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P. Leconte, G. Truchet, J.-F. Vidal, A. Santamarina, P. Blaise. Validation of the Apollo2.8 code package for the calculation of  $\beta_{EFF}$  and  $\Lambda$  kinetics parameters and the reactivity versus reactor period relationship. PHYSOR 2016, May 2016, Sun Valley, United States. cea-02438724

**HAL Id: cea-02438724**

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Submitted on 28 Feb 2020

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# VALIDATION OF THE APOLLO2.8 CODE PACKAGE FOR THE CALCULATION OF $\beta_{\text{EFF}}$ AND $\Lambda$ KINETICS PARAMETERS AND THE REACTIVITY VERSUS REACTOR PERIOD RELATIONSHIP

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## SUMMARY

This paper presents the analysis of kinetics parameters experiments performed in the IPEN/MB-01 mock-up with the deterministic APOLLO2 code. Comparisons of measurements and calculations are presented on the effective delayed neutron fraction  $\beta_{\text{eff}}$ , prompt neutron generation  $\Lambda$  and on the relationship between the reactivity and the period. The impact of the calculation scheme and of the input nuclear data library is tested and discussed. Comparisons with TRIPOLI4 continuous energy Monte-Carlo calculations have been done for numerical validation purpose.

The study shows the significant impact of uncertainties associated with delayed neutron abundances and decay constants on the reactivity prediction, ranging from 4 to 6% in the  $[0 - 0.5\%]$  range. One of the main results is also the overprediction of  $\beta_{\text{eff}}$  by  $3 \pm 0.7\%$ , using the JEFF-3.1.1 data, consistent with the overprediction of the reactivity of 4-6% over the whole positive period range. The ENDF/B-VII.0, in spite of a better estimate of  $\beta_{\text{eff}}$ , leads to an underestimation of the reactivity reaching up to 13%.

## 1. INTRODUCTION

The effective kinetics parameters of a nuclear reactor, namely the effective fraction of delayed neutrons  $\beta_{\text{eff}}$  and the prompt neutron generation time  $\Lambda$ , are of one of the fifteen design parameters which need to be validated for the APOLLO2.8/CEA2005V4 code package [1] used by CEA and its industrial partners EDF and AREVA. A more accurate validation of the individual groups of kinetics parameters is also needed to validate the relationship between the reactivity and the reactor period. This relation, just like the determination of the  $\beta_{\text{eff}}$ , are used in many applications of reactor physics, one of the main being the measurement of neutron absorber reactivity worth. Until very recently, the validation of kinetics parameters was difficult to assess due to few reported data in thermal systems. Moreover, the only internationally available data were based on critical configurations far from being representative of the neutron spectrum met in PWR.

Thanks to an extensive work performed by the team from Nuclear and Energy Research Institute (IPEN) in Brazil, in the IPEN/MB01 critical mock-up facility, it is now possible to validate the delayed neutron parameters associated to each time group. Indeed, by developing an innovative experimental technique, they obtain the effective delayed neutron parameters and also a set of  $\beta_i$  and  $\lambda_i$  parameters in a purely experimental way.

The purpose of this paper is to contribute to the validation APOLLO2.8/CEA2005V4 code package, based on the JEFF-3.1.1 nuclear data library, for the calculation of individual and effective delayed neutron parameters, just like the relationship between the reactivity and the reactor period. Both REL2005 optimized scheme and SHEM-MOC reference scheme will be used, in order to evaluate the impact of cross section collapsing and refinement of the spatial mesh used by the 2D-MoC solver. 3D calculations based on the continuous energy Monte Carlo code TRIPOLI4 will be presented either. Comparisons of several nuclear data files will be performed, in order to evaluate the impact of the eight-fold precursor groups adopted in JEFF-3.1.1, in agreement with the recommendation of WPEC Subgroup 6, whereas JEF-2.2 and ENDF/B-VII.0 library still use six groups.

