Methods and Issues for the Combined Use of Integral Experiments and Covariance Data: Results of a NEA International Collaborative Study

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The Working Party on International Nuclear Data Evaluation Cooperation (WPEC) of the OECD NEA Nuclear Science Committee established in 2009 a Subgroup (called "Subgroup 33") on "Methods and issues for the combined use of integral experiments and covariance data." The first stage has been devoted to producing the description of different adjustment methodologies and assessing their merits. A detailed document related to this first stage has been issued. Nine leading organizations (often with a long and recognized expertise in the field) have contributed: ANL, CEA, INL, IPPE, JAEA, JSI, NRG, IRSN and ORNL. In the second stage a practical benchmark exercise was defined in order to test the reliability of the nuclear data adjustment methodology. Comparison of the results obtained by the participants and major lessons learned in the exercise are discussed in the present paper that summarizes individual contributions which often include several original developments not reported separately.

The paper provides the analysis of the most important results of the adjustment of the main nuclear data of 11 major isotopes in a 33-group energy structure. This benchmark exercise was based on a set of 20 well defined integral parameters from 7 fast assembly experiments. The exercise showed that using a common shared set of integral experiments but different starting evaluated libraries and/or different covariance matrices, there is a good convergence of trends for adjustments. Moreover, a significant reduction of the original uncertainties is often observed. Using the a-posteriori covariance data, there is a strong reduction of the uncertainties of integral parameters for reference reactor designs, mainly due to the new correlations in the a-posteriori covariance matrix. Furthermore, criteria have been proposed and applied to verify the consistency of differential and integral data used in the adjustment. Finally, recommendations are given for an appropriate use of sensitivity analysis methods and indications for future work are provided.

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CONTENTS

I. FRAMEWORK AND BACKGROUND

A. Scope and Objectives

Nuclear data uncertainty impact studies [1–3] have pointed out that present uncertainty on the nuclear data should be significantly reduced, in order to get full benefit from the advanced modeling and simulation initiatives that have been launched worldwide in recent years. Only a parallel effort in advanced simulation and in nuclear data improvement will be able to provide designers with more general and well validated calculation tools that would be able to meet design target accuracies.

Tight design target accuracies, required in order to comply with safety and optimization requirements and objectives, can only be met if very accurate nuclear data are used for a large number of isotopes, reaction types and energy ranges.

The required accuracies on the nuclear data are difficult to meet using only differential experiments, even if innovative experimental techniques are used.

The use of integral experiments has been essential in the past to ensure enhanced predictions for power fast reactor cores. In some cases, these integral experiments have been documented in an effective manner and associated uncertainties are well understood.

A combined use of scientifically based covariance data and of integral experiments can be made using advanced statistical adjustment techniques (see, *e.g.* [4–6]). These techniques can provide in a first step adjusted nuclear data for a wide range of applications, together with new, improved covariance data and bias factors (with reduced uncertainties) for the required design parameters, in order to meet design target accuracies.

Moreover, the role for cross section adjustment is more and more perceived as that of providing useful feedback to evaluators and differential measurement experimentalists in order to improve the knowledge of neutron cross sections to be used in a wider range of applications.

Despite its recognized potential, the adjustment process has raised legitimate questions related both to physical meaning of the individual (*i.e.*, by isotope, reaction type and energy range) "adjustments", and to possible compensation effects since integral experiments depend

on a large number of parameters. Moreover, the first adjustments relied on uncertainty data essentially based on physicists' judgment and not on any formal approach.

It has also been pointed out that there exists no clear definition of the application domain of the adjusted multigroup data sets. When a new reactor concept is investigated, it is difficult to define what is the mathematical/physical extrapolation method (if any) to be used together with the previously adjusted data library. In any case, since the adjustments are performed at the multigroup level, they will also be related to the weighting function used to produce the original multigroup library and no unique procedures can be used to transfer the adjustments from the broad group level (where the adjustments are usually performed) to a fine group level or, even preferable, to the continuous energy level. Similarly, self-shielding effects are not necessarily accounted for explicitly.

Finally, the use of the a posteriori covariance matrix (both variances and correlations) is not a self-evident exercise and in fact in many cases use is made only of a posteriori variances.

The Working Party on International Nuclear Data Evaluation Cooperation (WPEC) of the OECD Nuclear Energy Agency Nuclear Science Committee recognized the importance of these issues and established a Subgroup (called "Subgroup 33") on "Methods and issues for the combined use of integral experiments and covariance data". In its mandate "it is proposed for this WPEC Subgroup to study methods and issues of the combined use of integral experiments and covariance data, with the objective of recommending a set of best and consistent practices in order to improve evaluated nuclear data files. Indication should be provided on how to best exploit existing integral experiments, define new ones if needed, provide trends and feedback to nuclear data evaluators and measurers".

The Subgroup activity has been completed and a final report is being assembled. The present paper summarizes and discusses the main results and recommendations.

B. Activities of the Subgroup

In summary, the general understanding of the adjustment methods, their theory and application, suggests a number of potential difficulties that have to be examined carefully, in order to agree on the best approach which would allow taking full benefit from the potential of the method. This has been the general objective of the activity of the Subgroup.

The first step of the Subgroup activity has been the compilation of a detailed report [7] with the assessment and comparison of the methodologies that the different participants to this Subgroup employ for adjustment of neutron cross section data using the observed discrepancies between calculated and measured values of integral experiments. To this purpose a documentation of the used adjustment methodologies, developed during more than three decades from the early sixties to the late nineties, has been provided by ANL, CEA, INL, IPPE, IRSN, JAEA, JSI, NRG, and ORNL. The report also includes the identification of merits and drawbacks of the existing adjustment methodologies, a comparison of mathematical formulation and specific features, and the criteria used for assessing the different methodologies.

In order to better understand the performance of these methodologies, the robustness of the results, their extrapolability and the impact of the uncertainties (not only on nuclear data but also on experiments and on methods) it has been decided to have the different organizations to participate to a common benchmark adjustment exercise that allows studying these specific issues. In particular it was agreed that the main objective of the benchmark was to test different methods of nuclear data adjustment/assimilation and different sets of covariance data, for the purpose of reducing *e.g.* the design uncertainties of a particular type of sodium-cooled fast reactor. The benchmark makes use of a single, limited set of selected integral experiments with fast neutron energy spectra and each organization used their own calculation methods and data.

C. The Adjustment Methodologies

As indicated above, the data statistical adjustment methods principles and mathematical formulations have been compared in a document [7]. Most of the methods, as reminded below, use practically the same mathematical formulation and that formulation is briefly summarized hereafter.

Let $\vec{E} = \vec{E}_i$ $(i = 1, \ldots, N_E)$ denote some experimental integral variables, and let $\vec{\sigma} = \vec{\sigma}_j$ $(j = 1, \ldots, N_\sigma)$ denote the multi-group parameters defining the model used to simulate these integral experiments, and $\vec{C}(\sigma)$ the associated calculated values to be compared with $\vec{E}$. Let $\vec{\sigma}_m$ and M_σ define the a priori expectation and covariance matrix of the multi-group parameters, and M_E define the experimental covariance matrix, including modeling covariance information when appropriate (*i.e.*, $M_E = V_e + V_m$). The evaluation of posterior expectation and covariances is done by finding the minimum of the following cost function (a generalised least-square)

$$\begin{aligned} \chi^2_{GLS} &= (\vec{\sigma} - \vec{\sigma}_m)^t M_\sigma^{-1} (\vec{\sigma} - \vec{\sigma}_m) \\ &+ (\vec{E} - \vec{C}(\sigma))^t M_E^{-1} (\vec{E} - \vec{C}(\sigma)). \end{aligned} \quad (1)$$

Information related to integral simulations is included in the $\vec{C}$ values as well as in their derivatives with respect to the multi-group parameters. Using a first order approximation, one can write

$$\vec{C}(\sigma) = \vec{C}(\sigma_m) + S \cdot (\vec{\sigma} - \vec{\sigma}_m)\,, \quad (2)$$

where S is a matrix $(N_E \times N_\sigma)$ of calculated derivatives supposed to be constant (when the cross sections slightly

change). Most of the time, S is referred to relative sensitivity coefficients

$$S_{ij} = \frac{\delta C_i / C_i}{\delta \sigma_j / \sigma_j}. \quad (3)$$

From a mathematical point of view, the method is quite general and has been extensively used for many kinds of inverse problems. In the field of reactor physics, this approach has been already applied to validate and/or further improve the nuclear data used in the simulation of thermal and fast reactors.

As indicated above, the formulations used by the different participants have been compared in [7].

The following observations can be made:

- Seven organisations (ANL, CEA, INL, IPPE, JAEA, JSI and IRSN) apply equivalent equations for the adjustment, though the names of the theory differ.
- ORNL uses similar equations as the above organisations. However, a correction factor ($F_{m/k}$) is applied to the covariance matrix of integral experiments to account for the C/E discrepancy.
- The NRG approach is completely different. It is based on the Total Monte Carlo method to produce thousands of TALYS-based evaluated files using MC sampling of nuclear parameters. The method used by NRG solves the inverse problem of nuclear data adjustment by selecting the optimal combination of random files that best reproduce all integral experiments.

D. The Benchmark Exercise

Every participant to the benchmark exercise used the same integral experiment values (E) and uncertainties, but their own calculated values (C), sensitivity coefficients, and adjustment/assimilation methods. The benchmark consisted of a three-phase exercise:

- Phase I. All participants used their own initial cross sections, own nuclear data covariance, with integral experiment and method correlation.
- Phase II. Some participants used their own initial cross sections, but a different nuclear data covariance matrix. This step allows a better understanding of the impact of the nuclear data covariance on the adjustment.
- Phase III. Verification of the impact of the adjustments on a few "Target Systems."

Finally, the addition of a set of integral experiments allowed a test of the robustness of the previous adjustments (stress tests).

1. Benchmark input

In order to limit the calculation effort and to allow pointing out major trends in more clear way, the number of isotopes to be adjusted has been limited to ten: ^{16}O, ^{23}Na, ^{56}Fe, ^{52}Cr, ^{58}Ni, ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu plus ^{10}B for testing. On the contrary, all major reactions have been considered. Finally, several covariance data sets have been used.

A unique energy group structure (given in Table I) has also been adopted.

TABLE I. 33 energy group structure (eV).

Group	Upper Energy	**Group**	Upper Energy	**Group**	Upper Energy
1	1.96×10^7	**12**	6.74×10^4	**23**	3.04×10^2
2	1.00×10^7	**13**	4.09×10^4	**24**	1.49×10^2
3	6.07×10^6	**14**	2.48×10^4	**25**	9.17×10^1
4	3.68×10^6	**15**	1.50×10^4	**26**	6.79×10^1
5	2.23×10^6	**16**	9.12×10^3	**27**	4.02×10^1
6	1.35×10^6	**17**	5.53×10^3	**28**	2.26×10^1
7	8.21×10^5	**18**	3.35×10^3	**29**	1.37×10^1
8	4.98×10^5	**19**	2.03×10^3	**30**	8.32×10^0
9	3.02×10^5	**20**	1.23×10^3	**31**	4.00×10^0
10	1.83×10^5	**21**	7.49×10^2	**32**	5.40×10^{-1}
11	1.11×10^5	**22**	4.54×10^2	**33**	1.00×10^{-1}

2. Nuclear data

The following nuclear data were explicitly considered:

- Elastic scattering infinite-dilution cross section,
- Total inelastic scattering infinite-dilution cross section,
- Capture infinite-dilution cross section (this includes ^{10}B(n,α) reaction),
- Fission infinite-dilution cross section,
- Average prompt fission neutron multiplicity ($\bar{\nu}$),
- Normalized prompt fission neutron spectrum,
- Average cosine of elastically scattered neutrons ($\bar{\mu}$),
- Average delayed fission neutron multiplicity ($\bar{\nu}_d$), as an optional adjustable parameter (on a voluntary basis). This proposal was driven by consideration of the impact of $\bar{\nu}_d$ on the integral C/E ratio value and uncertainty for Na void reactivity (measured in dollars). When not adjusting $\bar{\nu}_d$, the participants should have added the corresponding uncertainty to the C/E value of Na void reactivity in order to reduce their statistical weight.

The spectra of inelastically scattered neutrons have not been part of the benchmark exercise.

3. Nuclear covariance data

All participants used their own nuclear covariance data (Phase I, see above). However, in Phase II of the exercise, for comparison purposes and to disentangle effects from different a priori cross sections or covariance data, one common set of covariance data would be used by some of the participants, in addition to their own specific sets. The 33-group COMMARA-2.0 covariance data, developed by BNL-LANL collaboration (see section III), has been made available for that purpose.

E. Selection of Integral Experiments

The selection of fast neutron spectrum integral experiments has been based on the availability of well documented specifications and experimental uncertainties and possibly of some indication of uncertainty correlations. The selected experiments cover a wide range of fast neutron energy spectra, and include critical masses, spectral indices and, when available, selected Na void reactivity coefficients. In the notation used for spectral indices, Fij (or Cij) is the fission (or capture) rate of the isotope 23j of the element 9i (*i.e.*, U, Np, Pu for i=2,3,4, respectively), *e.g.*, F37 is the ^{237}Np fission rate. Detailed specifications on these integral experiments were taken from [8–10]:

- Jezebel ^{239}Pu configuration: 1 critical mass, 3 spectral indices: F28/F25, F49/F25, F37/F25,
- Jezebel ^{240}Pu configuration: 1 critical mass,
- Flattop Pu configuration: 1 critical mass, 2 spectral indices: F28/F25, F37/F25,
- ZPR6-7 standard configuration: 1 critical mass, 3 spectral indices: F28/F25, F49/F25, C28/F25,
- ZPR6-7 High ^{240}Pu content: 1 critical mass,
- ZPPR-9: 1 critical mass, 3 spectral indices: F28/F25, F49/F25, C28/F25, 2 Na void configurations: central void and leakage-dominated configurations,
- JOYO: 1 critical mass.

A specific activity has been devoted to the assessment of integral experiment covariance data that will be described in section IV.

F. Corrective Factors

The strategy proposed in order to avoid a full reanalysis of all experiments by the participants to the adjustment exercise has been to provide corrective factors obtained as a ratio between a very detailed (reference) calculation and a simplified one. Hence the C/E (Calculated/Experimental value) is obtained as

$$\frac{C}{E} = \frac{C^s C^f}{E}, \tag{4}$$

where E is the experimental value, C^s is the result coming from the simplified model calculation, and C^f is the corresponding corrective factor.

II. SENSITIVITY ANALYSIS

A major ingredient of any adjustment process is the sensitivity analysis. A number of theoretical developments and applications have been performed since the pioneering work of Usachev [11] that generalized the standard Wigner approach for critical nuclear reactors. In general these methods and approximations used in practical applications (*e.g.*, the use of first order sensitivity analysis) are well understood. However, the present activity offered a unique opportunity to perform a detailed international comparison on a set of well defined configurations. A number of issues were tackled and recommendations were formulated.

JAEA, INL, ANL, CEA and PSI have provided full sets of sensitivity coefficients for all integral parameters considered in the benchmark. Sensitivity coefficients for the effective multiplication factor $k_{\rm eff}$ have also been generated in a consistent manner by JSI and IRSN. ORNL has provided data but on a different energy group structure.

A. Methodologies

Sensitivity methods are well established, however in practical applications one has to specify if deterministic or Monte Carlo methods have been used and a number of ambiguities/approximations have to be eliminated or well understood in order to compare effectively the sensitivity coefficient produced by different groups. The main features of the different methods used within the Subgroup can be summarized as follows:

(1) For $k_{\rm eff}$, deterministic values of the sensitivity coefficients have been obtained by Standard Perturbation-Theory (SPT) techniques using transport-theory except for JAEA that made use of diffusion theory. More precisely, the various analyses were carried out on the basis of:

- SAGEP code [12], in conjunction with JENDL-4 data at JAEA,
- ERANOS code [13] in conjunction with ENDF/B-VII.0 data at INL and ANL, and
- ERANOS in conjunction with JEFF-3.1.1 and JEFF-3.1 data at CEA and PSI, respectively.

In addition, in conjunction with ENDF/B-VII.0 data, the code SUSD3D [14] was used together with DANTSYS [15] at JSI.

At IRSN, stochastic values of the sensitivity coefficients based on a multi-group approach have been obtained by TSUNAMI-3D which uses an adjoint based technique and is part of SCALE [16] in conjunction with ENDF/B-VII.0 data. The sensitivity coefficients take into account that a change of a given cross section may also influence other cross sections through modifications of their shielding factors. Thus, the TSUNAMI sensitivity coefficients are computed with the total instead of the partial derivatives as

$$S_{\sigma_x^i(g)} = \frac{dk}{k} \Big/ \frac{d\sigma_x^i(g)}{\sigma_x^i(g)} = \frac{\partial k}{k} \Big/ \frac{\partial \sigma_x^i(g)}{\sigma_x^i(g)} + \sum_j \sum_y \sum_h \left\{ \left(\frac{\partial k}{k} \Big/ \frac{\partial \sigma_y^i(h)}{\sigma_y^i(h)} \right) \left(\frac{\partial \sigma_y^j(h)}{\sigma_y^j(h)} \Big/ \frac{\partial \sigma_x^i(g)}{\sigma_x^i(g)} \right) \right\} . \quad (5)$$

In the formula for these "complete" sensitivity coefficients [16], the space variable has been omitted and *e.g.* $\sigma_x^i(g)$ is the cross section of nuclide i for reaction x in energy group g. The first expression on the right hand side corresponds to the standard definition ("explicit" term), with the additional summations ("implicit" effects) as an indirect term.

(2) For the reaction rates at core center relative to ^{235}U fission (F25), *i.e.*, F49/F25, F28/F25, F37/F25 and C28/F25, Generalized Perturbation Theory (GPT) [11] has been consistently used in the deterministic calculations for obtaining their sensitivity coefficients.

(3) Equivalent Generalized Perturbation Theory (EGPT) [17] has been employed for determining the sensitivity coefficients of the void reactivity effects in ZPPR-9 (Na void Step 3 and Na void Step 5) except for JAEA that used the standard formulation of GPT [11].

