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LWR-UOx Doppler Reactivity Coefficient: Best Estimate Plus (nuclear and atomic sources of) Uncertainties

D. Bernard, A. Calame, J-M. Palau

Commissariat à l'Energie Atomique et aux Energies Alternatives
CEA, DEN, DER, SPRC, LEPh, Cadarache, Bldg. 230
F-13108 Saint-Paul-Lez-Durance, France.
david.bernard@cea.fr

Abstract - *The negative Doppler reactivity coefficient of Light Water Reactors (LWR) is a major safety coefficient. Its calculation according to the full temperature range (from Cold Zero Power -CZP- to Hot Zero Power -HZP- or to Hot Full Power -HFP- or even accidental conditions) has to be precisely done.*

In the first part, this paper aims at estimating the various approximations of standard calculation routes: the uniform temperature spatial distribution versus the parabolic shape, the free gas model (FGM) broadening for absorption cross section even by using effective theories in place of the accurate cristal lattice model. And finally, the double differential scattering treatment in the neutron epithermal range (crude asymptotic kernel assumption versus more accurate Double Differential Cross Section (DDXS) Doppler broadening accounting for resonant up-scattering within the free gas model) will be discussed. More of that, a tentative to account for cristal lattice effects is proposed.

The second part is dedicated to the estimation of the Doppler coefficient uncertainty. The two discussed components are the nuclear data, namely the width channel parameters (neutron and γ) for the low energy ^{238}U+n resonances and the atomic data by propagating the phonon Density Of States uncertainty within the frame of the Cristal Lattice Model (CLM). This leads to ±6% for the global Doppler coefficient uncertainty.

I. INTRODUCTION

It is known that the atomic motion ostensibly and apparently modifies the nuclear cross section when the neutron incident energy (E) is within the order of magnitude of the kinetic energies of the targets. Consequently, neutron absorption and neutron scattering events has to be Doppler broadened according to the velocity distribution of the targeted atom. The general formula for the Doppler broadening of an absorption cross section σ at the temperature T is as follow:

$$\sigma^{T}_{(n,abso)}(E) = \int_0^{+\infty} dE' \sigma^{0\,Kelvin}_{(n,abso)}(E') \times S(E,E',T) \quad (1)$$

The spectroscopic function S accounts for the atomistic and neutron kinetics of the neutron entrance channel.

The Exact Perturbation Theory allows us to breakdown the low-enriched UOx-LWR reactivity worth into isotopes and cross sections. Indeed, such theory provides the split of reactivity effects between two neutronic states (represented by fluxes Φ_0 for low -300K- and Φ_1 for high -900K- fuel temperature) by using the integration of Boltzmann operators variations ΔH, leading to bilinear (forward and adjoint fluxes quoted '*') reaction rates:

$$\rho_{Dop} \propto \langle \Phi_0^*, \Delta H \Phi_1 \rangle \quad (2)$$

Rather than using "absolute" units of reactivity ($\Delta k/k$ or 'pcm'), we decided to normalize each bra-ket component to ρ_{Dop}. Isotopic and reactions contributions (then in %) are shown in Table I for a classical fuel pin (3% ^{235}U(w/o) enriched, Zr cladded, D=8cm of diameter) in a square lattice pitch of 1.26cm. This particular LWR case will be considered for the whole calculations in this paper.

Table I. LWR Doppler reactivity worth breakdown [%].

^{238}U	+109.7
^{235}U	-0.1
^{16}O	-9.6
Total	100.0

$\sigma_{(n,\gamma)}$	$\sigma_{(n,f)}$	$\sigma_{(n,n)}$	$\sigma^{E\to E'}_{(n,n)}$	Total
+110.8	-0.4	-1.1	-9.3	100.0

One can notice that ^{238}U(n,γ) is the main contributor to the Doppler worth (and will be the central component analyzed in this paper), especially in the first peripheral 800μm (60% of the Doppler worth) of the pellet (rim effect), see details in Fig. 1. Ten times lower, the thermal spectrum shift effect as seen on the ^{16}O scattering component tends to decrease the Doppler reactivity worth.

