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Biases ans uncertainties in Doppler reactivity worth calculations

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DE LA RECHERCHE À L'INDUSTRIE

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Biases and Uncertainties in Doppler reactivity worth calculations

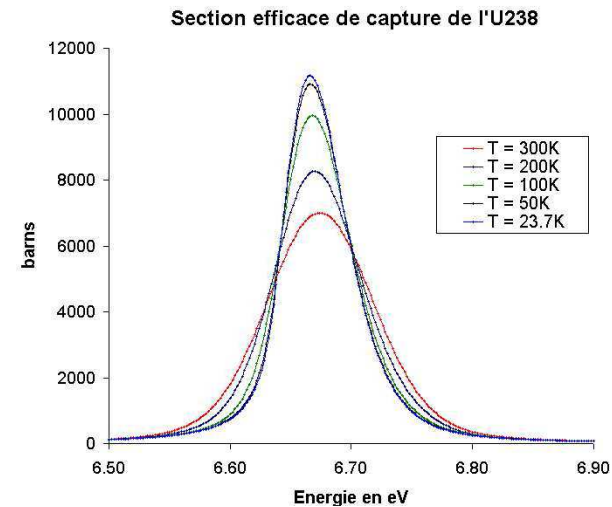
UAM-9 Workshop

20-22 May 2015

A. Santamarina, D. Bernard

➤ **The Fuel Reactivity Temperature Coefficient**

➤ **Challenges and biases in Doppler deterministic calculations**



➤ **Uniform effective temperature T_{eff} to account for pellet Temperature profile**

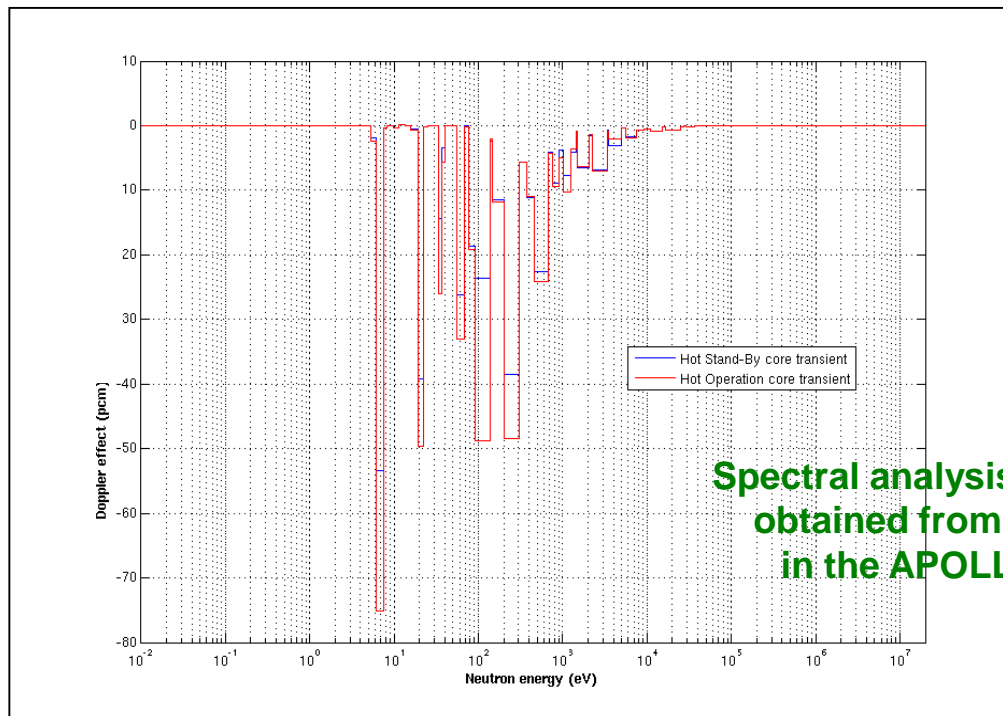
➤ **Effective temperature T_{eff}^{RI} to account for Crystal Lattice binding in UO₂ fuel**

➤ **Up-scattering effect in resonances**

➤ **Recommendations and Conclusion : Uncertainty in standard Doppler calculations**

The Fuel Reactivity Temperature Coefficient (FTC)

- 90% of the Fuel Temperature reactivity worth is due to $^{238}\text{U}(n,\gamma)$ broadening
 - ^{235}U component is weak (0.1%), due to cancellation of (n,f) and (n, γ) contributions
 - $^{16}\text{O}(n,n)$ positive component amounts to 10 % (thermal spectrum shift effect).
-
- 35% of $^{238}\text{U}(n,\gamma)$ Doppler effect comes from the first 3 resonances broadening.
 - 60% of $^{238}\text{U}(n,\gamma)$ Doppler effect comes from $E_n = [60\text{eV}; 2\text{keV}]$, unless capture rate is only 20%

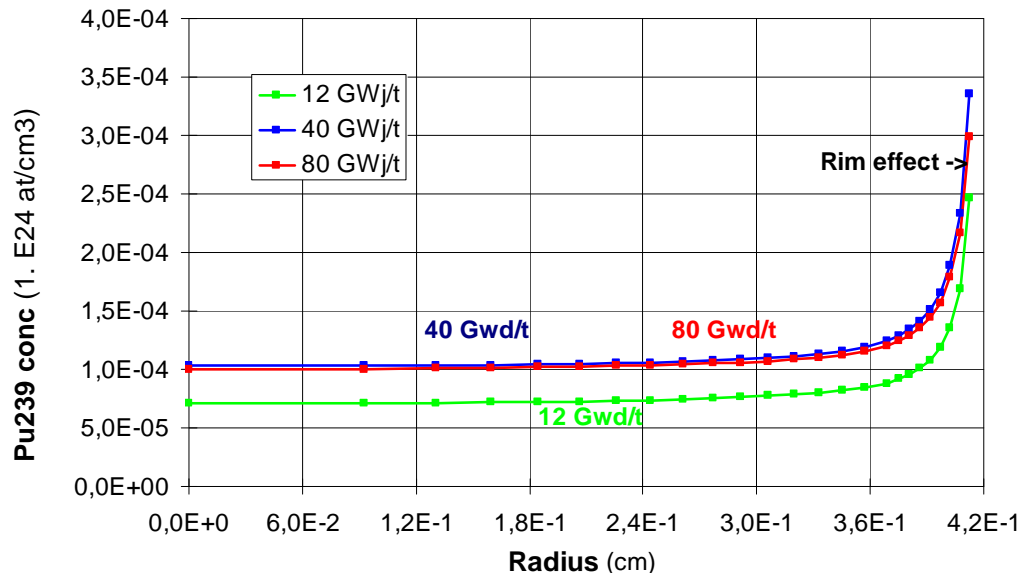


Spectral analysis of ^{238}U Doppler worth
obtained from Perturbation Theory
in the APOLLO2 transport code