B. Analysis of Sensitivity Profiles

1. k_{eff}

The sensitivity coefficients of the actinides related to the two JEZEBEL bare spheres and to the sodium-cooled systems, *i.e.*, the two ZPR6-7 cores, ZPPR-9, and JOYO, show very good consistency among the participants, *e.g.* as seen in Fig. 1. The sensitivity coefficients are almost independent of the code (deterministic SAGEP, ERANOS, DANTSYS/SUSD3D and TSUNAMI-1D, stochastic TSUNAMI-3D) and basic nuclear data (JENDL-4, ENDF/B-VII.0 or JEFF-3.1) being used.

As far as the sensitivity coefficients for the structural materials, sodium, oxygen, and those for the scattering reactions of the actinides (see examples in Figs. 2–4), consistency is also shown for most cases.

In the case of the sensitivity coefficients for the FLATTOP core, some of the energy profiles are characterized by larger discrepancies. However, most of these discrepancies are well understood. Thus, for the JAEA solution,

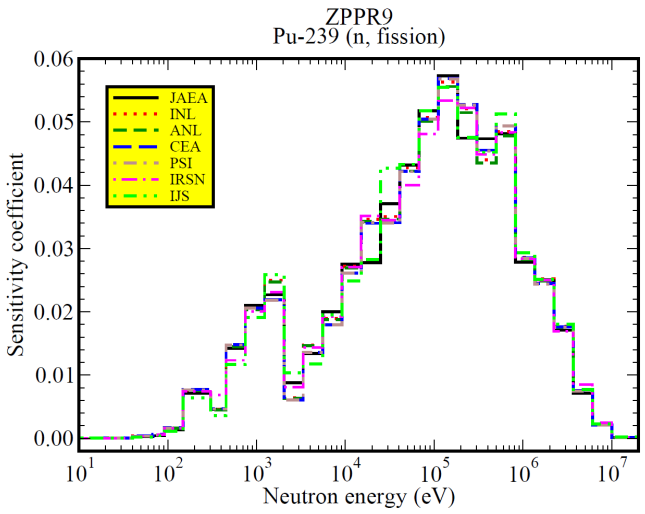

FIG. 1. Sensitivity profiles of ^{239}Pu fission cross section for ZPPR-9 k_{eff}.

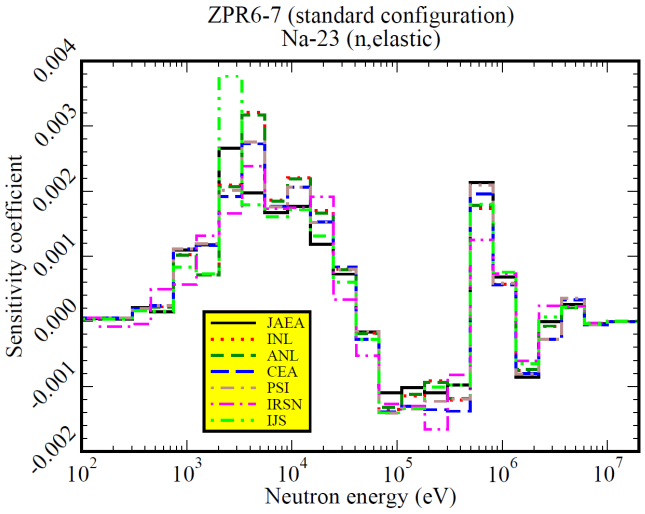

FIG. 2. Sensitivity profiles of ^{23}Na elastic cross section for ZPR6-7 k_{eff}.

it is largely attributed to the use of a 2D (r,z) model with diffusion theory instead of spherical geometry in conjunction with transport theory used by the other participants. This is causing much larger modeling effect for FLATTOP than for the other systems under investigation.

A further investigation was performed comparing Monte Carlo and deterministic methods. In particular, results for the sensitivities of the multiplication factor of the FLATTOP-Pu benchmark to perturbations of the ^{238}U elastic cross section were investigated. The results obtained by participants to the benchmark exercise are shown in Fig. 5 (top), including the JSI deterministic solution obtained by a refined P3 approximation for both the elastic as well as inelastic scattering cross sections. In addition, Fig. 5 (bottom) displays JSI Monte Carlo

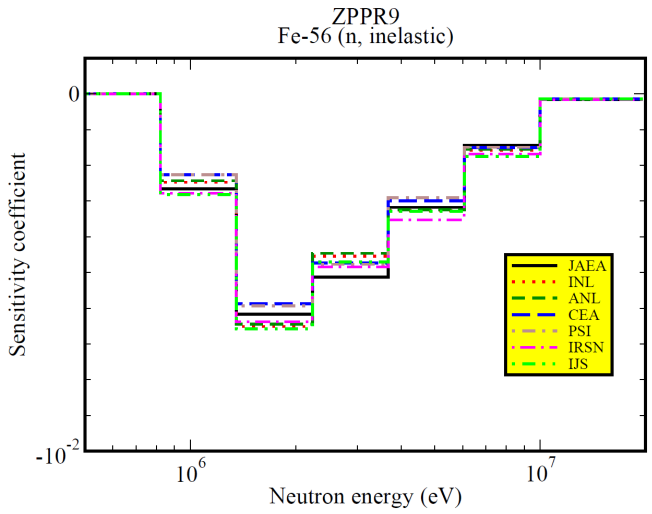

FIG. 3. Sensitivity profiles of ^{56}Fe inelastic cross section for ZPPR-9 $k_{\rm eff}$.

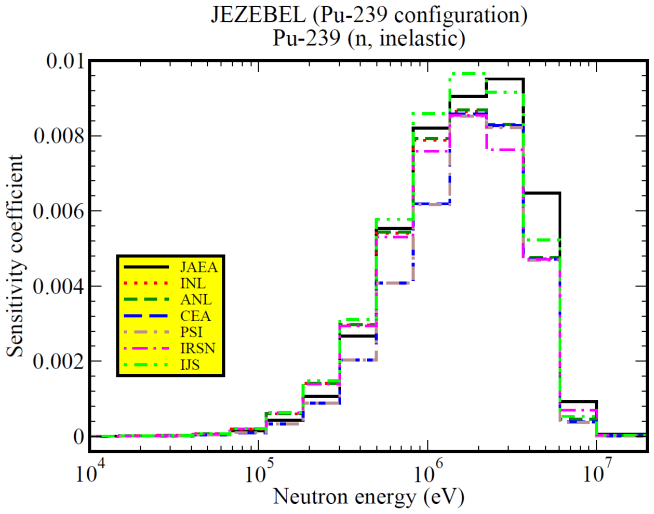

FIG. 4. Sensitivity profiles of ^{239}Pu inelastic cross section for JEZEBEL $k_{\rm eff}$.

results and data taken independently from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) handbook. The results show the following features:

(a) The reference JSI deterministic values (P1 approximation) are the largest, especially above 0.3 MeV coinciding with groups 1-8, and peak at higher energy. Using the P3 approximation largely removes this difference and leads to agreement for energies up to about 1 MeV with the bulk of the other solutions.

(b) The continuous energy Monte Carlo solution also agrees, by bearing in mind that "small" sensitivity coefficients such as for energies below 60 keV and above 5 MeV, are clearly difficult to calculate.

(c) The ORNL values provided in 238 groups are found

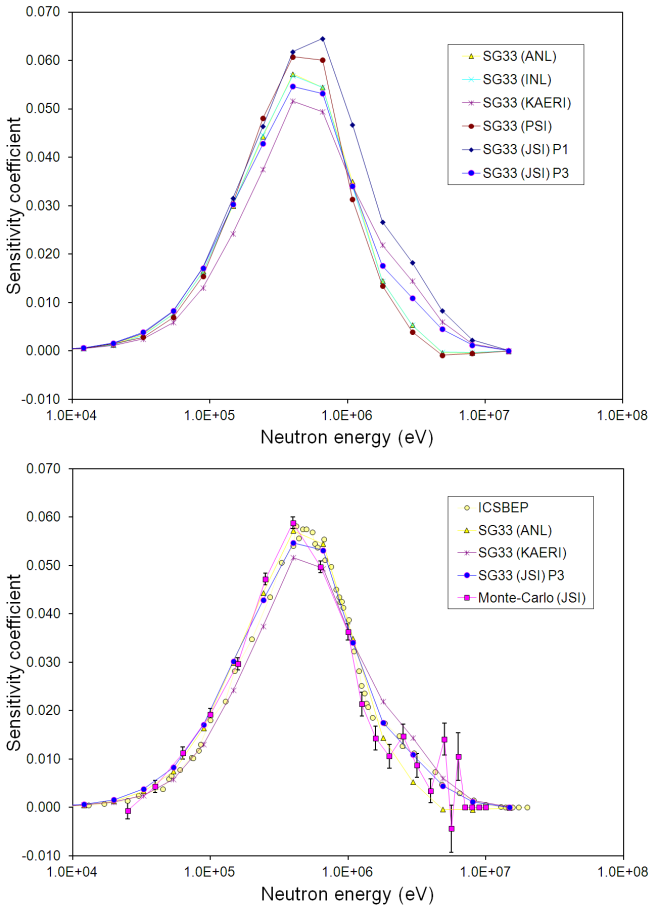

FIG. 5. Sensitivity profiles of ^{238}U elastic cross section for FLATTOP-Pu $k_{\rm eff}$ (see text).

consistent with ICSBEP, which in turn appear consistent with the INL and ANL solutions for energies up to about 1.5 MeV, whereas the PSI values are higher near the peak around 0.5 MeV and the KAERI values are systematically lower for energies < 0.6 MeV.

2. *Spectral indices F49/F25, F28/F25, F37/F25 and C28/F25*

The GPT was used by JAEA, INL, ANL, CEA, and PSI to calculate the sensitivity coefficients of spectral indices for JEZEBEL, ZPR6-7 and ZPPR-9 configurations. The results obtained by the participants are consistent, including those for the structural materials, oxygen and sodium in the case of ZPR6-7 and ZPPR-9. Some examples are given in Figs. 6–8.

3. *Reactivity effects*

The Na void (Step 3) and Na void (Step 5) in the ZPPR-9 experiment have been considered.

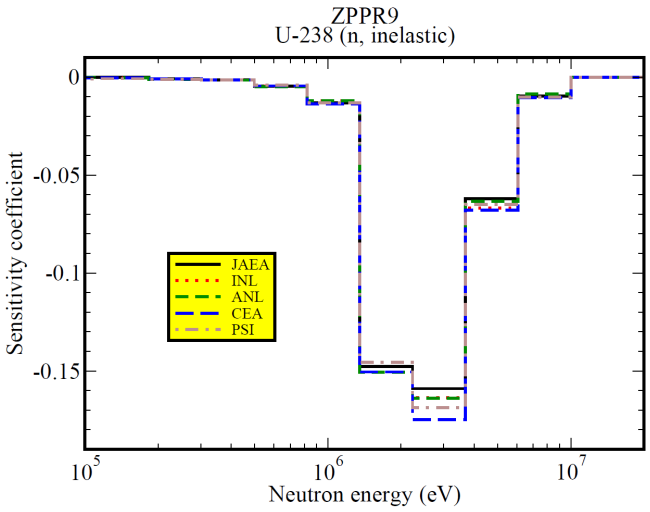

FIG. 6. Sensitivity profiles of ^{238}U inelastic cross section for ZPPR-9 F28/F25 spectral index.

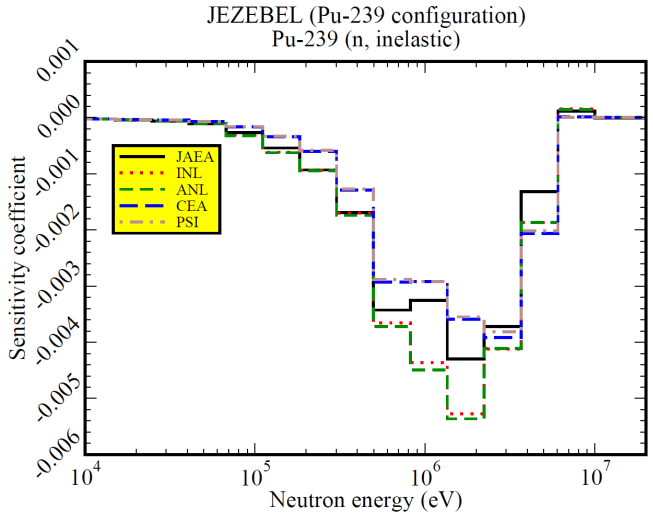

FIG. 7. Sensitivity profiles of ^{239}Pu inelastic cross section for JEZEBEL F37/F25 spectral index.

In general, good consistency is shown among the participants (JAEA, INL, ANL, CEA, and PSI) providing for ZPPR-9 deterministic solutions based upon the EGPT methodology (see Fig. 9) except for JAEA (see above). However, some differences can be seen for ^{240}Pu close to the threshold and for the sodium inelastic scattering cross section.

C. Summary of Major Recommendations

Calculation of sensitivity coefficients is now part of the standard calculation routes in many modern code systems. The agreement among results obtained by different methods is remarkable. However, a number of recommendations can be formulated on the basis of the comparisons described above:

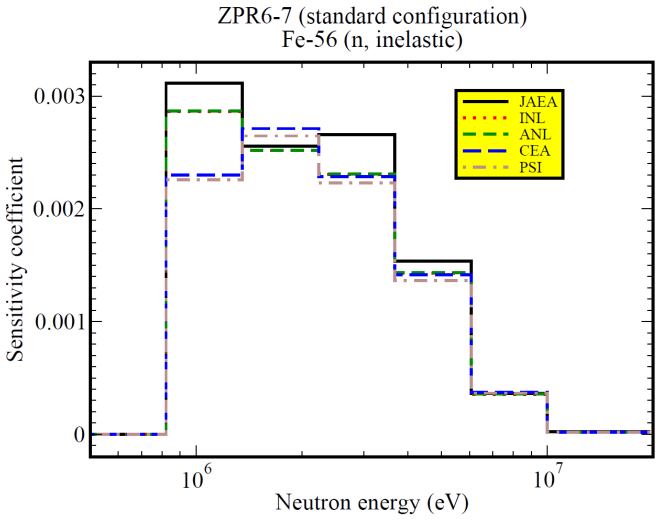

FIG. 8. Sensitivity profiles of ^{56}Fe inelastic cross section for ZPR6-7 C28/F25 spectral index.

- Sensitivity coefficients calculated, *e.g.* for the multiplication factor and reaction rate ratios with different deterministic methods and codes agree well among them, but one should be careful in specifying definitions and model approximations, such as *e.g.* the exact detector position and volume in the case of Generalized Perturbation Theory (GPT) for sensitivity coefficients of reaction rate ratios.
- "Small" sensitivity coefficient values are to be used with care, since in these cases errors can arise from numerical problems, such as those associated with the local convergence of the importance function.
- Resonance shielding effects, which appear not too important for the present exercise, should be considered with appropriate algorithms.
- Anisotropy of scattering should be accounted for at high energies when calculating sensitivity coefficients to elastic and probably also inelastic scattering cross sections.
- EGPT provides a powerful tool to calculate sensitivity coefficients for reactivity effects.
- Adjoint based and direct Monte Carlo techniques provide an interesting alternative to deterministic methods in particular for complex geometries. However, both methodologies are computationally very intensive. In addition, especially when using the direct method, care must be taken in carrying out the calculations with a sufficient precision. The sensitivity coefficients are computed by means of differences between two independent calculations,

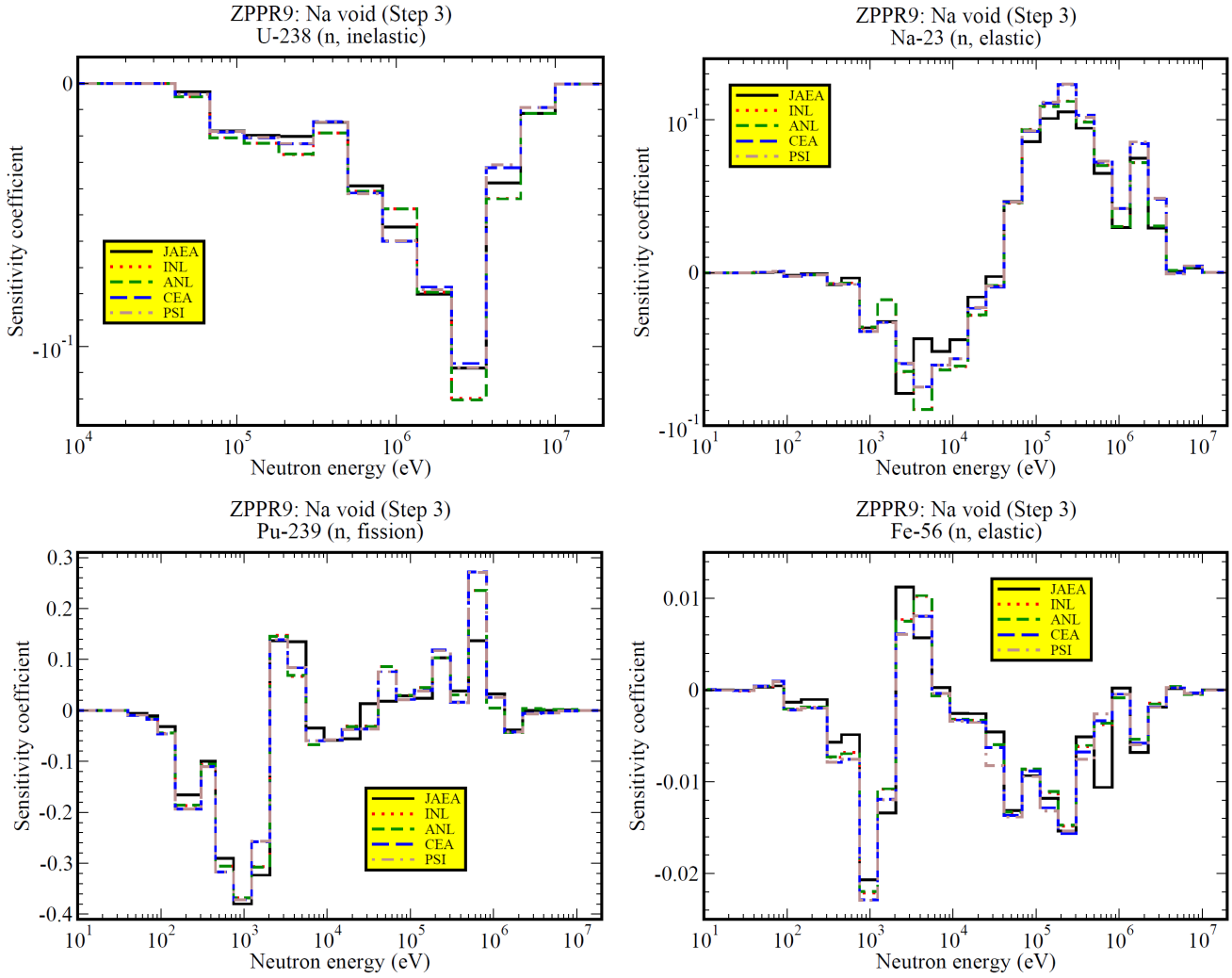

FIG. 9. Sensitivity profiles of various cross sections for ZPPR-9 Na voiding.

and sufficiently large perturbations of the cross sections must be introduced to ensure obtaining statistically significant differences of the results and at the same time avoiding non-linearity.

