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DARWIN2 LOW BURNUP VALIDATION FOR BURNUP CREDIT USING SFCOMPO PIE DATABASE – VERIFICATION OF ICF VALUES

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ABSTRACT

The DARWIN package, developed by the CEA and its French partners (AREVA and EDF), provides the parameters required for fuel cycle applications, especially fuel inventory. It is widely used in the French Burnup Credit (BUC) calculation route, based on the connection of the depletion code DARWIN and the Criticality-Safety Package CRISTAL.

The experimental validation process of BUC nuclides provided by DARWIN2.3 package consists in the comparison between JEFF-3.1.1-based calculated values of isotopic concentrations and experimental values obtained from the chemical analysis of PWR fuel rod cuts. As a complement to the extensive validation using the French PIE database, specific PIE data chosen for their quality were selected and analyzed in the SFCOMPO database of NEA. A set of 56 samples chosen in PWR-UO₂ experiments was selected, with initial ²³⁵U enrichment between 2.7% and 4.1% and local burnup estimated from ¹⁴⁸Nd measurement varying between 7 and 35 GWd/t_{HM}.

This paper provides an overview of calculation – experiment comparison obtained in Takahama-3 17x17, Trino-Vercellese 15x15 and Obrigheim 14x1 for uranium, plutonium isotopes, as well as available fission products contributing to the assembly reactivity. Consistent biases compared to SCALE5 results were obtained.

From these results, an analysis is driven using 15 selected samples with low burnup, selected among asymptotic rods of irradiated fuels at 1 or 2 cycles. This paper shows the consistency of the calculation - experiment biases obtained with DARWIN2.3 towards previously defined penalized biases used for the Isotopic Correction Factors (ICF) in BUC applications.

KEYWORDS

BUC, DARWIN, PWR UO_x, ICF, low BU

1. INTRODUCTION

The DARWIN package, developed by the CEA and its French partners (AREVA and EDF), provides the parameters required for fuel cycle applications, especially fuel inventory. It is widely used in the French Burnup Credit (BUC) calculation route [1] (Fig.1), based on the connection of the depletion code DARWIN [2] and the Criticality-Safety Package CRISTAL [3]. DARWIN Package calculates the concentrations of isotopes at the end of irradiation or after cooling times. Then, these concentrations, to which a correction factor can be applied [4,5], are used as input data in the Criticality- Safety Package CRISTAL, which provides the effective multiplication factor associated to the calculated situation. Part of this work was discussed within the French BUC Working Group, involving experts from IRSN, AREVA, EDF, ANDRA and CEA [6].