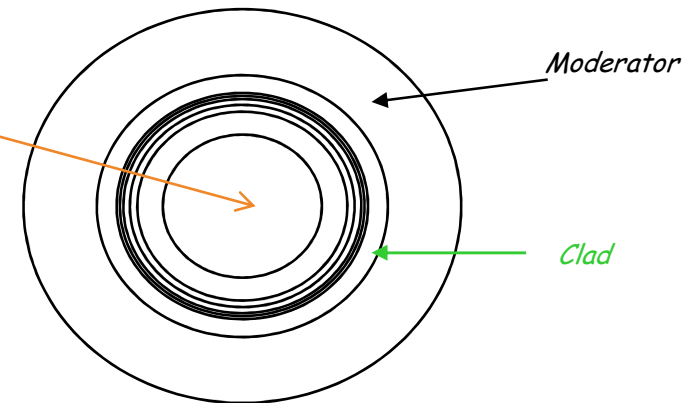
- The Fuel Reactivity Temperature Coefficient
- **Challenges and biases in Doppler deterministic calculations**
- Uniform effective temperature T_{eff} to account for pellet temperature profile
- Effective temperature T_{eff}^{RI} to account for Crystal Lattice binding in UO₂ fuel
- Up-scattering effect in resonances
- **Recommendations and Conclusion : Uncertainty in standard Doppler calculations**

Spatial self-shielding

- Resonance energetic self-shielding comes with fuel rod spatial self-shielding
- ^{238}U resonances are more self-shielded at the center of fuel pellet (shadow effect)
 \Rightarrow ^{238}U capture and ^{239}Pu build-up is higher on pellet boundary \Rightarrow thermomechanic 'rim effect' (Bu is twice !)



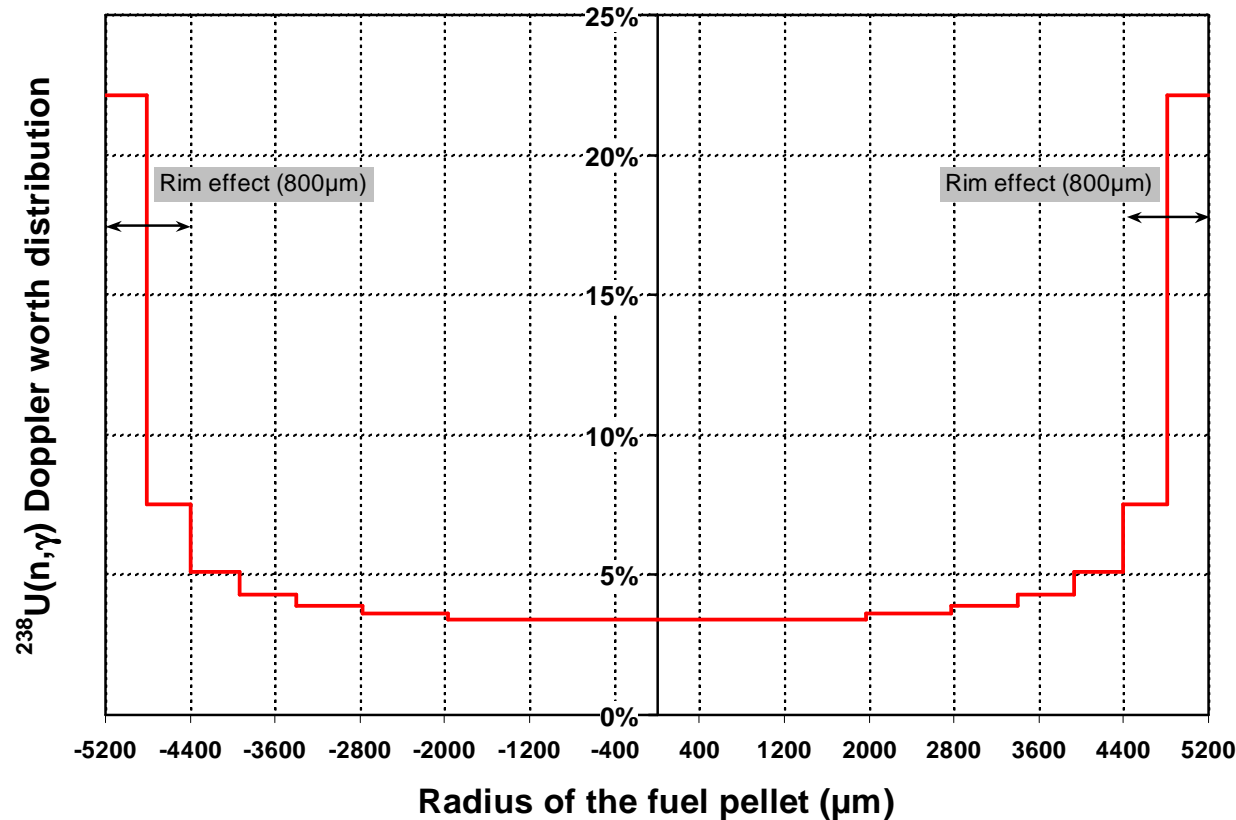
Fuel :
4 'self-shielded regions' needed



- Space-dependent self-shielding is required for accurate LWR calc.
- **4 concentric rings :**
5%, 15%, 30%, 50% in volume

Exact Perturbation Theory supplies the following spatial informations:

- 60% of the $^{238}\text{U}(n,\gamma)$ Doppler effect comes from the first 800 μm of the pellet
- The rim effect is significant in the Doppler worth:
both $\tau^{238}\text{U}(n,\gamma)$ and $\Delta\tau^{238}\text{U}(n,\gamma)$ present a non-uniform spatial distribution



Thus, the temperature model have to take into account the actual surface temperature.