III. NUCLEAR DATA COVARIANCES

Nuclear data covariances represent one of the important parameters in the cross section adjustment procedure. Generally, the covariance matrix of a scattered data set, x_i $(i = 1, \ldots, n)$ with the average value $m_{0i} = \langle x_i \rangle$, is defined as follows [18]:
variance

$$\mu_{ii} = var(x_i) = \langle (x_i - m_{0i})^2 \rangle \text{ for } i = 1, \ldots, n, \quad (6)$$

standard deviation (STD)

$$\sigma_i = std(x_i) = \sqrt{var(x_i)}, \quad (7)$$

covariance

$$\mu_{ij} = cov(x_i, x_j) = \langle (x_i - m_{0i})(x_j - m_{0j}) \rangle, \quad \text{for } i, j = 1, \ldots, n \text{ with } i \neq j, \quad (8)$$

and correlation factor $(-1 \leq \rho_{ij} \leq 1)$

$$\rho_{ij} = \frac{\mu_{ij}}{\sqrt{\mu_{ii}\mu_{jj}}} = \frac{cov(x_i, x_j)}{std(x_i)std(x_j)}. \quad (9)$$

The covariance matrix must be symmetric and positive-definite. In this section, first, the methodologies used to evaluate the nuclear data covariances are briefly reviewed. Next, some of the actual covariance data are illustrated. Comparisons are made among JENDL-4.0 (J-4.0 hereafter [19, 20]), and COMMARA-2.0 (C-2.0 hereafter [21]) which is to be used together with the ENDF/B-VII.0 central values [22], and the CEA COMAC [23]. More detailed comparisons can be found in Ref. [24].

A. Covariance Data Used in the Subgroup 33 Adjustment Exercise

Different covariance data have been developed in recent years and some of them have been used by the participants of Subgroup 33. For the evaluation of covariance data, different techniques have been used; in particular, a generalized least-square method to combine large experimental data bases [25, 26] or the Kalman-filter method, see for example [27]. The basic idea of this method is to optimize the nuclear model parameters by the inclusion of the cross section measurement information with the Bayesian parameter estimation. Specific techniques have been used to assess covariance data in the resonance region [28–31]. Further discussion on the different methods can be found in the quoted references and in the final report of Subgroup 33 [24].

Increases in computing power have made it feasible to evaluate nuclear data and their associated covariances using Monte Carlo (MC) methodology [32, 33]. One of the advantages of the MC-based method is that it does not need the sensitivity of nuclear model parameters, which frees it from the assumption of linearity. The MC method does however require a fairly large amount of computing time to obtain sufficiently small statistical uncertainties, as well as the need of the prior model parameter uncertainty, shape and correlation for random sampling. These methods face the difficulty to take into account deficiencies in the nuclear reaction models, and the quality and quantity of the cross section measurements.

Table II summarizes the features of various covariance data treated in the Subgroup 33 exercise. In total, 5 covariance libraries were used.

B. Comparison of Covariance Data

Most of the covariance data (diagonal values and by and large also correlation coefficients) used in the different participants data sets, are comparable in magnitude. However, a closer examination points out differences, sometimes associated with covariance data evaluation methods. To give some examples we will first show some discrepancies among the CEA COMAC library, the COMMARA-2.0 and the JENDL-4 covariances for ^{239}Pu and ^{241}Pu fission and ^{238}U inelastic scattering.

Figs. 10–12 show the diagonal values of ^{239}Pu and ^{241}Pu fission and ^{238}U inelastic scattering cross sections. The uncertainty on the ^{239}Pu fission cross section is small in all cases. However, there is approximately a factor of two difference between the COMAC values and the JENDL or COMMARA values. This difference is at the origin of very significant uncertainty value on most $k_{\rm eff}$ of Pu-fueled integral experiments (see section V). Also, in the case of the fission of ^{241}Pu, there are large differences between the COMAC values and, on the other side, the JENDL or COMMARA values in the energy region below ∼10 keV. These differences in uncertainty do not play a very important role in the present exercise, but can have a much stronger impact on core design and fuel cycle parameters of large Fast Reactor cores with softer spectra. Finally, the difference observed in the ^{238}U inelastic scattering cross section uncertainties has a significant impact on many key integral parameters since it will affect the slowing down characteristics of most cores, according to core composition, conversion ratio values, *etc.*

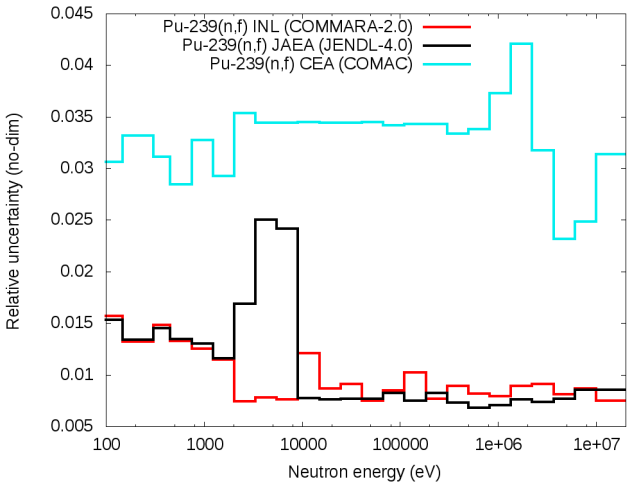

FIG. 10. Relative uncertainties of ^{239}Pu(n,f) cross sections.

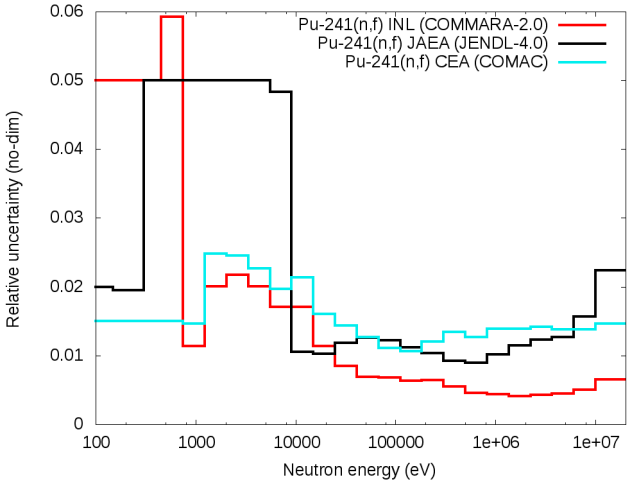

FIG. 11. Relative uncertainties of ^{241}Pu(n,f) cross sections.

C. Further Comparison of JENDL-4.0 and COMMARA-2.0 Covariance Libraries

One can say that in general, for the 11 isotopes treated in the Subgroup 33 exercise, that is, ^{10}B, ^{16}O, ^{23}Na, ^{56}Fe, ^{52}Cr, ^{58}Ni, ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, and ^{241}Pu, their associated covariance data are found to be rather similar between the two libraries, probably due to the use of similar

TABLE II. Features of covariance data used in the Subgroup 33 adjustment exercise.

Covariance library	Evaluated Isotopes	Covariance data included	Methodology applied to evaluate covariance data	Other features
COMMARA-2.0 (BNL,LANL)	- 12 light nuclei (coolants and moderators) - 78 structural materials and fission products - 20 actinides	- Reaction cross sections + $\bar{\nu}$ for 20 actinides + PFNS of ^{238,239,240}Pu + $\bar{\mu}$ of ^{23}Na, ^{56}Fe	- Generalized least-square method - Resonance R-matrix analysis - Kalman-filter method - Kernel approximation	- 33-energy group structure - To be used together with the ENDF/B-VII.0 central values - Released in October 2010 [21]
JENDL-4.0 (JAEA)	95 nuclides, including ^{10,11}B, ^{14,15}N, ^{16}O, ^{23}Na, ^{48}Ti, ^{52,53}Cr, ^{55}Mn, ^{56}Fe, ^{59}Co, ^{58,60}Ni, ^{90}Zr, ^{209}Bi, and all actinides	- Reaction cross sections + $\bar{\mu}$ for 16 light nuclei and structural materials - Reaction cross sections + $\bar{\nu}$ + PFNS + $\bar{\mu}$ for 79 actinides	- Generalized least-square method - Resonance R-matrix analysis - Kalman-filter method	- ENDF standard format - File 33 is given for resonance energy region - Released May, 2010 [19, 20]
COMAC(CEA) + JENDL/ENDF for some isotopes	- 24 light and intermediate nuclei - 15 actinides	Reaction cross sections + $\bar{\nu}$ (from JENDL-4) + PFNS (from JENDL-4)	- Generalized least-square - Resonance R-matrix and Optical Model analysis - Marginalization of systematic experimental uncertainties	33-energy group structure
TENDL (NRG)	^{235,238}U and ^{239}Pu	No covariance files but random ENDF files based on TENDL-2010 [34]	Monte Carlo-based method: TMC + selection based on distance minimization	Pointwise cross sections
SCALE 6.1 (ORNL)	- 2 isotopes in structural materials - 8 actinides (^{234,235,238}U, ^{237}Np, ^{239,240,241,242}Pu)	Reaction cross sections + $\bar{\nu}$ + PFNS	- Generalized least-square method - Delta chi-square filter method	- Initially a 44-energy group structure, collapsed to a 33-group structure - Released in June 2011 [35]

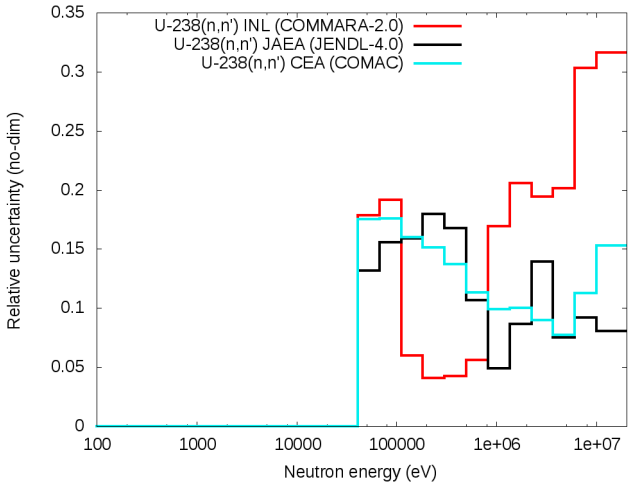

FIG. 12. Relative uncertainties of ^{238}U(n,n') cross sections.

evaluation methodology such as the full or simplified R-matrix analysis, the Bayesian estimation connected with some theoretical nuclear model codes, or the simultaneous evaluation for fission data of major actinides, *etc.* Furthermore, experimental cross section data from the international library EXFOR are commonly used to fit nuclear reaction model parameters.

However, there are some isotope-reaction-energy regions where the covariance data of the two libraries are notably different. Three examples will be examined in detail.

1. ^{235}U capture in 3-300 keV energy region

As seen in Fig. 13, the standard deviation (STD) of C-2.0 is exactly ±20%, while that of J-4.0 is very small around ±2-4%. Further, the correlations of C-2.0 are almost perfectly positive, but those of J-4.0 are only partially positive. The difference of the capture cross section center values between ENDF/B-VII.0 and J-4.0 is around -10 to +5% in this energy range. From Refs. [19–21], C-2.0 applied the Bayesian code KALMAN with the GNASH code for the covariance evaluation, on the other hand, JENDL-4.0 used the generalized least square code GMA. It seems unlikely that these two methods generate such a large difference, if both methods adopt the same experimental information. More analysis seems to be needed to assess the covariance in the fast energy region of ^{235}U capture reaction.

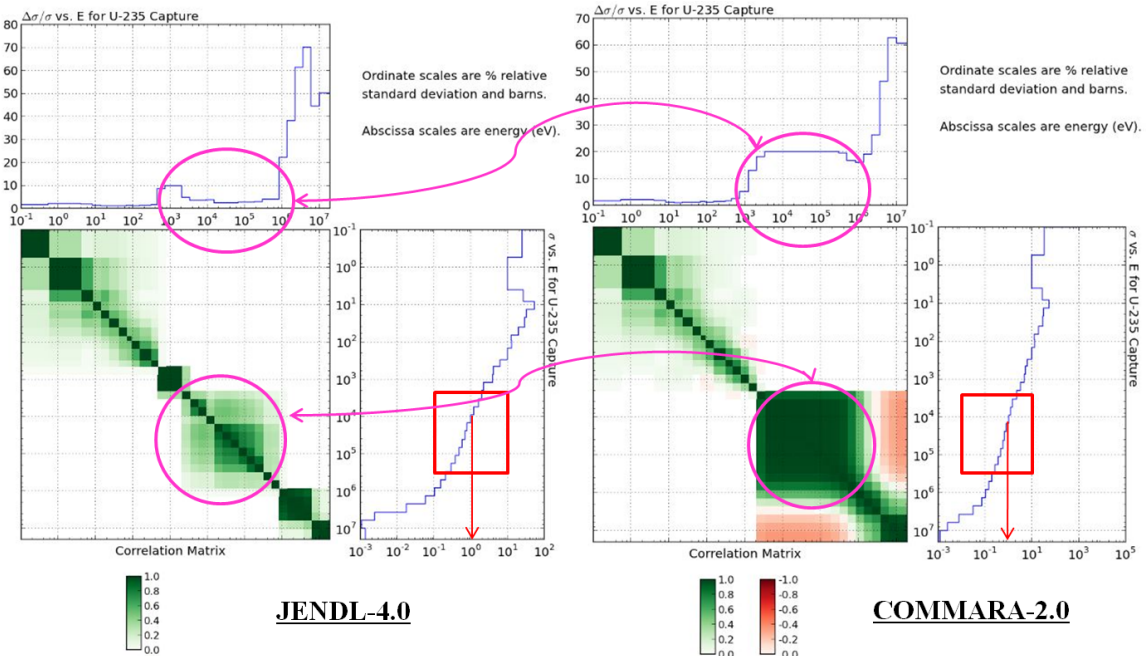

FIG. 13. Comparisons of JENDL-4.0 and COMMARA-2.0 covariance for ^{235}U neutron capture.

2. ^{23}Na elastic scattering data around 2 keV

At this energy, there appears a giant resonance peak which affects significantly the sodium-voiding reactivity in sodium-cooled fast reactor cores. As found in Fig. 14, the shape of the standard deviation is extremely different between two libraries; that is, the minimum STD value occurs at the cross section peak energy in C-2.0, and on the contrary, the maximum appears there in J-4.0. With a simple consideration, the trend of C-2.0 seems more natural, since the larger cross sections would be more accurate due to the small statistical uncertainty in the measurement. The correlations are also quite different. In the C-2.0 covariance, the 2 keV peak has no correlations with other energy, while J-4.0 is partially positive everywhere above 100 eV. The covariance of C-2.0 is evaluated by the EMPIRE/KALMAN combination, where the prior resonance model parameter uncertainties are derived from Mughabghab [31]; on the other hand, J-4.0 applies the GMA code with some corrections to meet the measured cross sections with the evaluated ones of J-4.0 which is based on the multi-level Breit-Wigner formula with rather old resonance parameter values recommended by BNL in 1981. The cross section difference between ENDF/B-VII.0 and J-4.0 is -17 to +4% around 2 keV, therefore, the difference of STDs might be reasonable if we take into account the corrections given to J-4.0 covariance.

3. ^{56}Fe elastic scattering in 0.3-25 keV energy range

The central values of the ^{56}Fe elastic scattering cross section in the resonance region from 10^{-5} eV through 850 keV are almost identical for ENDF/B-VII.0 and JENDL-4.0, since the resonance parameters adopted in both libraries are based on a common evaluation around 1990. The covariance data of C-2.0 and J-4.0 were, however, independently evaluated. In the C-2.0 covariance, the resonance region of ^{56}Fe up to 850 keV was evaluated with the kernel approximation and data from Mughabghab [31]; on the other hand, the covariance data of J-4.0 were firstly estimated from the experimental data with the GMA code. Then the estimated variances were modified by considering the difference between the average of the experimental data and that of JENDL-4 [19]. The differences of the STD shapes and the correlations in Fig. 15 might stem from these utterly different methodologies of their covariance evaluations, though the energy-averaged STD values seem rather similar with each other, that is, ±5.6% in C-2.0 and ±4.5-11% in J-4.0.