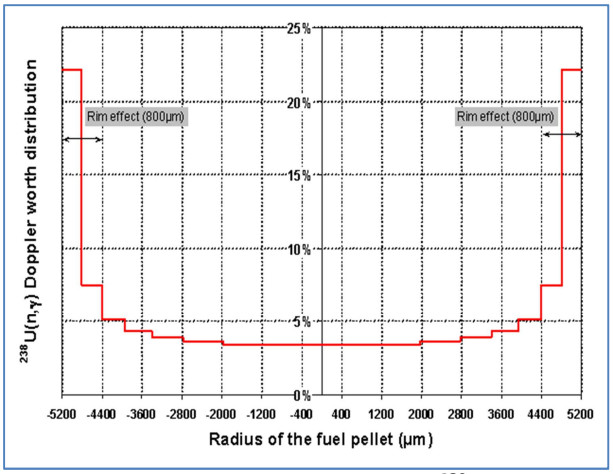

Fig. 1. Fuel pellet radial breakdown of the ^{238}U(n,γ) Doppler reactivity worth in the pellet.

The analysis of ^{238}U(n,γ) component can be done further as a function of the neutron energy (see Fig. 2) for the energy-cumulative sum of the linear reaction rate for state 0, the cumulative sum of its variation, and the cumulative sum of reactivity (bilinear rate) net effect from state 0 to state 1.

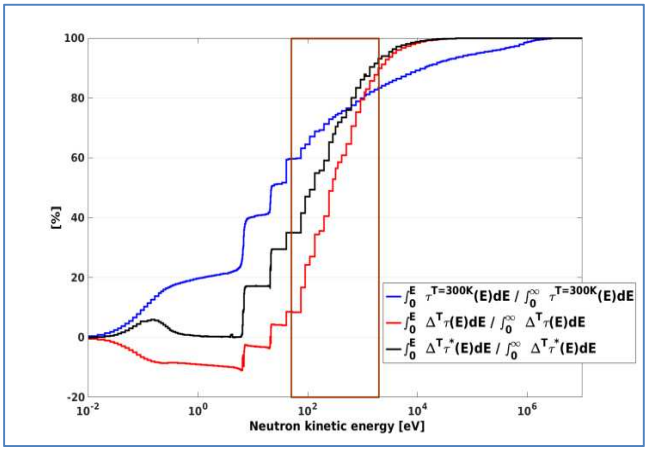

Fig. 2. Energy breakdown of the ^{238}U(n,γ) reaction rate, its variation with temperature and its Doppler reactivity worth.

Because of their high self shielding factors, first ^{238}U(n,γ) resonances from 50eV to 2keV contribute only to 20% of the capture rate but are involved in 60% of its variation in temperature and of the ^{238}U(n,γ) Doppler worth.

II. ASSOCIATED APPROXIMATIONS AND BIAIS

This chapter is devoted to the quantification of approximations done when calculating the Doppler worth.

1. Uniform temperature

The use of a uniform radial temperature in the pellet is often made for design calculations or even fuel cycle reactor follow-up calculations. This temperature has to account for the "rim effect" of ^{238}U capture reaction rates (for plutonium build-up prediction for instance but this temperature is not fitted for the rate variation, *i.e.* Doppler worth). Rowlands [1] proposed to weight peripheral $T_{surface}$ and central T_{center} temperatures of the pellet respectively by 10/18 and 8/18 for cylindrical geometries. This correction was generalized for accidental conditions by Chabert and Santamarina [2] by using the following effective and uniform temperature supposing the conservation of the ^{238}U(n,γ) reaction rates: ($\bar{T}$ stands for the volume-averaged actual temperature)

$$T_{eff} = \bar{T} - \frac{1}{18}\left(T_{center} - T_{surface}\right) \quad (3)$$

The Rowlands temperature from one hand and the Chabert-Santamarina one from the other hand become similar when assuming a parabolic radial shape in the pellet, *i.e.* for classical operating conditions but not for accidental ones.