FTC components in LWR UO2 assemblies

Isotopic components obtained from Perturbation Theory : $\delta\rho = \frac{1}{I_f} \langle \phi^*, \delta H \phi \rangle$

The Rim effect induces 30% Doppler contribution for the 5% pellet periphery
 ⇒ temperature at fuel surface should be accounted for

UOX fuel	Fuel region 1	Fuel region 2	Fuel region 3	Fuel region 4	Full Fuel
²³⁸ U	-42.9	-36.2	-38.2	-29.4	-146.7
²³⁵ U	+0.1	0.0	0.0	0.0	+0.1
¹⁶ O					+12.9
Total	-42.8	-36.2	-38.2	-29.4	-133.7

Thermal spectrum shift due to temperature of fuel's Oxygen

(n,γ)	(n,f)	(n,n)	$\sigma_s^{g' \rightarrow g}$	Total
-148.2	+0.6	+1.5	+12.4	-133.7

1st calculation challenge : space-dependent self-shielding formalisms require crossed probability tables to account for non-uniform temperatures

FTC components in LWR MOX assemblies

- ^{238}U broadened resonance contribution almost the same in MOx and UOx fuels
- **Doppler level increases by about 30% due to ^{240}Pu broadening**

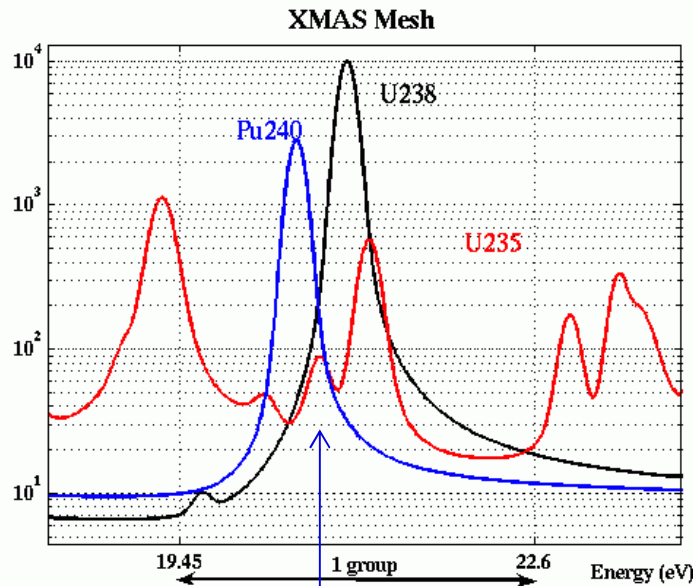
MOX Sample	Fuel region 1	Fuel region 2	Fuel region 3	Fuel region 4	Full Fuel
^{238}U	-42.9	-36.1	-42.1	-31.7	-152.8
^{240}Pu	-23.2	-22.8	-19.0	-6.6	-71.6
^{239}Pu	-0.6	-0.2	-0.1	0.0	-0.9
^{242}Pu	-0.5	-0.3	-0.1	0.0	-0.9
^{241}Pu	+0.1	+0.1	0.0	0.0	+0.2
^{235}U	+0.1	0.0	0.0	0.0	+0.1
^{16}O					-6.6
Total	-67.0	-59.3	-61.3	-38.3	-232.5

^{239}Pu : cancellation between (n,f) and (n, γ) strong components

Thermal spectrum shift due to temperature of fuel's Oxygen : becomes negative

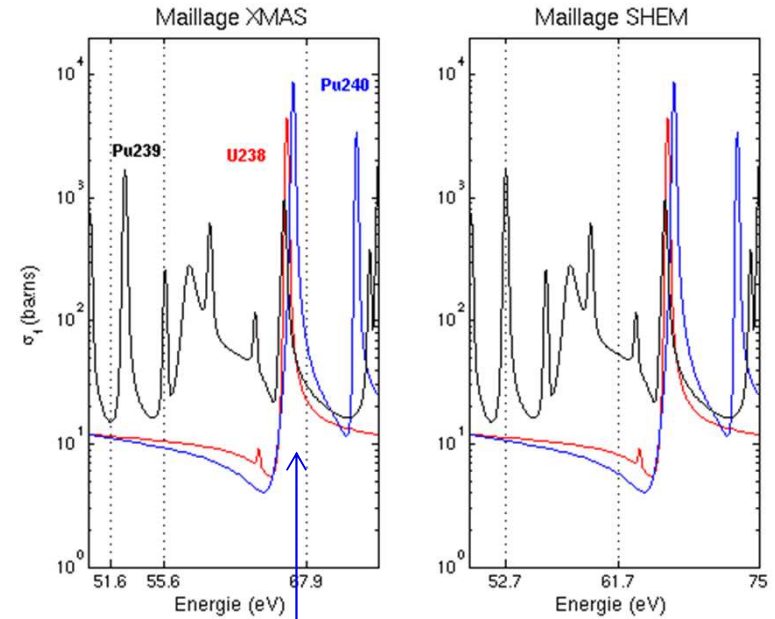
(n, γ)	(n,f)	(n,n)	$\sigma_s^{g' \rightarrow g}$	Total
-272.9	+42.4	+4.6	-6.6	-232.5

Resonance overlap in MOX: 2nd Doppler calc challenge



$^{238}\text{U}/^{240}\text{Pu}/^{235}\text{U}$ overlap at $E=20\text{eV}$

Mutual shielding taken into account by the fine mesh of SHEM

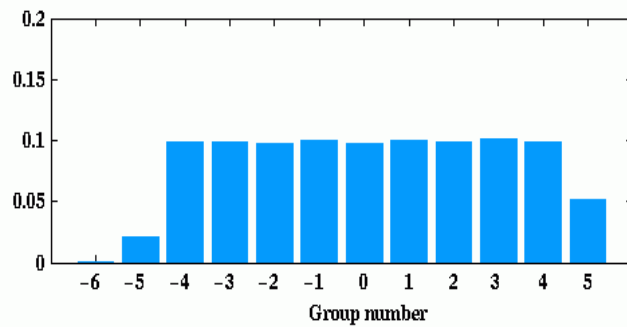
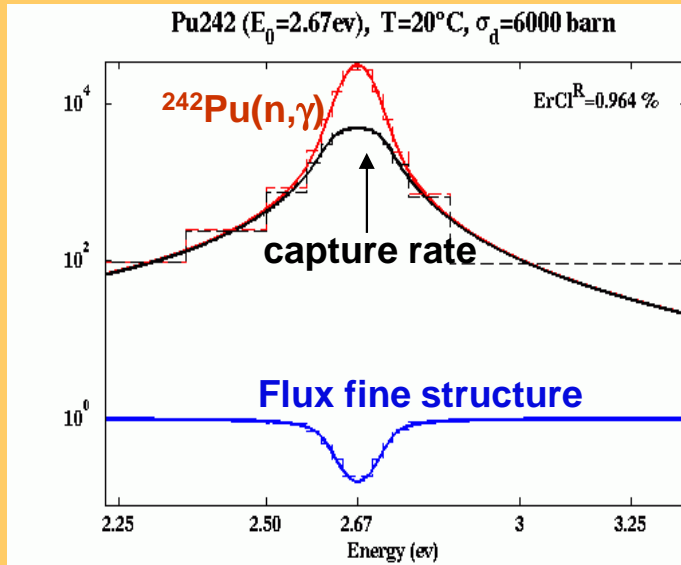