## 2. OVERVIEW OF THE EXPERIMENTS

IPEN/MB-01 is a zero power (<100W) research reactor located in São Paulo, Brazil. The core configuration is a 28x26 lattice of stainless steel clad fuel pins made of 4.35 wt.% enriched uranium oxide. The reactor is fully flooded with light water when it is operated, the critically being adjusted by the insertion of 2 groups of 12 AgInCd control rods. The square pitch of the core was chosen to be close to the optimum moderation ratio.

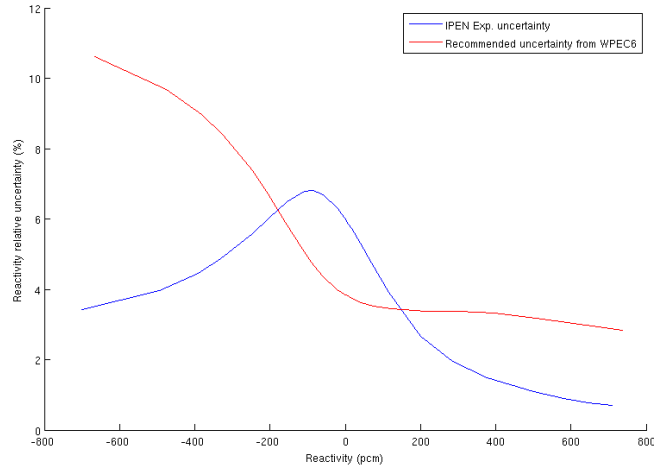
Experimental data related to Kinetics Measurements are evaluated in the IRPhE database, under the following classification: IPEN(MB01)-LWR-RESR-001 [2]. Measurements of delayed neutron parameters are based on a combination of macroscopic and microscopic noise techniques.

On the one hand, macroscopic noise experiments are used to solve the low frequency range (<1 Hz) of the auto-power spectral density (APSD) and cross-power spectral density (CPSD). The method is based on a least-square fit of both APSD and CPSD. On the other hand, microscopic noise experiments were used to obtain the effective delayed neutron fraction  $\beta_{\text{eff}}$ , the prompt neutron generation time  $\Lambda$  and their ratio  $\beta_{\text{eff}}/\Lambda$ . The experimental methodology uses a combination of Rossi- $\alpha$  and Feynman- $\alpha$  techniques. Compared with other methods, this one leads to a purely experimental evaluation of effective delayed neutron parameters.

In the IRPhE report, a benchmark is proposed to validate the reactivities from the one region inhour equation. The benchmark covers eight reactivity values from -0.76\$ to 0.78\$. Instead of discrete values, we have decided to compare the calculations of the inhour equation based on continuous values of  $T$ , in order to cover a range of -1\$ to 1\$. To do so, we have recalculated the reactivity values based on the  $(\beta_i, \lambda_i)$  provided by the IRPhE report. Moreover, we decided to represent the reactivity in pcm instead of dollar because when reactivities are measured in dollars, they are always converted in pcm to be compared with calculations. By doing this, we remove a correlation which exists between the numerator and the denominator in the inhour equation, so we obtain:

$$\rho_{pcm} = \Lambda/T + \sum_{i=1}^{n_{prec}} \frac{\beta_i}{1+\lambda_i T} \quad (1)$$

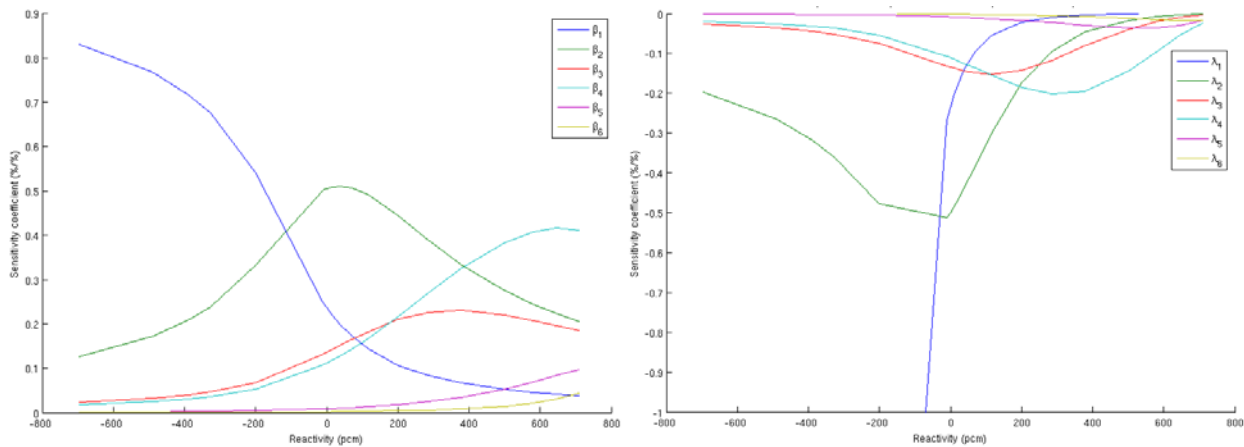
The relative uncertainty on  $\rho_{pcm}$  has been calculated with a Monte-Carlo method and is illustrated in Figure 1. It is compared to the recommended uncertainties by WPEC6 [3] on the abundances of delayed neutron from  $^{235}\text{U}$  and  $^{235}\text{U}$  fission.