We performed Monte Carlo TRIPOLI4 [3] calculations of the Doppler worth between HFP conditions and power excursion state (2274K in the center and 774K at surface of the pellet):

- one by using actual parabolic radial temperature profile (dividing the pin volume into 13 concentric volumes),
- one by using the effective Chabert-Santamarina flat temperature profile.

The results show how the effective approximation is reasonable for predicting HFP ^{238}U capture rates. The difference between the effective temperature flat distribution and the actual temperature profile is less than +2.4±1.7% for average pin rate and high temperature and less than +0.9% for its variation as its Doppler worth (+1.4±1.0%). Associated uncertainties are due to inherent statistical convergence of the TRIPOLI4 Monte Carlo code.

We can deduce that this effective theory assuming the modification of ^{238}U temperature (for all channels and even for others isotopes such as ^{235}U or ^{16}O in the fuel pin) give accurate results for the Doppler worth calculation.

2. Accounting for actual atomic motion to Doppler-broaden absorption cross sections

The Doppler kernel (Eq. 1) is often reduced to a Gaussian function (Free Gas Model -FGM- or assumption) for the velocity distribution convoluted to a Lorentzian for a single level cross section description (performing the so-called ψ/φ classical Voigt functions or Fadeeva functions for multipole description of cross sections [4]) but if we consider UO_2 fuel lattice, the harmonic motion of the uranium atoms has to be accounted for. It is possible to perform Cristal Lattice Model (CLM) Doppler broadening by using nuclear data evaluation codes such as SAMMY [5,6] or CONRAD [7] for instance.

These two use rigorous Van Hove theory [8]:

$$S_{CLM}(E,E',T) = \frac{1}{2\pi}\int_{+\infty}^{+\infty} dt\, e^{iE't+\frac{E}{A+1}[\gamma(t)-\gamma(t=0)]} \quad (4)$$

With the use of the following function of the Density Of atomic States (DOS) $\rho(\hbar\omega)$:

$$\gamma(t) = \int_0^{+\infty} d(\hbar\omega)\frac{\rho(\hbar\omega)}{\hbar\omega}\left[coth\left(\frac{\hbar\omega}{2k_BT}\right)\cos(\hbar\omega t) + isin(\hbar\omega t)\right] \quad (5)$$

The CLM spectroscopic function is developed and gives the so-called classical phonon expansion formula for numerical issues:

$$\gamma(t) - \gamma(0) = \sum_{\nu=1}^{\infty}\frac{x_\nu}{\nu!}(it)^\nu \quad (6)$$

With, complex odd and real even following terms:

$$x_{2\nu-1} = \int_0^{\infty} d(\hbar\omega)(\hbar\omega)^{2\nu-2}\rho(\hbar\omega)$$
$$x_{2\nu} = \int_0^{\infty} d(\hbar\omega)(\hbar\omega)^{2\nu-1}\rho(\hbar\omega)\ coth\left(\frac{\hbar\omega}{2k_BT}\right) \quad (7)$$

We first notice the poor robustness (namely the order ν of phonon expansion see Fig. 3 (36.7eV ^{238}U+n capture cross section), considering classically 40 and 1000 phonons exchange) of such algorithms and we will then advise to account for a minimum of 1000 phonons exchange for absorption cross section reconstruction within temperature. The convergence is ensured by comparison with a 10,000 phonon exchange calculation.

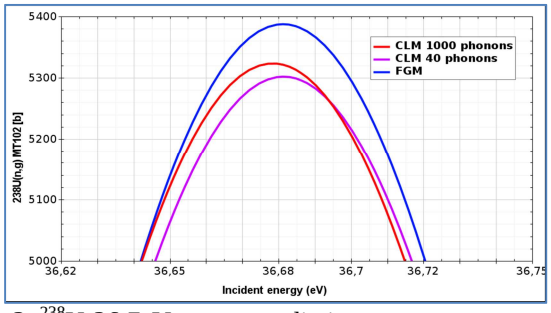

Fig. 3. ^{238}U-36.7eV neutron radiative capture cross section for different spectroscopic functions.