IV. COVARIANCES OF EXPERIMENTAL INTEGRAL PARAMETERS

A. Experimental Covariance Matrix Definition

Experimental uncertainties of an integral parameter are usually given by the experimenters in the form of components. However, correlations between integral parameters are scarcely found in the experiment reports; therefore, we have to estimate them from the experimen-

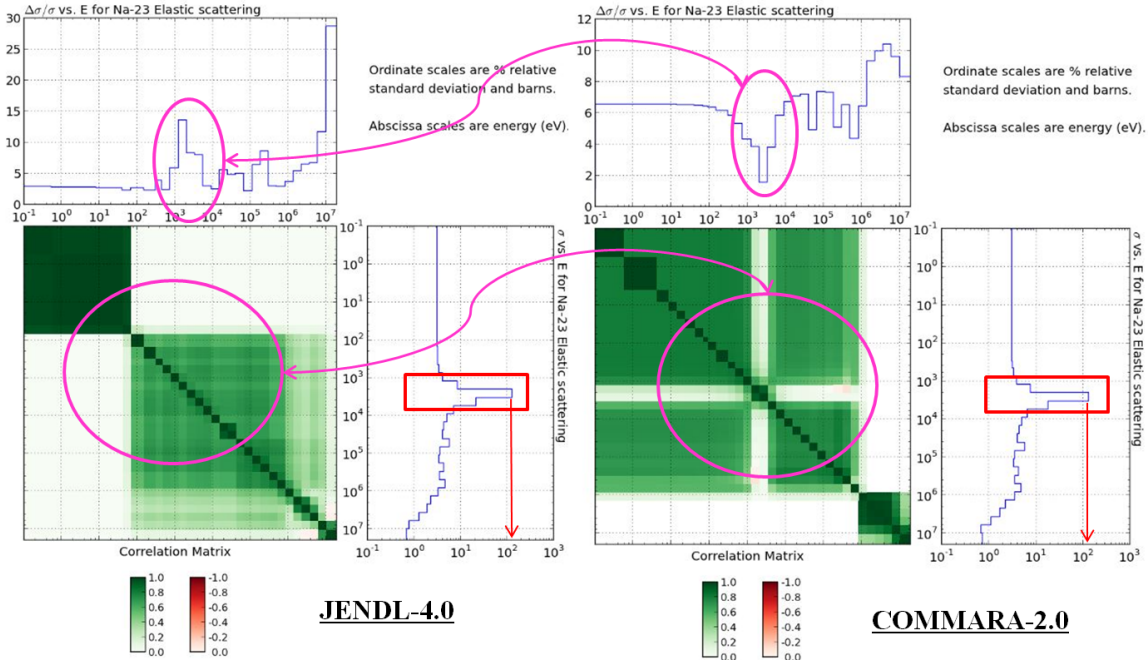

FIG. 14. Comparisons of JENDL-4.0 and COMMARA-2.0 covariance for ^{23}Na neutron elastic scattering.

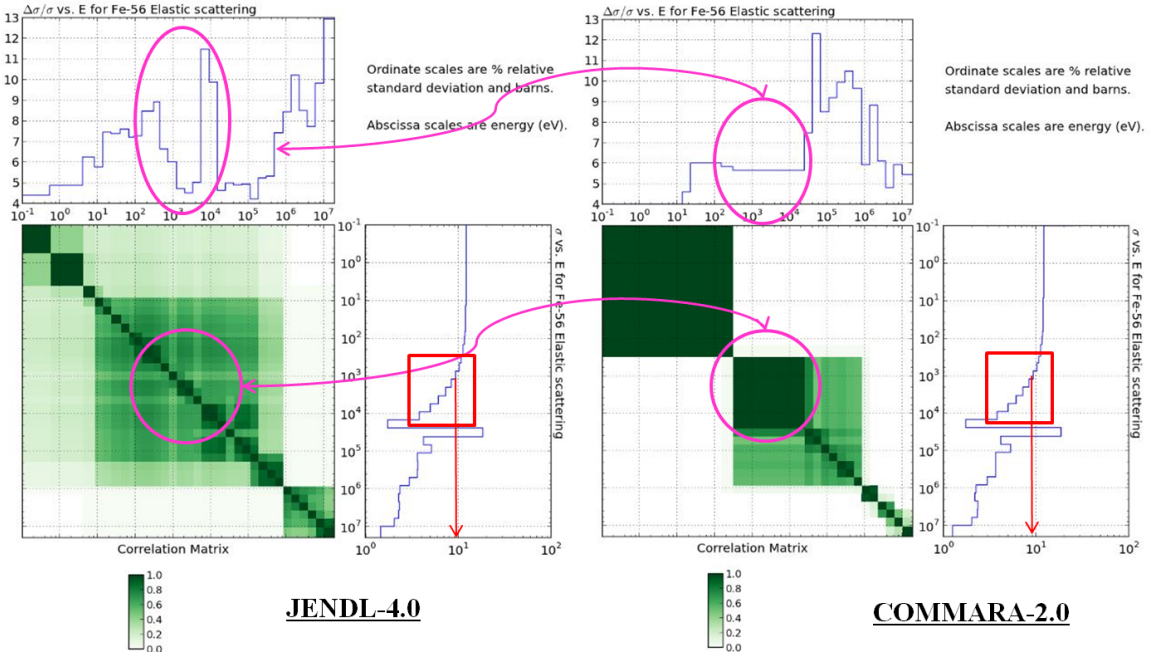

FIG. 15. Comparisons of JENDL-4.0 and COMMARA-2.0 covariance for ^{56}Fe neutron elastic scattering.

tal information available. The method adopts the following three steps.

(1) Classification of Uncertainty Components to either Common or Independent (step 1). In this step one identifies all components of the experimental uncertainties for "Data A" and "Data B" for which quantitative values were reported, and each of them is put into a category "Common uncertainty (*i.e.*, the correlation factor is 1.0) between Data A and B", or into a category "Independent uncertainty (*i.e.*, the correlation factor is 0.0)". If an uncertainty component is judged as a mixture of common and independent uncertainties, that is, the correlation factor is not considered as either 1.0 or 0.0, then the uncertainty component must be divided into more detailed subcomponents until the uncertainty component becomes either common or independent uncertainty.

(2) Summing up of Common and Independent Uncertainties (step 2). The common and independent uncertainties respectively are summed-up statistically to obtain standard deviation, σ_{Total}, the diagonal term of ma-

trix. The statistical treatment is justified by the assumption that all uncertainty components are already divided until there are no correlations between any uncertainty items in the measurement of an integral parameter. The total uncertainty of a data set A, $\sigma_{Total,A}$, *i.e.*, the diagonal term of uncertainty matrix V_e (see Eq. (1)), is given by the summation in quadrature of common and independent uncertainties

$$\sigma_{Total,A} = \sqrt{\sigma^2_{Common,A} + \sigma^2_{Independent,A}}, \qquad (10)$$

where σ_{Common} is the sum of all common uncertainty components and $\sigma_{Independent}$ is the sum of all independent uncertainty components.

(3) Evaluation of Correlation Factor (step 3). The correlation factor, non-diagonal term, of data sets A and B, $\rho_{A,B}$, is derived as the ratio of common uncertainties to the total uncertainties as

$$\rho_{A,B} = \frac{\sum_i \sigma_{Common,A,i} \times \sigma_{Common,B,i}}{\sigma_{Total,A} \times \sigma_{Total,B}}, \qquad (11)$$

where suffix i is the common uncertainty components between data set A and set B. Steps 1 to 3 must be repeated for all matrix elements to generate a full experimental covariance matrix as the input of adjustment exercise. Note that, for example, the correlation factors among several sodium void reactivity measurements would be changed depending on the combination of void steps, even in the same experimental core.

B. Full Experimental Covariance Matrix in Subgroup 33 Exercise

Applying the above-mentioned methodology, the full covariance matrix for the 20 experiments treated in the Subgroup 33 exercise is summarized in Table III. Additional comments are given below:

(1) The correlation factors of the Reaction Rate Ratios (RRRs) in Jezebel ^{239}Pu, Flattop and ZPR6-7 are borrowed from those of ZPPR-9, since the denominator of the RRRs, F25, is common in these experiments, and there is scarce information for the former three experiments to evaluate the common and independent components of the RRRs. The F37/F25 ratio is assumed to possess similar characteristics with F28/F25 which has a threshold feature versus neutron energy.

(2) From the fuel composition tables of [37, 38], the plutonium fuel plates used in ZPR6-7, ZPR6-7 High ^{240}Pu content and ZPPR-9 experiments were found to be the same. This means at least that the criticality of these three cores must be correlated through the composition uncertainties. In Table III, the evaluated correlation factors with the sensitivity coefficients of core compositions are added. The correlations among other parameters of these three cores are neglected here, since the effects of common core material to other parameters are usually small compared with that of criticality.

C. Modeling Covariance Matrix

The evaluation methodology of the modeling covariance, V_m (see Eq. (1)), depends on the method adopted to obtain the calculation value of an integral experiment. Here, we consider three kinds of methods: (1) Continuous-energy Monte Carlo method based on the as-built experimental geometry and compositions (MC method, hereafter), (2) Deterministic method based on the combination of the standard calculation and the corrections by the most-detailed models (Deterministic method), and (3) Combination of the deterministic calculation based on the simplified geometry and the correction by the Monte Carlo calculation with as-built geometry (Combined method). The resulting matrix for the selected experiments is given in Table IV. A full description can be found in [24].

V. COMPARISON OF INTEGRAL EXPERIMENT INITIAL C/E'S, UNCERTAINTIES AND TARGET SYSTEM UNCERTAINTIES

A. Introduction

In this section we will inspect the results provided by the benchmark participants regarding the initial $C/E's$, uncertainties associated to the integral experimental analysis (both experimental and calculation), as well those related to nuclear data, and target systems uncertainties (nuclear data related). The integral experimental analysis results have been provided by the following organizations:

- ANL: ENDF/B-VII.0 cross sections, MCNP5 for experiment analysis, and ERANOS system and COMMARA-2.0 covariance data for uncertainty analysis.
- CEA: JEFF-3.1.1 cross sections, ERANOS/PARIS (in conjunction with corrective factors) for experimental analysis, and ERANOS/PARIS and COMAC covariance data for uncertainty analysis.
- INL: ENDF/B-VII.0 cross sections, MCNP5 for experiment analysis, and SANDRA code and COMMARA-2.0 covariance data for uncertainty analysis.
- IRSN: ENDF/B-VII.0 cross sections, SCALE-6 for experiment analysis, and BERING code and COMMARA-2.0 covariance data for uncertainty analysis (only k_{eff} quantities provided).
- JAEA: JENDL-4 cross sections, MVP for experimental analysis, and SAGEP code and JENDL-4 covariance data for uncertainty analysis.
- JSI: ENDF/B-VII.0 cross sections, DANTSYS for experiment analysis, and SUSD3D system and

TABLE III. Experimental covariance matrix of integral parameters V_e applied in the Subgroup 33 exercise. Diagonal values are 1σ uncertainties in %, non-diagonal values are correlation factors (between -1 and $+1$).

No.	Core	Parameter	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	Jezebel-Pu239	keff	0.2																			
2		F28/F25	0	1.1																		
3		F49/F25	0	0.23	0.9																	
4		F37/F25	0	0.23	0.32	1.4																
5	Jezebel-Pu240	keff	0	0	0	0	0.2															
6	Flattop	keff	0	0	0	0	0	0.3														
7		F28/F25	0	0	0	0	0	0	1.1													
8		F37/F25	0	0	0	0	0	0	0.23	1.4												
9	ZPR6-7	keff	0	0	0	0	0	0	0	0	0.23											
10		F28/F25	0	0	0	0	0	0	0	0	0	3.0										
11		F49/F25	0	0	0	0	0	0	0	0	0	0.23	2.1									
12		C28/F25	0	0	0	0	0	0	0	0	0	0.23	0.32	2.4								
13	ZPR6-7 Pu240	keff	0	0	0	0	0	0	0	0	0.13	0	0	0	0.22							
14	ZPPR-9	keff	0	0	0	0	0	0	0	0	0.31	0	0	0	0.30	0.117						
15		F28/F25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2.7					
16		F49/F25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.23	2.0				
17		C28/F25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.23	0.32	1.9			
18		Central Na void	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.9		
19		Large Na void	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.41	1.9	
20	Joyo	keff	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.18

COMMARA-2.0 covariance data for uncertainty analysis (only k_{eff} quantities were provided with the exclusion of JOYO MK-I). P1 and S4 with the built-in Gaussian quadrature constants were used in DANTSYS transport calculations.

- KAERI: ENDF/B-VII.0 cross sections, DANTSYS for experiment analysis, DANTSYS/SUSD3D system and COMMARA-2.0 covariance data for uncertainty analysis (only k_{eff} quantities provided for uncertainty evaluation).
- ORNL: ENDF/B-VII.0 cross sections, TSUNAMI-1D for experiment analysis, and TSURFER code and ORNL covariance data for uncertainty analysis (only 1D results analyzed).
- PSI: JEFF-3.1 cross sections, ERANOS (in conjunction with corrective factors) for experimental analysis, and ERANOS and COMMARA-2.0 covariance data for uncertainty analysis.

In the following sections inspection and analysis of the participants' results is provided.

B. C/E's

Table V compares the $(E-C)/C$ results provided by the participants expressed in %. For all k_{eff} values, with exception of KAERI, the discrepancies between experimental and calculation results lie in a quite narrow range of ~250 pcm. This indicates that the current cross section libraries are in very good agreement for the set of experiments selected for the exercise, that are often used for the validation of these cross section data sets.

However, one has not to forget that k_{eff} is an integral quantity and therefore the agreement can be the result of cancellation of uncertainties. One exception is F28/F25 of ZPR6-7.

The spectral indices discrepancies are contained in a more widespread range of 4%. It is not clear why there is little agreement between CEA and PSI results, which both used the JEFF-3.1 cross section set. It could be due to differences during the cell calculations with the ECCO code. It is also interesting to note that the general tendency for all cross section sets is to underestimate the fission spectral indices results.

TABLE IV. Modeling covariance matrix V_m used in the Subgroup 33 exercise (all calculations based on continuous-energy Monte Carlo method). Diagonal values are 1σ uncertainties in %, non-diagonal values are correlation factors (between -1 and $+1$).

No.	Core	Parameter	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	Jezebel-Pu239	keff	0.03																			
2		F28/F25	0	0.9																		
3		F49/F25	0	0.5	0.8																	
4		F37/F25	0	0.5	0.5	0.8																
5	Jezebel-Pu240	keff	0	0	0	0	0.03															
6	Flattop	keff	0	0	0	0	0	0.03														
7		F28/F25	0	0	0	0	0	0	0.8													
8		F37/F25	0	0	0	0	0	0	0.5	0.7												
9	ZPR6-7	keff	0	0	0	0	0	0	0	0	0.03											
10		F28/F25	0	0	0	0	0	0	0	0	0	2.2										
11		F49/F25	0	0	0	0	0	0	0	0	0	0.5	1.4									
12		C28/F25	0	0	0	0	0	0	0	0	0	0.5	0.5	1.2								
13	ZPR6-7 Pu240	keff	0	0	0	0	0	0	0	0	0	0	0	0	0.03							
14	ZPPR-9	keff	0	0	0	0	0	0	0	0	0	0	0	0	0	0.02						
15		F28/F25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2.1					
16		F49/F25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.5	1.2				
17		C28/F25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	1.4			
18		Central Na void	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5.3		
19		Large Na void	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5.0	
20	Joyo	keff	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.03

Finally, for sodium void results the discrepancy spread is within a ∼6% range. It is interesting to observe that both ENDF/B-VII.0 and JEFF-3.1 cross section sets have different sign between the spectral component experiment (Step 3) and the leakage component one (Step 5), while JENDL-4 overestimates in both cases.

C. Experimental and Calculation Uncertainties on C/E's

Table VI shows the (quadratic) combination of experimental and calculation uncertainty on the C/E as provided by the participants. All the participants, as indicated in the exercise, have adopted the same experimental uncertainties provided in the original documentation of the experiment benchmark models; therefore, the observed differences have to be attributed to the diverse assumptions the participants have taken on their calculation values. However, the following organizations have chosen not to apply any calculation uncertainties: CEA, JSI, and KAERI. IRSN has applied a constant 0.1% calculation uncertainty to seven $k_{\rm eff}$, the only quantities they have considered for the exercise.

In general the uncertainties are relatively low and quite consistent among the different participants. There are a few exceptions. For the sodium void reactivity, participants that have adopted the Monte Carlo (instead of deterministic) codes have quite high uncertainties (∼7%). This is due to the intrinsic (statistical) difficulty that stochastic methods encounter when confronted with small reactivity variations. It has to be kept in mind that for a reliable adjustment it is needed that both experimental and calculation uncertainties stay as low as possible.

Low experimental uncertainties provide good quality results, thus giving credibility to the adjustment process. Low calculation uncertainties prevent the adjustment from compensating for shortcomings present in the calculation route. In other words, if the calculation uncertainties are high, there is the danger that the changes in the cross sections coming from the adjustment are not physical, but the result of an artificial compensa-

tion. However, the integral data which have large calculation uncertainty do not harm the adjusted results, since the weight of the data become small and give less effects to the cross section changes. The risk is to underestimate the calculation uncertainty because, in such case, the cross sections are not physically changed to force the adjusted C/E values to be 1.0.

D. Nuclear Data Uncertainties

Table VII illustrates the nuclear data uncertainties evaluated by the participants on the experimental quantities considered for the adjustment exercise. ORNL used ENDF/B-VII.0 covariance information that was collapsed to fit the 33-group format of the exercise. Six organizations (ANL, INL, IRSN, JSI, KAERI, and PSI) have used the same covariance data matrix, COMMARA-2.0. As one would expect there is good agreement among the results of these organizations with the exception of KAERI. The problem is likely related to the sensitivity coefficients (see related discussion in section II devoted to this subject).

In general JENDL-4 shows consistently lower uncertainty values than COMMARA-2.0. Exceptions are the spectral indices of fission ^{239}Pu and ^{238}U capture, indicating that for these two reactions JENDL-4 has larger variances than COMMARA-2.0. Uncertainties calculated by CEA using the COMAC covariance matrix are higher than corresponding results using COMMARA-2.0. The only exception is for ^{237}Np fission spectral indices. Quite remarkably, the k_{eff} uncertainty values span a range from ∼1500 to ∼2000 pcm. Relatively high values (up to more than 10%) are associated to the ^{238}U fission spectral indices.

Finally, concerning the uncertainties attached to the sodium reactivity coefficients, there is a fairly good agreement among all the participants. ZPPR-9 Step 3 results lie in the range between 6 and 7%, and Step 5 results between 7 and 10%.

E. Uncertainty Consistency for Adjustment

In this section we examine the consistency of the combined experimental, calculation, and nuclear data uncertainties with the observed discrepancies between experimental and calculated results. In order to establish this consistency, we define the adjustment margin AM

$$AM = U_{ND} + U_{C/E} - \left| \frac{E-C}{C} \right|, \tag{12}$$

where $U_{ND} = \sqrt{SM_\sigma S^t}$ is the uncertainty associated to nuclear data, $U_{C/E} = \sqrt{V_e + V_m}$ is the quadratic combination of the experimental and calculation uncertainty, E is the experimental result and C the calculated result. The AM quantity establishes if in the adjustment there is enough room provided by the nuclear data uncertainty to accommodate the C/E discrepancy. Of course, the C/E discrepancy has to take into account its associated uncertainty. If the AM values are negative, this implies that there is not enough uncertainty for the adjustment in the one sigma range. This will be reflected, afterwards, in the χ^2 values. One could interpret the appearance of negative values as a sign of some inconsistency in the covariance matrix (usually due to too low uncertainties associated to specific cross sections).