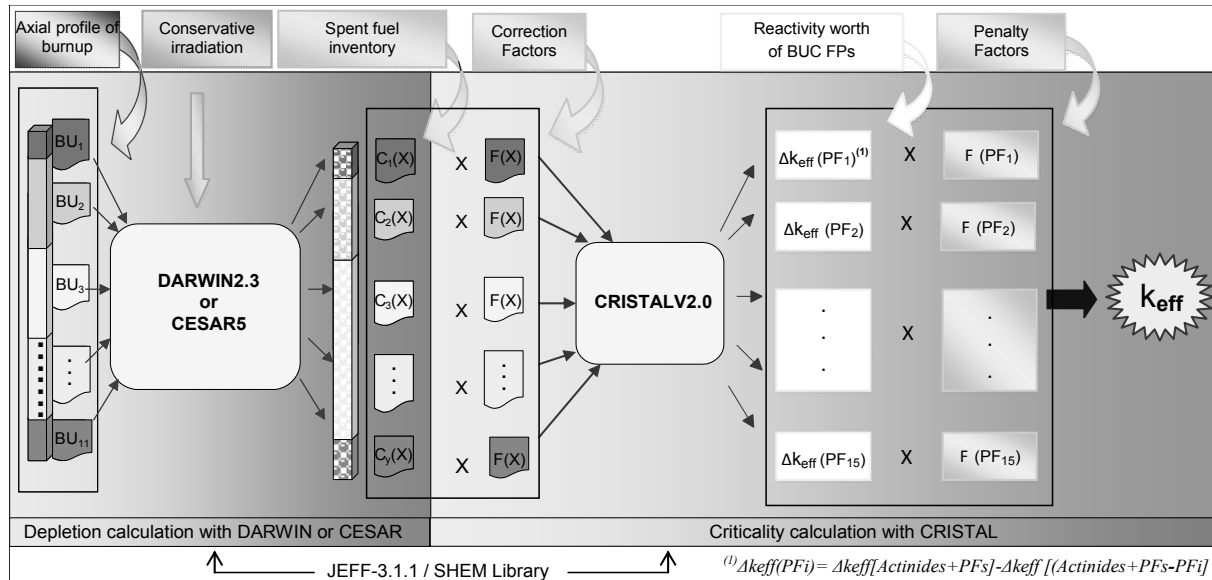


Figure 1 The French BUC calculation route

The CEA – AREVA BUC methodology, accounts for:

- 15 poisoning Fission Products (FPs), stable and non-gaseous, in addition to the actinides [7], following the recommendations of the benchmark Phase-I of the OECD BUC Expert Group [8],
- conservative hypotheses for the depletion calculations,
- experimental validation of the spent fuel inventory obtained with DARWIN and of the reactivity worth of BUC nuclides calculated with CRISTAL,
- a bounding axial burnup profile of spent fuel assemblies. A recommended bounding profile for PWR LEU spent fuel assemblies (SFA) applications has been previously described.

A specific BUC program [9] has been developed at Cadarache Centre in the framework of the CEA-AREVA collaboration in support of this methodology. This program involves two kinds of experiments:

- Chemical analyses and microprobe measurements of PWR spent fuel rods to obtain the fuel inventory (Actinides and FPs);
- Reactivity worth measurements of each BUC nuclide by oscillation in the MINERVE reactor of UO_2 samples involving the separated-FP.

The experimental validation process of BUC nuclides provided by DARWIN2.3 Package consists in the comparison between calculated values of isotopic concentrations using the industrial scheme ‘CYCLE 2008’ [10] with the European evaluation JEFF-3.1.1 [11] and experimental values obtained from the chemical analysis of fuel rod cuts. As a complement to the extensive validation using the French PIE database [12], specific P.I.E. (Post Irradiated Examination) data chosen for their quality were selected in the SFCOMPO NEA database and analyzed. This paper provides an overview of calculation – experiment comparison obtained in Takahama-3 17x17, Trino-Vercellese 15x15 and Obrigheim 14x14 for BUC nuclides. From these results, an analysis is driven using 15 selected samples with low burnup, selected among asymptotic rods of irradiated fuels at 1 or 2 cycles. The consistency of the C/E biases, towards previously defined penalized biases used for the Isotopic Correction Factors (ICF) in BUC applications [13], is analyzed in the third section.

2. DARWIN VALIDATION FOR BUC NUCLIDES USING SFCOMPO P.I.E. DATA

2.1. Industrial Scheme ‘CYCLE 2008’ (calculation model of the depleted fuel)

The new ‘REL2005’ optimized and validated scheme for PWR UO_x calculation is based on the recent package APOLLO2.8 [14] developed by CEA. In the specific case of fuel cycle studies, a consistent scheme ‘CYCLE2008’ has been developed and validated using the benefit of the validation program of the ‘REL2005’ APOLLO2.8 scheme [15]. It provides self-shielded cross sections used by PEPIN2 in order to give BUC isotopes concentrations of the depleted fuel. The neutron energy spectrum is calculated in the 2D assembly geometry, using a Pij multicell model: the UP1 Interface Current method based on linearly anisotropic interface fluxes. The fuel pellets are split into 4 rings (UOX) in order to give an accurate representation of absorption of ²³⁸U as well as FPs concentration profile. Local spectrum calculation is performed in the SHEM 281 energy group structure [16]. Space-dependent self-shielding (used only above 23 eV that is the upper limit of the fine mesh in SHEM) is repeated at recommended burnup steps, optimized consistently with the ‘REL2005’ recommendations. Refined burnup steps are used for the depletion calculation.