$^{238}\text{U}/^{240}\text{Pu}/^{239}\text{Pu}$ overlap at $E=66\text{eV}$

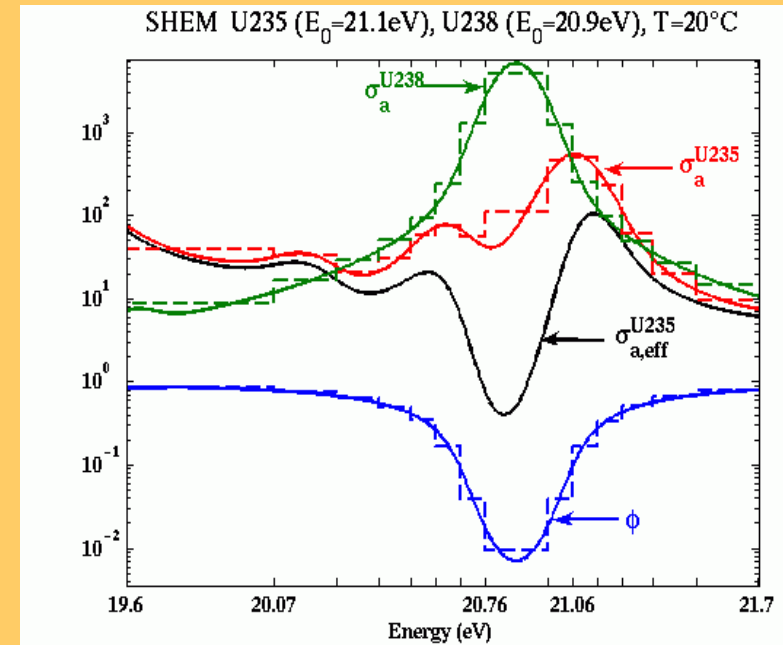
Mutual shielding taken into account by SHEM-361g (used for Sub-Group method)

