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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

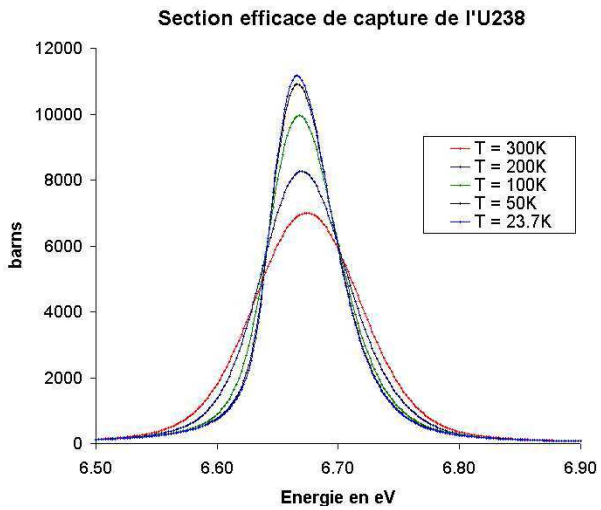
UAM-9 Workshop

20-22 May 2015

A. Santamarina, D. Bernard

Summary

- **The Fuel Reactivity Temperature Coefficient**
- **Challenges and biases in Doppler deterministic calculations**

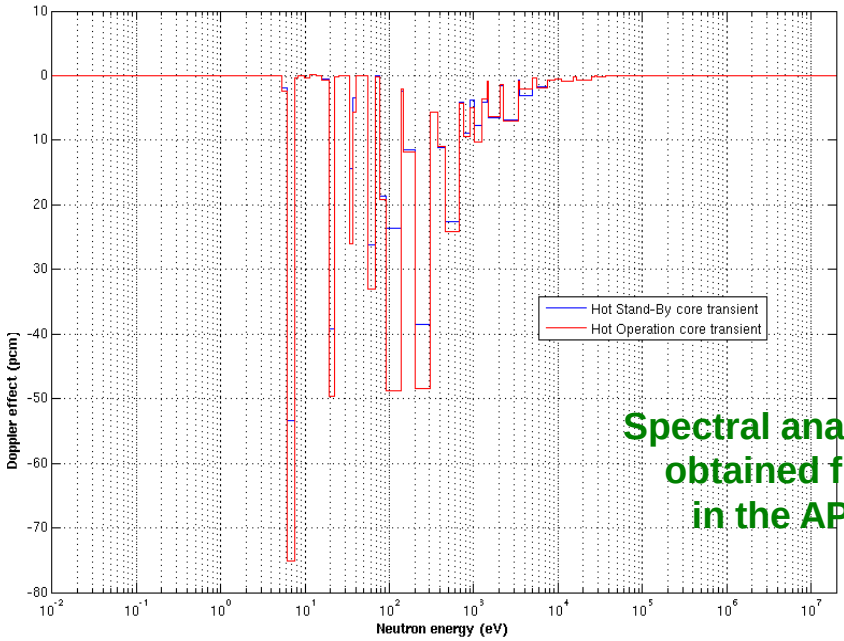


- **Uniform effective temperature Teff to account for pellet Temperature profile**
- **Effective temperature $Teff^{RI}$ to account for Crystal Lattice binding in UO2 fuel**
- **Up-scattering effect in resonances**
- **Recommendations and Conclusion : Uncertainty in standard Doppler calculations**

The Fuel Reactivity Temperature Coefficient (FTC)

- **90% of the Fuel Temperature reactivity worth is due to ^{238}U(n,γ) broadening**
- **^{235}U component is weak (0.1%), due to cancellation of (n,f) and (n,γ) contributions**
- **^{16}O(n,n) positive component amounts to 10 % (thermal spectrum shift effect).**

- **35% of ^{238}U(n,γ) Doppler effect comes from the first 3 resonances broadening.**
- **60% of ^{238}U(n,γ) Doppler effect comes from E_n = [60eV;2keV],**unless capture rate is only 20%



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

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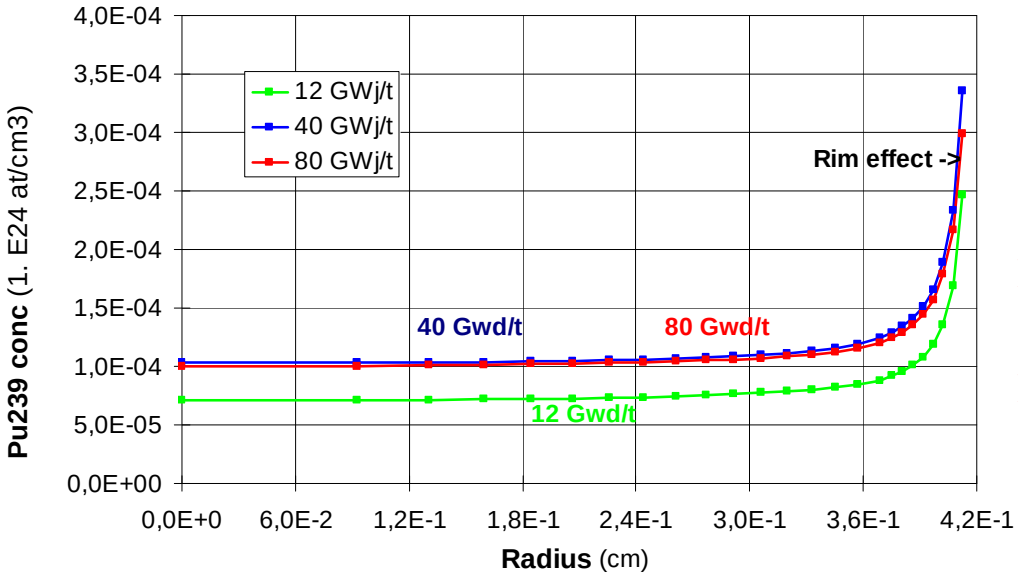
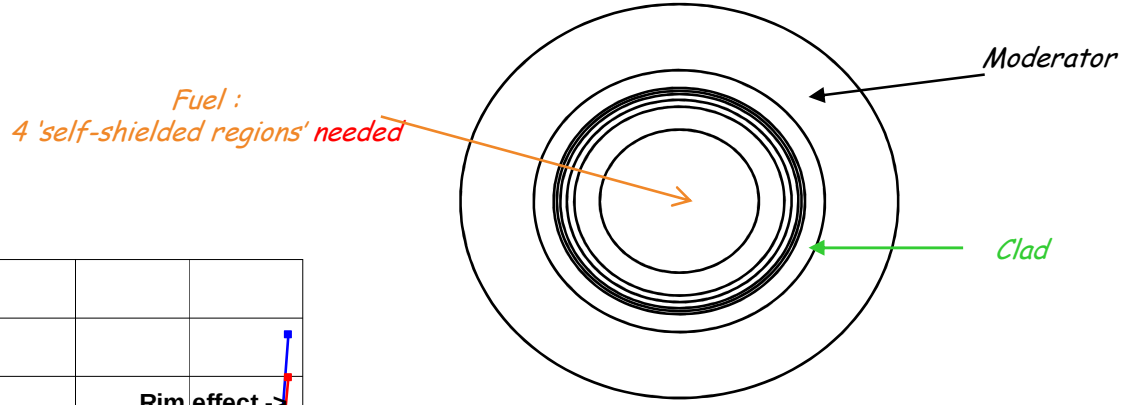
Spatial self-shielding