This scheme is also used in calculation of BUC nuclides concentrations using DARWIN2 package for BUC applications (Fig.2). The PEPIN2 evolution module uses the results provided by APOLLO2, self-shielded cross-sections and multigroup spectra, to make up the collapsed library with burnup dependent cross-sections required in the depletion chains.

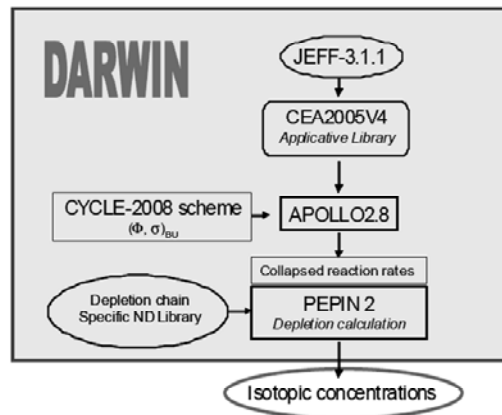


Figure 2 Sequence including the DARWIN2 ‘CYCLE 2008’ Scheme in BUC calculations

2.2. PIE data selection in SFCOMPO database

A set of 56 samples chosen in PWR-UO₂ experiments was selected in the SFCOMPO database of the NEA [17], with initial ²³⁵U enrichment between 2.72% and 4.11% and local burnup estimated from ¹⁴⁸Nd measurement varying between 7 and 35 GWd/t_{HM}, detailed in Table I. This database allows the calculation of a wide range of PWR assemblies, as a complement to the extensive validation using the French P.I.E. database, especially with samples irradiated at low burnup (1 or 2 cycles). Moreover, calculated biases can be compared with published results of other laboratories involved in depletion calculation of BUC nuclides [18].

Table I. PWR UO₂ selected samples in SFCOMPO P.I.E. database

Reactor	Assembly	IE (%)	Rods	Samples	BU (GWd/t _{HM})	Analysed Isotopes
TRINO	509-049	2.72	J8, L5	9, 10, 11, 12, 13, 14, 13, 14, 15, 16, 17, 18	8 - 15	U, Pu, Am, Cm, ¹³⁴⁻¹³⁷ Cs, ¹⁵⁴ Eu, ¹⁰⁶ Ru, ¹⁴⁴ Ce, Kr, Xe
	509-032	3.13	E11, H9, Q15 (n°8)	1, 2, 3, 4, 5, 6, 7, 8	7 - 18	
	509-069	3.13	A1, E5, E11, J9, L5, L11	19 to 36	13 - 27	
TAKAHAMA	NT3G23 UO ₂ Gd ₂ O ₃	4.11	SF95	SF95-1 to SF95-5	14 - 35	U, Pu, Am, Cm, Nd, Cs, ¹⁵⁴ Eu, ¹⁰⁶ Ru, ¹²⁵ Sb
			SF96	SF96-1 to SF96-5	9 - 30	
OBRIGHEIM	BE124	3	D1, E3, G7, M14	1, 4, 7, 8, 9, 10, 11, 13, 14, 16	15 - 31	U, Pu, Am, Cm, ¹³⁴⁻¹³⁷ Cs, ¹⁵⁴ Eu, ¹⁴⁸ Nd, Kr, Xe

2.3. General trends obtained with DARWIN 2.3

The trends on the (C-E)/E biases are summarized in Table II for main actinides involved in BUC studies. The calculation burnup is adjusted using the experimental indicator, namely the ¹⁴⁸Nd. ²³⁵U seems slightly overestimated at low burnup (mean +3%) as shown in Fig.3, although it is well calculated using French experiments. The slight overestimation of ²³⁹Pu (mean +3%) shown in Fig.3, is less than the result obtained using SCALE5 [19] (mean +5%). Both DARWIN2 and SCALE5 ²⁴⁰Pu C/E sample results are varying between -8% / +8%, depending on the type of assembly, although it is calculated within 2% accuracy from French experiment.

