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# EXPERIMENTAL VALIDATION OF THE CRISTAL V2.0 FRENCH CRITICALITY CALCULATION PACKAGE

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## ABSTRACT

A new version of the CRISTAL criticality calculation package, named CRISTAL V2.0 [1], has been developed by IRSN and CEA, in collaboration with AREVA. Four calculation routes are now available, using nuclear data issued from the JEFF-3.1.1 evaluation: two multigroup routes based on 281 groups cross-sections (APOLLO2 – MORET 5 or APOLLO2-S<sub>n</sub> calculations), a pointwise Monte Carlo route (TRIPOLI-4®) and a criticality standard calculation route.

The CRISTAL V2.0 package benefits from a broad validation database covering almost all areas of criticality-safety applications, from fuel fabrication to reprocessing, including transportation. 3,127 critical experiments, corresponding to 342 series, either issued from the OECD/ICSBEP Handbook or performed in French facilities (confidential data) were selected for the CRISTAL V2.0 validation database. Currently, more than 2,300 experiments are already part of the validation database.

This validation work does not highlight significant (C - E) discrepancies and inter-comparisons between the different calculation routes mainly show good agreements on a large set of common experiments.

## KEYWORDS

Validation – CRISTAL – APOLLO2 – MORET 5 - TRIPOLI-4

## 1. INTRODUCTION

Since more than 20 years, CRISTAL is the French package for Criticality-Safety. Carried out in a joint project between CEA, IRSN and AREVA, CRISTAL benefits from the recent advances of calculation codes and from the current knowledge concerning nuclear data. In the V2.0 version, in addition of up to date calculation schemes, the new LATEC workbench brings to users many new capabilities.

Regarding all the CRISTAL versions, validation was always a major point of interest with a continuous work in order to improve more and more the level of confidence in the CRISTAL package. For the

CRISTAL V2.0 version, a significant effort has been done to increase the representativeness and the number of experiments in the validation database. Thus, the CRISTAL validation database, which was initially made up of more than 500 critical experiments (CRISTAL V0) and thereafter of 2,132 experiments (CRISTAL V1), is being extended to 3,127 experiments.

## 2. CRISTAL V2.0 CALCULATION ROUTES

The CRISTAL V2.0 package [1] is composed of four calculation routes which use JEFF-3.1.1 nuclear data [2]:

- A multigroup Monte Carlo route involving the multigroup nuclear data library CEAV5.1.2 (derived from JEFF-3.1.1 evaluation), the APOLLO2.8-3.C [3] cell code (used for self-shielding, flux calculations, collapsing and homogenization with  $P_{ij}$  calculations) and the MORET 5.B.1 [4] Monte Carlo code (for 3D calculation with a general  $P_n$ -like anisotropy treatment),
- A multigroup deterministic route involving the  $S_n$  method implemented in the APOLLO2.8-3.C code, the multigroup nuclear data library CEAV5.1.2 (derived from JEFF-3.1.1 evaluation) and the APOLLO2 cell code (used for self-shielding, flux calculations, collapsing and homogenization with  $P_{ij}$  calculations),
- A pointwise route using the TRIPOLI-4.8.1@ [5] Monte Carlo code with the continuous energy CEAV5.1.2 library (derived from JEFF-3.1.1 evaluation),
- A criticality standard route founded on iterative APOLLO2- $S_n$  (multigroup deterministic route) calculations and also including the LATEC Workbench [6] capability to simply check the deterministic calculation results. Thus, the validation of this route is directly linked to the multigroup deterministic and the pointwise routes validations.

A major improvement of the V2.0 version is the update of the cross sections library, from JEF-2.2 to JEFF-3.1.1. The APOLLO2 and TRIPOLI-4 libraries based on the JEFF-3.1.1 evaluation and called CEAV5.1.2 are generated by the French nuclear data processing system GALILEE [7], that relies on the NJOY nuclear data code for pointwise and multigroup cross sections and on the CALENDF code for probability tables. A noticeable feature of the GALILEE system is that the APOLLO2 library used by multigroup Monte Carlo and deterministic routes are built in a fully consistent way with the pointwise library for the TRIPOLI-4 Monte Carlo code.