- 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 !)





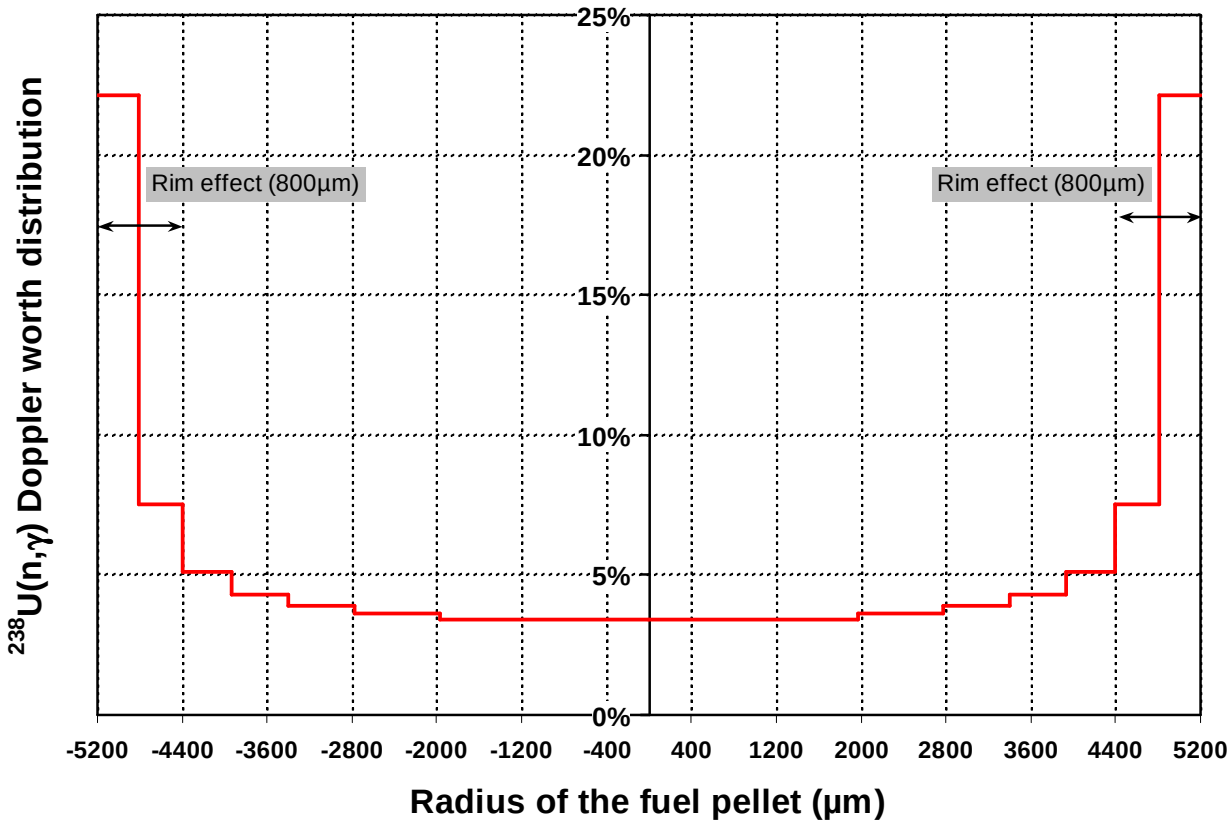
- Space-dependent self-shielding is required for accurate LWR calc.
- **4 concentric rings : 5%, 15%, 30%, 50% in volume**

Rim effect

***Exact Perturbation Theory** supplies the following spatial informations:*

- **60% of the $^{238}U(n,\gamma)$ Doppler effect comes from the first 800µm of the pellet**

- The rim effect is significant in the Doppler worth:
  both $\tau^{238}_{U(n,\gamma)}$ and $\Delta\tau^{238}_{U(n,\gamma)}$ 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 : $\delta\rho = \frac{1}{I_f} < \phi^*, \delta H \phi >$

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)	$\sigma_s^{g'\to g}$	Total
-148.2	+0.6	+1.5	+12.4	**-133.7**