**Figure 1.** Uncertainty on the absolute reactivity in pcm, for positive and negative periods

For  $\rho_{\S}$  close to 1, Equation (16) shows that the uncertainty on  $\rho_{pcm}$  is mainly coming from  $\beta_{eff}$ , which explains the asymptotic level at 0.7% on the blue curve, while using uncertainties on individual parameters  $\beta_i$ , we would reach 2.5% from IPEN experimental uncertainties (blue curve) and 3% with the ones from WPEC6 (red curve). For  $\rho_{\S}$  close to 0, the uncertainty on  $\rho_{pcm}$  is the combination of all the delayed neutron parameters ( $\beta_i, \lambda_i$ ), with an asymptotic value of 6% from IPEN experiment and 3.5% with the data from WPEC6.

For a more quantitative estimation of the impact of each parameter on the reactivity, we have evaluated the sensitivity coefficients from each family. They have been calculated assuming a 1% increase on each of the 12 parameters ( $\beta_i, \lambda_i$ ) based on equation (4). The corresponding plots are presented hereafter (Figure 2). One can notice the very high sensitivity of the first decay constant in the negative period range: it means that when the reactor is shut down, the level of subcriticality may be highly dependent on how accurate the decay of  $^{87}\text{Br}$  is known.



**Figure 2.** Sensitivity coefficients of the reactivity to  $\beta_i$  (left side) and  $\lambda_i$  (right side)

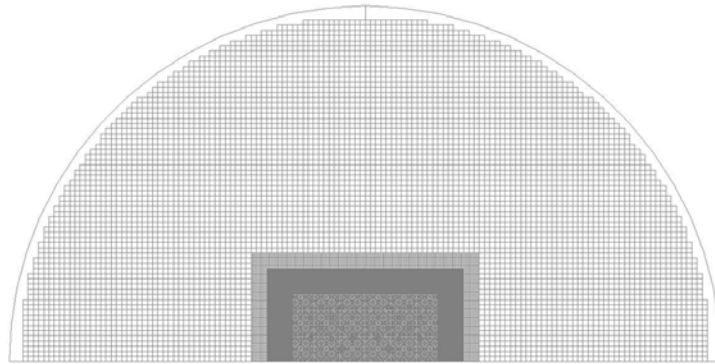
### 3. ANALYSIS OF DATA

#### 3.1. Calculation methods and evaluated delayed neutron data

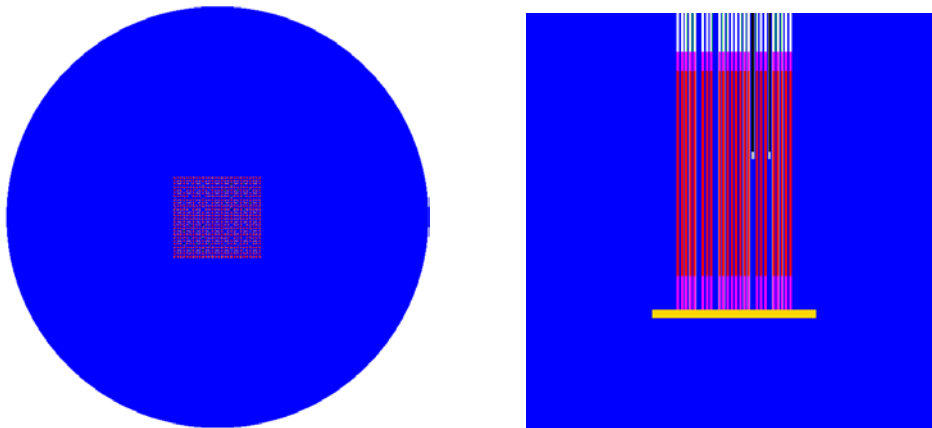
The experimental data were analysed with the APOLLO2.8 deterministic code [1], through two different calculation schemes, both based on a 2D modeling of the full core configuration (Figure 3):

- The SHEM-MOC reference scheme for LWR assemblies performs a self-shielding calculation above 23 eV on a multicell pattern, followed by a heterogeneous exact-2D flux calculation of the full core, based on the Method of Characteristics and using 281 energy groups.
- The optimized REL2005 is a two-step calculation scheme: in the first step, both self-shielded cross-sections ( $E > 23$  eV) and the neutron energy spectrum are calculated in the 2D assembly geometry; in the second step, the exact-2D MoC calculation is carried out, using collapsed cross sections from the first step, in an optimized 26-group mesh.

A TRIPOLI-4 input file was also generated, based on the exact 3D geometry (Figure 4). Calculations have been performed with the recently implemented IFP method in order to provide adjoint-weighted kinetic parameters [4]. Additional developments were realized for this study in order to obtain the adjoint-weighted delayed neutron parameters ( $\beta_i$ ,  $\lambda_i$ ) for each family.