The APOLLO2 multigroup library is based on the 281-group energy mesh SHEM [8] optimized for LWR and which avoids the resonance self-shielding approximation below 23 eV.

## 3. VALIDATION METHODOLOGY

The CRISTAL validation methodology is based on the following steps:

- A validation working group defines a set of experiments of interest (Validation database) addressing the needs expressed by the users.
- Criticality calculations are performed with the different calculation routes of the CRISTAL package to provide the  $k_{\text{eff}}$  value for each selected experimental configuration, exclusively using validated schemes and procedures that are recommended for CRISTAL V2.0 users.
- Calculation - Experiment (C – E) discrepancies and their related uncertainties are estimated and analyzed.

### 3.1. Validation Database

Validation is based on calculation-experiments comparisons. The observed discrepancies are then interpreted and eventually transposed to actual configurations. Therefore critical experiments were selected to investigate all the operations encountered in the nuclear fuel cycle (including fabrication, transport, storage, and reprocessing).

The different criteria of the database selection were:

- Wide variety of fissile media covering those encountered in the nuclear fuel cycle,
- Diversity of configurations (to cover a wide moderation ratio range and to validate different materials),
- Variety of laboratories (to avoid eventual experimental biases and correlations between experiments),
- Quality of data provided in benchmarks.

The main sources of the benchmarks selection are, on the one hand, the OECD/ICSBEP Handbook [9] and, on the other hand, experiments performed by IRSN in the CEA Valduc facilities (Apparatus B, MARACAS), some of them with the financial support of the AREVA company, as well as experiments performed by CEA in Saclay (Alecto) and in Cadarache (Eole and Minerve reactors).

Thus, the CRISTAL validation database is being extended for the new V2.0 version:

- To enhance the consistency between the selected experiments of each route,
- To take into account the needs highlighted for the last few years,
- To have a better statistic, a larger diversity of laboratories,
- To investigate inconsistencies detected in the CRISTAL V1 validation studies.

The final selection of experiments for each route is the responsibility of the entity supporting its validation (CEA or IRSN), but a CRISTAL validation working group ensures the coordination of all and publishes a dedicated report with the complete validation data base.

Finally, the CRISTAL V2.0 experimental validation database is composed of 3,127 critical experiments (342 series) amongst which 2,714 were selected for the APOLLO2-MORET 5 multigroup route; 793 for the APOLLO2-S<sub>n</sub> multigroup deterministic route and 1,350 for the TRIPOLI-4 pointwise route (see Table I).