1rst 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

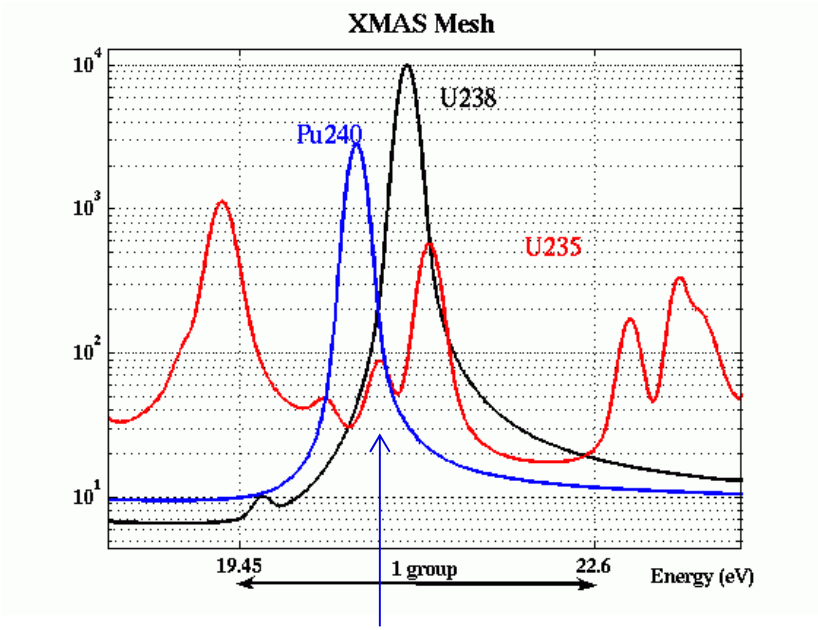
MOX Sample	Fuel region 1	Fuel region 2	Fuel region 3	Fuel region 4	Full Fuel
^{238}U	-42.9	-36.1	-42.1	-31.7	**-152.8**
^{240}Pu	-23.2	-22.8	-19.0	-6.6	**-71.6**
^{239}Pu	-0.6	-0.2	-0.1	0.0	**-0.9**
^{242}Pu	-0.5	-0.3	-0.1	0.0	**-0.9**
^{241}Pu	+0.1	+0.1	0.0	0.0	**+0.2**
^{235}U	+0.1	0.0	0.0	0.0	**+0.1**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

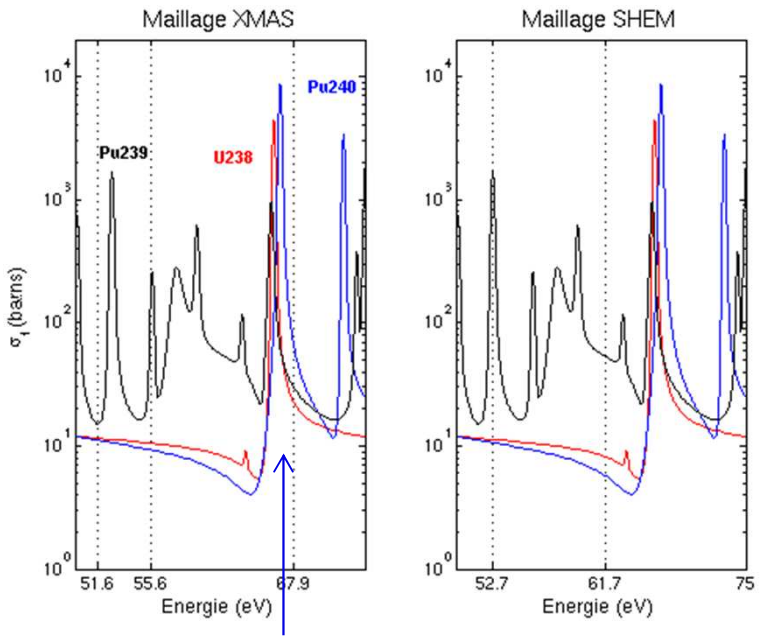
(n,γ)	(n,f)	(n,n)	$\sigma_s^{g'\rightarrow g}$	Total
-272.9	**+42.4**	+4.6	-6.6	**-232.5**

Resonance overlap in MOX: 2nd Doppler calc challenge



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

Mutual shielding taken into account by the fine mesh of SHEM



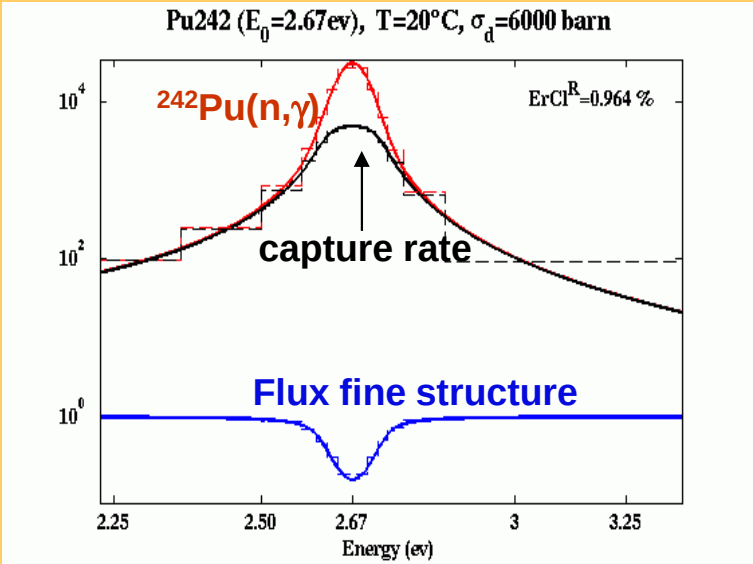
^{238}U/^{240}Pu/^{239}Pu overlap at E=66eV

