USE OF DIFFERENT LIBRARIES IN THE ANALYSIS OF THE DOPPLER MEASUREMENTS OF THE SEFOR REACTOR: ASSESSMENT OF THE DOPPLER EFFECT OF THE ASTRID CORE.

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ABSTRACT

For the next generation of fast reactors, global objectives are required in terms of safety, sustainability, waste minimization and non-proliferation issues. Concerning safety issues, particular efforts have been made in order to obtain core designs that can be resilient to accidental transients. In that frame, the CEA held R&D program toward a GEN-IV-like core concept that could meet those requirements: the ASTRID project. Based on heterogeneous core geometry (axial inner fertile layer, large upper sodium plenum) the ASTRID core shows improved behavior in case of unprotected loss of flow. It has been found that Doppler Effect plays a dominant role for the considered transients to deal with in the safety demonstration. The prediction of the Doppler Effect by neutronic simulation codes require experimental validation, the reason for which static tests conducted within SEFOR (South-West Experimental Fast Oxide Reactor) – a fast reactor fueled with mixed PuO$_2$-UO$_2$ and cooled with sodium – are being used. The SEFOR experimental tests are being analyzed with the ERANOS code package using nuclear data libraries of different evaluations: JEFF-3.1.1, JEFF-3.2, ENDF-B/VII.1 and JENDL4. The C/E values on the SEFOR Doppler Effect range from 1.01 to 1.07 with an experimental uncertainty of ±0.06. With the use of perturbation break down in energy and isotope, this paper identifies the reasons for such large C/E spread and identifies the differences and similarities of the SEFOR Doppler Effect with the ASTRID one.

KEYWORDS: ASTRID SFR, Doppler Effect, SEFOR experiment, Nuclear Data uncertainty

1. INTRODUCTION

The SEFOR Doppler experiments have unique and valuable features of measuring whole core Doppler reactivity effect induced in various situations, such as steady-state at power levels of 20 MW, oscillation tests and prompt critical transients up to 10,000 MW. The core is driven super-critical with the removal of boron carbide assembly, and its criticality is managed with reflector assemblies positioning. The
experimental program was conducted by the American General Electric Company (GE) and the West German Karlsruhe Laboratory (KFK) from 1969 to 1972 [1].

SEFOR presents characteristics similar to sodium fast reactors, such as ASTRID [2]; this paper describes analyses and results obtained for the SEFOR Doppler coefficient, obtained with several nuclear data libraries, and their relevance regarding ASTRID Doppler one. The reactivity variation was measured by the reflector positions. Reactivity effects due to increment of temperature can be divided into two components, one being the thermal expansion – sodium & structures – the other being the Doppler Effect. In the rapid transient tests, the fuel temperature alone is modified (from uniform temperature state of 677K to 1365K±100K) and its effects on reactivity relates directly to the core Doppler constant.

The Doppler reactivity coefficient is determined on two different cores: the first core (Core I) contains a BeO pin at the center of fuel assemblies, to soften the neutron spectrum and increase the Doppler Effect; in the second core (Core II), moderators subassemblies are replaced with stainless steel, with a consequent hardening in the neutron spectrum. Core I fuel assembly layout is illustrated in Figure 1 (left). Core II fuel assembly dimensions and geometry are identical to Core I [1].

![Figure 1. SEFOR Core I fuel assembly layout (left) & its representation in ECCO (right)](image)

Previous analyses have been conducted with ENDF/B-III & JEF-2 [3]. In order to set aside modelling effects from nuclear data effects, the ECCO/ERANOS [4] model from reference [3] is used in this study. Figure 1 (right) presents the ECCO model used at lattice step to calculate the fuel assembly cross-section for core calculations. Two observations can be made:

1. The steel side rods and tightenner sleeve composition have been homogenized with the inner sodium;
2. Some B$_4$C is present in the outermost sodium sheet.