D. Bernard - A. Santamarina, Conf. M&C2003, Gatlinburg, April 6-11

Rigorous method:
iterative algorithm for optimal discretisation



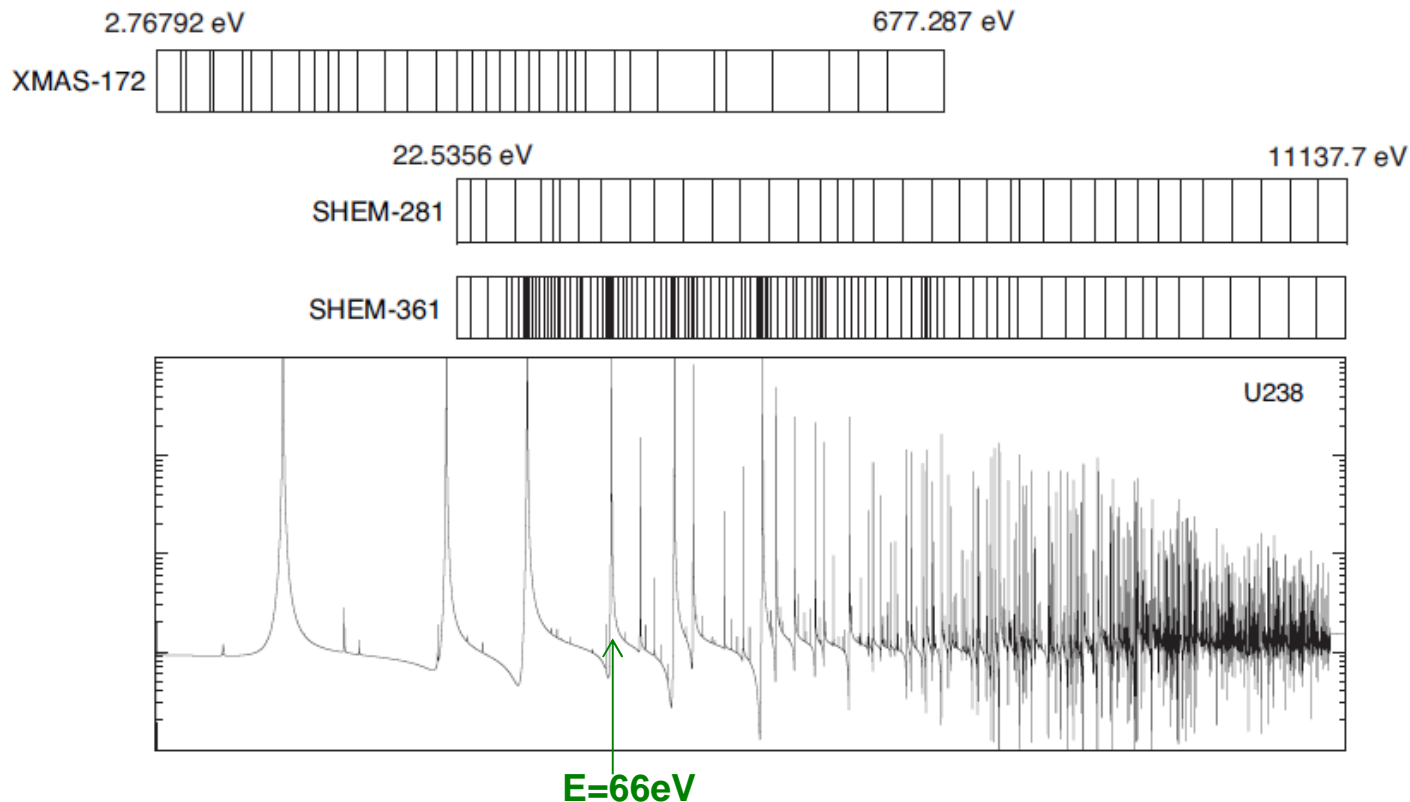
U238/U235 overlap 20eV



N. Hfaiedh - A. Santamarina, Conf. M&C2005, Avignon, Sept 12-15

SHEM-361g for Sub-Group self-shielding

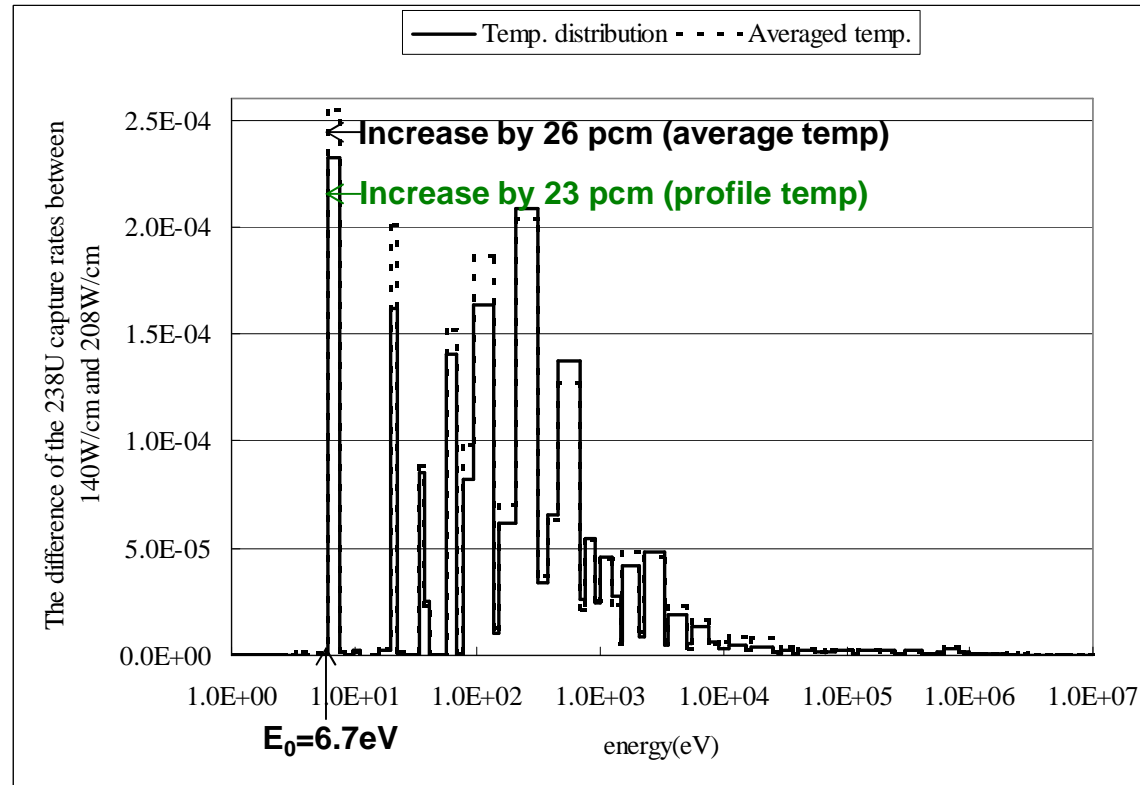
- From SHEM-281g to SHEM-361g to allow NR assumption in SG method
⇒ refine discretization between 24eV and 3keV → 80 supplementary groups



- Moreover, resonance overlap ^{238}U / ^{239}Pu is explicitly described

- The Fuel Reactivity Temperature Coefficient
- Challenges and biases in Doppler deterministic calculations
- **Uniform effective temperature T_{eff} to account for pellet temperature profile**
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Spectral distribution of the ^{238}U capture increase with fuel temperature



The average temperature model overestimates the ^{238}U capture increase particularly in the first large resonances (because true temperature is lower in the rim)

Consideration of temperature profile (cylindrical pellet)

- At least, Rowlands formula should be used :

$$T_{eff} = \frac{4}{9}T_c + \frac{5}{9}T_s$$

- We propose the more accurate effective temperature (also suited for transients):

$$T_{eff} = \bar{T}_{therm} - \frac{1}{18}(T_c - T_s)$$

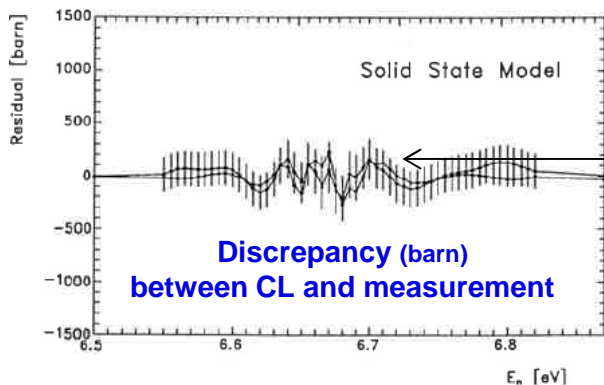
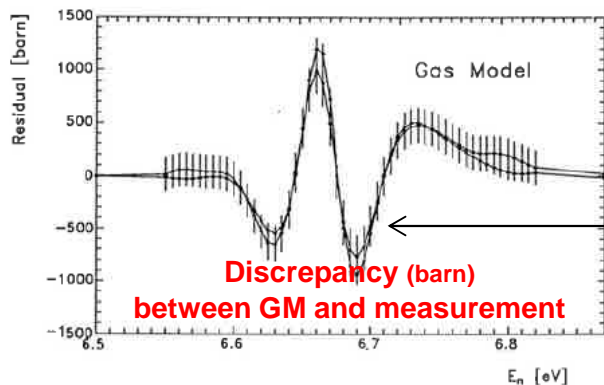
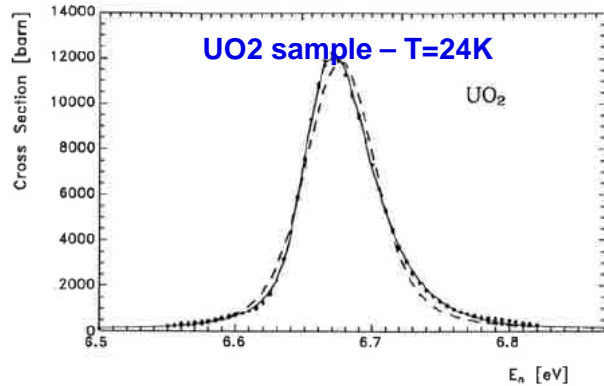
with: $\bar{T}^{therm} = \int T(r) dr / \int dr$

A. Santamarina, Report CEA/SPRC/02-03, 2002

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Doppler broadening of ^{238}U in UO_2 fuels