The SAMMY calculation using 40 and 1000 phonon is used to process a new Punctual Evaluated Nuclear Data File to TRIPOLI4 up to various neutron energies (470eV@T=300K, 240eV@600K and 160eV@900K) because of other numerical problems (above those energies, cross sections go down to zero). Then, taking classical 40 instead of 1000 phonon's exchange will lead to an error by about +1.5% to -2.3% (±1%) on the LWR-Doppler worth (see Table II). TRIPOLI4 Monte Carlo calculations show a difference by about (+4.3±1)% for the Doppler (from 300K to 600K) reactivity worth by comparing the converged Van Hove Cristal Lattice calculations to FGM for a flat temperature distribution.

Table II. Doppler worth errors by using CLM and FGM.

Temperature Variation [K]	Models compared	Doppler worth relative difference [%] (Associated 1σ stochastic uncertainty)
300-600	CLM(40ph) vs CLM(1000ph)	+1.47 (0.91)%
	FGM vs CLM(40ph)	+2.80 (0.96)%
	FGM vs CLM(1000ph)	+4.31 (0.95)%
300-900	CLM(40ph) vs CLM(1000ph)	-0.19 (0.52)%
	FGM vs CLM(40ph)	+2.27 (0.52)%
	FGM vs CLM(1000ph)	+2.07 (0.52)%
600-900	CLM(40ph) vs CLM(1000ph)	-2.27 (1.21)%
	FGM vs CLM(40ph)	+1.58 (1.20)%
	FGM vs CLM(1000ph)	-0.72 (1.16)%

Cristal lattice effects tend rationally to decrease the Doppler worth and are decreasing as a function of the temperature.

To bypass such complex CLM calculations, the user often perform cross section Doppler broadening with effective theories. The latter uses free gas model by modifying the applied temperature in order to preserve:

- the cross section: the approximate Lamb theory [9] (within severe assumptions such as the weak binding of uranium in the lattice which is not fulfilled for the resonances involved in the LWR Doppler coefficient, *i.e.* lower than 2keV), assuming a Debye density of electronic states or as proposed by Butland [10] by assuming an actual phonon spectrum measured by Thorson and Jarvis. This theory is the reduction of Eq. (7) at the first order of development.
- The capture rate such as Meister-Santamarina effective and pragmatic theory [11], but valid for rather low temperature (<1200K).

To give an example (see Fig. 4), the corrections to be applied to temperatures within the two theories are plotted in Fig. 4. If we basically suppose the Doppler worth proportional to $\sqrt{T_1} - \sqrt{T_0}$, the difference between the two theories can reach 7% at low temperature. But, once again, the Lamb theory is not applicable in LWR cases.

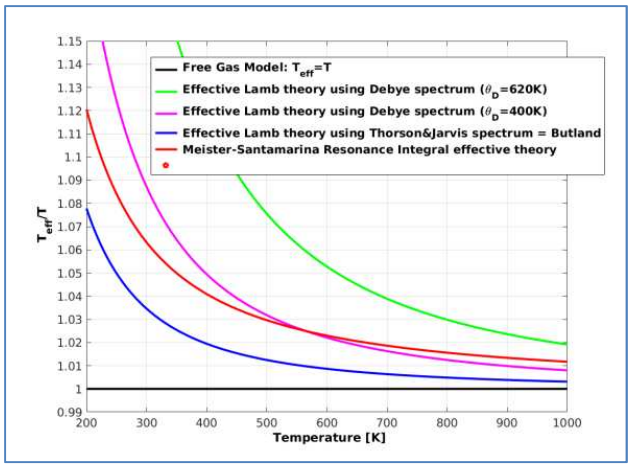

Fig. 4. Effective temperatures to be used in FGM Doppler broadening to account for cristal lattice effects.