The first item is due to the ECCO cell code limitations in geometrical descriptions. The second is due to the RZ representation of the full core in ERANOS: since the B$_4$C rods are not explicitly represented (and to reduce spatial effects), their compositions have been homogenized with the outer sodium region. Previous CEA interpretation (with ERANOS/JEF2) for the reactivity effects of sharp transient change in fuel temperature gave C/E$_{SEFOR I}$ = 0.96±0.15 and C/E$_{SEFOR II}$ = 1.05±0.15 [3]. The goal of this paper is to provide a systematic study of evaluated nuclear data impact on global quantities (Doppler Effect) and, using perturbation theory, identify which nuclear data isotopes are responsible for the differences and hence provide feedbacks to nuclear data evaluators. In addition, a study quantifies to which extent the SEFOR analyses are relevant to the ASTRID core concept.
2. REACTIVITY AND DOPPLER EFFECT’S C/E

This section concerns the validity of Experimental and Calculated value. Previous work [3] has shown errors in experimental data treatment. Calculated quantities with different nuclear data libraries are given and C/E are discussed.

2.1. Experimental Values for SEFOR I and II Cores

Experimental values of the SEFOR core reactivity can be found in references [1] and [5]. It has however been found that fuel thermal conductivity coefficient requires attention. GE experimental values were then revisited [3] and induce revisited Doppler constants as shown in Table I. $\beta_{\text{eff}}$ values were obtain with Keppin’s evaluation. The re-evaluated Doppler constant is 3 or 5% larger than the original GE evaluation. In addition, the experimental uncertainty is significantly reduced from 15% to 6%.

Table I. Reevaluated Experimental Doppler constant by Hazama & Tommasi

| Core | Doppler constant ($) $\beta_{\text{eff}}$ (pcm) | Experimental Doppler constant (pcm) | Experimental standard deviation (%) |
|------|------------------------------------------------|-----------------------------------|-----------------------------------|
| I    | -2.61 327                                     | -853.5                            | 6                                 |
| II   | -2.03 330                                     | -670.0                            | 6                                 |

2.2. Calculated Values for SEFOR I and II Cores

This study uses the same model (geometry and composition) as in reference [3] for lattice and core steps, so that discrepancies between calculations with different libraries can be attributed to nuclear data only. The calculation scheme in use is detailed in 2.2.1 and results are given in 2.2.2.

2.2.1. Calculation scheme and nuclear data libraries

Calculations were performed with the ERANOS code system. The main features of the calculation scheme are as follows. Several nuclear data libraries are used (JEFF-3.1.1 [6], JEFF3.2 [7], JENDL4 [8], ENDF/BVII.1 [9]), with fine (1968 energy groups) and broad structure (33 groups). The cell calculations are performed with the ECCO module, using a 2D heterogeneous model of the fuel subassemblies and a fine energy mesh (1968 groups); nuclear data are condensed in 33 groups for the core calculations, performed then in S8 transport with the BISTRO finite difference Sn transport module (P1 scattering anisotropy) in a RZ core geometry.

The nuclear data library introduced as “JEFFhyb” in the following study is the JEFF-3.1.1 library for all isotopes, except for the $^{23}$Na that was taken from JEFF-3.2. It should be noticed that JEFF-3.2 $^{23}$Na data uses recent differential measurements and remove some deficiencies of previous evaluations [10].

The JEFF-3.3 library is not considered in this paper; the study undertaken here is meant to be a preliminary review to a revisited SEFOR 3D model with the APOLLO3-RNR [11] code system, on which the JEFF-3.3 library is not available yet.

2.2.2. Calculated Doppler constants and C/E

Differences in processing, data type used (integral or microscopic) and additional experimental data will lead to disparities in evaluated nuclear data libraries, which will yield – for an identical calculation scheme – notable variations in neutronic quantities of interest, such as reactivity and Doppler effect.
For each library and the two configurations, the core’s reactivity is evaluated in its “cold” state (iso-thermal, at 677K) and in its “hot” state (corresponding to prompt transient, with the fuel sub-assemblies at 1365K, the rest at 677K). Table II gathers the calculated Doppler constants according the tested libraries.