Gelina meas. of resonance $E^{U^{238}}=6.7\text{eV}$



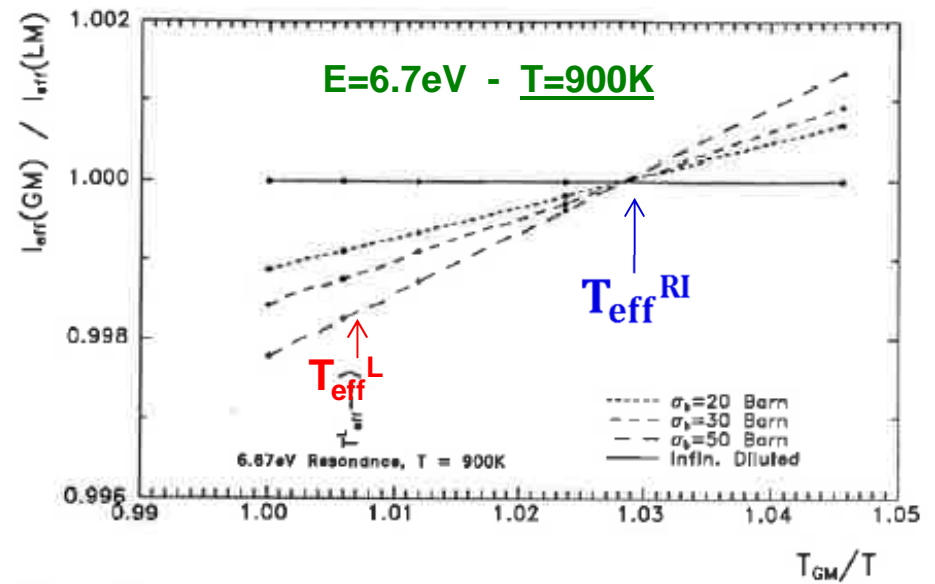
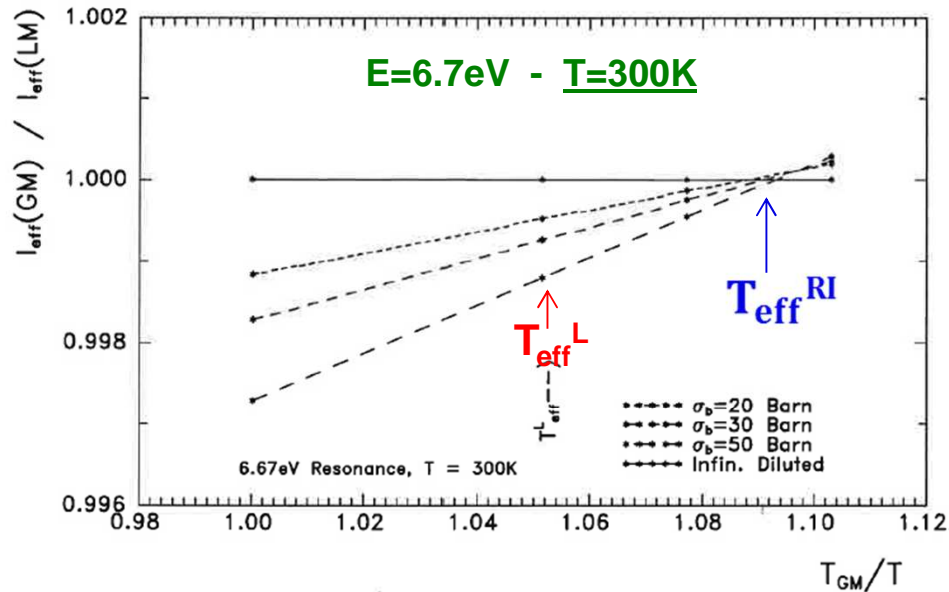
- Thermal motion of fuel atoms → Free Gas Model (GM)
- **But** atoms are actually embedded in a solid state
- Lamb has shown that in a 'weak binding' assumption, the Doppler broadening can be approximated by GM, using an effective temperature $T_{\text{eff}}^L (= \langle \mathcal{E} \rangle / k_B)$
- The 'weak binding' approx is not relevant for $E_n < 1\text{keV}$
 ⇒ **GM using T_{eff}^L does not fit ^{238}U first resonances**
- We use **Cristal Lattice Model(LM)**, with 2 lattice vibration frequencies (acoustic and optical mode):

$$\rho(\hbar\omega) = 0.9 \cdot \delta(\hbar\omega - 13.4\text{meV}) + 0.1 \cdot \delta(\hbar\omega - 51.8\text{meV})$$
 ⇒ **describe accurately ^{238}U resonances in UO_2**

A. Meister et al., Conf. ND'97, Trieste, May 19-24

Determination of the actual effective temperature

- The real effective temp $T_{\text{eff}}^{\text{RI}}$ has to preserve the ^{238}U capture rate (thus I_{eff} Res. Integral)
- Solving the flux fine structure equation (both for σ_{238}^{GM} and σ_{238}^{LM}) supplies I_{eff}
- Then we solved the following equation : $I_{\text{eff}}^{\text{GM}}(T_{\text{eff}}^{\text{RI}}) = I_{\text{eff}}^{\text{LM}}(T)$

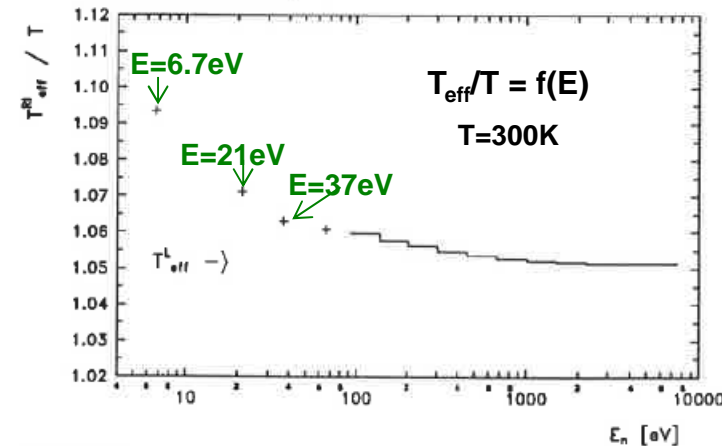


- $T_{\text{eff}}^{\text{RI}}$ is quite independent from Geometry/Concentration

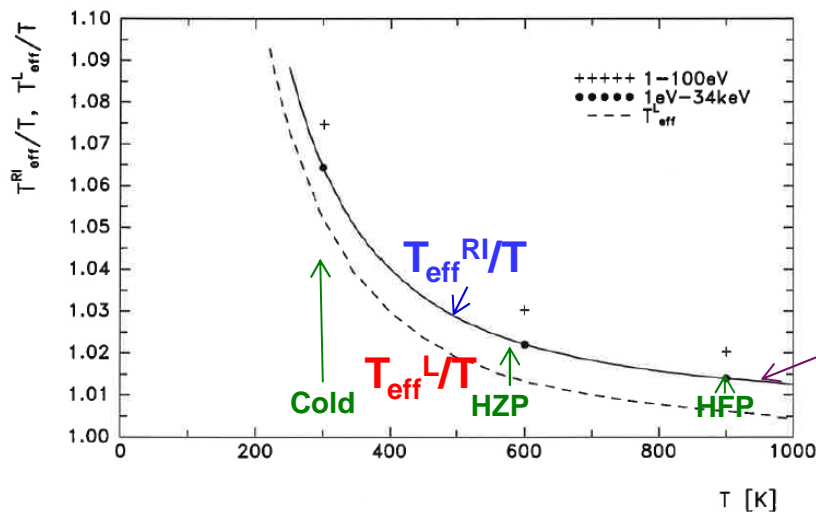
A. Meister and A. Santamarina, Conf. PHYSOR98, Long Island, May 19-24