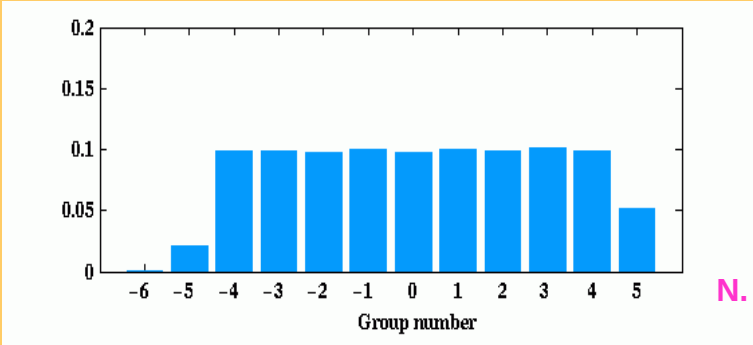
Mutual shielding taken into account by SHEM-361g (used for Sub-Group method)

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

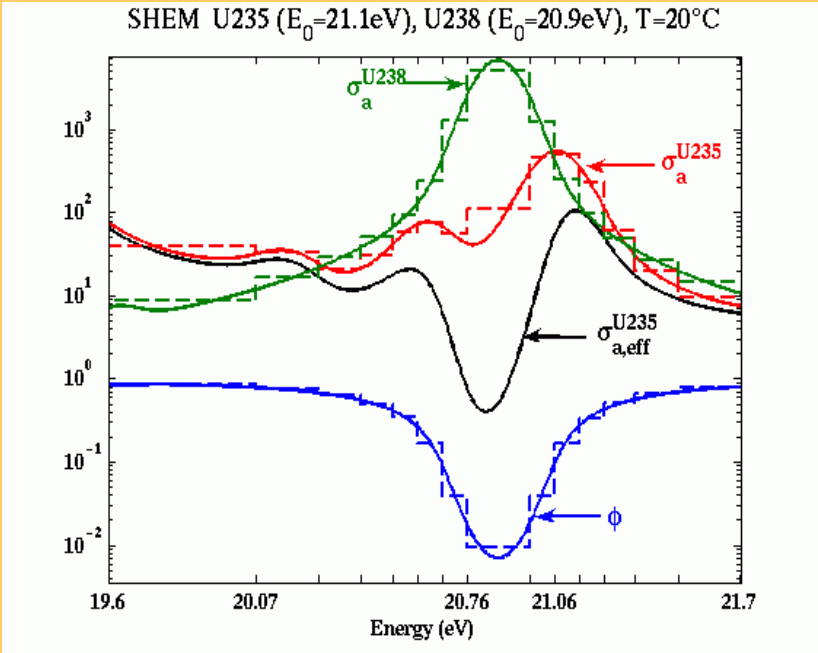
SHEM optimized mesh : resonances ^{242}Pu and ^{238}U

Rigourous method:
iterative algorithm for optimal discretisation





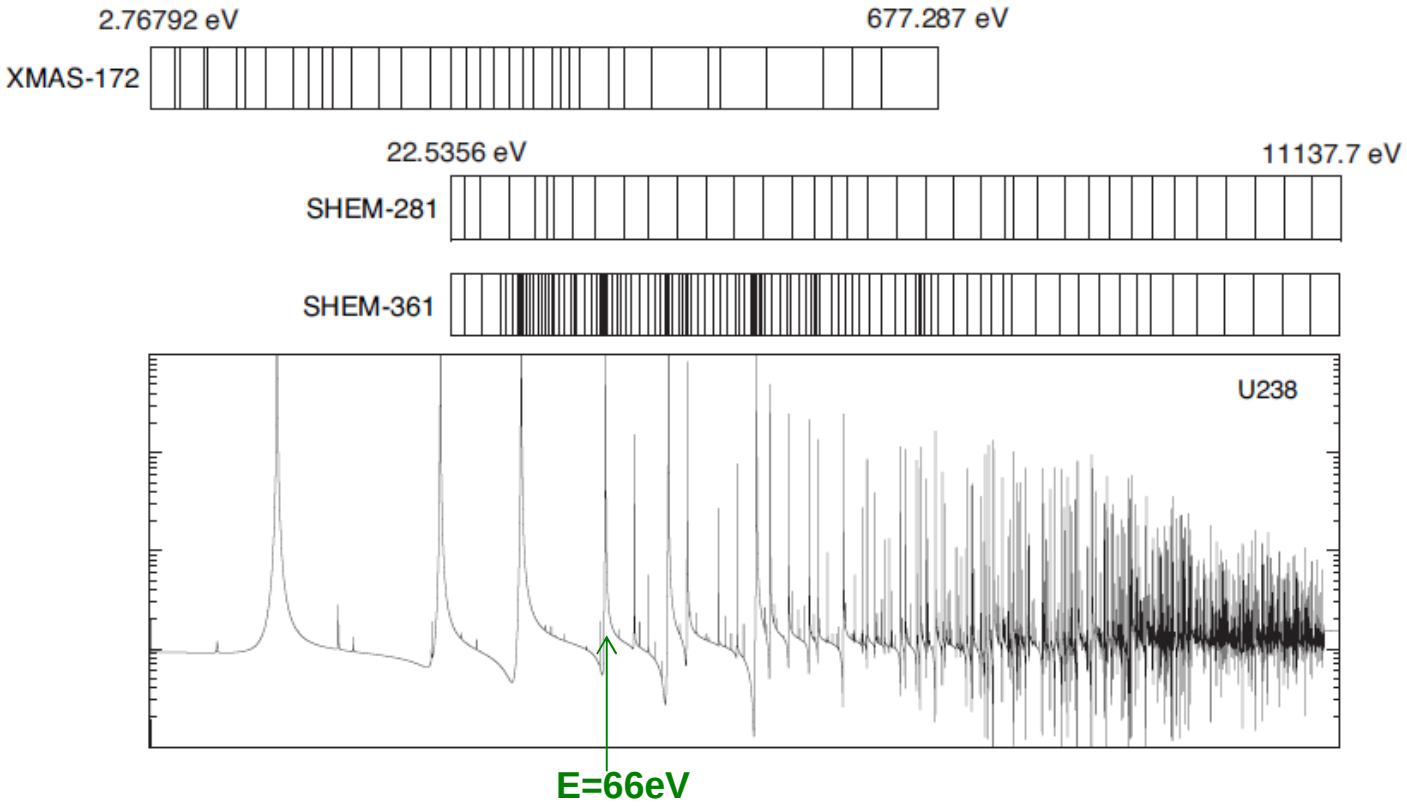
U238/U235 overlap 20eV



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 / ^{i}Pu is explicitely described**