Similarly, the Doppler worth relative difference between realistic Meister-Santamarina theory and FGM without effective temperature should be -3.6% between 300K and 600K. Table II give research tracks of validation of the Meister-Santamarina theory with a decrease of -4.3(1.0)% between the converged CLM calculation and the same FGM calculation.

3. Treatment of neutron thermalization on resonant isotopes

Last but not least concerns the kinematic equations treatment in transport codes, generally distinguishing thermalization of neutrons for a rather low energy range (few eV) and slowing down above. In general, for the second range, the assumption (called Asymptotic Kernel: AK) is to suppose a fixed target. But, recent developments have been done to account for resonant up scattering in Monte Carlo and deterministic codes. As proposed by Rothenstein and Dagan [12], the Doppler Broadening Rejection Correction (DBRC) is now implemented for the broadening of the DDXS (accounting for both entrance and outgoing neutron channels) in the TRIPOLI4 code [13]. This correction is not yet fully used for reactor studies and could modify the differential Doppler coefficient up to 18% at high temperature, *i.e.*, when target velocities are high enough to up scatter the neutron in the higher part of the left wing of the capture cross section (see Fig. 5 and Fig. 6).

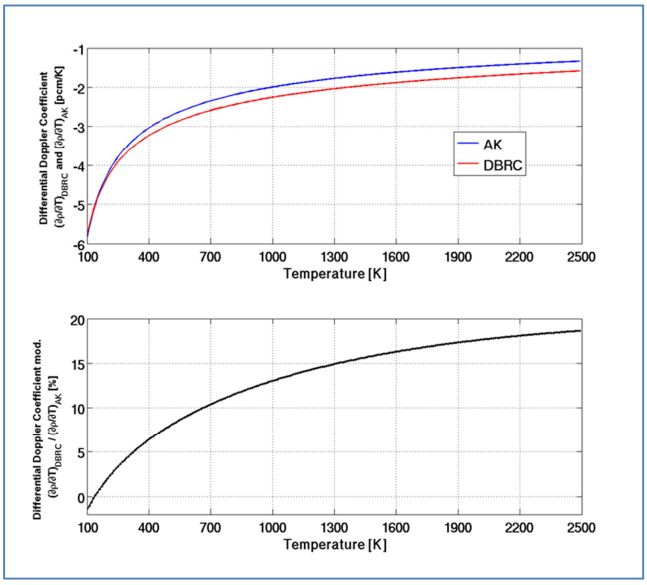

Fig. 5. DBRC modification of the Doppler worth.

Indeed, the main modification concerns resonances with high $g_J\Gamma_n$ values (such as E_0=36.7eV for ^{238}U+n for half of the total reactivity modification):

- Fig. 6 shows the consequence on the capture rate now fully asymmetric (neutron flux is increased in the left wing), and,
- the modification (up to 18% at high temperature) of the differential Doppler worth plotted in Fig. 5 by using classical Asymptotic Kernel and the recently implemented DBRC model for a typical LWR fuel pin as a function of the temperature) from 0eV to 1MeV for the ^{238}U+n DDXS treatment.

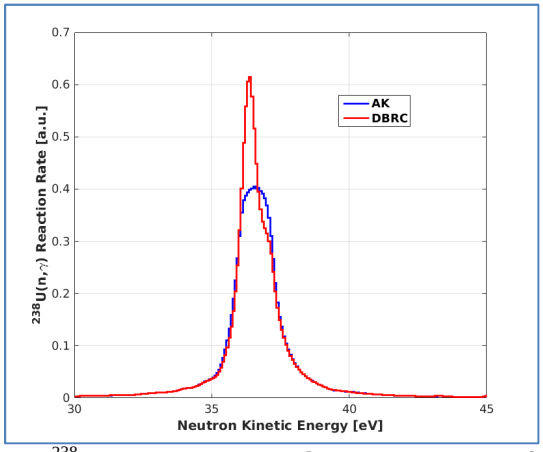

Fig. 6. ^{238}U-36.7eV neutron radiative capture rate when accounting for DDXS Doppler DBRC broadening vs Asymptotic Kernel treatment at T=1174K.