The total uncertainties (1σ) correspond to the combination of uncertainties on chemical assays (from SFCOMPO when available or deduced from published analysis of the selected experiments [19]) and of the determination of the rod-cut burnup derived from ¹⁴⁸Nd content. Technological uncertainties (fuel and moderator temperature) are also included.

Consistent biases, towards foreigner laboratories using SCALE5, were then obtained from these samples, although inconsistent results can be highlighted for some samples providing high technological uncertainties. The comparison of total uncertainties associated to each sample with those of the French P.I.E. database in Table III enhances the quality of the later one. Therefore, a careful choice of accurately characterized samples should be done among this selected sample set to derive the BUC ICFs.

Table II. Trends of the DARWIN2.3 experimental validation using SFCOMPO PWR experiments

Isotope	SFCOMPO 7 – 40 GWd/t DARWIN2.3 / SCALE5.1	Previous work [12] French PWR C-E ± 1σ (%)
²³⁵ U	+3% / +2%	0 ± 2%
²³⁶ U	-7% / -4.5%	-1% ± 1%
²³⁹ Pu	+3% / [0 - +10]%	-2% ± 1%
²⁴⁰ Pu	[+3 - +8]% / [+4 - +13]% Takahama	0% ± 2%
²⁴¹ Pu	[-9 - +9]% / idem	-1% ± 3%

Table III. Uncertainty ranges (%) obtained for actinides, comparison with French P.I.E. data

Reactor	TRINO	TAKAHAMA	OBRIGHEIM	DARWIN French PIE (20 GWd/t)
Isotope	σ min / σ max	σ min / σ max	σ min / σ max	mean (%)
^{235}U	2.6 / 2.8	0.6 / 2.6	4 / 5.3	2
^{239}Pu	2.3 / 2.5	1.1 / 3.6	0.7 / 0.8	0.6
^{240}Pu	3.2 / 3.6	1.7 / 3.8	0.6 / 2.6	2
^{241}Pu	3.3 / 4.7	2.1 / 5.2	1.7 / 5.1	2.5
^{242}Pu	5.8 / 7.1	4.2 / 8.3	6.9 / 7.7	4

