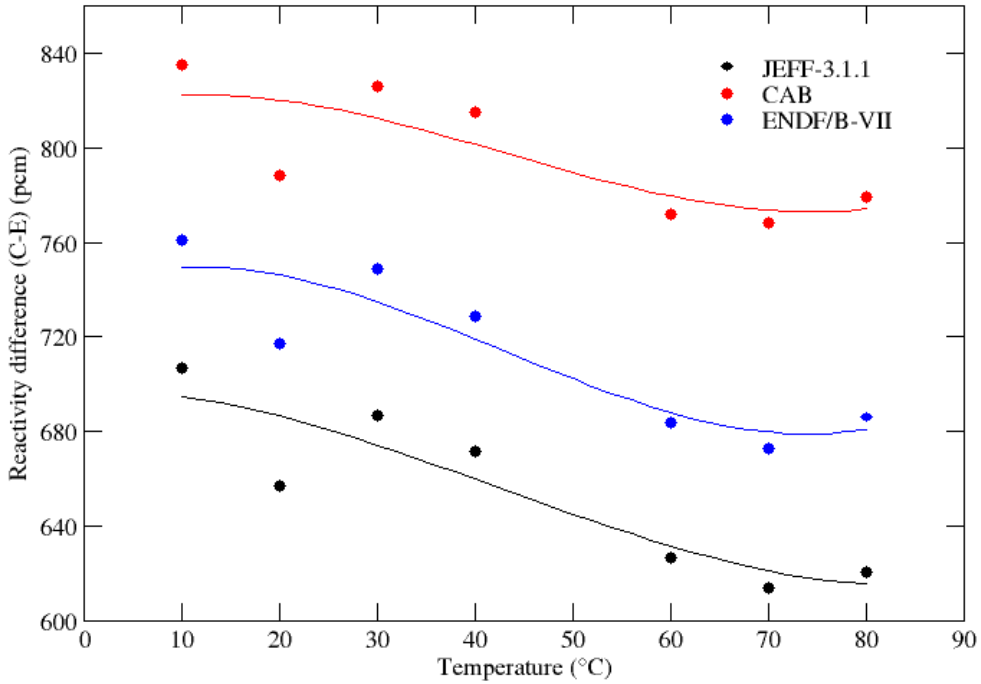
RESULTS: MISTRAL-3

Mistral-3 reactivity difference C-E $\Delta\rho$(pcm)

- TRIPOLI4 code + JEFF-3.1.1
- TRIPOLI4 code + CAB
- TRIPOLI4 code + ENDF/B-VII.1

Third order polynomial fitting

$$\Delta\rho = AT^3 + BT^2 + CT + D$$



Same trend as Mistral-2.

✓ Mean difference between CAB and JEFF-3.1.1 = +140 pcm. (equivalent to Mistral-2)

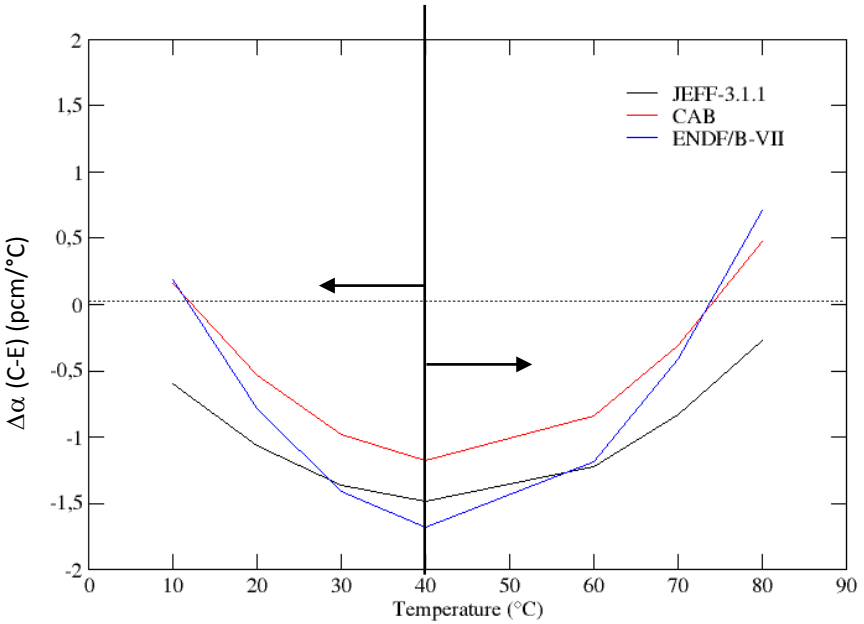
✓ Mean difference between ENDF/B-VII and JEFF-3.1.1 = +60 pcm (same result as Mistral-1 and Mistral-2).

RESULTS: MISTRAL-3

Mistral-3 reactivity temperature coefficient error $\Delta\alpha$(pcm/°C)

- TRIPOLI4 code + JEFF-3.1.1
- TRIPOLI4 code + CAB
- TRIPOLI4 code + ENDF/B-VII.1
- APOLLO2 code+JEFF-3.1.1

$$\Delta\alpha = \frac{d(\Delta\rho)}{dT}$$



Mistral - 3 RTC error (C-E) pcm/°C			
	10°C to 40°C	40°C to 80°C	10°C to 80°C
Uncertainties	*±0.5*	*±0.5*	*±0.4*
JEFF - 3.1.1	-1.2	-1.1	-1.1
CAB	-0.7	-0.7	-0.7
ENDF/B-VII.1	-1.0	-1.0	-1.0

✓ Still the same tendency for all TSL.

✓ Like $\Delta\alpha$ in Mistral-2, there is underestimation of RTC throughout all temperature range, except at 10°C and 80°C (biggest uncertainties in these measures).

✓ For MOX lattices, the spectral component of the RTC error is correctly predicted (T<40°C) ➡ supports change in $\sigma_\gamma/\sigma_f(Pu^{239})$ in thermal range of JEFF-3.1 library.

CONCLUSIONS

✓ Mean RTC error in pcm/°C (10°C – 80°C)

- Mistal-1benchmark (representative of a UOX slightly over moderated lattice).
  - JEFF-3.1.1 = -0.3 ± 0.3
  - ENDF/B-VII.1 = -0.5 ± 0.3
  - CAB model = 0.0 ± 0.3
- Mistal-2benchmark (representative of a MOX slightly over moderated lattice).
  - JEFF-3.1.1 = -0.8 ± 0.3
  - ENDF/B-VII.1 = -1.0 ± 0.3
  - CAB model = -0.7 ± 0.3
- Mistal-3benchmark (representative of a MOX over moderated lattice).
  - JEFF-3.1.1 = -0.9 ± 0.4
  - ENDF/B-VII.1 = -0.8 ± 0.4
  - CAB model = -0.5 ± 0.4

✓ The spectral component of the discrepancy in the reactivity coefficient remains between acceptable margins for Mistral-2 and Mistral-3.

✓ A different approach for creating TSL files, molecular dynamics simulation, was assessed. For all tested TSL, similar trends are achieved → IKE model used in JEFF - 3.1.1 library is quite satisfactory.

Slight improvements of the integral trends by using the TSL data files obtained with the CAB model