### Table II. Calculated Doppler constants (pcm) and related C/E values for SEFOR Core I & II using different evaluated nuclear data libraries.

| Core configuration | JEFF-3.1.1 | JEFFhyb | JEFF-3.2 | JENDL-4 | ENDF-B/VII.1 |
|--------------------|------------|---------|----------|---------|-------------|
| Core I Doppler constant | -874.1 | -869.2 | -917.4 | -879.9 | -887.6 |
| Core II Doppler constant | -682.1 | -676.7 | -708.4 | -682.6 | -692.1 |
| Core I C/E | 1.024 | 1.019 | 1.075 | 1.031 | 1.040 |
| Core II C/E | 1.018 | 1.010 | 1.057 | 1.019 | 1.033 |

The main contribution to the Doppler coefficient in a fast oxide reactor, such as SEFOR, comes from neutrons in the energy range between 0.5 keV and 10 keV. The Doppler reactivity effect is thus more important in Core I than in Core II, the spectrum being noticeably softer [2] (as shown in Figures 3) with the presence of BeO subassemblies at the center of fuel assemblies. The C/E values on the SEFOR Doppler Effect range from 1.01 to 1.07 with an experimental uncertainty of ±0.06. The reasons for such large C/E spread will now be analyzed with the use of perturbation theory and differences and similarities of the SEFOR Doppler Effect with the ASTRID one will be identified.

### 3. ANALYSES USING PERTURBATION THEORY

As its name indicates, the perturbation theory [12] links a small variation of the Boltzmann operator \( \delta H = \delta A - \frac{\delta F}{k} \) (e.g. concentrations, cross-sections, temperatures) to its effects on an observable, macro quantity (e.g. reactivity, sodium void reactivity worth, Doppler Effect). Its use is particularly suitable for analyzing differences in isotopes’ contribution to the calculated Doppler Effect emerging from disparities in evaluated nuclear data libraries.

\[
\delta \rho_{g,r,i} = -\frac{\langle \Phi^+, \delta A_{g,r,i} \rangle}{\langle \Phi^+, F_{g,r,i} \rangle} \quad ; \quad \Phi^+ \text{ and } \Phi^+ \text{ direct and adjoint fluxes} \\
A \text{ the disparition operator} \\
F \text{ the apparition operator}
\]

\[(1)\]

#### 3.1. SEFOR and ASTRID Doppler Effects

At first, direct and adjoint fluxes of the SEFOR I & II cores are compared with those of the ASTRID core to have a qualitative idea of the physics at play in the different cores. Figure 2 displays 33-energy-group mean direct fluxes, with the means adjoint fluxes in lighter colors. Flux level have been normalized for a better display (ASTRID flux level is of the order 10^{15} \text{ cm}^{-2} \text{s}^{-1} while SEFOR is around 10^{6} \text{ cm}^{-2} \text{s}^{-1}).

ASTRID presents:
- A softer spectrum than SEFOR I (which contains BeO moderator) and even softer than SEFOR II, with no moderator but steel rods. SEFOR cores exhibit a lower Pu content than ASTRID’s.
- A higher flux in the lower part of the spectrum, between 10 eV to ~3 keV which affects the Doppler Effect.
- A dip at ~3 keV due to the large resonance of 23Na.
Figure 2. Direct and Adjoint flux comparison between SEFORs’ and ASTRID’s core

Adjoint fluxes (light colored curves) convey the importance of a neutron of energy $E_g$ to the reactivity. It can be seen that in both SEFOR configurations, the slope of the adjoint flux at high energy (above 10 keV) is less pronounced than in ASTRID, due to the less degraded Pu vector as seen in Table III. The ASTRID Pu fuel contains numerous nuclides with fission thresholds.

Table III. Atomic fraction of elements in the fuel (in %) for SEFOR Core I & II and ASTRID Core

| Isotope     | SEFOR I | SEFOR II | ASTRID |
|-------------|---------|----------|--------|
| Fe (natural)| 24.2    | 28.3     | 23.8   |
| $^{23}$Na   | 11.3    | 11.6     | 11.3   |
| $^{16}$O    | 34.3    | 31.1     | 37.4   |
| Pu enrichment | 20.3 | 20.3     | 26.7   |
| Pu vector   |         |          |        |
| $^{238}$Pu  | $-^1$   | $-^1$    | 3.8    |
| $^{239}$Pu  | 91.7    | 91.7     | 39.9   |
| $^{240}$Pu  | 8.3     | 8.3      | 35.3   |
| $^{241}$Pu  | $-^1$   | $-^1$    | 7.9    |
| $^{242}$Pu  | $-^1$   | $-^1$    | 13.1   |