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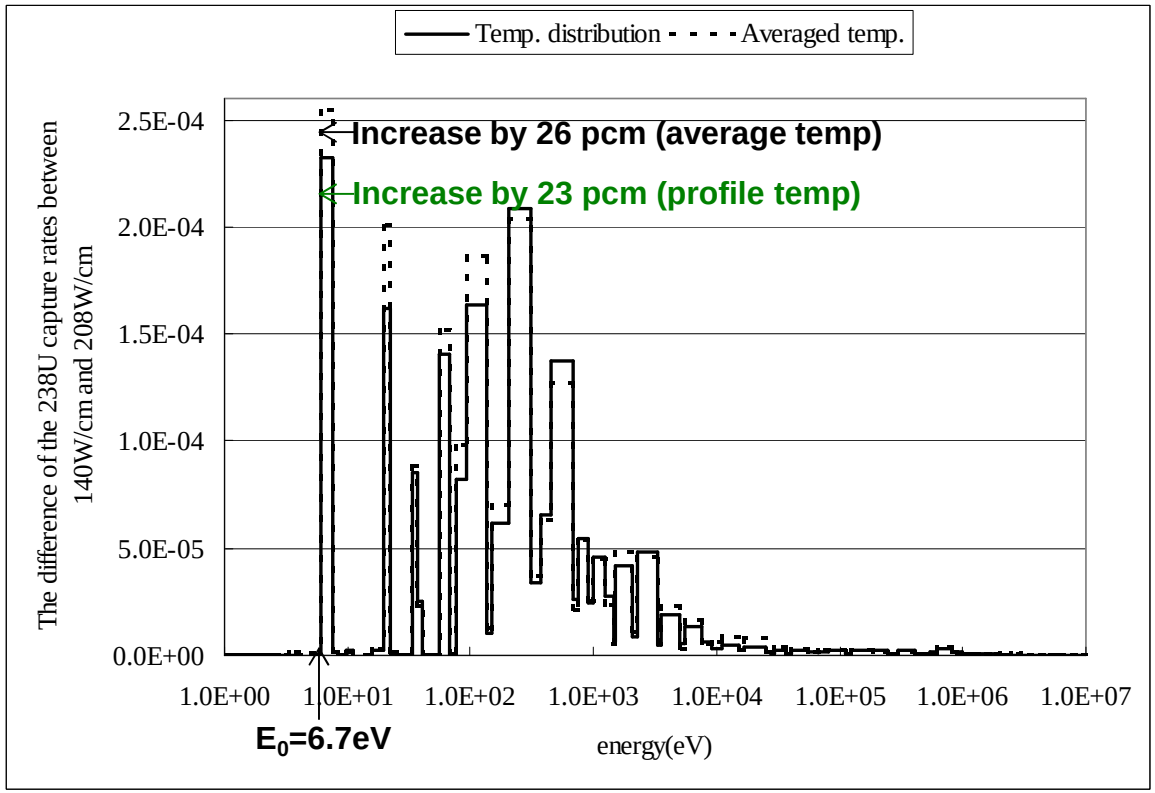
^{238}U capture increase with power (140 W/cm → 208 W/cm)

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)

A. Santamarina – T. Takeda, Conf. PHYSOR2002, Seoul, October 7-10

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):**

$$\boxed{T_{eff} = \overline{T}_{therm} - \frac{1}{18}\left(T_c - T_S\right)}$$

with: $T^{therm} = \int T(\mathbf{r})\, d\mathbf{r} \,/\, \int d\mathbf{r}$

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

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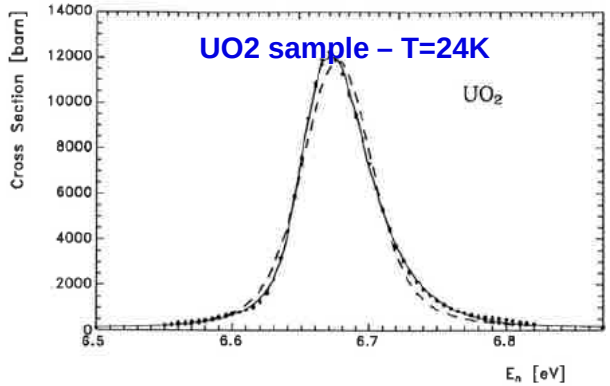
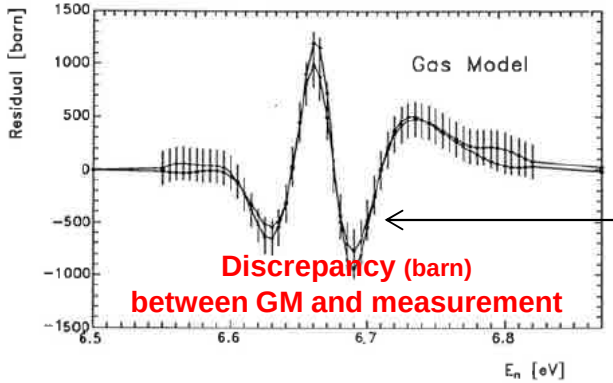
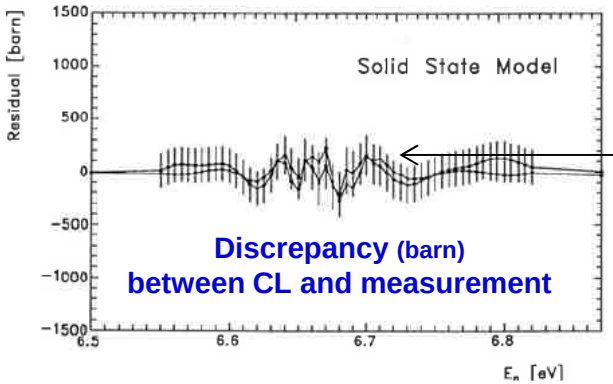
Doppler braodening of ^{238}U in UO_2 fuels