**Figure 3.** 2D model of the full core of IPEN/MB-01 for the APOLLO2/MoC solver (REL2005)



**Figure 4.** 3D model of the full core of IPEN/MB-01 for TRIPOLI-4® code

Various delayed neutron data were tested: JEF-2.2, ENDF/B-VII.0 and JEFF-3.1.1. For the latter, the historic 6-group structure was changed to a 8-group structure, following the recommendations of the NEA/WPEC6 group [3]. The main reasons for adopting this new delayed neutron group structure are the need for a more consistent description of the delayed neutron emission from the longest lived precursors and the the advantage of using a single set of precursor half-lives (for all fissile isotopes and incident neutron energies) in calculations of reactor kinetics. Therefore, data in the new structure can be used without approximation in reactor kinetics calculations by solving only nine differential equations, on the contrary, classical six group structure (characterized by different sets of half-lives for different isotopes and for different incident neutron energies) in principle required the solution of six differential equations for each fissionable isotope and for each different incident neutron energy. Table 1 summarizes the main delayed neutron data from JEFF-3.1.1.

**Table 1.** Delayed neutron parameters from JEFF-3.1.1, in the 8-group model

Group	Precursor	Half-life (s)	Group Average (s)	$\lambda_i$ (s <sup>-1</sup> )	<sup>235</sup> U	<sup>235</sup> U	<sup>238</sup> U
					thermal fission	fast fission	fast fission
					$\beta_i$ (pcm) (*)	$\beta_i$ (pcm) (*)	$\beta_i$ (pcm) (*)
1	<sup>87</sup> Br	55.6	55.6	0.0124667	21.80 ± 13%	22.63 ± 2%	12.84 ± 16%
2	<sup>137</sup> I	24.5	24.5	0.0282917	102.35 ± 4%	99.82 ± 2%	159.05 ± 18%
3	<sup>88</sup> Br	16.3	16.3	0.0425244	60.74 ± 10%	65.95 ± 3%	57.35 ± 21%
4	<sup>138</sup> I	6.46	5.21	0.1330420	130.93 ± 12%	133.09 ± 2%	209.51 ± 20%
	<sup>93</sup> Rb <sup>89</sup> Br	5.93 4.38					
5	<sup>94</sup> Rb	2.76	2.37	0.2924570	219.98 ± 2%	207.62 ± 2%	449.61 ± 18%
	<sup>139</sup> I	2.30					
	<sup>85</sup> As	2.08					
	<sup>98m</sup> Y	2.00					
6	<sup>93</sup> Kr	1.29	1.04	0.6664877	60.01 ± 5%	61.95 ± 4%	302.80 ± 26%
	<sup>144</sup> Cs	1.00					
	<sup>140</sup> I	0.86					
7	<sup>91</sup> Br	0.542	0.424	1.634781	53.97 ± 2%	57.96 ± 5%	195.75 ± 19%
	<sup>95</sup> Rb	0.384					
8	<sup>96</sup> Rb	0.203	0.195	3.5546	15.22 ± 41%	15.97 ± 4%	142.38 ± 143%
	<sup>97</sup> Rb	0.170					
Sum					665.00	664.99	1529.29