1 Some $^{238,241,242}$Pu were present in low amount in SEFOR’s fuel (respectively 0.015%, 0.68% and 0.034% of the total Pu vector) and were assimilated to $^{240}$Pu for the $^{238,242}$Pu and $^{239}$Pu for the $^{241}$Pu in the experimental program results [1]
In the end, those differences induce differences on the Doppler Effect contribution, in reactivity, broken down by energy for the two main relevant reactions – Capture and Fission – as seen in Figure 3, thanks to (1) derived from the Perturbation Theory [12].

![Figure 3. Doppler Effect breakdown in reactivity for SEFOR cores I & II and ASTRID core](image)

SEFOR cores I & II display compensations between total capture and fission reactions while this effect is practically nonexistent for ASTRID: in a softer spectrum, fission cross sections broadening of nuclides with fission thresholds doesn’t affect the reactivity as much.

**Table IV. Doppler reactivity effect breakdown into nuclides’ contribution (in pcm) using JEFF-3.1.1**

| Isotope | SEFOR I | SEFOR II | ASTRID |
|---------|---------|---------|--------|
| $^{239}$Pu | 12.6 | 15.8 | 3.1 |
| $^{240}$Pu | -9.1 | -7.3 | -33.3 |
| $^{241}$Pu | - | - | -13.8 |
| $^{235}$U | -0.2 | -0.1 | -0.1 |
| $^{239}$U | -609.2 | -477.5 | -456.0 |
| $^{56}$Fe | -3.0 | -3.8 | -6.1 |
| $^{23}$Na | -0.8 | -0.9 | -0.7 |
| $^{16}$O | -3.5 | -3.1 | -1.2 |
| **Total** | -613.2 | -478.3 | -514.7 |

It can be seen in Table IV – obtained using (1) – that the main contributor to the Doppler Effect is, as expected, the $^{239}$U. In SEFOR cores I & II, the relatively small positive effect induced by the broadening
of the $^{239}\text{Pu}$ fission cross-section is balanced by the increase of captures by the $^{240}\text{Pu}$. This compensation is however dependent on the neutronic spectrum and on the fuel’s plutonium vector: for ASTRID and its degraded Pu vector, the $^{240}\text{Pu}$ has a prominent role in the Doppler Effect contribution.

In addition, thanks to the calculated sensitivity vector, uncertainties on the Doppler Effect due to nuclear data and the representativeness ratio between SEFOR cores and ASTRID can be calculated with (2) from [12] – with the JEFF-3.1.1 nuclear data library and associated COMAC-V1 [14] dispersion matrix.

$$r = \frac{s_{\text{AST}}^T M s_{\text{SEF}}}{\sqrt{s_{\text{AST}}^T M s_{\text{AST}} \cdot s_{\text{SEF}}^T M s_{\text{SEF}}}}; \text{ with } s_{\text{SEF}} \text{ the sensibility vector of SEFOR }$$

$$s_{\text{AST}} \text{ the sensibility vector of ASTRID }$$

$$M \text{ the associated covariance matrix }$$

SEFOR core I and II representativeness regarding the ASTRID core are, respectively, of 0.809 and 0.813. One needs to thread lightly with the transferability of the SEFOR experiment toward ASTRID; this is mainly due to the vastly different Pu vector and fuel enrichment between both cores.

Uncertainties due to nuclear data on the calculated Doppler Effect are of 3.96% for SEFOR1 and 4.32% for SEFOR2; uncertainties for the ASTRID core Doppler Effect amounts to 4.41%.