Gelina meas. of resonance E^{U238}=6.7eV







- 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_{eff}^{L} (= $\langle\varepsilon\rangle/k_B$)
- The 'weak binding' approx is not relevant for E_n<1keV
  ⇒ 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):

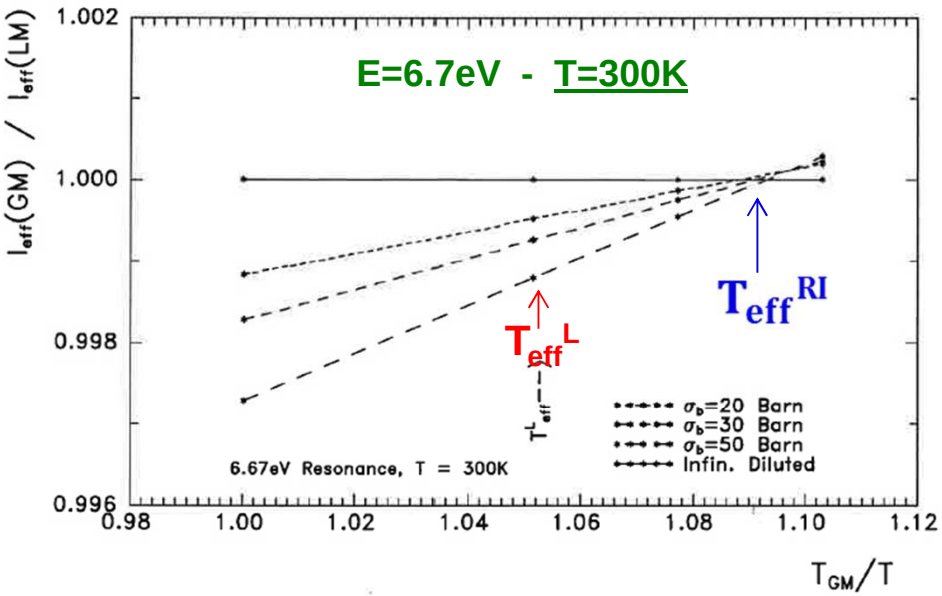
$$\rho(\hbar\omega) = 0.9 \cdot \delta(\hbar\omega - 13.4\text{meV}) + 0.1 \cdot \delta(\hbar\omega - 51.8\text{meV})$$

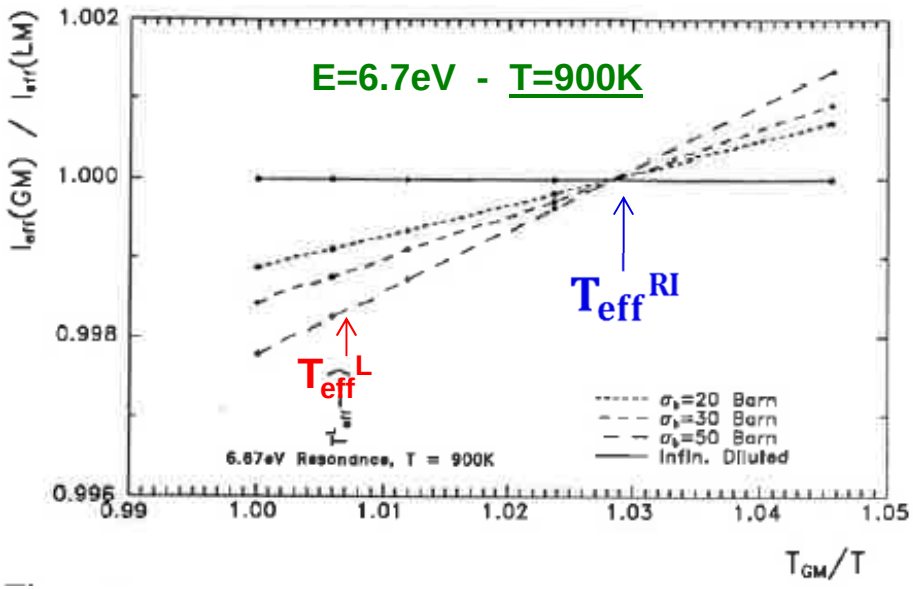
  ⇒ describe accurately ^{238}U resonances in UO_2

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

Determination of the actual effective temperature

- The real effective temp T_{eff}^{RI} has to <u>preserve the ^{238}U capture rate</u> (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 : $I_{eff}^{GM}(T_{eff}^{RI}) = I_{eff}^{LM}(T)$