(\*) the relative uncertainties are the ones recommended by WPEC6 report [3] **Erreur ! Source du renvoi introuvable.** but are not reported in the JEFF-3.1.1 nuclear data library

### 3.2. C/E comparison on the effective delayed neutron fraction and prompt generation time

The comparison of calculated and measured effective kinetics parameters are given in Table 2.

**Table 2.** Calculated vs Experimental effective kinetics parameters:  $C/E - 1 \pm \delta E/E$  (%)

Effective kinetic parameter	TRIPOLI-4.9DEV JEFF-3.1.1	APOLLO2.8 SHEM-MOC JEFF-3.1.1	APOLLO2.8 REL2005 JEFF-3.1.1	APOLLO2.8 REL2005 ENDF/B-VII.0	APOLLO2.8 REL2005 JEF2.2
$\beta_{\text{eff}}$ (pcm)	$3.2 \pm 0.7$	$3.1 \pm 0.7$	$2.9 \pm 0.7$	$0.1 \pm 0.7$	$4.9 \pm 0.7$
$\Lambda$ ( $\mu\text{s}$ )	$-4.7 \pm 3.3$	$-3.6 \pm 3.3$	$4.2 \pm 3.3$	$4.5 \pm 3.3$	$4.1 \pm 3.3$

The TRIPOLI-4.9 results indicate an overestimation of the  $\beta_{\text{eff}}$  of around 3%, using delayed neutron abundances from JEFF-3.1.1, a trend which is consistent with APOLLO2.8 calculations using the same data. The substitution of the nuclear data library by JEF-2.2 increases the C/E discrepancy by almost 2%, in agreement with what was expected, as the delayed neutron multiplicity  $\nu_{235U}^d$  was reduced when the JEFF-3 file was built. The substitution of JEFF-3.1.1 by ENDF/B-VII.0 leads to a significant improvement in the prediction of IPEN experiments, with a consistency within 1 $\sigma$  uncertainty. The impact of the calculation scheme in APOLLO2 has been shown negligible.

The prompt neutron generation time is slightly underestimated by TRIPOLI4.9 calculations, but remains in the range of 2 $\sigma$  uncertainty. The result is consistent with MCNP6 results reported in [5] where the (C-E)/E was  $-3.8 \pm 4.6\%$ . The APOLLO2.8 calculations based on SHEM-MOC leads to the same trend with an underestimation of 3.6%. The REL2005 calculation of  $\Lambda$  is about 8% higher than with the SHEM-MOC scheme. This difference may occur because of the 26-group collapsing of effective cross sections, involving a collapsing of multigroup values of the inverse average velocity, defined as follows in APOLLO2:

$$\langle 1/v \rangle_g = \frac{\int d\vec{r} \int dE \frac{1}{v(E)} \Phi(E, \vec{r})}{\int d\vec{r} \int dE \Phi(E, \vec{r})} \quad (1)$$