### 3.2. Doppler Effect Comparison using Different Libraries for the Different Cores.

In table V, Doppler Effects using different evaluated nuclear data libraries, for the 3 cores, are presented.

|                | JEFF-3.1.1 | JEFFhyb | JEFF-3.2 | JENDL-4 | ENDF/B-7.1 |
|----------------|------------|---------|----------|---------|------------|
| SEFOR core I   | -613.2     | -609.9  | -634.4   | -617.4  | -622.9     |
| SEFOR core II  | -478.3     | -474.6  | -496.5   | -478.7  | -485.7     |
| ASTRID core    | -514.7     | -511.7  | -512.7   | -497.9  | -530.9     |

Switching between JEFF-3.1.1 and JEFF-3.2 has a significant impact for both SEFOR cores (-4.7% for Core I and -3.7% for Core II) while the ASTRID Doppler is not affected.

Since $^{238}\text{U}$ is the main contributor to the Doppler Effect, it is interesting to investigate the impact of this library change between the different cores with a breakdown by isotope into reactions and energy group. With JANIS [15], no differences were found on $^{238}\text{U}$ cross sections between the different evaluations. Hence, the Doppler reactivity differences when using different evaluations is due to indirect effects, i.e. spectrum changes due to changes in cross sections of other nuclides.

By computing Doppler Effect sensitivities to cross sections changes (via Equivalent Generalized Perturbation Theory) and one-group cross section variations between JEFF-3.1.1 and JEFF-3.2, one can obtain Doppler Effect variation between the two libraries. The change on the Doppler Effect between SEFOR Core I and ASTRID core when moving from JEFF-3.1.1 to JEFF-3.2 is due to $^{239}\text{Pu}$ fission (0.6%), $^{240}\text{Pu}$ capture (0.6%) and $^{25}\text{Na}$ elastic (0.6%). Of course, as $^{240}\text{Pu}$ does not exist significantly in SEFOR Core I, it can be only partially responsible for the differences of capture cross sections above 100 keV. JEFF-3.2 $^{25}\text{Na}$ elastic – which remains the reference – also induces a change on Doppler Effect through spectrum changes in the 1 keV region (it can be seen as a direct change between JEFF-3.1.1 and JEFFhyb which is JEFF-3.1.1 + $^{25}\text{Na}$ JEFF-3.2). The impact on Doppler is similar on the three cores.

But the change on $^{239}\text{Pu}$ fission cross section (specifically between 1 keV and 63 keV) between the 2 nuclear data evaluations JEFF-3.1.1 and JEFF-3.2 induces a differential change on the Doppler reactivity effect of SEFOR 1 & 2 on one side and ASTRID on the other side. The JEFF-3.2 $^{239}\text{Pu}$ fission cross section change is not supported by integral data assimilation and should be further investigated.
4. CONCLUSION

The prediction of the Doppler Effect by neutronic simulation codes require experimental validation, the reason for which transient tests conducted within SEFOR (South-West Experimental Fast Oxide Reactor), a fast reactor fueled with mixed PuO$_2$-UO$_2$ and cooled with sodium are being used. The SEFOR experimental tests are being analyzed with the ERANOS code package using nuclear data libraries of different evaluations: JEFF-3.1.1, JEFF-3.2, ENDF-B/VII.1 and JENDL4. The C/E values on the SEFOR Doppler Effect range from 1.01 to 1.07 with an experimental uncertainty of ±0.06. With the use of perturbation break down in energy and isotope, this paper identifies the reasons for such large C/E spread and identifies the differences and similarities of the SEFOR Doppler Effect with the ASTRID one. A fine analysis has been conducted on the origins of such bias in complement to integral data assimilation work which has shown that JEFF-3.1.1 is a good starting point for all nuclides, except $^{23}$Na for which JEFF-3.2 should be used. JEFF-3.2 changes relative to JEFF-3.1.1 on $^{239}$Pu fission affects significantly the Doppler Effect, changes which are not supported by the integral data assimilation work. Hence, JEFFhyb is the better choice for calculating Doppler Effect – which is supported by the best C/E value (1.018 and 1.010 respectively for SEFOR I and SEFOR II) of all tested nuclear data sets. The representativeness approach gives values slightly above 0.8 with COMAC-V1, meaning that SEFOR I and II are representative enough of ASTRID to grasp the physics involved, yet conclusions from SEFOR should not be directly applied to the ASTRID core (not the same Pu vector). A more thorough analysis on a 3D model of the SEFOR cores with the APOLLO3-RNR code system is undergoing.

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