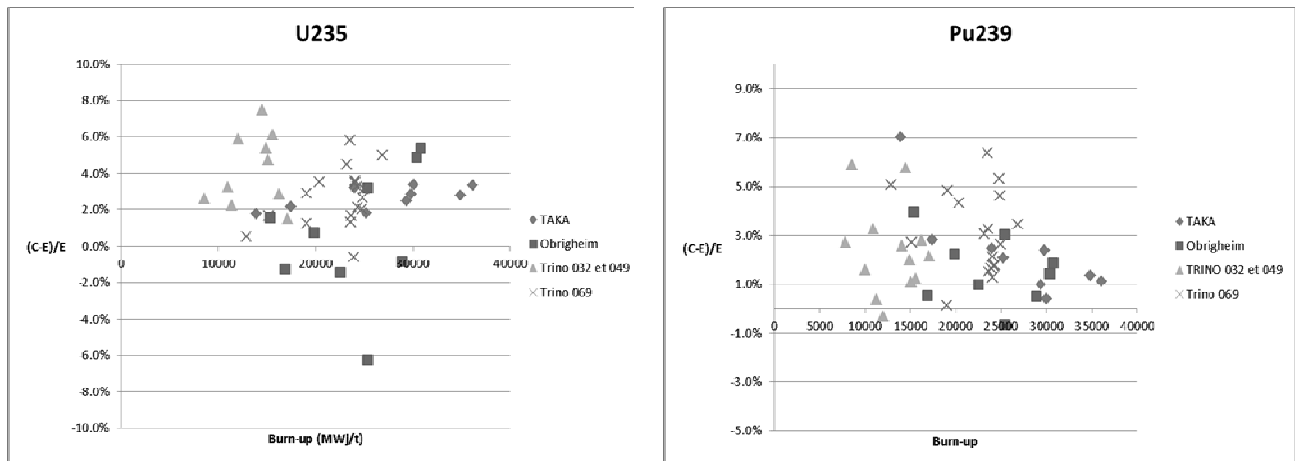


Figure 3 C/E bias (in%) obtained for ^{235}U and ^{239}Pu in SFCOMPO P.I.Es

3. COMPARISON WITH PENALIZED BIAS USED FOR ICF IN BUC APPLICATIONS

3.1. Selected samples for BUC application

From these results, an analysis is made using 15 selected samples at low burnup, selected among asymptotic rods of irradiated fuels at 1 or 2 cycles (Table IV). They are chosen for the quality of the measurement data, the availability of BUC isotopes among the chemical analysis, the number of irradiation cycles and the location of the rod / sample (flat BU zone of the fissile column, middle of the assembly to avoid environment perturbations).

Table IV. Selected rod cuts for BUC application

Reactor	Assembly	$E_{U^{235}}$ (%)	Rods	Samples	BU (GWd/t _{HM})	Analysed Isotopes (BUC interest)
TRINO	509-049	2.72	J8, L5	13, 14, 17	14 - 15	U, Pu, Am, ¹³⁴⁻¹³⁷ Cs,
	509-032	3.13	E11, H9	2, 3, 5, 6	16 - 17	¹⁵⁴ Eu
TAKAHAMA	NT3G23 UO ₂ Gd ₂ O ₃	4.11	SF96, SF95	SF95-1, SF96- 2 to SF96-5	9 - 30	U, Pu, Am, Nd, Cs, ¹⁵⁴ Eu, ¹⁰⁶ Ru
OBRIGHEIM	BE124	3	E3, G7	7, 9, 10, 11	17 - 31	U, Pu, Am, ¹³⁴⁻¹³⁷ Cs, ¹⁵⁴ Eu, ¹⁴⁸ Nd

3.2. ICF derivation methodology

Isotopic Correction Factors (ICFs) are applied to the BUC nuclide densities to ensure the conservatism of the irradiated fuel inventory in criticality studies. They take into account two sources of errors :

1- The bias between calculated values of isotopic concentration (using the industrial scheme 'CYCLE 2008') and experimental values obtained from accurate chemical analyses of well characterized fuel rod cuts, selected in the French P.I.E (Post Irradiated Examination) database ;

2- The total uncertainty obtained by combining the various uncertainty components : measurement uncertainty associated with the chemical assays; fuel coolant/moderator temperatures during irradiation; local Burnup estimation; initial content in ²³⁵U; reactor cycle follow-up.

The JEFF3.1.1 ICFs values, to be implemented in PWR UO₂ applications to guarantee the conservatism of the SFA inventory, were already derived from the experimental validation of DARWIN2.3 [13] [1]. The purpose of this work is to check the consistency of these Penalized (C-E)/E values towards recent results obtained from experimental values of the SFCOMPO database at low burnup.

In order to obtain the Penalized (C-E)/E values, the C/E biases obtained from SFCOMPO rod cut measurements are increased by the 95% one-sided confidence interval of the total experimental uncertainty (Tab. III) :

- burnup determination ($\pm 2\%$ at 1σ) from ¹⁴⁸Nd adjustment;
- moderator temperature ($\pm 2^\circ\text{C}$), at 1σ ;
- fuel temperature ($\pm 50^\circ\text{C}$),
- reactor cycle follow-up
- chemical analysis uncertainties.

These independent uncertainties are then combined.

3.3. BUC actinides and FP results

In this work C/E results are compared with the penalized bias associated to each BUC nuclide, in order to verify the consistency of the linear trend at low burnup ($< 30 \text{ GWd/t}_{\text{HM}}$) derived from DARWIN2 experimental validation [13].