The AM quantity is similar to the χ quantity used by JAEA as explained in [7]. The χ for every integral parameter is defined as

$$\chi = \frac{|E-C|}{\sqrt{U_{ND}^2 + U_{C/E}^2}} \tag{13}$$

and is used with a three sigma range criterion for deciding the elimination of an experiment from the adjustment.

Moreover, other methods can be suggested to verify the consistency of a set of integral experiments and parameter uncertainties. For example, the Cook's distance is used in statistics to estimate the influence of a data point when performing least squares analysis. Data points with large residuals (outliers) and/or high uncertainties may distort accuracy of the adjustment as well as its conclusions. Points with a large Cook's distance are to be carefully checked. Some results of this type of analysis can be found in [24] and in section VI D.

The present analysis has been performed using the rather simple and intuitive formulation of Eq. (12).

Table VIII reports the AM values for the different solutions provided by the participants.

There are only seven negative values (indicated in shaded cells). The KAERI FLATTOP k_{eff} would be challenging to adjust in view of the associated quite large negative AM (-521 pcm). This is the result of different contributions: a quite unusually large initial C/E discrepancy (almost 1000 pcm), no calculation uncertainty provided, and, finally, the sensitivity coefficient problem previously mentioned. PSI has a relative high negative AM for the ^{239}Pu fission spectral index in ZPR6-7, and one should expect some difficulty in adjusting this integral parameter, but this cannot be proven as PSI has not yet performed the adjustment.

The ANL and INL four negative values are relative to the ^{239}Pu fission spectral indices and are likely due to the low uncertainty associated by COMMARA-2.0 to ^{239}Pu fission. The only negative value for CEA is associated to the fairly low uncertainty on ^{237}Np fission for COMAC previously observed in section V.4. For these entire five negative AM values one should expect, after adjustment, a difficulty for the C/E to reach the unity value even including the new evaluated associated uncertainty in the one sigma range. This is indeed the case if one inspects such quantities after adjustment (see related section). The impact on χ^2 is not expected to be large for two reasons. First the negative AM values are relatively low (<1% for spectral indices), and then, because

TABLE V. (E-C)/C results provided by the participants expressed in %.

Core	Parameter	ANL	CEA	INL	IRSN	JAEA	JSI	KAERI	ORNL	PSI
JEZEBEL239	k_{eff}	0.014	0.187	0.014	0.051	0.130	-0.091	-0.296	-0.001	0.059
JEZEBEL239	F28/F25	2.351	0.026	2.354	-	3.242	-	1.630	2.232	1.791
JEZEBEL239	F49/F25	2.534	1.412	2.533	-	1.667	-	2.019	2.570	1.539
JEZEBEL239	F37/F25	1.319	1.526	1.317	-	2.103	-	2.680	1.244	-0.013
JEZEBEL240	k_{eff}	0.019	-0.255	0.019	0.051	0.160	-0.235	-0.267	-0.079	-0.373
FLATTOP-PU	k_{eff}	-0.100	0.020	-0.097	-0.112	0.140	-0.953[a]	-0.944	-0.255	0.071
FLATTOP-PU	F28/F25	1.811	1.034	1.812	-	2.323	-	1.278	3.030	1.386
FLATTOP-PU	F37/F25	0.446	1.535	0.442	-	0.756	-	1.469	0.989	-0.697
ZPR6-7	k_{eff}	-0.040	-0.270	-0.043	-0.216	-0.527	-0.188	-0.091	-	-0.144
ZPR6-7	F28/F25	-0.446	4.207	-0.448	-	-3.251	-	1.183	-	-0.441
ZPR6-7	F49/F25	3.761	3.752	3.756	-	2.145	-	-1.320	-	4.244
ZPR6-7	C28/F25	-0.973	-0.445	-0.970	-	-1.643	-	-2.387	-	-0.467
ZPR6-7 240	k_{eff}	0.060	-0.221	0.063	-0.099	-0.329	-0.171	-0.003	-	-0.091
ZPPR-9	k_{eff}	0.080	0.005	0.078	-0.133	-0.210	-0.160	-0.133	-	0.004
ZPPR-9	F28/F25	2.985	3.664	2.987	-	1.750	-	0.948	-	4.104
ZPPR-9	F49/F25	1.956	2.417	1.958	-	0.080	-	1.131	-	2.480
ZPPR-9	C28/F25	-0.918	-0.334	-0.921	-	-1.845	-	-2.586	-	-0.372
ZPPR-9	Na Void Step 3	-1.887	-3.401	-1.884	-	-6.385	-	-4.585	-	-2.804
ZPPR-9	Na Void Step 5	2.752	3.126	2.754	-	-4.970	-	-6.978	-	2.759
JOYO MK-I	k_{eff}	0.249	0.083	0.255	0.219	0.180	-	-0.504	-	0.056

[a] Results are very sensitive to $S_N P_N$ order ($S_6P_1 : -0.81$, $S_8P_1 : -0.48$, $S_{12}P_1 : -0.24$, $S_{16}P_1 : -0.15$, $S_{48}P_3 : -0.17$).

TABLE VI. Combination of experimental and calculation uncertainties on the $C/E's$ (%).

Core	Parameter	ANL	CEA	INL	IRSN	JAEA	JSI	KAERI	ORNL	PSI
JEZEBEL239	k_{eff}	0.201	0.200	0.201	0.224	0.202	0.200	0.200	0.200	0.224
JEZEBEL239	F28/F25	1.421	1.100	1.421	-	1.447	-	1.100	1.100	1.487
JEZEBEL239	F49/F25	0.949	1.400	0.949	-	1.172	-	0.900	0.900	1.345
JEZEBEL239	F37/F25	1.432	0.900	1.432	-	1.612	-	1.400	1.400	1.720
JEZEBEL240	k_{eff}	0.201	0.200	0.201	0.224	0.202	0.200	0.200	0.200	0.224
FLATTOP-PU	k_{eff}	0.303	0.300	0.302	0.316	0.302	0.300	0.300	0.300	0.316
FLATTOP-PU	F28/F25	1.860	1.100	1.860	-	1.384	-	1.100	1.100	1.487
FLATTOP-PU	F37/F25	1.432	1.402	1.432	-	1.561	-	1.400	1.400	1.720
ZPR6-7	k_{eff}	0.230	0.230	0.230	0.251	0.231	0.230	0.230	-	0.250
ZPR6-7	F28/F25	3.499	2.100	3.499	-	3.744	-	3.000	-	3.162
ZPR6-7	F49/F25	2.524	3.000	2.524	-	2.541	-	2.100	-	2.326
ZPR6-7	C28/F25	2.683	2.400	2.683	-	2.692	-	2.400	-	2.600
ZPR6-7 240	k_{eff}	0.221	0.220	0.221	0.242	0.222	0.220	0.220	-	0.241
ZPPR-9	k_{eff}	0.120	0.117	0.117	0.154	0.119	0.117	0.117	-	0.153
ZPPR-9	F28/F25	2.915	2.700	2.915	-	3.414	-	2.700	-	2.879
ZPPR-9	F49/F25	2.119	2.000	2.119	-	2.338	-	2.000	-	2.236
ZPPR-9	C28/F25	1.992	1.900	1.992	-	2.354	-	1.900	-	2.147
ZPPR-9	Na Void Step 3	7.737	1.900	7.737	-	5.593	-	1.900	-	4.225
ZPPR-9	Na Void Step 5	7.543	1.900	7.543	-	5.311	-	1.900	-	4.133
JOYO MK-I	k_{eff}	0.181	0.180	0.181	0.206	0.182	-	0.180	-	0.206

the $\chi^2$is normalized to (divided by) the number of experiments (degrees of freedom). Having only one or two small inconsistencies will not show up in an adjustment with 20 experiments.

Let us continue our analysis observing that in Eq. (12), a not negligible role is played by the $U_{C/E}$ term. As indicated in section V.3, the desirable situation is to have this quantity as low as possible in order to provide a reliable adjustment. Let's define the experiment merit EM, where in Eq. (12) we suppress the term U_{ND}. What we want to spot now are positive values. Positive EM will indicate that the experiment is not providing enough useful information (*i.e.*, has not enough merit to be included in the adjustment) because there is too much uncertainty associated with respect to the observed C/E. In practice, these experiments could be excluded from the adjustment because they are not valuable either for poor experimental quality and/or because the employed calculation analysis carries too much uncertainty, or kept in order to provide a constraint that should not be changed

TABLE VII. Uncertainties due to nuclear data (%).

Core	Parameter	ANL	CEA	INL	IRSN	JAEA	JSI	KAERI	ORNL	PSI
JEZEBEL239	k_{eff}	0.640	2.072	0.636	0.611	0.693	0.658	0.117	1.186	0.511
JEZEBEL239	F28/F25	3.720	7.342	3.696	-	3.198	-	-	3.311	2.426
JEZEBEL239	F49/F25	0.830	2.811	0.823	-	0.625	-	-	0.809	0.719
JEZEBEL239	F37/F25	2.390	1.483	2.354	-	1.505	-	-	7.204	1.604
JEZEBEL240	k_{eff}	0.660	1.763	0.656	0.540	0.649	0.634	0.123	0.982	0.579
FLATTOP-PU	k_{eff}	0.760	1.913	0.764	0.519	1.257	0.719	0.123	1.128	0.829
FLATTOP-PU	F28/F25	3.120	7.885	3.093	-	2.936	-	-	2.616	1.948
FLATTOP-PU	F37/F25	2.050	1.585	2.034	-	1.444	-	-	7.076	1.421
ZPR6-7	k_{eff}	0.970	1.586	0.968	0.972	0.816	0.943	0.313	-	0.972
ZPR6-7	F28/F25	6.400	9.959	6.395	-	4.819	-	-	-	6.400
ZPR6-7	F49/F25	0.840	2.378	0.836	-	1.147	-	-	-	0.833
ZPR6-7	C28/F25	1.510	3.916	1.512	-	2.004	-	-	-	1.493
ZPR6-7 240	k_{eff}	0.970	1.559	0.971	0.970	0.812	0.948	0.311	-	0.973
ZPPR-9	k_{eff}	1.180	1.666	1.191	1.202	0.902	1.183	0.384	-	1.203
ZPPR-9	F28/F25	7.850	10.688	7.896	-	5.277	-	-	-	7.742
ZPPR-9	F49/F25	0.870	2.387	0.870	-	1.152	-	-	-	0.846
ZPPR-9	C28/F25	1.550	3.894	1.545	-	2.030	-	-	-	1.521
ZPPR-9	Na Void Step 3	7.670	6.493	7.563	-	5.950	-	-	-	7.228
ZPPR-9	Na Void Step 5	9.920	8.543	9.679	-	7.311	-	-	-	9.157
JOYO MK-I	k_{eff}	0.890	1.416	0.863	0.867	0.583	-	0.348	-	0.878

TABLE VIII. Adjustment Margin (AM) values expressed in %.

Core	Parameter	ANL	CEA	INL	IRSN	JAEA	JSI	KAERI	ORNL	PSI
JEZEBEL239	k_{eff}	0.827	2.085	0.823	0.784	0.764	0.767	0.021	1.385	0.676
JEZEBEL239	F28/F25	2.790	8.417	2.763	-	1.404	-	-	2.179	2.122
JEZEBEL239	F49/F25	-0.755	2.799	-0.761	-	0.129	-	-	-0.861	0.525
JEZEBEL239	F37/F25	2.503	0.857	2.469	-	1.014	-	-	7.360	3.311
JEZEBEL240	k_{eff}	0.842	1.708	0.83	0.726	0.691	0.598	0.056	1.103	0.430
FLATTOP-PU	k_{eff}	0.963	2.193	0.969	0.723	1.418	0.602	-0.521	1.173	1.075
FLATTOP-PU	F28/F25	3.169	7.950	3.141	-	1.997	-	-	0.686	2.048
FLATTOP-PU	F37/F25	3.036	1.452	3.024	-	2.249	-	-	7.487	2.444
ZPR6-7	k_{eff}	1.160	1.545	1.155	1.008	0.520	0.985	0.453	-	1.079
ZPR6-7	F28/F25	9.453	7.852	9.446	-	5.312	-	-	-	9.121
ZPR6-7	F49/F25	-0.397	1.626	-0.396	-	1.543	-	-	-	-1.085
ZPR6-7	C28/F25	3.220	5.871	3.225	-	3.053	-	-	-	3.6
ZPR6-7 240	k_{eff}	1.131	1.559	1.129	1.116	0.705	0.997	0.528	-	1.123
ZPPR-9	k_{eff}	1.220	1.778	1.230	1.224	0.811	0.957	0.368	-	1.352
ZPPR-9	F28/F25	7.780	9.724	7.825	-	6.941	-	-	-	6.516
ZPPR-9	F49/F25	1.033	1.970	1.031	-	3.410	-	-	-	0.602
ZPPR-9	C28/F25	2.625	5.460	2.616	-	2.539	-	-	-	3.296
ZPPR-9	Na Void Step 3	13.520	4.995	13.416	-	5.158	-	-	-	8.649
ZPPR-9	Na Void Step 5	14.711	7.317	14.468	-	7.653	-	-	-	10.531
JOYO MK-I	k_{eff}	0.822	1.513	0.789	0.854	0.585	-	0.024	-	1.029

by the adjustment.

In total fairness, in terms of usefulness of an experiment, correlations in the experimental uncertainties should be established and one should look also at the case where only the experimental uncertainty is considered. In fact, the calculation uncertainty component depends on circumstances independent from the experiment. Besides, another criterion for retaining or discarding an experiment would be to look at their correlation through the cross product of sensitivities weighted with the covariance matrix (the so-called representativity factor). If the correlation factor is very close to 1, one of the two experiments should be discarded as it provides redundant information (unless the configurations are not experimentally correlated), and kept only for a posteriori verification with the new adjusted cross sections and covariance matrix data.

On the other hand, because EM values neglect the uncertainty coming from the nuclear data U_{ND}, this could, in some circumstances, mislead in concluding about the usefulness of an experiment. In particular, let's consider the case where there is a very good agreement between calculation and experimental results so that the $(E-C)/C$ is almost zero, and, therefore, EM is posi-

tive. If the initial nuclear data uncertainties are greater than the $U_{C/E}$, still the resulting a posteriori uncertainty will be reduced, after adjustment, for the experiment under consideration. Therefore, one has to be very careful in drawing conclusions, and, for sure, this subject of experimental selection deserves further investigations.

EM values corresponding to the benchmark solutions provided by participants are shown in Table IX. Inspection of this table provides the following conclusions regrouped by type of integral parameters:

- Critical Masses – For organizations using ENDF/B-VII.0 cross sections only the JOYO experiment provides a useful contribution to the adjustment. This can be readily seen looking at the column of IRSN that has considered only critical masses. The reason for this is the excellent performance of ENDF/B-VII.0 for Pu fuelled fast cores, while the significant amount of ^{235}U in JOYO requires an adjustment (in particular for the capture, as it will be seen in the section VI on adjustment). On the contrary, organizations using JEFF-3.1 (CEA, and PSI) and JENDL-4 (JAEA) perform well for JOYO. CEA will take advantage of adjustment associated to the discrepancies in $k_{\rm eff}$ of JEZEBEL ^{239}Pu (and strangely enough not ^{240}Pu), FLATTOP but not for the softer cores (ZPR6-7, ZPPR-9). Exactly the contrary is true for JAEA (good agreement for harder cores, adjustment needed for softer cores). It is not clear why for PSI, that uses JEFF-3.1, the Pu fuelled cores seem not to need any adjustment.

- Spectral Indices – ^{238}U capture spectral indices have positive *EM* values for everybody (with exception of KAERI), and, therefore, it seems not to provide any contribution to the adjustment except as a constraint. For the fission spectral indices the situation is more complex. ^{238}U fission spectral indices require adjustments in harder cores practically for all participants, while JEFF-3.1 needs it also for softer cores. ^{239}Pu fission indices need adjustment in all cores. One exception is JAEA that has positive *EM* values for the ZPR6-7 and ZPPR-9 cores, indicating that the adjustment needed for the Pu fuelled softer cores $k_{\rm eff}$ do not concern the ^{239}Pu fission but some other reactions (or isotope). For ^{237}Np fission spectral indices the situation is mixed. These spectral indices are not important for the adjustment of ENDF/B-VII.0 users, while action is needed for CEA on both JEZEBEL and FLATTOP, and JAEA (but only for JEZEBEL). The fact that PSI has positive *EM* values for these indices indicate that probably is using a version of JEFF-3.1 with different ^{237}Np cross sections with respect to CEA.

- Sodium Void Reactivity Coefficients – ENDF/B-VII.0 does not benefit from these experiments, the main reason being the high uncertainties associated to the C/E's. JAEA will use the information from the experiment dominated by the central component, while CEA will also benefit from that dominated by the leakage component. There is no agreement on the *EM* values of CEA and PSI. This time the indication is that they are probably using different ^{23}Na cross sections.

Conversely to *EM* let's now define the Theoretical Adjustment Margin (*TAM*) where in Eq. (12) we suppress the $U_{C/E}$ term. This corresponds to the ideal situation where we have perfect measured experiment and perfect calculation tools with no error or uncertainty associated. Even though this is more an academic exercise, the negative *TAM* values can provide stronger recommendations for the quality of the covariance data. Again negative *TAM* will point out the inability of the covariance data to accommodate the adjustment, where now all the discrepancies have to be attributed to shortcomings in the nuclear data. Table X shows the *TAM* values for the solutions provided by the participants. As expected, there are more negative *TAM* values than *AM* ones. If one excludes the columns of KAERI and ORNL (very low or zero U_{ND} values for the reasons previously indicated), it is quite striking that the rows for the ^{239}Pu fission spectral indices have practically all negative *TAM* values. This indicates that all cross section files have overly optimistic uncertainties for ^{239}Pu fission cross sections.