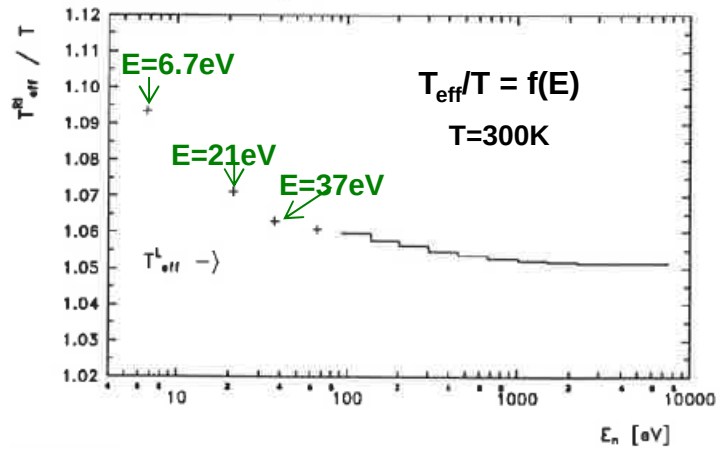


- T_{eff}^{RI} is quite independent from Geometry/Concentration

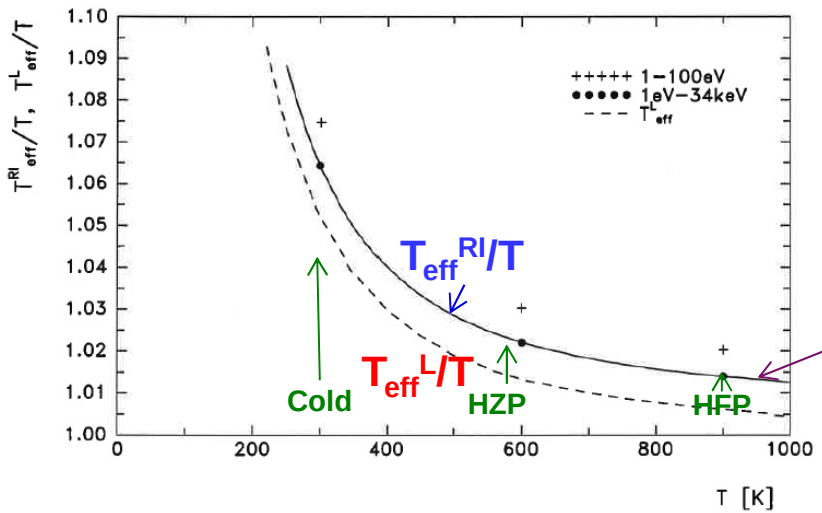
A. Meister and A. Santamarina, Conf. PHYSOR98, Long Island, May 19-24

The accurate effective temperature T_{eff}^{RI}

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



- Therefore we proposed T_{eff}^{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<1000K):

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

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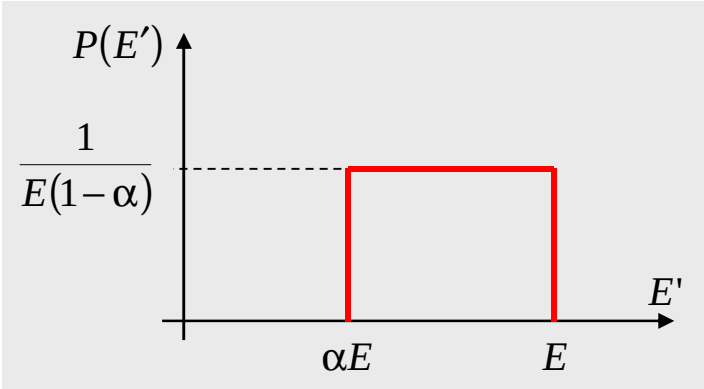
Doppler boadening – approx elastic Scattering Kernels

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

$$P(E \rightarrow E')\,dE' = \frac{1}{(1-\alpha)E}\,dE'$$

with

$$\alpha = \left(\frac{A-1}{A+1}\right)^2$$



→ **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: $p(V,\mu_t) = \dfrac{\sigma_s(v_r,0)v_r g(V)}{2\sigma_s(E,T)v}$ $\quad$ $\sigma_S(v_r)$=constant + Gaz Model $\Rightarrow p(V,\mu_t) \propto \dfrac{\sqrt{v^2+V^2-2\mu_t V v}}{v+V}\left[V^3 e^{-\beta^2 V^2} + vV^2 e^{-\beta^2 V^2}\right]$

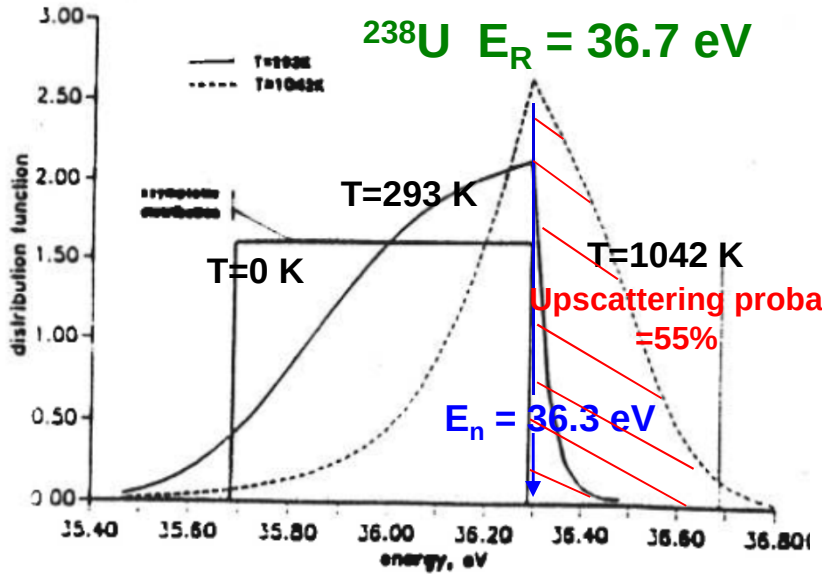
SVT algorythm : μ uniformly sampled in [-1;+1] - target velocity V sampled - then Rejection applied to sampled pair (μ_i,V_i)