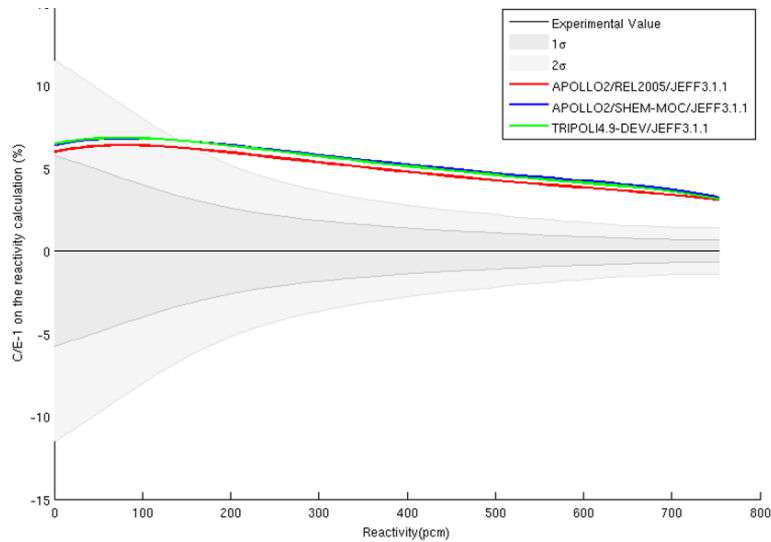
Indeed, the collapsing used in APOLLO2 is not supposed to preserve the velocity mean values from a fine mesh to a coarse mesh. In addition to this, the weighting method should use the  $\Phi(E, \vec{r}) \cdot \Phi^+(E, \vec{r})$  product instead of only the forward flux, to preserve the generation time after the collapsing of 281 to 26 groups.

By the way, the 8% higher prompt neutron generation time from REL2005 calculations involves a 4% overestimation compared with the experiment, a trend which, luckily, also stays within the range of 2 $\sigma$  uncertainty.

### 3.3. C/E comparison on the inhour relation

The agreement between the calculated and measured relationship between the reactivity and the reactor period was tested on a wider range than the one considered in [5]0. To do so, we had to re-estimate the experimental values based on the measured delayed-neutron parameters and to evaluate the propagated uncertainty, as described in §2.5. We have followed the same procedure to evaluate the Inhour relation based on computed kinetic parameters.

Firstly, we have computed the inhour relation based on the same data library (JEFF-3.1.1) but using different calculation methods. The curves in Figure 5 give the (C-E)/E values on the reactivity prediction as a function of the reactivity. It shows that a very small impact occurs by using TRIPOLI4 or APOLLO2 and even with the optimized scheme using collapsed cross sections: the maximum difference is less than 1%. The same comparison was performed for the negative reactivity range with equivalent conclusions.



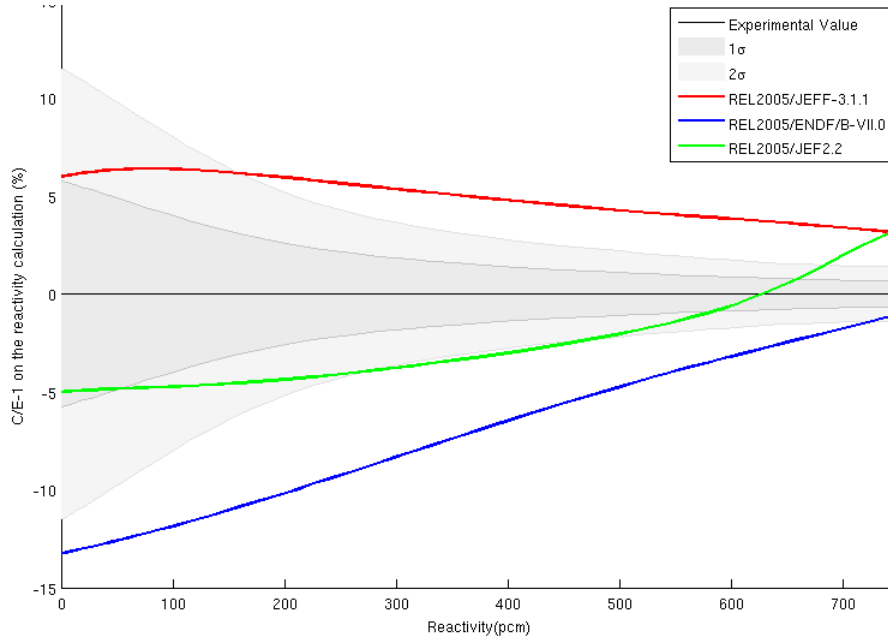
**Figure 5.** Comparison of various calculation methods based on JEFF-3.1.1 delayed neutron data for the prediction of the inhour relation in the positive reactivity range

Then the agreement between the calculated and measured inhour relation is presented in Figure 6 for APOLLO2/REL2005 calculations based on different libraries.