Another good reason for looking at *TAM* values is the following consideration: if the method uncertainty is very large, the *AM* and χ, quoted above, would suggest that an experiment is still useful for the adjustment, despite the fact that the use of better methods (*e.g.*, with fewer approximations) would make clear that the specific experiment is not useful. In other words, why should one compensate weaknesses of the calculation methods with cross section modifications? This was an early criticism to any statistical adjustment method.

One should simply remember that the method uncertainty reduction is a necessary condition in order to provide unambiguous indications on the integral experiment selection. This is also consistent with the fact that in most cases what we call "method uncertainty" is in fact more a systematic uncertainty or even a bias, with rather limited "statistical" meaning. This is especially true when deterministic methods are used in the experiment analysis. When stochastic methods are used the uncertainty is more statistical in nature, provided that the Monte Carlo code employed in the analysis has no errors or computational approximations (such as the treatment of unresolved resonances in early versions of MCNP4).

VI. ANALYSIS OF THE ADJUSTMENTS

In this section the results of the adjustments are discussed. First the so-called Phase I (*i.e.*, all participants use their own initial cross sections, own nuclear data covariance, with integral experiment and method correla-

TABLE IX. Experiment Merit (EM) values expressed in %.

Core	Parameter	ANL	CEA	INL	IRSN	JAEA	JSI	KAERI	ORNL	PSI
JEZEBEL239	k_{eff}	0.187	0.013	0.187	0.173	0.072	0.109	-0.096	0.199	0.165
JEZEBEL239	F28/F25	-0.930	1.074	-0.933	-	-1.795	-	-0.530	-1.132	-0.305
JEZEBEL239	F49/F25	-1.585	-0.012	-1.584	-	-0.496	-	-1.119	-1.670	-0.193
JEZEBEL239	F37/F25	0.113	-0.626	0.115	-	-0.491	-	-1.280	0.156	1.707
JEZEBEL240	k_{eff}	0.182	-0.055	0.182	0.186	0.042	-0.035	-0.067	0.121	-0.149
FLATTOP-PU	k_{eff}	0.203	0.280	0.205	0.204	0.162	0.188	-0.644	0.045	0.245
FLATTOP-PU	F28/F25	0.049	0.066	0.048	-	-0.939	-	-0.178	-1.930	0.100
FLATTOP-PU	F37/F25	0.986	-0.133	0.990	-	0.805	-	-0.069	0.411	1.023
ZPR6-7	k_{eff}	0.190	-0.040	0.187	0.035	-0.296	0.042	0.139	-	0.106
ZPR6-7	F28/F25	3.053	-2.107	3.051	-	0.493	-	1.817	-	2.721
ZPR6-7	F49/F25	-1.237	-0.752	-1.232	-	0.396	-	0.780	-	-1.918
ZPR6-7	C28/F25	1.710	1.955	1.713	-	1.050	-	0.013	-	2.133
ZPR6-7 240	k_{eff}	0.161	-0.001	0.158	0.143	-0.107	0.049	0.217	-	0.150
ZPPR-9	k_{eff}	0.040	0.112	0.039	0.021	-0.091	-0.226	-0.016	-	0.149
ZPPR-9	F28/F25	-0.070	-0.964	-0.071	-	1.664	-	1.752	-	-1.225
ZPPR-9	F49/F25	0.163	-0.417	0.161	-	2.257	-	0.869	-	-0.244
ZPPR-9	C28/F25	1.075	1.566	1.071	-	0.509	-	-0.686	-	1.775
ZPPR-9	Na Void Step 3	5.850	-1.501	5.853	-	-0.792	-	-2.685	-	1.421
ZPPR-9	Na Void Step 5	4.791	-1.226	4.789	-	0.341	-	-5.078	-	1.374
JOYO MK-I	k_{eff}	-0.068	0.097	-0.074	-0.013	0.002	-	-0.324	-	0.150

TABLE X. Theoretical Adjustment Margin (TAM) values expressed in %.

Core	Parameter	ANL	CEA	INL	IRSN	JAEA	JSI	KAERI	ORNL	PSI
JEZEBEL239	k_{eff}	0.626	1.885	0.622	0.560	0.562	0.567	-0.179	1.185	0.453
JEZEBEL239	F28/F25	1.369	7.317	1.342	-	-0.043	-	-	1.079	0.635
JEZEBEL239	F49/F25	-1.704	1.399	-1.710	-	-1.042	-	-	-1.761	-0.820
JEZEBEL239	F37/F25	1.071	-0.043	1.037	-	-0.599	-	-	5.960	1.591
JEZEBEL240	k_{eff}	0.641	1.508	0.637	0.502	0.489	0.398	-0.144	0.903	0.207
FLATTOP-PU	k_{eff}	0.660	1.893	0.667	0.407	1.116	0.462	-0.821	0.873	0.759
FLATTOP-PU	F28/F25	1.309	6.850	1.281	-	0.613	-	-	-0.414	0.562
FLATTOP-PU	F37/F25	1.604	0.050	1.592	-	0.688	-	-	6.087	0.724
ZPR6-7	k_{eff}	0.930	1.315	0.925	0.757	0.289	0.755	0.223	-	0.828
ZPR6-7	F28/F25	5.954	5.752	5.947	-	1.568	-	-	-	5.958
ZPR6-7	F49/F25	-2.921	-1.374	-2.920	-	-0.998	-	-	-	-3.411
ZPR6-7	C28/F25	0.537	3.471	0.542	-	0.361	-	-	-	1.026
ZPR6-7 240	k_{eff}	0.910	1.339	0.908	0.871	0.483	0.777	0.308	-	0.882
ZPPR-9	k_{eff}	1.100	1.661	1.113	1.069	0.692	0.840	0.251	-	1.198
ZPPR-9	F28/F25	4.865	7.024	4.909	-	3.526	-	-	-	3.637
ZPPR-9	F49/F25	-1.086	-0.030	-1.088	-	1.072	-	-	-	-1.634
ZPPR-9	C28/F25	0.632	3.560	0.624	-	0.185	-	-	-	1.149
ZPPR-9	Na Void Step 3	5.783	3.095	5.679	-	-0.434	-	-	-	4.424
ZPPR-9	Na Void Step 5	7.168	5.417	6.925	-	2.341	-	-	-	6.398
JOYO MK-I	k_{eff}	0.641	1.333	0.608	0.648	0.402	-	-0.156	-	0.823

tion) results are investigated with focus on specific cases of interest. A typical result of Phase II (*i.e.*, use of own initial cross sections, but a different nuclear data covariance matrix) is then discussed. The impact of adjustments and of a posteriori correlations (Phase III) is successively analyzed.

Finally, the results of some "stress tests" performed in order to verify the robustness of the adjustment procedures, are also reported.

A. Use of Different Nuclear Data and Associated Covariances (Phase I)

1. General comments

A few general comments can be made.

In most results, no incoherent trends are found when compared to initial uncertainties. Fig. 16 illustrates this major effect for some typical examples.

One other important point is that variances are not that much reduced between prior and posterior cross sections uncertainties (except for CEA where initial uncer-

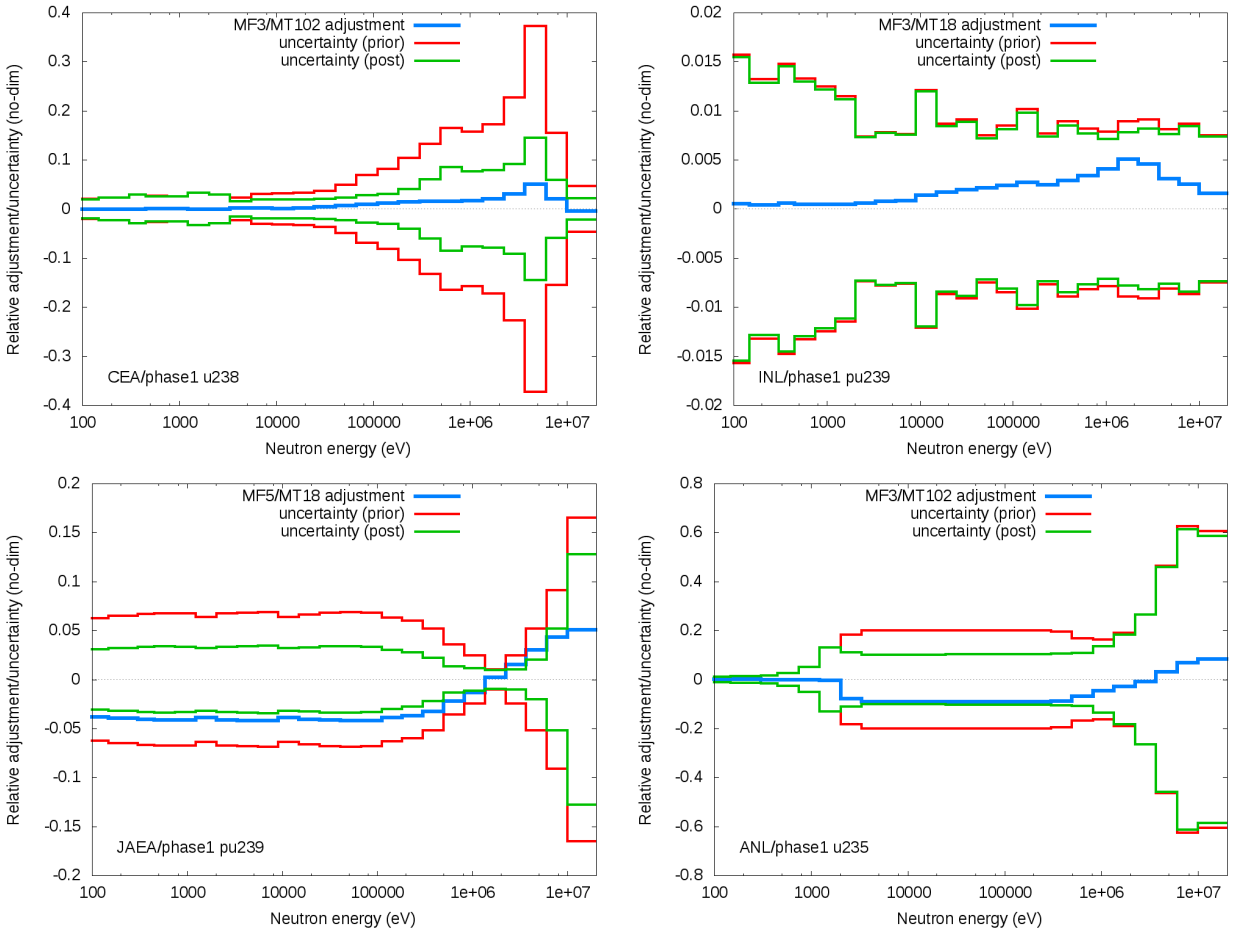

FIG. 16. Example of adjustment trends for major isotopes. The results are consistent with a priori and a posteriori uncertainties.

tainties for some isotopes may be found pessimistic and some minor cross sections). It means that the final overall uncertainty reductions on benchmarks calculation or concept calculation are mainly due to correlations created by the adjustment. This point will be investigated in the next paragraph.

A final additional general comment on these results is the fact, that it appears that only a few (∼5) initial isotopes are involved in the adjustment procedure. ^{58}Ni, ^{52}Cr, ^{10}B do not contribute to the data adjustment.

2. *Specific adjustment analysis*

A first investigation of the adjustment results for some selected data as obtained by JAEA (using their own nuclear data and covariance data set J-4.0), INL (using their own nuclear data and covariance data set COMMARA-2.0) and CEA (using their own nuclear data and covariance data set COMAC) is given below:

(a) ^{239}Pu capture (Figs. 17–19)

- In the energy range ∼3-500 keV the uncertainties in the three covariance data sets (J-4.0, COMAC, COMMARA-2.0) are rather similar and the uncertainty is in the range ∼6-9% to 7-12%. As for the adjustments, they are consistently indicating an increase of the capture cross section by ∼1-2% up to a maximum of ∼10%.
- In the range ∼5-50 keV, the suggested increase of the capture cross sections in the three files are such that even the adjusted data look very consistent and still close to each other as before adjustment.

(b) ^{239}Pu inelastic scattering cross section and prompt fission neutron spectrum (Fig. 20).

- ^{239}Pu(n,n') is an important reaction (*i.e.*, large sensitivities) when ^{239}Pu is a major component of the core (*e.g.*, JEZEBEL and FLATTOP), in particular for k_{eff} and F28/F25.
- In general, some decrease of (n,n') is suggested for each file. For example, this trend allows to get a better agreement with F28/F25, which is underestimated for both JEZEBEL and FLATTOP by all groups, since negative sensitivity coefficients for the F28/F25 parameter to variations of the ^{239}Pu(n,n')

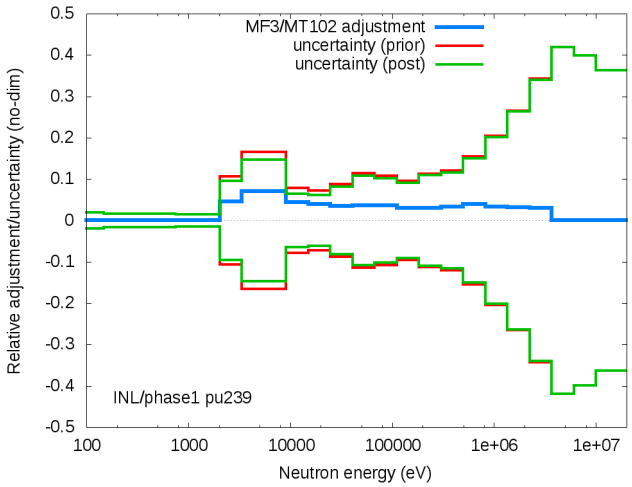

FIG. 17. INL ^{239}Pu neutron capture adjustments.

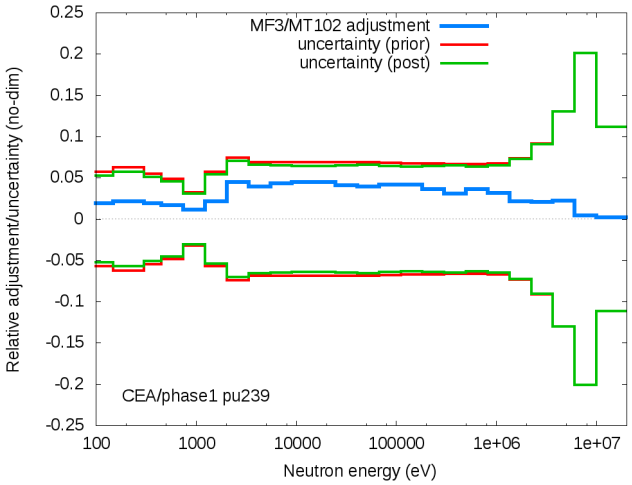

FIG. 18. CEA ^{239}Pu neutron capture adjustments.

are calculated as expected (even if not in perfect agreement) by all groups.

- However, the changes of the inelastic cross section are the highest for INL and the lowest for CEA.

Even if after adjustment a rather better agreement is found among the three data sets, a good understanding of the trends is obtained only if the ^{239}Pu inelastic cross section adjustments are considered together with the prompt fission neutron spectrum adjustments. In fact, only JAEA and CEA results show significant adjustments for that parameter while INL and ANL show very small adjustments. The lower adjustment (decrease) of (n,n') in the JAEA and CEA results is partly compensated by the decrease of the energy fission spectrum below ∼3.5 MeV suggested both in the JAEA and in the CEA results. When a smaller decrease of the inelastic cross section is suggested, this is associated with a higher reduction of the prompt fission neutron spectrum

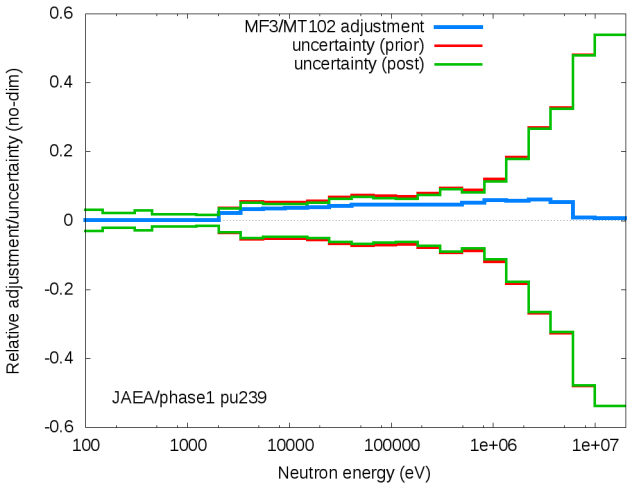

FIG. 19. JAEA ^{239}Pu neutron capture adjustments.

(see CEA with respect to JAEA adjustments of the two parameters). In fact a lower inelastic cross section at high energy allows fewer neutrons below, *e.g.* 1-2 MeV, and the same effect is produced by a lower amount of prompt fission neutrons in that energy range. In other words, since both adjustments of the JAEA and CEA results (*i.e.*, decrease of (n,n') and harder fission spectrum) consistently harden the neutron spectrum and help to improve the C/E of F28/F25 in FLATTOP and JEZEBEL, in the INL adjustment a larger (n,n') decrease is needed since a smaller decrease (JAEA and CEA) is "compensated" by the fission spectrum hardening. In summary, the net result is better C/E values (*i.e.*, closer to 1) for the FLATTOP and JEZEBEL F28/F25 (and F37/F25) with the three adjustments (JAEA, CEA and INL). Finally, the suggested change of the prompt neutron fission spectrum both in the JAEA and in the CEA cases, are very consistent.

(c) ^{238}U inelastic scattering and fission cross sections (Figs. 21–23).

- The uncertainty values for the inelastic scattering cross section in the three files are rather different in magnitude and energy trend. For example, in the range 1-20 MeV the COMMARA-2.0 uncertainties are 2-3 times higher than in the J-4.0 (and in the CEA-COMAC) covariance dataset. Below ∼1 MeV that trend is inversed between the two files.

- The ^{238}U inelastic cross section adjustments of the present benchmark are in any case rather small and often much smaller than the uncertainties, and the a posteriori cross sections are only marginally more consistent than the a priori values. Anyway CEA and INL/ANL exhibit the need to reduce this reaction.