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

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

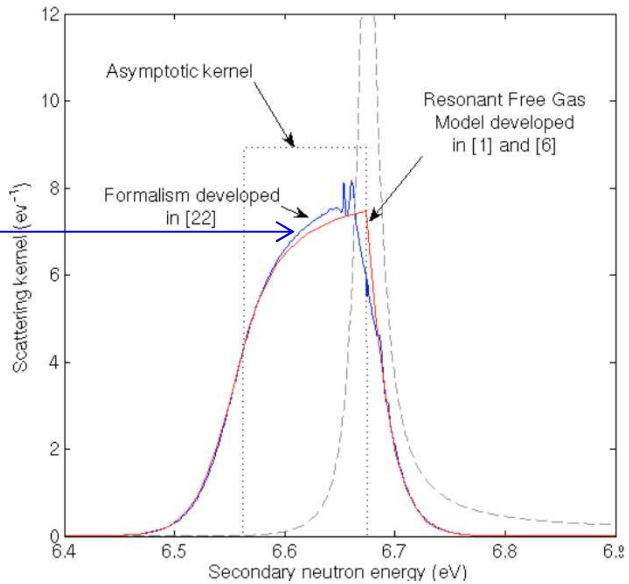
Resonance Elastic Kernel and Up-scattering

- **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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Biases in LWR Doppler coeff calc. (using $T_{thermal}$, and AK)

	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 UO_2 fuels is particularly important at room temperature
- On the contrary, resonant up-scattering is particulary 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%

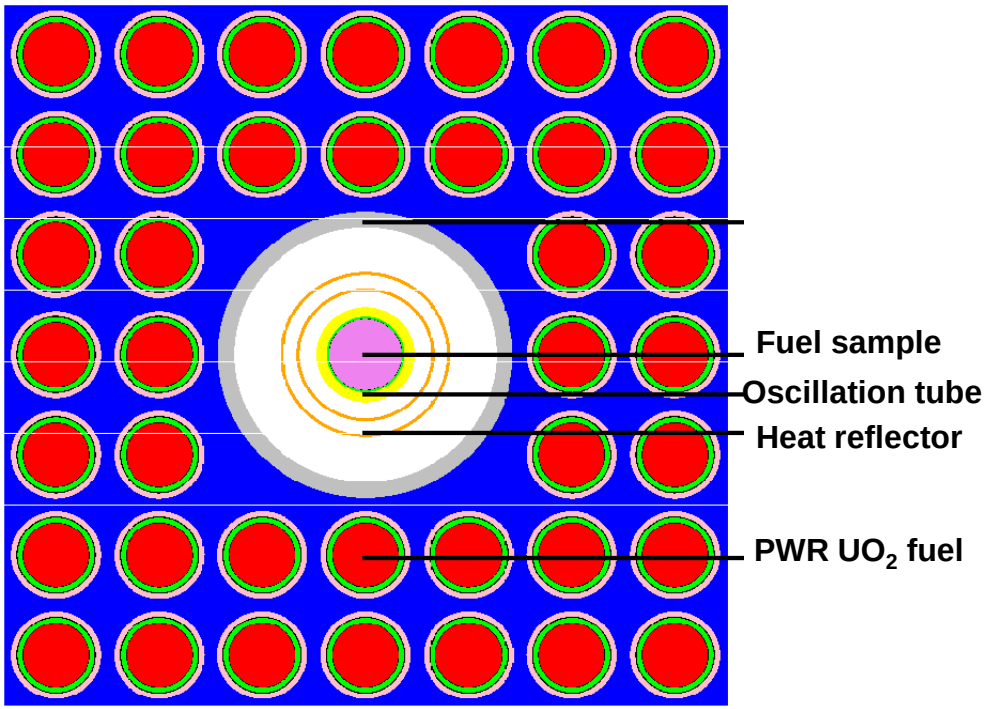
- **FTC uncertainty due to nuclear data is small:**

$^{238}U(n,n')$	H(n,n)	$^{238}U\ \Gamma_n,\Gamma_\gamma$	Total Unc. 1σ
0.6%	0.5%	1.0%	1.3%

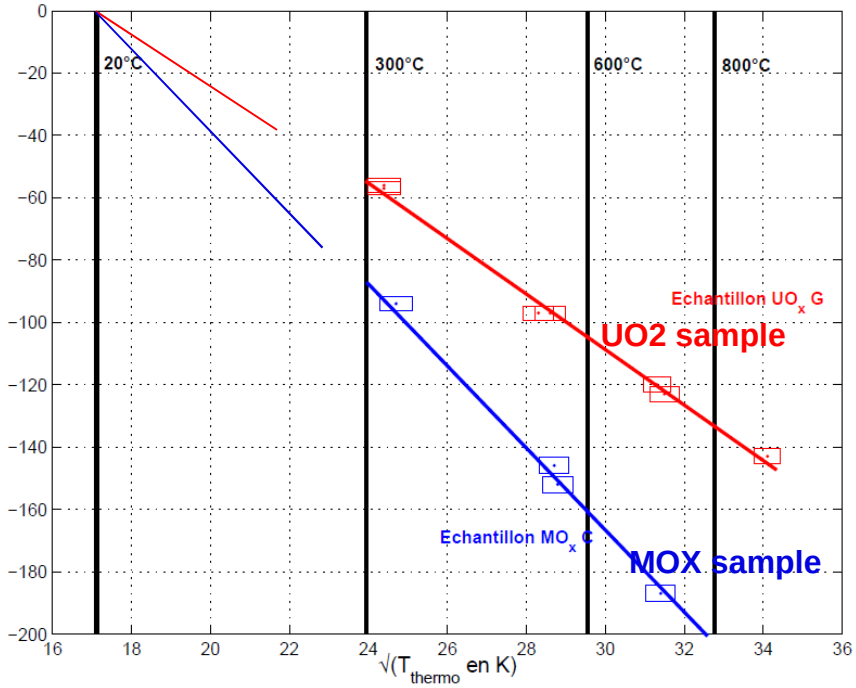
⇒ **The total uncertainty on FTC best-estimate calculation amounts to 4%**

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%(1σ)**
- 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℃ up to 900℃**
  4 UO2 fuel samples (E_{U235} = 0.2; 0.7; 3.0; 5.1%) & 6 MOX fuel samples
  ⇒ **TRIPOLI4-DRBC: (C-E)/E = +3% ± 3%(1σ)**



Measured Fuel Temp. reactivity worth vs √T



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Merci pour votre attention