Unfortunately, DBRC technique is assuming a FGM broadening. We will now attempt to account for a cristal-effective theory as proposed by Courcelle and Rowlands [14]. Indeed, for the time being, no formal theory is available for the Doppler broadening of double differential energy-resonant cristal scattering cross section. Courcelle and Rowlands (noted CR) demonstrate that an approximate formula could be proposed to treat such solid state effects in neutron-cristal scattering resonant interactions through the following DDXS:

$$\frac{d^2\sigma_s^T(E)}{d\Omega dE'} = \frac{1}{4\pi}\frac{k_f}{k_i} \times S_{CLM}\left(\vec{k}_f - \vec{k}_i; E' - E\right) \times \sigma_{s,FGM}^{T(1+\mu)/2}\left(\frac{E+E'}{2} - \frac{E\mu}{A}\right) \quad (8)$$

Where $k_{i,f}$ stand for initial and final neutron wave numbers and μ the cosine scattering angle in the center of mass of the system (A is the mass of the target relative to the mass of the projectile). This effective FGM theory is then based on two parameters:

- an effective temperature $T^{CR} = T(1+\mu)/2$ to be applied only for scattering events (not for absorption cross sections for instance), and
- the shift of the compound nucleus energy $E^{CR} = \left(\frac{E+E'}{2} - \frac{E\mu}{A}\right)$.

We propose to use the DBRC technique (to provide E' and μ) and the FGM-Dopplerized spectroscopic function (avoiding so the complex problem of the CLM phonon expansion technique). We propose to account for the

Courcelle Rowlands effective theory by modifying the neutron weights ($W \rightarrow W'$) in the TRIPOLI4 code:

$$\left[\frac{d^2\sigma_s^T(E)}{d\Omega dE'}\right]_{CR} \sim \left[\frac{d^2\sigma_s^T(E)}{d\Omega dE'}\right]_{DBRC} \times \frac{W'}{W} \quad (9)$$

with:

$$\frac{W'}{W} = \frac{\sigma_s^{T^{CR}}(E^{CR})}{\sigma_s^T(E)} \quad (10)$$

Assuming now a Single Level Breit and Wigner description for low energy s-waves, one can use the simplified equation for the scattering cross sections (and notations) given in [15] "with the help of a '50' points Gauss-Hermite quadrature" considering the first order ψ/φ Voigt convolution:

$$\frac{W'}{W} \approx \frac{4\pi a^2 + \sum_i \frac{2a}{\lambda\!\!\!^{-CR}} \sigma_0(E^{CR}) \varphi(E^{CR},T^{CR}) + \frac{\Gamma_{n,i}}{\Gamma_{t,i}} \sigma_0(E^{CR}) \psi(E^{CR},T^{CR})}{4\pi a^2 + \sum_i \frac{2a}{\lambda\!\!\!^{-}} \sigma_0(E) \varphi(E,T) + \frac{\Gamma_{n,i}}{\Gamma_{t,i}} \sigma_0(E) \psi(E,T)} \quad (11)$$

with the potential scattering cross section $4\pi a^2 = 9.4b$ for ^{238}U+n, $\lambda\!\!\!^{-}$ the neutron reduced wave length, $\sigma_0(E) = 4\pi\lambda\!\!\!^{-2} g_J \frac{\Gamma_{n,i}}{\Gamma_{t,i}}$ where $\Gamma_{n,t,i}$ stand for neutron and total width, and g_J and the statistical spin factor for a given resonance i.