Table I. CRISTAL validation database

Fissile Medium	ICSBEP Categories	Number of cases					
		Multigroup route « APOLLO2-MORET 5 »		Multigroup route « APOLLO2 S <sub>n</sub> »		Pointwise route « TRIPOLI-4 »	
		Target	Already calculated	Target	Already calculated	Target	Already calculated
PU (70 series)	PU-COMP-INTER	1	1	0	0	0	0
	PU-COMP-MIXED	34	34	0	0	6	6
	PU-MET-FAST	66	53	26	26	53	53
	PU-MET-INTER	1	0	0	0	1	1
	PU-SOL-THERM	310	283	119	119	235	235
HEU (104 series)	HEU-COMP-FAST	5	0	0	0	0	0
	HEU-COMP-INTER	0	1	8	8	0	0
	HEU-COMP-MIXED	26	26	0	0	12	12
	HEU-COMP-THERM	121	20	0	0	25	25
	HEU-MET-FAST	237	180	94	47	141	141
	HEU-MET-INTER	4	4	0	0	4	4
	HEU-MET-MIXED	4	3	2	2	4	4
	HEU-MET-THERM	70	112*	4	4	68	68
HEU-SOL-THERM	295	220	156	156	180	180	
IEU (21 series)	IEU-COMP-FAST	1	0	0	0	0	0
	IEU-COMP-INTER	18	4	0	0	0	0
	IEU-COMP-THERM	4	2	0	0	2	2
	IEU-MET-FAST	11	9	6	6	0	0
	IEU-SOL-THERM	44	1	18	0	0	0
LEU (88 series)	LEU-COMP-THERM	681	550	93	93	273	273
	LEU-MET-THERM	34	31	0	0	30	30
	LEU-MISC-THERM	60	46	44	44	11	11
	LEU-SOL-THERM	112	109	37	33	96	96
U233 (9 series)	U233-COMP-THERM	9	0	0	0	0	0
	U233-MET-FAST	1	1	1	0	3	3
	U233-SOL-INTER	6	6	6	0	11	11
	U233-SOL-THERM	36	36	7	0	28	28
MIX (46 series)	MIX-COMP-INTER	0	0	1	1	0	0
	MIX-COMP-THERM	323	318	59	59	60	60
	MIX-MET-FAST	28	28	31	31	2	2
	MIX-MET-INTER	2	0	0	0	0	0
	MIX-MET-MIXED	0	0	1	1	0	0
	MIX-MISC-THERM	104	73	61	61	58	58
MIX-SOL-THERM	60	67**	19	19	47	47	
SPEC (4 series)	SPEC-MET-FAST	6	3	0	0	0	0
<b>TOTAL</b>		<b>2714</b>	<b>2221</b>	<b>793</b>	<b>710</b>	<b>1350</b>	<b>1350</b>

\* Two benchmark models are included in the database for HEU-MET-THERM-011

\*\* Seven experiments of a non ICSBEP series have been transferred to MIX-MISC-THERM, when evaluated for ICSBEP.

### 3.2. Validation Process

First of all, the validation work consists in calculating the C-E value exclusively using schemes and procedures that are recommended for CRISTAL V2.0 users. C-E value is given by calculated  $k_{\text{eff}}$  minus benchmarks  $k_{\text{eff}}$ , and its combined standard deviation ( $\sigma = \sqrt{\sigma_{\text{calculation}}^2 + \sigma_{\text{benchmark}}^2}$ ).

Calculations are considered in good agreement with the benchmark when the discrepancies are in the uncertainties margins (depending on the combined standard deviation and on the confidence interval).

Comparisons with other available experimental programs in the same field (similar media, materials and/or configurations) allow highlighting eventual experimental biases.

In a second step, (C - E) discrepancies are analyzed in order to uncouple the different sources of calculation biases and so, have a feedback to the nuclear data and/or to the calculation schemes using inter-code comparisons:

- Between the different CRISTAL V2 routes, with the benefit of a consistent evaluation process for the nuclear data libraries generation, and with possibility of using other cross-section libraries (as ENDF-B/VII.0) with the TRIPOLI-4 pointwise code,
- Using other available calculation results from international codes (MCNP, SCALE, MONK, etc...).

In a final step, (C - E) discrepancies are analyzed in order to identify areas for further investigations, which can conduct to an extension of the validation database.

## 4. MAIN RESULTS

The main results of the validation are presented by medium type hereafter.

### 4.1. Solutions

#### 4.1.1. Low-enriched uranium solutions

The experimental programs involve low enriched  $\text{UO}_2(\text{NO}_3)_2$  and  $\text{UO}_2\text{F}_2$  solutions with an uranium concentration ranging from 168 g/l to 980 g/l. Different tanks and reflectors were studied.