The accurate effective temperature $T_{\text{eff}}^{\text{RI}}$

- $T_{\text{eff}}^{\text{RI}}$ depends strongly on resonance energy:
 - In large resonances $E < 100$ eV, the solid state effect is stronger than Lamb ($T_{\text{eff}}^{\text{RI}} > T_{\text{eff}}^{\text{L}}$)
 - Above 1 keV, $T_{\text{eff}}^{\text{RI}}$ tends towards $T_{\text{eff}}^{\text{L}}$



➤ Therefore we proposed $T_{\text{eff}}^{\text{RI}}/T$ corrections for the various energy domains



➤ However, the I_{eff} preservation on the whole resonance range (useful for **thermal reactors**) gives the **Meister-Santamarina formula** ($T < 1000\text{K}$):

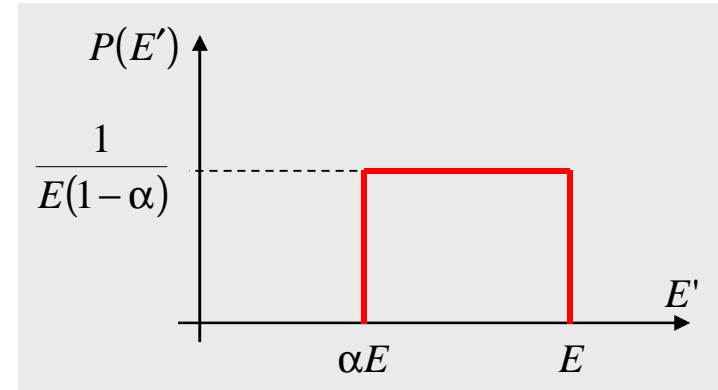
$$\frac{T_{\text{eff}}}{T} = 1 + \frac{8.6}{T} + \frac{3100}{T^2} \quad (T \text{ en K})$$

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- **The Asymptotic Kernel (AK): T = 0K - target at rest**

$$P(E \rightarrow E') dE' = \frac{1}{(1-\alpha)E} dE' \quad \text{with} \quad \alpha = \left(\frac{A-1}{A+1} \right)^2$$

→ Used in deterministic resonance self shielding calculation



- **Sampling the Velocity of the Target (SVT) → Used in Monte Carlo codes**

$$\sigma_s(E \rightarrow E', \omega \rightarrow \omega', T) = \frac{1}{v} \int_{V: v_r > 0} v_r \sigma_s(v_r, 0) P(v, V \rightarrow E', \omega') M_T(V) dV$$

joint Probability Density: $p(V, \mu_t) = \frac{\sigma_s(v_r, 0) v_r g(V)}{2\sigma_s(E, T) v}$ $\sigma_s(v_r) = \text{constant}$ + $\Rightarrow p(V, \mu_t) \propto \frac{\sqrt{v^2 + V^2 - 2\mu_t V v}}{v + V} [V^3 e^{-\beta^2 V^2} + v V^2 e^{-\beta^2 v^2}]$
Gaz Model

SVT algorithm : μ uniformly sampled in [-1;+1] - target velocity V sampled - then Rejection applied to sampled pair (μ_i, V_i)

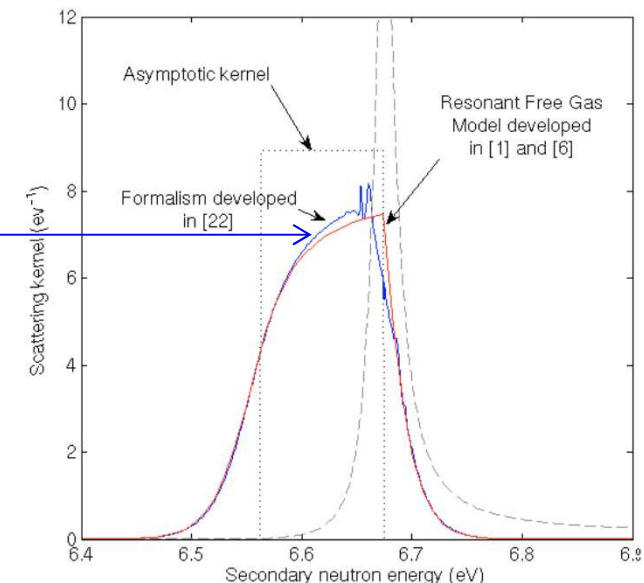
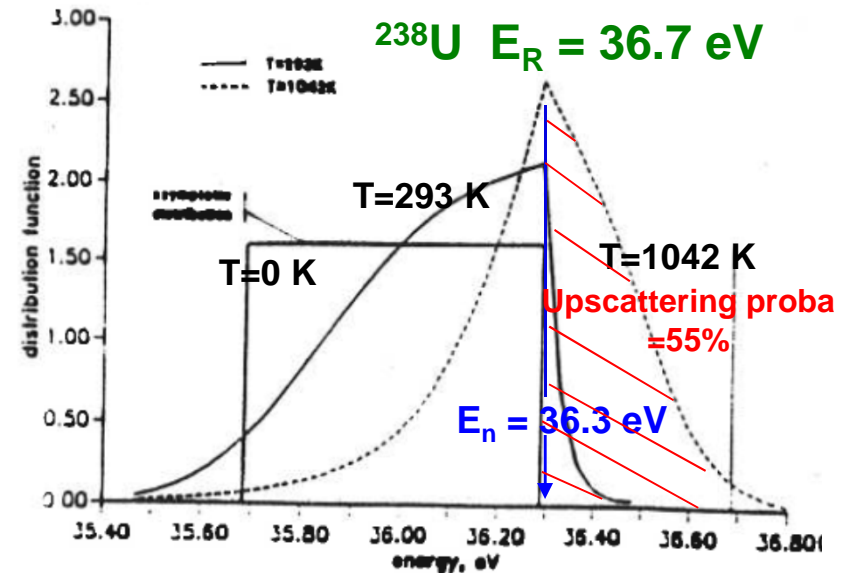
$$R_{SVT} = \frac{\sqrt{v^2 + V^2 - 2\mu_t V v}}{v + V} = \frac{v_r}{v + V} \leq 1$$

When (μ_i, V_i) known, the two-body kinematic equations for energy and momentum are solved \Rightarrow scattered neutron properties