An overestimation of the reactivity prediction is observed ranging from 3.8 to 6.5% over the [0-1\$] reactivity range, using either APOLLO2 or TRIPOLI-4 calculations based on JEFF-3.1.1. The C/E differences remains below  $2\sigma$  uncertainty only for reactivities of less than 150 pcm. These results are consistent with the overestimation of  $\beta_{eff}$  discussed before: a systematic reduction of the delayed neutron abundances by 3% would improve the reactivity prediction within  $2\sigma$  uncertainty over the full range of positive periods. The relatively constant behavior of the curve indicates a



good estimation of the relative delayed neutron abundances which prevents reactivity-dependent bias, producing canceling effects when two reactivities of the same order are compared.



**Figure 6.** Comparison of various delayed neutron data (APOLLO2.8/REL2005 calculations) for the prediction of the inhour relation in the positive reactivity range

The change of JEFF-3.1.1 input library to JEF-2.2 or ENDF/B-VII.0 produces significantly different behaviors. Using JEF-2.2, very small reactivities (<50pcm) are predicted below 1σ uncertainty and we stay below 2σ till 650 pcm. Nevertheless, these apparently better results should be balanced by the worse prediction of the effective delayed neutron fraction which is overestimated by 5% compared with IPEN experiments. The overestimation is equivalent to a shift of the curve to lower values, which would make most of the reactivity prediction out of the 2σ uncertainty range.

The results obtained with ENDF/B-VII.0 are even worse, reaching a maximum bias of 13% for small reactivities of less than 10 pcm. A linear trend is observed with a decrease of the bias to almost 0 close to prompt reactivity which indicates a possible bias on the relative values of individual delayed neutron data. This can be confirmed by the calculation of the mean delayed neutron lifetime

$\bar{\tau} = \frac{\sum \beta_i \tau_i}{\sum \beta_i}$ , as for low reactivities, the inhour equation can be approximated in the following form:

$$\rho_{pcm} \approx \frac{\beta_{eff} \bar{\tau}}{\Lambda} \quad (2)$$

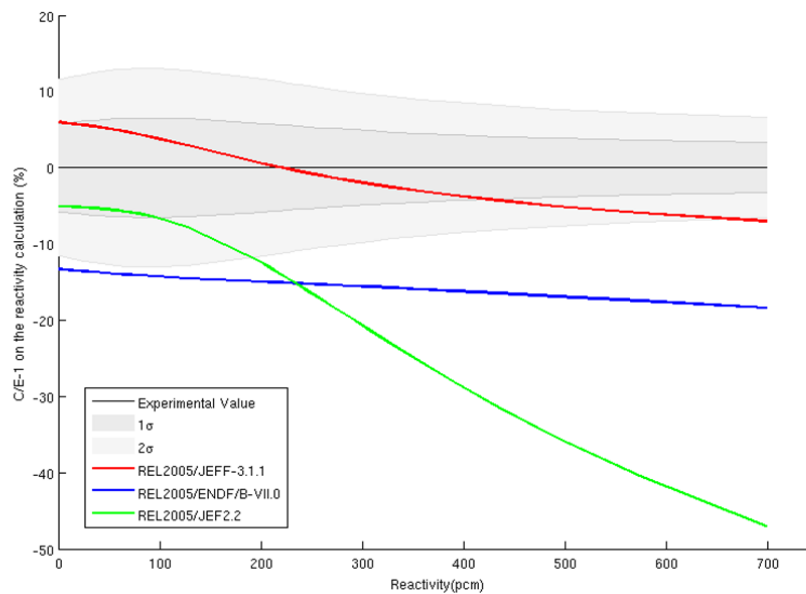
Table 3 presents the comparison of calculated and measured  $\bar{\tau}$  values. It clearly indicates that the best set of  $\tau_i$  values is the one from JEFF-3.1.1. The strong underestimation of  $\bar{\tau}$  with JEF-2.2 or

ENDF/B-VII.0 data is clearly responsible for the underprediction of the inhour relation in the low reactivity range (<100 pcm).