- For CEA, there is an adjustment of the fission cross section of ^{238}U (a slight decrease of ∼1% in the en-

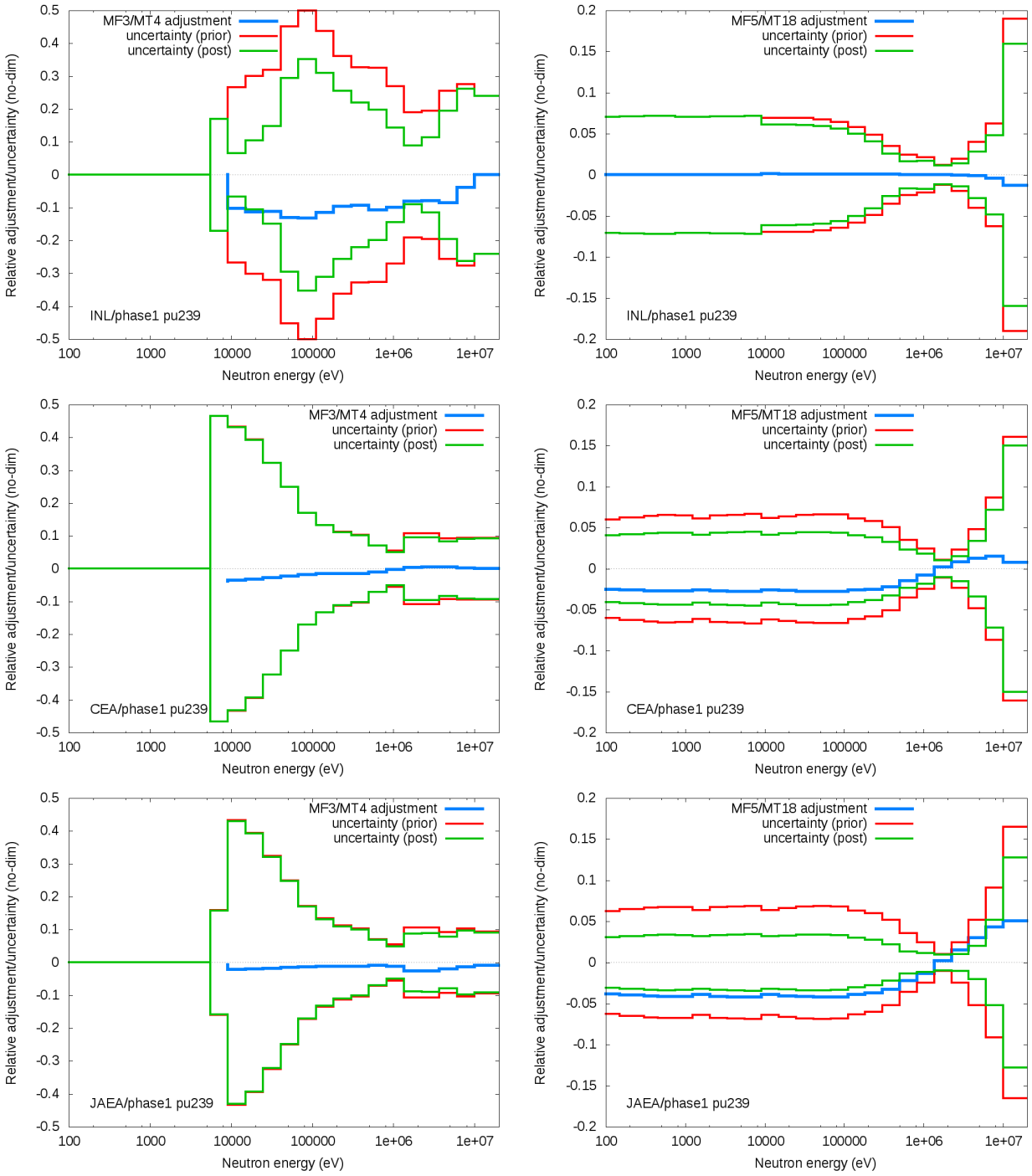

FIG. 20. ^{239}Pu(n,n') cross section and prompt fission spectrum adjustments.

ergy range ∼400 keV - 1 MeV), while the INL adjustment shows a slight decrease of $\bar{\nu}$. CEA variance is too pessimistic and INL/CEA difference outside the scope INL/CEA relative difference.

(d) ^{235}U capture (Fig. 24).

The uncertainty values on this parameter are significantly different among the different covariance data files (see section III C).

The larger uncertainties in COMMARA-2.0 (and in CEA covariance data) allow a significant decrease of the cross section, essentially to improve the k_{eff} under prediction of INL. Finally, the JAEA adjustment is a decrease of the capture cross section only at very high energy where the J-4.0 uncertainties are higher. Elsewhere, the low uncertainty data in J-4.0 do not allow any significant decrease of the ^{235}U capture data.

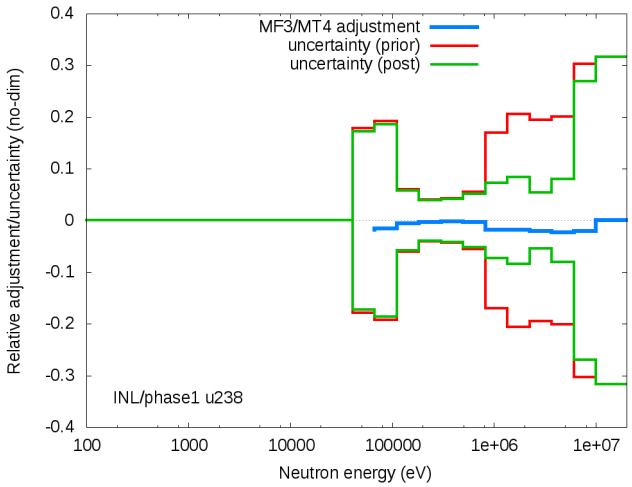

FIG. 21. INL ^{238}U inelastic scattering cross section adjustments.

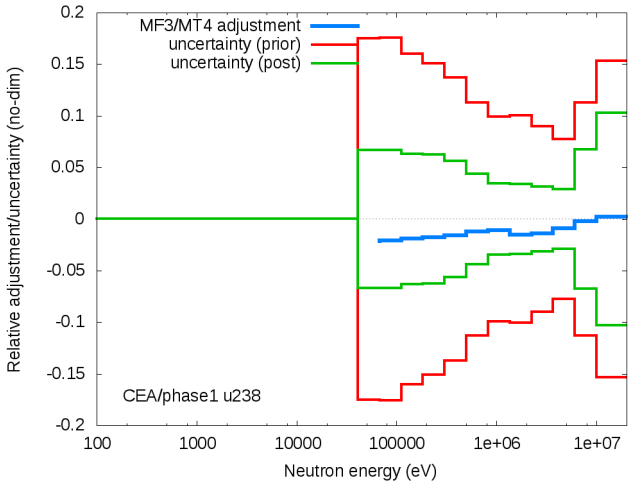

FIG. 22. CEA ^{238}U inelastic scattering cross section adjustments.

It is worth noting that most teams (INL/ANL, CEA, IRSN and JAEA) point out the necessity of decreasing the ^{235}U capture cross section. An equivalent conclusion was given by WPEC Subgroup 29.

(e) For other data, *e.g.* ^{23}Na inelastic and elastic, ^{56}Fe inelastic scattering cross sections, the adjustments are rather small and it is rather difficult to extract clear common trends.

In summary, the analysis of these examples suggests that:

- Adjustment should include all significant parameters in order to provide meaningful indication (see case of inelastic scattering and prompt fission spectrum of ^{239}Pu), and a wide range of integral experiments with different sensitivity profiles.

- Very different covariance data give rise to different adjustments (case of ^{238}U(n,n') and ^{235}U capture). This point reinforces the need to produce very reliable covariance data and to understand the impact of very small variance data and of correlations (in energy, among reactions, *etc.*).

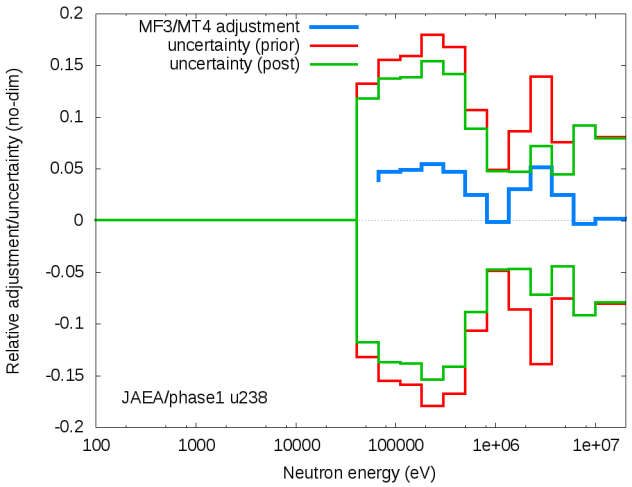

FIG. 23. JAEA ^{238}U inelastic scattering cross section adjustments.

B. Impact of Replacing Covariance Data on the Adjustment (Phase II).

In principle, the central cross section values and the corresponding covariance data of a library must be consistent. However, here we intentionally replace the covariance data used in the adjustment procedure, though we use the same values of other adjustment parameters, especially the C/E values which completely depend on the central cross sections, to analyze the pure effects of the different covariance data to the adjusted results. Two adjustment cases are surveyed as follows:

- Case J (Phase I): This is the reference adjustment case. Cross sections and covariance data are both based on the JENDL-4.0 library (J-4.0, Refs. 19-20).

- Case B (Phase II): The covariance data are taken from C-2.0 and no J-4.0 covariance data are supplemented. The other adjustment parameters are identical with Case J.

To investigate the effect of different covariance data, the cases of criticality and the sodium void reactivity have been investigated. Here we will focus on the case of criticality ($k_{\rm eff}$).

Fig. 25 compares the $k_{\rm eff}$ C/E changes of the two cases due to the adjustment. It is found that the adjusted C/E values of the two cases are almost identical for $k_{\rm eff}$ of small through large cores. In detail, however, there are

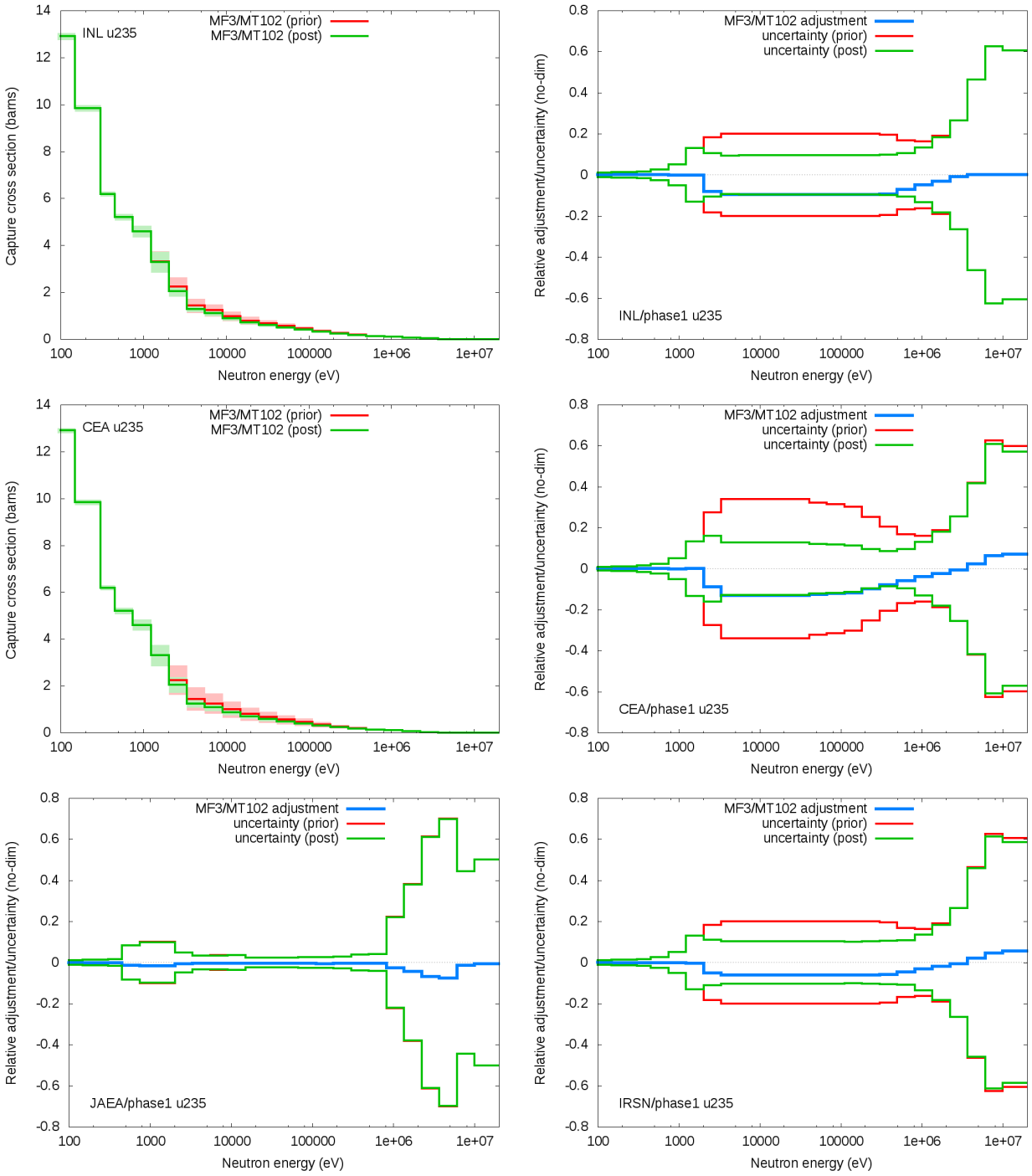

FIG. 24. Adjustment of ^{235}U neutron capture cross section obtained by INL (top), CEA (middle), JAEA and IRSN (bottom).

some differences between Case J and Case B for the k_{eff} of the JOYO Mk-I core which contains the ^{235}U fuel as well as plutonium, while the other cores do not include ^{235}U in fuel. The use of C-2.0 shows better improvement of JOYO C/E values than J-4.0.

The contribution of ^{235}U capture cross section adjustment in case B (Phase II) is significantly different by ∼400 pcm between the J-4.0 and C-2.0 covariance data, while those of ^{23}Na and ^{56}Fe elastic scattering are smaller (∼70 pcm each) but opposite in sign. The overall k_{eff} correction is of the order of ∼200 pcm and makes the C/E agreement much better.

As for the most important contribution, *i.e.*, ^{235}U capture, the difference of STDs between C-2.0 and J-4.0 significantly affected the changing rate of the cross section. The small STD of J-4.0 must constrain the alteration of

the cross section by the adjustment. The large STD of C-2.0 allows the large changing rate of the ^{235}U capture cross sections to improve the C/E value of JOYO k_{eff} by the adjustment.

One can see in Fig. 25 that the initial a priori covariance *does not seem to influence the final C/E values* as well as their uncertainties.

This final point is due to the form of generalized least square equations. Let us remind the form of the equation for a posteriori covariances

$$M'_\sigma = M_\sigma - M_\sigma S^t \left(M_E + S M_\sigma S^t\right)^{-1} S M_\sigma. \quad (14)$$

If $SM_\sigma S^t >> M_E = V_e + V_m$, then the posterior uncertainties on experiments due to the new cross section data, $SM'_\sigma S^t$, is almost equal to M_E. V_e stands for integral experiments covariances and V_m for modeling covariances.

C. Effect of Uncertainties and Correlations (prior/posterior) on "Target System" Uncertainties (Phase III)

In order to investigate the impact of adjustments and in particular of a posteriori correlations, two "Target Systems" have been defined on which the effect of the adjustment is tested. This corresponds to what is expected to be done in practice: one wants to verify the impact of an adjustment in terms of reduction of uncertainties. Two target systems have been defined: the JAEA Fast Breeder Reactor (FBR) defined in Ref [40] and the ANL Advanced Burner Reactor (ABR), described in Ref. [41]. For this last system, a metal and oxide core fuel versions have been considered, and for the oxide core, also a recycled fuel core version has been considered.

We evaluated the impact of correlations before and after adjustment on the target systems k_{eff} uncertainties. Only the COMAC-V0 covariance matrices were used. The following uncertainty propagation calculations were performed:

- Case 1: Full prior/posterior covariance matrix.
- Case 2: Remove, from previous case, correlations between different isotopes (*e.g.*, no correlation between ^{235}U and ^{238}U).
- Case 3: Remove, from previous case, correlations on reactions for each isotopes (*e.g.*, inelastic and elastic scattering for ^{238}U).
- Case 4: Keep only variances.

The results are shown in Table XI.

For all target systems, the uncertainty using prior and posterior covariance matrices converge to rather similar values when correlations are deleted. Moreover, one can see that:

TABLE XI. Impact of correlations on the k_{eff} uncertainty of the "Target Systems."

ABR Oxide	Prior covariances	Posterior covariances
Case 1	1550 pcm	170 pcm
Case 2	1550 pcm	510 pcm
Case 3	1720 pcm	680 pcm
Case 4	1200 pcm	820 pcm
JAEA FBR	Prior covariances	Posterior covariances
Case 1	1310 pcm	220 pcm
Case 2	1310 pcm	490 pcm
Case 3	1560 pcm	610 pcm
Case 4	1170 pcm	900 pcm
ABR Metal	Prior covariances	Posterior covariances
Case 1	1740 pcm	250 pcm
Case 2	1740 pcm	560 pcm
Case 3	2020 pcm	730 pcm
Case 4	1290 pcm	850 pcm
ABR Oxide Recycled	Prior covariances	Posterior covariances
Case 1	1250 pcm	260 pcm
Case 2	1250 pcm	490 pcm
Case 3	1400 pcm	590 pcm
Case 4	1080 pcm	820 pcm

- Correlations among isotopes (after adjustment) are important and contribute to the uncertainty reduction by a factor 2-3 in terms of target system uncertainties.
- Correlations among reactions for each isotope are significant, as well as correlation between energy groups for each reaction.
- As for the prior covariance matrix, taking into account cross-correlations (between reactions and energy groups) tends to give an overall uncertainty of the same order of magnitude (Case 4 → Case 1), except for ABR Metal core. But, the effect of energy correlations is an increase of the uncertainty (Case 4 → Case 3) and the effect of constraint on reactions tends to lower this uncertainty (Case 3 → Case 2 = Case 1).
- As for the posterior covariance matrix, the introduction of correlations gives always a reduction of uncertainty Case 4 → Case 3 → Case 2 → Case 1.