Resonance Elastic Kernel and Up-scattering

- ▶ **Ouisloumen & Sanchez (NSE 1991)** : energy distribution of scattered neutrons at resonance energy is strongly affected by nuclei thermal motion
- ▶ **Bouland & Rowlands (Conf ND1994)** developed the TRAMP code and quantified resonant scattering effect. At LWR HZP:
 - +1% on ^{238}U capture rate
 - +9% on Doppler coefficient
- ▶ **A. Courcelle, R. Dagan, J. Rowlands** tried to consider **solid state effects on resonance scattering** : small impact vs GM

Dagan, Rowlands, Courcelle (Conf ND2007, Nice)



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	Cold → HZP 293K 560K	HZP → HFP 560K 900K
Flat Temperature Profile	0%	+8.0%
UO ₂ binding : GM vs LM	+4.0%	+1.3%
AK vs Resonant Upscat	-6.0%	-9.4%

- It is mandatory to take into account the temperature profile at LWR operating condition
- **Crystal binding** in UO₂ fuels is particularly important at **room temperature**
- On the contrary, **resonant up-scattering** is particularly **important for large linear power** (however, the -9% AK bias on Doppler worth is assessed in the Free Gaz approximation)

Uncertainty in FTC neutronic calculations

- Using the previous recommended T_{eff} and the resonant scattering kernel, the **calculation uncertainty components** (1σ) are:

Flat Temp	UO ₂ binding	Up-scattering	Total Unc. 1σ
2%	0.3%	3%	3.6%

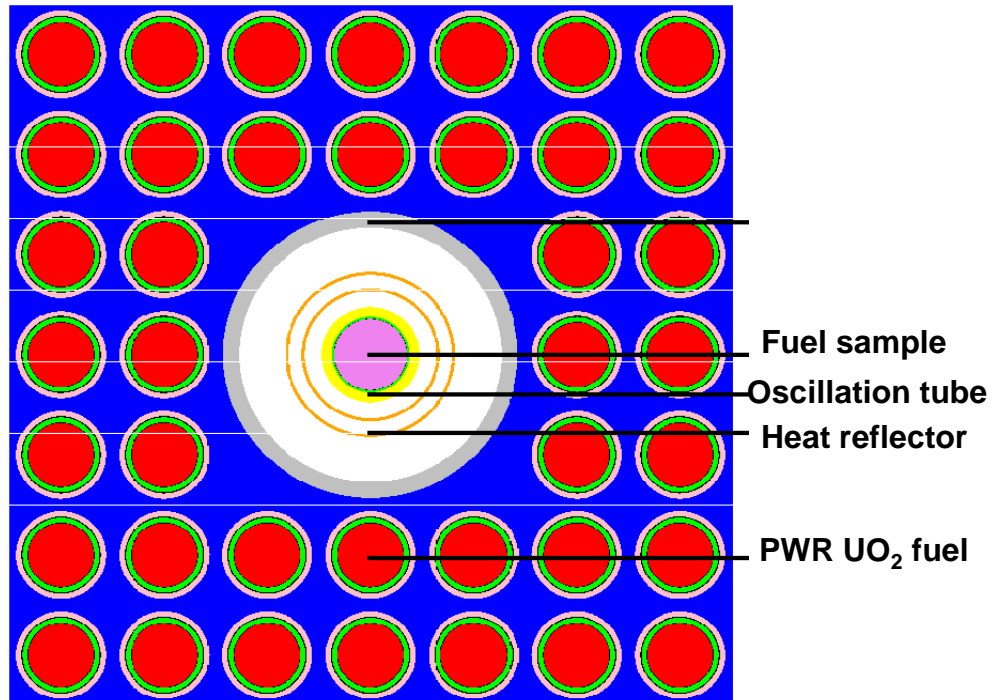
- **FTC uncertainty due to nuclear data is small:**

²³⁸ U(n,n')	H(n,n)	²³⁸ U Γ_n, Γ_γ	Total Unc. 1σ
0.6%	0.5%	1.0%	1.3%

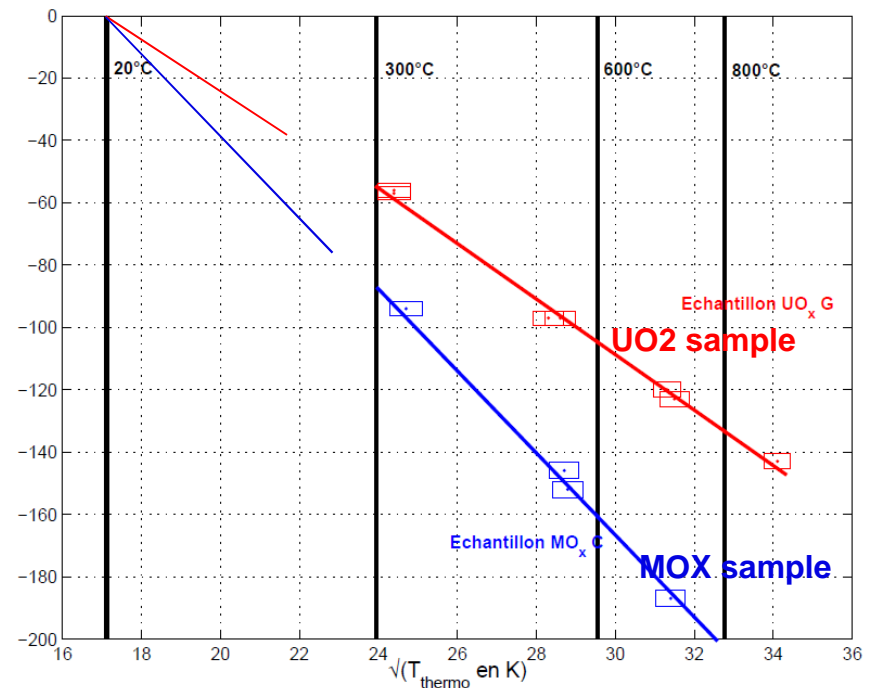
⇒ **The total uncertainty on FTC best-estimate calculation amounts to 4%**

Conclusions

- Modeling assumptions in FTC neutronic calculation generate high biases : **2% to 10%**
- Total uncertainty (bias uncert + ND) in FTC best-estimate calculation amounts to **4%(1 σ)**
- Supplementary deterministic biases can occur in MOX due to resonance shielding
- Fuel Temp Coeff measured in the PWR lattice at MINERVE in 1978 from 20°C up to 900°C
4 UO₂ fuel samples ($E_{U235} = 0.2; 0.7; 3.0; 5.1\%$) & 6 MOX fuel samples
⇒ TRIPOLI4-DRBC: **(C-E)/E = +3% \pm 3%(1 σ)**



Measured Fuel Temp. reactivity worth vs \sqrt{T}



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Merci pour votre attention