Thus, applying JEFF-3.1.1 [16] resonance parameters, the neutron weight corrections ($\frac{W'}{W}$) is plotted below (see Figure 7) in blue close to the main resonance responsible of up-scattering events. Superimposed in red is the scattering cross section for ^{238}U+n. Calculations are done with $T = 1174K$.

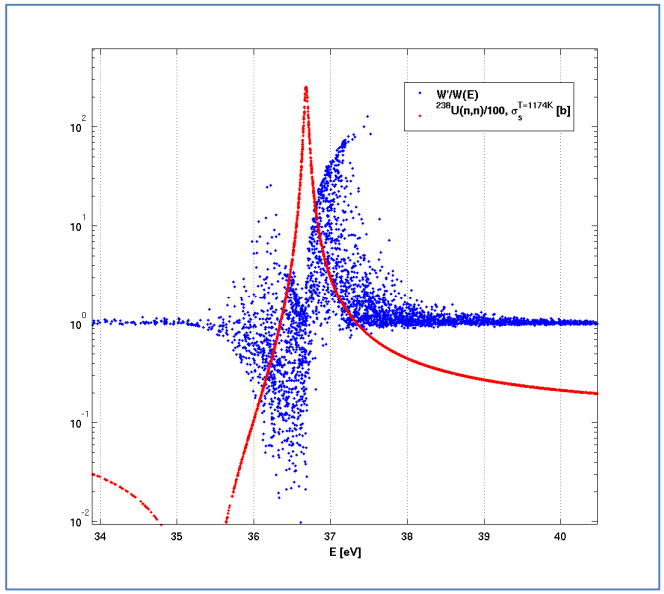

Fig. 7. Proposed weight correction in Monte Carlo calculations to account for CLM in DDXS Doppler broadening within the effective CR theory

We notice that, most of the time, the neutron weight should decrease in the left wing but should be increase in the right resonance wing, emphasizing so the down scattering and probably locally modify the neutron spectrum. Then, qualitatively speaking, resonant thermalization of neutron on uranium dioxide should be slightly overestimated versus the DBRC (FGM) model.

4. BEPU (Best Estimate Plus Uncertainties) approach

To conclude this section, we propose the calculation of the Best Estimate Doppler reactivity worth for the temperature distributed LWR fuel pin, including CLM broadening for ^{238}U capture cross sections and FGM for DDXS broadening (*i.e.* using the DBRC technique). By comparing this result to the less accurate model (uniform Chabert-Santamarina effective temperature and FGM for integrated cross section, *i.e.* without DBRC) we can give an estimation of the potential bias done for classical design calculations of HZP to HFP conditions.
The results are -2.62(0.01)pcm/K and -2.75(0.01)pcm/K for the two Doppler coefficients Monte Carlo calculations respectively.

The potential error (or model defect) when calculating Doppler Coefficient without recent theories (DBRC, CLM for capture) is estimated to be about 5%.

III. DOPPLER COEFFICIENT UNCERTAINTY

One can distinguish two kinds of uncertainties. The first one is associated to nuclear reactions properties (namely resonance parameters for instance) and the other one is associated to atomic data (the density of state governing the uranium motion in the UO_2 cristal). These two propagated uncertainties will be discussed in the following sections.

1. Uncertainties raise with the DBRC model

As shown previously, low energy neutron+target kinematics laws through DDXS Doppler broadening are crucial for reactivity worth calculations. Consequently, one has to be confident into scattering cross sections (namely $g_J\Gamma_n$ value, especially for the ^{238}U+n 36.7eV resonance). Indeed, as shown is Fig. 6, up-scattered neutron average energy is about $\overline{E'} \sim E_0 - 350meV$. The averaged incident energy is estimated: $\bar{E} = \overline{E'}\left[1 + \frac{(A-1)^2}{(A+1)^2}\right]/2 \sim 36.05eV$, where the potential and resonant components start interfering. One can show that this destructive interference is very sensitive to Γ_n values. One can show by derivating the Single Level Breit and Wigner description with respect to the parameter Γ_n that the cross section value could be affected by 180% (at the interference hole) for only 1% modification of this resonance parameter. Finally, the

estimated uncertainty of this particular $g_J\Gamma_n$ value leads to 2.4% uncertainty on the up-scattering rate in this elastic cross section left wing, leading to less than 0.2% on the Doppler reactivity worth of this 36.7eV resonance. But this can also depend on the temperature.