3.3.1. ²³⁵U penalized bias and C/E results

The recent ICF value versus burnup of ²³⁵U was derived from the DARWIN2.3/JEFF-3.1.1 experimental validation, giving a penalized bias $\Delta = (C-E)/E - 1.65\sigma$ shown in Fig.4. At high burnup it is mainly driven by a strong uncertainty component due to burnup determination, the depletion of ²³⁵U being accurately

predicted by DARWIN2.3 package within 1% accuracy for low burnup ranges (< 30 GWd/t). For criticality studies, the penalized bias equals to -3.2% at 30 GWd/t_{HM}. An ICF value of 1.033 applied to the ²³⁵U JEFF3.1.1-based concentration can be therefore recommended at 30 GWd/t_{HM}, in order to guarantee its conservativeness in criticality calculations.

The results obtained from SFCOMPO rod cuts measurements at low burnup confirm the relevancy of the retained penalized bias using JEFF-3.1.1, as shown in Fig.4. The C/E result obtained from Sample n°10 of Obrigheim experiment is covered by the large experimental uncertainty; the ¹³⁷Cs result shows an overestimation by +3%, to be compared with the -3.5% general tendency obtained in previous work [12], which explains the under estimation of ²³⁵U.

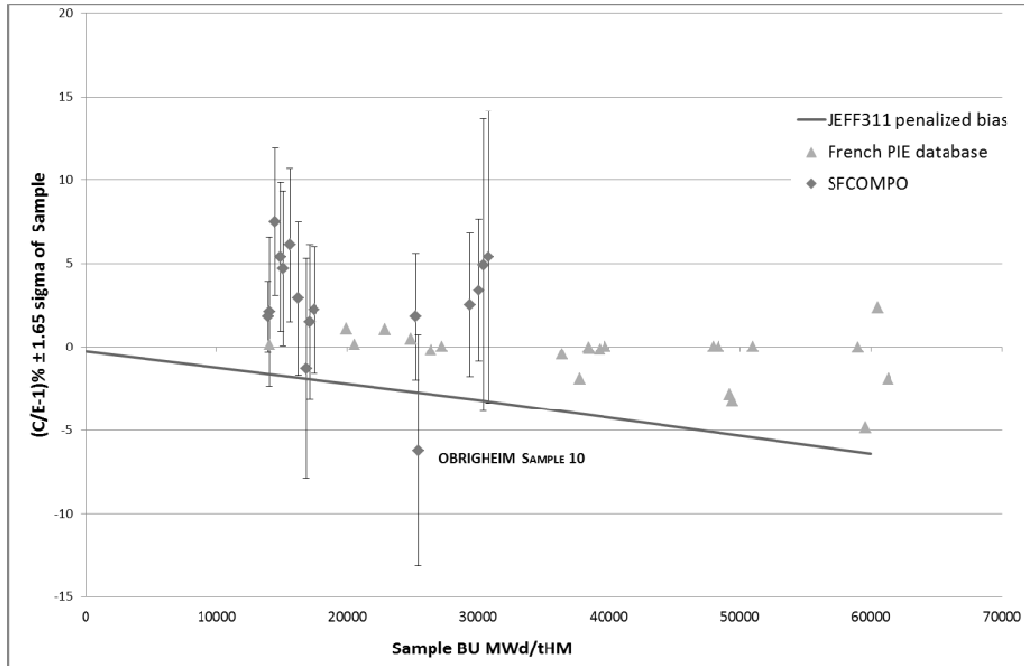


Figure 4 Confirmation of penalized bias of ²³⁵U using SFCOMPO P.I.E. data at low Burnup

3.3.2. ²⁴¹Pu penalized bias and C/E results

The recent ICF value of ²⁴¹Pu is derived from the DARWIN2.3/JEFF-3.1.1 experimental validation, giving a penalized bias $\Delta = (C-E/E) - 1.65\sigma$ shown in Fig.5. It is partly driven by experimental uncertainties around 3% and the slight underestimation of the ²⁴¹Pu building. The penalized bias associated to the ²⁴¹Pu concentration amounts to -6.4% at 30 GWd/t_{HM}.

The C/E results obtained from SFCOMPO P.I.E. data at low burnup using 1.65 σ uncertainty confirm the relevancy of the retained bias using JEFF-3.1.1: every C/E value is less penalizing than the retained bias for criticality studies as shown in Fig.5.