As previously with the CRISTAL V1.2 package, a good  $k_{\text{eff}}$  prediction with a very slight over-estimation (about 0.2 %) can be pointed out for all cases, except for LEU-SOL-THERM-001 series ( $\text{UO}_2\text{F}_2$  with an uranium concentration of about 980 g/l), which leads to an over-prediction of about 1.5 %. As this over-prediction is higher than the experimental uncertainties and as similar results are obtained with other codes (MONK and MCNP) and libraries, this allows questioning either the quality of experimental data or the nuclear data of fluorine.

#### 4.1.2. High-enriched uranium solutions

The experiments involve mainly  $\text{UO}_2\text{F}_2$  and  $\text{UO}_2(\text{NO}_3)_2$  solutions. The uranium concentration ranges from 13 g/l to 730 g/l. Some of the solutions were poisoned with soluble gadolinium.

Good agreements are observed between the calculations and the experimental results. The previous CRISTAL V1.2 package had shown a general trend to  $k_{\text{eff}}$ 's over-prediction for high-Uranium

concentrations. The modification of the  $^{235}\text{U}$  capture cross section in the JEFF-3.1.1 evaluation used in CRISTAL V2.0 allows reducing significantly the discrepancies.

#### 4.1.3. Plutonium solutions

These experiments cover a broad range of isolated plutonium solutions or plutonium solutions in interaction with Pu concentrations from 10 g/l to 412 g/l and with various  $^{240}\text{Pu}$  contents.

Good agreements are observed between the calculations and the experimental results. The CRISTAL V1.2 package had shown a general trend to slightly over-predict  $k_{\text{eff}}$ . The modification of  $^{239}\text{Pu}$  unresolved resonance parameters and  $\bar{\nu}$  in the JEFF-3.1.1 evaluation allows reducing this over-prediction to a non-significant bias of about 0.2 %. There is no obvious trend, neither with plutonium concentration nor with the  $^{240}\text{Pu}$  content. As an over-estimation of almost 2 % can be noticed for the PU-SOL-THERM-019 benchmark involving a beryllium oxide reflector, the beryllium nuclear data could be responsible for this over-estimation.

#### 4.1.4. Mixed uranium and plutonium solutions

The experiments are carried out in different tanks with homogeneous mixed U-Pu nitrate solutions. The solutions are composed of low enriched uranium with different  $^{240}\text{Pu}$  contents and plutonium fractions.

An under-estimation of about 0.5 % is obtained, except for the MIX-SOL-THERM-003 benchmark, which led to contradictory results with an over-estimated  $k_{\text{eff}}$  of about 1 %, up to 1.3 %.

#### 4.1.5. $^{233}\text{U}$ solutions

For intermediate spectra, the experimental validation is based upon the U233-SOL-INTER-001 benchmark with uranium enriched at 98 % in  $^{233}\text{U}$ . An average under-estimation of about 1 % with a calculation-experiment discrepancy up to 3 % is observed. The use of nuclear data coming from the JEFF-3.1.1 evaluation with CRISTAL V2.0 leads to similar trends as those obtained with CRISTAL V1.2 and the JEF-2.2 evaluation. However, the standard deviation of calculation-experiment discrepancies is lower with CRISTAL V2.0.

For thermal spectra, the validation calculations are performed based upon uranium enriched at 98 % in  $^{233}\text{U}$  in  $\text{UO}_2(\text{NO}_3)_2$  solutions. The uranium concentration ranges from 45 g/l to 866 g/l. A good calculation-experiment agreement is observed with APOLLO2-MORET 5 and TRIPOLI-4 routes. However, a 2 %  $k_{\text{eff}}$  over-estimation for U233-SOL-THERM-013 case 15 is observed. Similar results for this case are obtained with the MCNP code and ENDF/B-V or ENDF/B-VI nuclear data, allowing expecting a potential experimental bias on this experimental configuration.