**Table 3.** Comparison of calculated and measured mean delayed neutron lifetime  $\bar{\tau} = \frac{\sum \beta_i \tau_i}{\sum \beta_i}$

IPEN/MB-01 experiments	APOLLO2.8/REL2005 JEFF-3.1.1		APOLLO2.8/REL2005 ENDF/B-VII.0		APOLLO2.8/REL2005 JEF2.2	
	$\bar{\tau}$ (s)	C/E-1	$\bar{\tau}$ (s)	C/E-1	$\bar{\tau}$ (s)	C/E-1
$12.17 \pm 0.69$	12.49	2.6±5.7%	10.52	-13.6±5.7%	11.0	-9.6±5.7%

Finally, we have tested the agreement between the calculated and measured inhour relation in the negative reactivity range. It is presented in Figure 7 for APOLLO2/REL2005 calculations based on different libraries (note than x-axis gives the absolute value of negative reactivities).



**Figure 7.** Comparison of various delayed neutron data (APOLLO2.8/REL2005 calculations) for the prediction of the inhour relation in the negative reactivity range

The comparison of JEFF-3.1.1 with ENDF/B-VII.0 and JEF2.2 shows even higher differences than in the positive period range. Calculations based on ENDF/B-VII.0 underestimate the reactivity by 13 to 18% over the full range of negative reactivities. JEF2.2 works slightly better, especially for reactivities of less than 200 pcm where the reactivity prediction stays within 2s uncertainty, but for higher values (i.e. period between -100 and 80s), we observe a divergent trend which reaches more than 40% close to -1\$ of reactivity. The JEFF-3.1.1 clearly gives the best agreement with the experiment and a relatively constant behavior over the reactivity range, which here again reduces the risk of bias when two reactivities are compared.

## 4. CONCLUSIONS

The analysis of the kinetic parameter experiments performed in the IPEN mock-up was used to extend the validation of the APOLLO2.8/CEA2005V4 code package. In addition to the validation of the effective delayed neutron fraction and prompt neutron generation time, these experiments provide a set of measured parameters of the delayed neutron abundances and decay constants which are useful to validate the relation between the reactivity and the reactor period. The main conclusions from this study are summarized hereafter:

- A significant impact of the delayed neutron parameter uncertainties was observed when they are propagated to the absolute reactivity in pcm through the inhour equation. Based on IPEN measurements of  $\beta_i$  and  $\lambda_i$ , an uncertainty of 3 to 6% ( $1\sigma$ ) is obtained on the typical reactivity range of [0; 0.5\$] where the reactors are operated, to be compared to 3-4% using the recommended data by WPEC6. It should be noted that the lack of correlation data in both data set may involve unrealistic uncertainties when they are propagated to the reactivity.
- The overprediction of  $\beta_{\text{eff}}$  obtained with the previous nuclear data library JEF-2.2 has been improved with JEFF-3.1.1 with the reduction of the delayed neutron multiplicity in the thermal fission of  $^{235}\text{U}$ . Nevertheless, a remaining overestimation of  $3 \pm 0.7\%$  indicates that more thermal experiments would be required to clarify the need to reevaluate these data.
- The ENDF/B-VII.0 delayed neutron data underestimate the reactivity, reaching up to 13% for low values (<100 pcm). A better behavior is obtained with JEFF-3.1.1, due to a more consistent evaluation of the mean delayed neutron lifetime. Here again, the trend on the in-hour relation based on JEFF-3.1.1 data would be consistent with a small decrease of the  $\beta_{\text{eff}}$ .

## 5. ACKNOWLEDGMENTS

The authors are grateful to A. Dos Santos and R. Diniz from IPEN for answering questions and providing detailed information on the measurement procedure. The authors would like also to acknowledge EDF and AREVA for the financial support of this study.

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