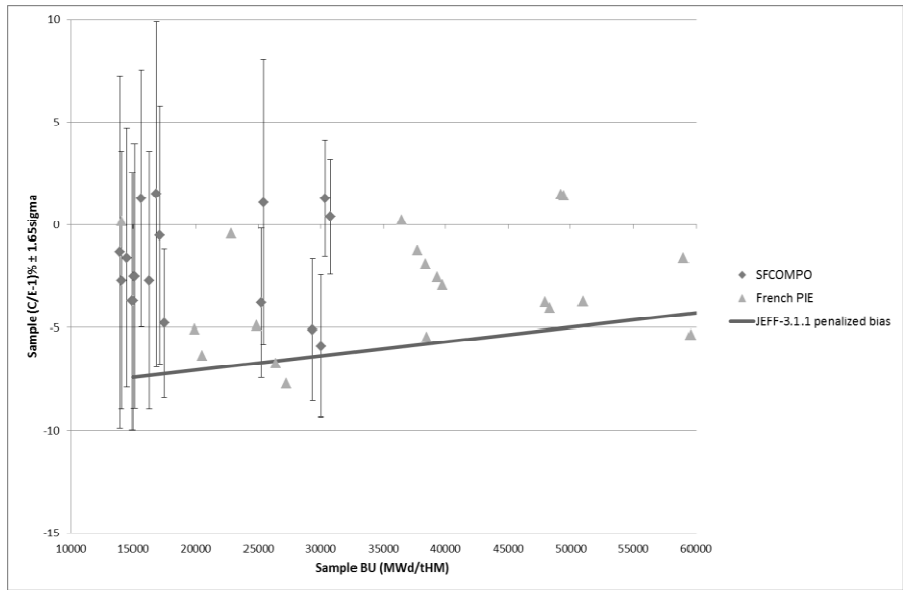


Figure 5 Confirmation of penalized bias of ^{241}Pu using SFCOMPO P.I.E. data at low Burnup

3.3.3. Absorber actinides ^{240}Pu and ^{242}Pu

The penalized bias derived from DARWIN2.3/ JEFF-3.1.1 C/E results for absorber isotopes is +1.8% for ^{240}Pu , which is accurately predicted with DARWIN2.3, and +1.6% for ^{242}Pu which is slightly underestimated [12, 13].

The underestimated ^{240}Pu C/E obtained for most samples clearly confirm the JEFF-3.1.1 retained bias, as shown in Fig.6. The Takahama-3 experiment shows quite inconsistent result, with a slight C/E overestimation, however covered by the large experiment uncertainty.

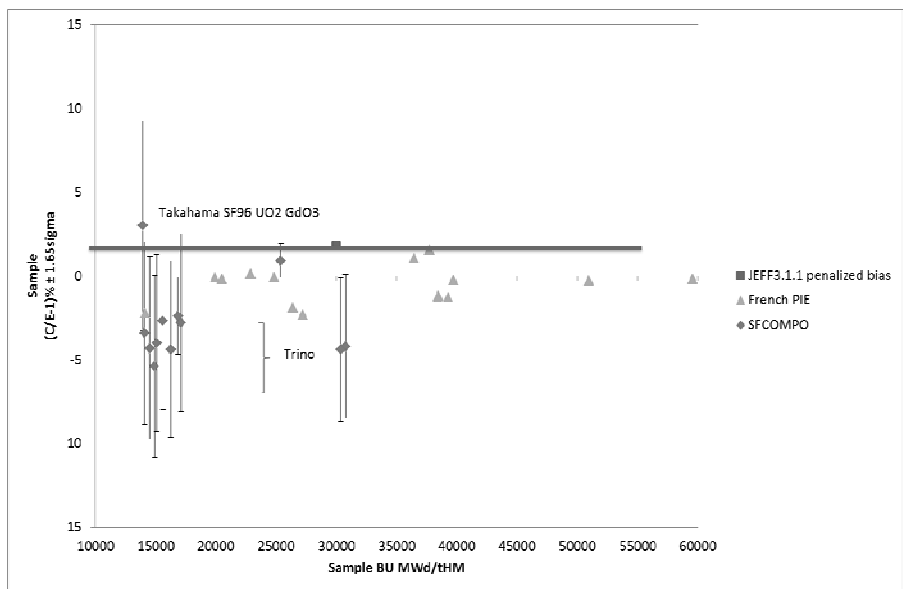


Figure 6 Confirmation of penalized bias of ^{240}Pu using SFCOMPO P.I.E. data at low Burnup