## 4.2. Powders

This category gathers experiments from the ICSBEP Handbook under the nomenclature LEU-COMP-THERM, HEU-COMP-MIXED and HEU-COMP-INTER. It concerns:

- Low-enriched uranium oxide powders with various moderation ratio, reflected by Plexiglas, concrete or polyethylene,
- Low-enriched (2 and 3 %)  $\text{UF}_4$  powder moderated by and reflected by various hydrogenous materials (paraffin, polyethylene, plexiglas),
- High-enriched (93 %) uranium oxide powder reflected by polyethylene,

- High-enriched (90 %) uranium hydride reflected by iron, beryllium or depleted uranium in epithermal spectrum,
- High-enriched (90 %) homogeneous Uranium/Boron/Graphite fissile medium in epithermal spectrum.

The calculations are in most cases in good agreement with the experimental  $k_{\text{eff}}$ ; in fact, most of the calculation-experiment discrepancies are in the uncertainty margins. Nevertheless, for some cases of LEU-COMP-THERM-045 involving boxes of  $\text{U}_3\text{O}_8$  powders interspersed with absorbing and hydrogenated materials, discrepancies up to around +1.5 % can be pointed out for the APOLLO2-MORET 5 and TRIPOLI-4 routes for concrete reflected cases, with an increasing tendency versus moderation.

When comparing with the former CRISTAL V1.2 package, a general improvement of the results can be outlined for experiments with highly enriched uranium. This is mainly due to the use of the JEFF-3.1.1 evaluation that benefits from corrections of the  $^{235}\text{U}$  capture cross sections.

### 4.3. Lattices of Fuel Rods

#### 4.3.1. $\text{UO}_2$ rods

The investigated experiments involve lattices of low-enriched  $\text{UO}_2$  pins. Different square and triangular lattices of water-moderated are considered in order to cover a wide range of moderation ratio. Some of these configurations involve soluble poisons (boron or gadolinium), absorbing canisters (borated steel, boral, hafnium, cadmium...) and different kinds of reflectors (water, polyethylene, concrete, steel, lead...).

For lattices of rods in water without absorbing canisters, a good agreement with experimental  $k_{\text{eff}}$  is obtained with a slight average +0.2 % over-estimation for multigroup routes, the pointwise Monte Carlo route offering a very good consistency with the experimental  $k_{\text{eff}}$ . The small observed bias is caused by the homogenization process in the APOLLO2  $P_{ij}$  cell calculation. It confirms the good results already obtained with the previous CRISTAL V1.2.

For lattices of rods in water surrounded by an absorbing canister, an average +0.5 % over-estimation is highlighted for multigroup routes, whereas a very good agreement with experimental  $k_{\text{eff}}$  is obtained when using the pointwise TRIPOLI-4 route. This behavior can be attributed, on the one hand, to the fact that the absorbing material and the water gap between the lattice and canister are not described in the APOLLO2  $P_{ij}$  cell calculation, which leads to an inaccurate calculated flux before the homogenization, and, on the other hand, to the multigroup treatment of the absorbing material cross sections.

For lattices of rods reflected by stainless steel and lead, an average +0.75% over-estimation (up to +1.5%) is highlighted for the multigroup routes, whereas a good agreement with experimental  $k_{\text{eff}}$  is obtained with the pointwise TRIPOLI-4 route. The discrepancy depends on the reflector thickness and also on the distance between the fissile unit and the reflector. The reason is, similarly as before, due to the multigroup treatment of  $^{56}\text{Fe}$  and lead in the reflector but the effect is sharper due to the fact that the depletion of flux in the vicinity of the reflector is larger. It leads to emphasize the multigroup treatment problem.

Nevertheless, a significant improvement, but not sufficient for thick reflector, is obtained with the new CRISTAL V2.0 package for  $\text{UO}_2$  rods with absorbing canisters, reflected by lead or stainless steel for multigroup routes thanks to the 281-group energy mesh and the self-shielding of structural materials.