2. ^{238}U+n Resonance parameter (RP) uncertainty propagation

According to RP available covariance matrices, the uncertainty propagation is carried out for the first ^{238}U+n s-waves. A straightforward modification of each individual neutron channel width (+10% up to E_n=200eV for which one half of the Doppler worth is involved) and the γ width (fixed 23.0meV for all resonances) in the ENDF file is propagated through Monte Carlo TRIPOLI4 calculations to estimate the sensitivities of the Doppler worth. The sensitivity is about -0.5 to -0.9%/% for Γ_n parameters depending on the resonance. The modification of all the Γ_γ to the value of 23meV (lower than 5% RP modification for few low energy s-waves) leads to a significant modification of about -6.0% (±0.3%) on the calculated Doppler worth.

Using then a proper covariance matrix for RP, the sandwich propagation rule can give us an uncertainty on the reactivity worth. Compared to the JEFF-3.1.1 evaluated nuclear data file, two sources [17, 18] of RP and RP uncertainties are shown below for the 36.7eV resonance.

Table III. RP and RP uncertainty values.

36.7eV res.	$g_J\Gamma_n$/meV	Γ_γ/meV	Correlation
JEFF-3.1.1 [16]	33.554	22.89	none
BNL [17]	33.8±0.2	22.9±0.3	0
EPJA [18]	33.592±0.02	22.264±0.024	-0.47

Reduced neutron widths are consistent between the last two references. But, associated uncertainties are different by a factor of 10. γ-widths are 3% different, this cannot be fully explained with their associated uncertainties about 1.3% for the first reference [17] and 0.11% (ten times lower) for the second [18]. The confidence in such matrices is not reached. Nevertheless, the high anticorrelation value mentioned in the second reference is expected between the two RP and should lead to a lower propagated uncertainty.

Then, to be pragmatic, we propose a nuclear (source of) uncertainty of about ±5% on the LWR-Doppler reactivity worth due to few ^{238}U+n s-waves-RP uncertainties.

3. Atomic data uncertainty propagation

An attempt to propagate the uncertainty of the phonon Density Of States in the cristal lattice model was done. To do so, we spread the energy of the phonon density by a factor 1.3 leading to much more constrain exchanges between the neutron and the cristal lattice. Compare to actual DOS, the Doppler worth was then modified by +2(±0.4)%, which is the order of magnitude of its uncertainty.

IV. CONCLUSIONS

We provided the Best Estimate Plus Uncertainty propagation (BEPU approach) for the main contributor of the LWR fuel reactivity coefficient, *i.e.* ^{238}U+n cross sections broadening. The latter could be biased by about -4% to +18% (depending on the temperature range; involving solid states effects for low temperature and resonant up scattering events for high temperature) in classical design calculations. Its associated uncertainty is estimated to about 6%.

As prospects, we can mention:

- the rigorous treatment of the thermal scattering law (through $S(\alpha,\beta,T)$ functions) for uranium dioxide instead of FGM treatment,
- the propagation of the uncertainty associated to the energy of resonances (E_0), and to indirect components for thermal and epithermal flux settings (prompt fission neutron spectra, ^{238}U(n,n'γ), elastic scattering of hydrogen…),
- an additional technological uncertainty which is the temperature knowledge itself, that affects directly absorption cross section broadening.

A new experimental program dedicated to the validation of the Doppler coefficient is wished for the whole range of the temperature range (T=100K for cristal binding effects and T>2000K for neutron thermalization treatment) as done in the past but in a more reduced range [19].

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