The underestimated ^{242}Pu C/E obtained for most samples confirm the JEFF-3.1.1 retained bias (Fig.7). One sample from Obrigheim seems not consistent at 26 GWd/t_{HM}, however covered by 1.65σ uncertainty.

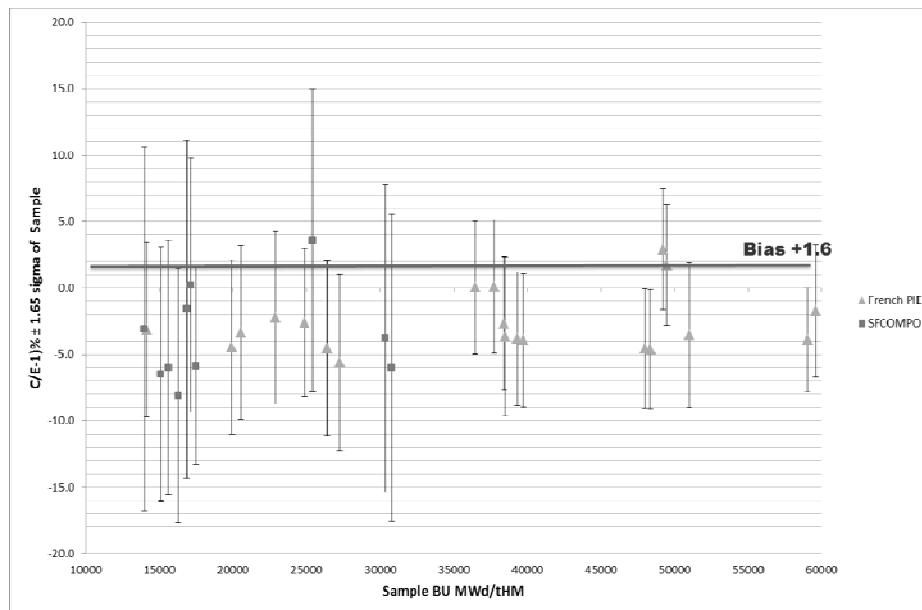


Figure 7 Confirmation of penalized bias of ^{242}Pu using SFCOMPO P.I.E. data at low Burnup

4. CONCLUSION

The SFCOMPO PIE database is of high interest for depletion calculation benchmarking. A large range of fuel design, enrichment, burnup, are available with a good associated statistic. However, uncertainties in chemical analysis and reactor data have to be carefully evaluated, which is the purpose of WPNCs Expert Group. In criticality applications, most actinides and burnup indicator are available.

This work has validated the extension of the DARWIN2 experimental validation to low burnup. The comparison with SCALE5 analysis results of the selected experiments has shown consistent results.

From this work, a key result can be derived for BUC application in PWR UO_2 :

- The Consistency of the calculation - experiment biases obtained with DARWIN2.3 towards previously defined penalized biases is demonstrated in this paper.
- Results obtained from 15 representative samples (asymptotic rods) for ^{235}U , ^{240}Pu , ^{241}Pu , ^{242}Pu confirm the relevancy of penalized biases derived from the French P.I.E. data.
- This study confirms the validity of JEFF-3.1.1 Isotopic Correction Factor at low burnup [10 – 30 GWd/t_{HM}].

These ICFs were applied in recent criticality calculation for BUC PWR applications, carried out using the French BUC calculation Route based on DARWIN2.3 and CRISTAL V2.0.

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