### 4.3.2. Lattices of UO<sub>2</sub>-PuO<sub>2</sub> rods

Four series of experiments available in the database of the three routes are selected for the analysis of tendencies. They involve mixed UO<sub>2</sub>-PuO<sub>2</sub> rods with a PuO<sub>2</sub> content varying from 3 % to 19.7 %, <sup>240</sup>Pu contents varying from 8.6 % to 22 % and with different moderation ratios. The lattices do not comprise absorber canisters.

A general good agreement with the experimental  $k_{\text{eff}}$  is obtained with the multigroup APOLLO2-MORET5 and the pointwise TRIPOLI-4 routes. For what concerns the APOLLO2-S<sub>n</sub> route, a +0.5 % over-estimation can be outlined, which might be due to cross sections collapsing.

In conclusion, CRISTAL V2.0 package is not source of significant improvement in the results since the former ones were in quite good accordance with the experimental  $k_{\text{eff}}$ .

### 4.4. Lattices of Slabs

This category gathers experiments from the ICSBEP Handbook under the nomenclature HEU-MET-THERM, HEU-MET-FAST and HEU-MET-INTER.

Five series of uranium experiments are considered for the slab arrays applications. Uranium is composed of highly enriched uranium (< 93 % <sup>235</sup>U). The experiments are calculated only with the APOLLO2-MORET 5 multigroup and the TRIPOLI-4 pointwise routes, except for one series (HEU-MET-THERM-006).

Regarding uranium metal slabs, a large dispersion of results is observed versus the moderator or the reflector nature. Without reflector, a tendency to slightly under-estimate  $k_{\text{eff}}$  can be pointed out, whereas a good agreement is obtained with a polyethylene reflector and a large over-estimation with Teflon.

Regarding fuel plates assemblies in water, a tendency to under-estimate  $k_{\text{eff}}$  up to -2 % is observed and a trend versus spacing between assembly plates can be highlighted. The homogenization of cross sections in the APOLLO2 p<sub>ij</sub> cell calculation tends to increase this trend.

Moreover, the use of the CRISTAL V2.0 package associated with the JEFF-3.1.1 library is source of a decrease of  $k_{\text{eff}}$  up to -1.5 % with the multigroup routes and TRIPOLI-4 for experiments in epithermal and thermal energy ranges. The JEFF-3.1.1 evaluation of <sup>235</sup>U explains such variation.

### 4.5. Fuel Rods Arrays in Fissile Solution

These experiments concern UO<sub>2</sub> or UO<sub>2</sub>-PuO<sub>2</sub> fuel rods in uranium, plutonium or mixed U-Pu nitrate solutions. Different lattices pitches and various solutions concentrations are tested.

These configurations allow validating the APOLLO2 calculation options for self-shielding, taking into account the resonant isotopes in both the fissile solution and the fuel rods.

For the two series involving UO<sub>2</sub> rods and calculated by the three routes, a general tendency to over-estimate  $k_{\text{eff}}$  by +0.5 % is observed with the APOLLO2-S<sub>n</sub> and APOLLO2-MORET5 routes. This is not the case with the TRIPOLI-4 route, for which a general good agreement is observed. This leads to identify a bias associated with the homogenization process and/or the multigroup treatment of cross sections. It should be noted that the observed trend is the same as for the CRISTAL V1.2 package. No improvement is done.

For two of the three series involving mixed UO<sub>2</sub>-PuO<sub>2</sub> rods in plutonium or mixed U-Pu solutions,  $k_{\text{eff}}$  is over-estimated on average by +0.4 % with the multigroup APOLLO2-MORET 5 code, by +0.7 % with the APOLLO2-S<sub>n</sub> multigroup code and by +0.3 % with the TRIPOLI-4 pointwise route. No bias due to the multigroup treatment of cross sections is therefore identified for the multigroup APOLLO2-MORET 5

route, which is not the case for the APOLLO2-S<sub>n</sub> code where a small +0.3 % bias is pointed out. This bias can be attributed to the 20-energy group collapsing of nuclear data for the deterministic calculation. A slight improvement of the results is obtained with the new CRISTAL V2.0 package.

For the series involving mixed UO<sub>2</sub>-PuO<sub>2</sub> rods in a mixed uranium/plutonium solution with gadolinium, a general tendency to under-estimate k<sub>eff</sub> is highlighted with all the codes. This tendency increases with the concentration of gadolinium in the solution.

#### 4.6. Metallic Systems

These experiments concern high-enriched uranium and plutonium metal systems with different <sup>240</sup>Pu contents. Different reflectors with varying thicknesses are investigated (none, water, polyethylene, steel, graphite, aluminum, beryllium).

Generally, improvements in the evaluation of <sup>235</sup>U, H in H<sub>2</sub>O (thermal scattering of hydrogen) with JEFF-3.1.1, and in the multigroup treatment of intermediate mass isotopes (<sup>56</sup>Fe) give satisfactory results in fast systems [2] [10]. Moreover, the under-estimation of unreflected plutonium metal systems observed with JEF-2.2 is reduced with the new <sup>239</sup>Pu evaluation (ν<sub>p</sub>, σ<sub>c</sub> and σ<sub>f</sub> thermal shapes) in JEFF-3.1.1.

##### 4.6.1. Multigroup treatment of intermediate mass isotope in metallic reflectors

Specific options are implemented in CRISTAL V2.0 (JEFF-3.1.1 / 281g) for the multigroup scattering cross sections treatment of intermediate mass isotopes (<sup>56</sup>Fe) in thick reflectors [10] [11], avoiding the former over-estimation of the reactivity with JEF-2.2 / 172g library.

With the CRISTAL V2.0 package, the results indicate a bias reduction on k<sub>eff</sub> amounting from 1 % to 2.5 % for multigroup calculations (APOLLO2-S<sub>n</sub> or APOLLO2-MORET 5) for thick reflector configurations (e > 5 cm), while thin reflectors (e < 5 cm) configurations are still precisely calculated (see Fig. 1). In these configurations, the TRIPOLI-4 Monte Carlo calculation is accurate, enhancing the residual scheme bias of around 1 % on the calculated k<sub>eff</sub> for thick reflectors with the multigroup solver S<sub>n</sub> and with the APOLLO2-MORET 5 route.

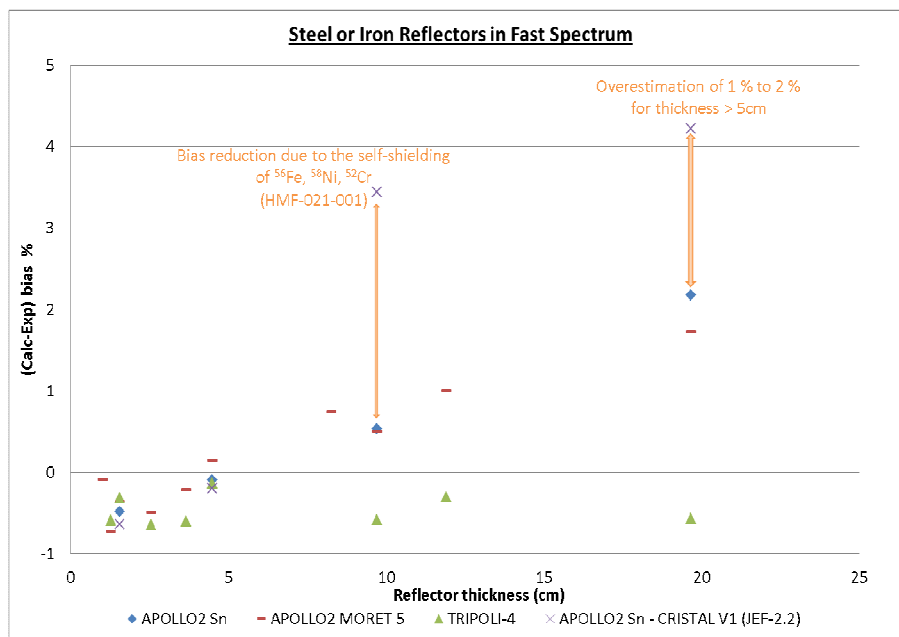
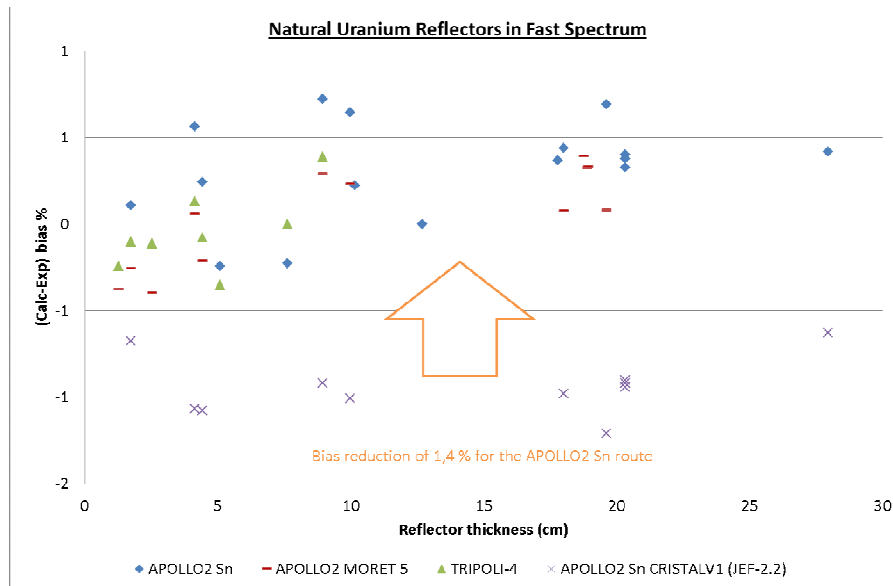


Figure 1 Experimental validation of CRISTAL V2.0 for steel / iron reflectors

#### 4.6.2. Impact of the JEFF-3.1.1 / 281g treatment of $^{238}\text{U}$

For configurations with natural uranium reflectors, the use of the 281-energy-group mesh instead of the former 172-energy-group mesh, designed to avoid self-shielding models for the resonances of major and minor actinides, and the fully validated evaluation JEFF-3.1.1, lead to a strong reduction of the former under-estimation of  $k_{\text{eff}}$  of fast spectrum configurations (see Fig. 2).



**Figure 2 Experimental validation of CRISTAL V2.0 for Natural Uranium Reflected configurations in Fast Spectrum**

## 5. CONCLUSIONS

The new version of the CRISTAL criticality calculation package, named CRISTAL V2.0, will be delivered soon to OECD/NEA data bank. It benefits from a broad validation database covering almost all areas of criticality-safety applications, from fuel fabrication to reprocessing, including transportation. 3127 critical experiments either issued from the OECD/ICSBEP Handbook or performed in French facilities (proprietary data) are selected for the CRISTAL V2.0 validation database. Currently, more than 2,300 experiments are already calculated with the different calculation routes of the CRISTAL package.

Validation studies, based on calculation-experiment discrepancies analyses and code to code comparisons, highlights the effect of the approximations used in the multigroup routes and the nuclear data accuracy. Thus, the improvements in both nuclear data and calculation schemes allow obtaining better calculation results than with the previous version V1.2. It is pointed out that the calculation results are generally in good agreement with the benchmark  $k_{\text{eff}}$  that ensure to the CRISTAL package a high level of performance for criticality-safety calculations.

Finally, it must be emphasized that the validation work is still in progress and that the validation database will be extended by adding available experiments involving specific isotopes, such as neptunium and thorium as well as structural materials (MIRTE program [12]) and poisoned fuel pins.

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