More results related to the impact of the adjustments on the "Target Systems" can be found in [24]. These results do confirm the trends and the conclusions given above.

D. Calculation of Cook Distance: Influence of Experiments

If the adjustment is done by discarding a chosen integral data point I, the results (adjusted cross sections) are noted: $\{\sigma_p^I\}$. The original adjustment is noted $\{\sigma_p\}$.

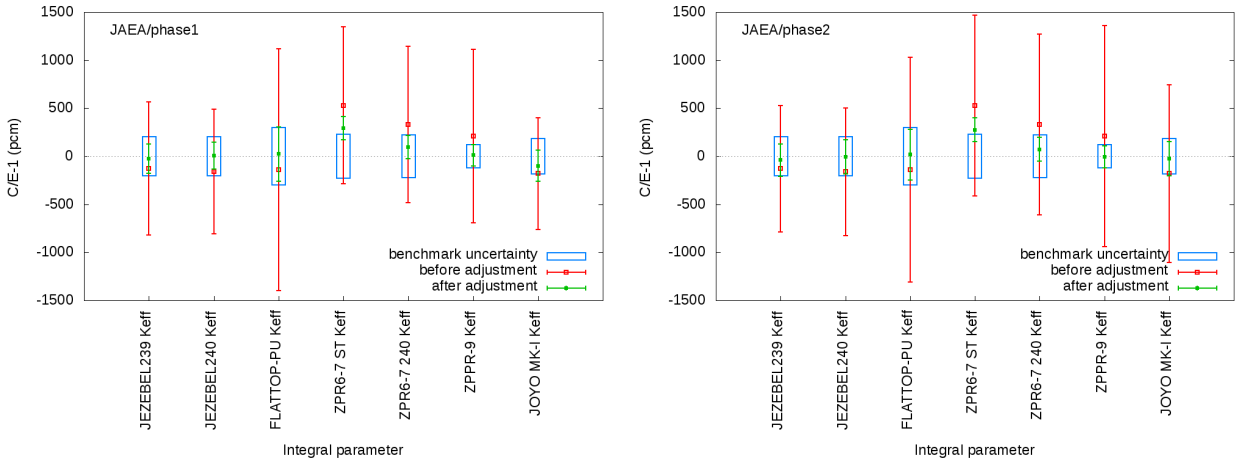

FIG. 25. Modifications of C/E of k_{eff} values due to adjustment.

The Cook distance is calculated using

$$D_I = \left(\sigma_p^I - \sigma_p\right)^t \left(M'_\sigma\right)^{-1} \left(\sigma_p^I - \sigma_p\right). \tag{15}$$

Low values of D shows a negligible impact of the remote data points. High values of D indicate very influential experiments. This last point may be due to very low experimental uncertainties as well as very important influence on final multigroup cross sections.

The calculation of Cook distance was carried out using COMAC-V0 covariances. The results (blue bars) can be seen on Fig. 26. The influence of each experiment is detailed by type:

- k_{eff}: JOYO is an important experiment in the adjustment for two reasons: all isotopes have an impact on the reactivity of the core (^{235}U + ^{239}Pu fuel) and the experimental uncertainty is rather small (180 pcm). If we change manually this specific uncertainty, from 180 pcm to 500 pcm, we obtain the red bars on Fig. 26, where the weight of JOYO is reduced by almost a factor 10 ; Jezebel ^{240}Pu and ^{239}Pu are the second and third experiments with the most leverage mostly because of the low experimental uncertainty; Flattop is 4 times less important than Jezebel ^{239}Pu because of its large experimental uncertainty (300 pcm instead of 200 pcm); ZPPR-9 has the same influence as Jezebel ^{239}Pu, thanks to its very small experimental uncertainty (118 pcm); ZPR6-7 and ZPR6-7 High ^{240}Pu content have a negligible impact, in comparison with ZPPR-9, mostly due to their experimental uncertainties (∼230 pcm).

- Sodium void reactivity: these experiments seem to be important (the same order of magnitude with Jezebel ^{240}Pu and JOYO). Structural material such as ^{23}Na and ^{56}Fe are more sensitive to this kind of experiment than to multiplication factor, which can explain the weight of sodium void in the adjustment. Also, the experimental uncertainties for ZPPR-9 Step 3 and Step 5 are quite low.

- Reaction rate ratios: for all cases, this type of integral experiment has a very limited impact in the adjustment because the sensitivities are mostly focused on only two reactions in the whole set of cross section parameters.

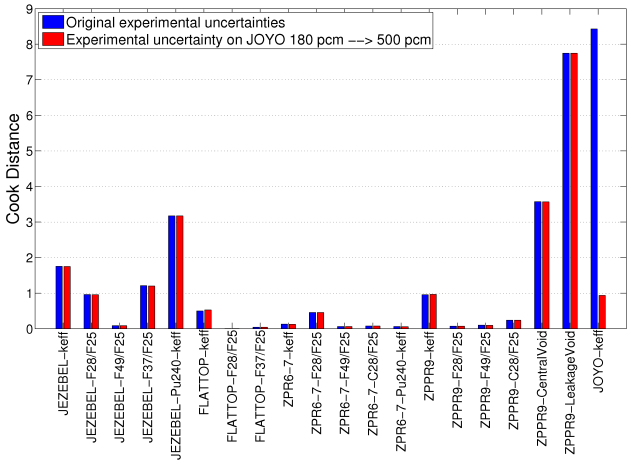

FIG. 26. Cook distance of experiments. The largest distances indicate the most influential integral parameters.

E. Stress Tests on the Adjustments

1. *Stress test specification*

In the previous paragraphs we have described the cross section adjustment exercise based on the selected 20 fast reactor experiment benchmarks as the reference case. As

seen in the previous discussion, the adjusted results of the reference case are quite satisfactory from both viewpoints of the integral and differential data. The objective of this section is to study the impact on the adjusted results when an integral experiment with different nature from the standard 20 experiments set is added to the reference case. This exercise was characterized as the "Stress test", *i.e.*, one specific integral experiment was added with a C/E value very different from 1 to 20 reference integral experiments, to find what would be the feedback on the adjusted results.

A larger number of cases are described in detail in Ref. [24], however here we will summarize only a typical result.

In particular, the following two adjustment cases have been analyzed:

1) Case J4: This is the reference adjustment case with the standard 20 integral data. Cross sections and covariance data are based on the JENDL-4.0 library (Refs.19-20).

2) "Stress test": One integral experiment, *i.e.*, the k_{eff} of the ZPR-9/34 core [39], is added to the reference Case J4. The unique features of the ZPR-9/34 core are:

- the core region consists of 93% enriched-uranium and iron,
- the height and diameter of the core are 1.8m and 1.2m, respectively,
- the core is surrounded by stainless steel reflector.

The experimental k_{eff} value and associated uncertainty of the stress test experiment is based on the ICSBEP handbook [8]. The k_{eff} value is calculated by a continuous-energy Monte Carlo code with two-dimensional homogenized (r,z) benchmark models, and applied with the corrective factors between the simplified RZ model and the as-built three-dimensional heterogeneous model which are supplied in the ICSBEP handbook. The modeling uncertainty is based on the uncertainty estimation associated with the "Monte Carlo transformation of model" correction factors to convert the simplified (r,z) model values to the as-built model which is also supplied in the ICSBEP handbook [8]. The Monte Carlo statistical uncertainties of the simplified (r,z) model calculation are also added to the modeling uncertainties, though they are negligible compared with the model transformation uncertainties.

2. Results of the stress test

As for the initial results, it is interesting to note that the k_{eff} value of ZPR-9/34 is overestimated by +1420 pcm; on the other hand, k_{eff} values of six cores treated in Case J4, numbers 1, 5, 6, 9, 13 and 20, are within only ±530 pcm. The objective of the "Stress test" is to verify whether the adjustment operation could manage the C/E value of ZPR-9/34 very different from 1 without harmful influence to other integral data and/or cross sections adjustment performances.

The C/E value changes for all integral data in Case J4 and "Stress test" are summarized in Tables XII and XIII. The "Stress test" does not seem to give any critical harm to the standard 20 integral data of Case J4. In fact in the "Stress test" case, the adjusted results are practically as good as in Case J4. Even the C/E value of the extra ZPR-9/34 k_{eff} which is newly added to the adjustment, changes to almost 1.00.

In both cases the χ^2 test gives an excellent indication of reliability of the adjustment (0.53 and 0.63, respectively). Moreover, the analysis of the impact of newly added experiment can be analyzed in terms of Eqs. (12) and (13). As for the diagnostics using Eq. (13), the values associated to each experiment in the case of JAEA, here chosen as example, are given in the last column of Tables XII and XIII. The ZPR-9/34 k_{eff} experiment shows an acceptable value (*i.e.*, $\chi = 1.21$ which is below 3 sigma). If we use the parameters defined in section V and based on Eq. (12), one obtains for the adjustment margin, $AM = -0.005$, the experiment merit, $EM = -1.16$, and the theoretical adjustment margin, $TAM = -0.17$. These values can be interpreted as follows: the new experiment will marginally contribute to the overall adjustment (*i.e.*, $AM \sim 0$); however there is merit in the newly added information ($EM < 0$); but the negative value of TAM indicates that nuclear data, important for that specific experiment, have associated uncertainties that are probably underestimated.

Finally, it is needed to confirm that the adjustment gives no harm not only in terms of integral data a posteriori values, but also in terms of differential cross sections. For this purpose, the nuclide- and reaction-wise contributions to the total k_{eff} modifications were investigated, comparing the cases with and without stress test

In the "Stress test" case, it is found that the large improvement of the C/E value, approximately -1300 pcm, is attained by the cross section changes of ^{56}Fe capture and elastic scattering reactions, which are considered to result in the negative reactivity of the absorption effect by the iron in the core region, and the neutron leakage enhancement by the stainless steel reflector. These two cross section adjustments are responsible for ∼700 and ∼600 pcm, respectively

Fig. 27 shows the cross section modifications for the ^{56}Fe capture reaction. In the reference Case J4, there are small changes of the cross sections. However, quite large cross section alterations occur in the "Stress test". The order of magnitude is +11% below 100 keV, which is very close to the STD value, ±10%. Changes of this magnitude might be close to or exceed the limitation of allowance from the viewpoint of the nuclear data evaluation.

Fig. 28 illustrates the changes of the ^{56}Fe elastic scattering cross sections. In the Case J4, there are small alterations. On the other hand, in the "Stress test", the ^{56}Fe elastic cross sections are decreased to adjust k_{eff} val-

TABLE XII. Results of the adjustment based on JENDL-4.0 (Case J4: Standard 20 integral data) – reduced $\chi^2 = 0.53$.

No.	Core	Integral parameter	C/E Value		Integral parameter uncertainty (%)		Nuclear-data-induced uncertainty (%)		Ratio of $\lvert C/E-1\rvert$ to prior total uncertainty[a]
			Before	After	Experiment ($\sqrt{V_e}$)	Modeling ($\sqrt{V_m}$)	Before ($\sqrt{SM_\sigma S^t}$)	After ($\sqrt{SM'_\sigma S^t}$)	
1	JEZEBEL239	$k_{\rm eff}$	0.9987	0.9997	0.20	0.03	0.69	0.15	0.18
2	JEZEBEL239	F28/F25	0.969	0.990	1.1	0.94	3.20	1.02	0.89
3	JEZEBEL239	F49/F25	0.984	0.987	0.9	0.75	0.63	0.47	1.23
4	JEZEBEL239	F37/F25	0.979	0.989	1.4	0.80	1.50	0.67	0.93
5	JEZEBEL240	$k_{\rm eff}$	0.9984	1.0001	0.20	0.03	0.65	0.14	0.24
6	FLATTOP-PU	$k_{\rm eff}$	0.9986	1.0002	0.30	0.03	1.26	0.28	0.11
7	FLATTOP-PU	F28/F25	0.977	0.998	1.1	0.84	2.94	0.97	0.70
8	FLATTOP-PU	F37/F25	0.993	1.001	1.4	0.69	1.44	0.72	0.35
9	ZPR6-7	$k_{\rm eff}$	1.0053	1.0029	0.23	0.03	0.82	0.12	0.62
10	ZPR6-7	F28/F25	1.034	1.029	3.0	2.24	4.82	1.85	0.55
11	ZPR6-7	F49/F25	0.979	0.976	2.1	1.43	1.15	0.83	0.75
12	ZPR6-7	C28/F25	1.017	1.011	2.4	1.22	2.00	1.12	0.50
13	ZPR6-7 240	$k_{\rm eff}$	1.0033	1.0010	0.22	0.03	0.81	0.12	0.39
14	ZPPR-9	$k_{\rm eff}$	1.0021	1.0001	0.117	0.02	0.90	0.11	0.23
15	ZPPR-9	F28/F25	0.983	0.977	2.7	2.09	5.28	2.02	0.27
16	ZPPR-9	F49/F25	0.999	0.996	2.0	1.21	1.15	0.83	0.03
17	ZPPR-9	C28/F25	1.019	1.013	1.9	1.39	2.03	1.12	0.60
18	ZPPR-9	Na Void Step 3	1.068	1.038	1.9	5.26	5.95	3.32	0.84
19	ZPPR-9	Na Void Step 5	1.052	1.014	1.9	4.96	7.31	4.04	0.58
20	JOYO MK-I	$k_{\rm eff}$	0.9982	0.9990	0.18	0.03	0.58	0.16	0.29

[a] Ratio of $|C/E-1|$ to prior total-uncertainty: $|C/E-1|/\sqrt{SM_\sigma S^t + V_e + V_m}$.

ues of the stainless steel or iron reflector core of ZPR-9/34. These cross section changes are quite large, but still within the STD values, which may be acceptable from the nuclear data viewpoint.

The fact that the required adjustments are so close to the STD values in the JAEA covariance matrix, can be associated to the negative, even if small value, of the *TAM* parameters, as discussed in the previous paragraph.

As far as the other cross sections, the stress test does not modify significantly the adjustment results obtained in the case J4. As an example, the adjustments of the ^{239}Pu capture cross sections are shown in Fig. 29. Both in Case J4 and in the "Stress test" case, the change is approximately +3-5%, which is within one standard deviation (STD) value of the JENDL-4.0 covariance, that is, ±6-9% in the dominant energy region.

In summary the example shown here and further stress tests reported in [24], tend to confirm the robustness of the adjustment procedures.

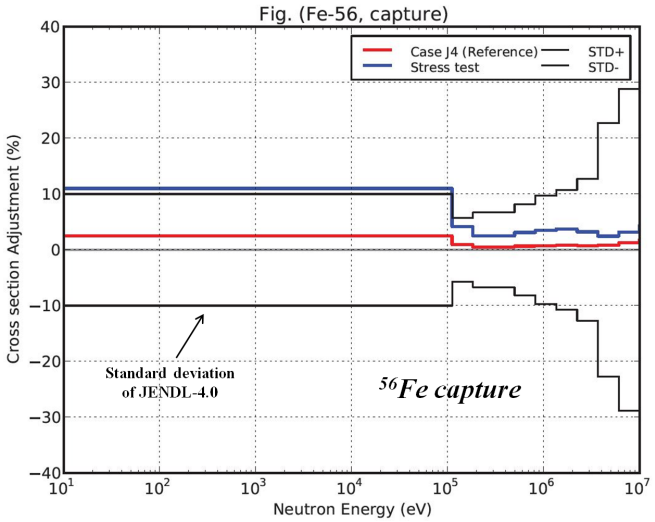

FIG. 27. Change of cross sections by adjustment: ^{56}Fe(n,γ).

F. Conclusion of Adjustment Results

This first analysis indicates that:

- Adjustment should include all significant parameters in order to provide meaningful indications (see case of inelastic scattering and chi of ^{239}Pu), and a wide range of integral experiments with different sensitivity profiles.
- Very different covariance data give rise to different adjustments (case of ^{238}U(n,n') and ^{235}U capture). This point reinforces the need to produce very reliable covariance data and to understand the impact of very small variance data and of correlations (in energy, among reactions, *etc.*).
- Initial C/E's are driving the path to adjustment in some cases (see example of CEA ^{238}U(n,n') trends depending on C/E's values in [24]).
- Experimental uncertainties have to be correctly

TABLE XIII. Results of the "stress test" adjustment with ZPR-9/34 added to the 20 integral data, (Case J4) – reduced $\chi^2 = 0.63$.

No.	Core	Integral parameter	C/E Value		Integral parameter uncertainty (%)		Nuclear-data-induced uncertainty (%)		Ratio of $\lvert C/E-1\rvert$ to prior total uncertainty[a]
			Before	After	Experiment ($\sqrt{V_e}$)	Modeling ($\sqrt{V_m}$)	Before ($\sqrt{SM_\sigma S^t}$)	After ($\sqrt{SM'_\sigma S^t}$)	
1	JEZEBEL239	$k_{\rm eff}$	0.9987	0.9997	0.20	0.03	0.69	0.15	0.18
2	JEZEBEL239	F28/F25	0.969	0.989	1.1	0.94	3.20	1.02	0.89
3	JEZEBEL239	F49/F25	0.984	0.987	0.9	0.75	0.63	0.47	1.23
4	JEZEBEL239	F37/F25	0.979	0.989	1.4	0.80	1.50	0.67	0.93
5	JEZEBEL240	$k_{\rm eff}$	0.9984	1.0000	0.20	0.03	0.65	0.14	0.24
6	FLATTOP-PU	$k_{\rm eff}$	0.9986	1.0007	0.30	0.03	1.26	0.28	0.11
7	FLATTOP-PU	F28/F25	0.977	0.997	1.1	0.84	2.94	0.97	0.70
8	FLATTOP-PU	F37/F25	0.993	1.001	1.4	0.69	1.44	0.72	0.35
9	ZPR6-7	$k_{\rm eff}$	1.0053	1.0028	0.23	0.03	0.82	0.12	0.62
10	ZPR6-7	F28/F25	1.034	1.033	3.0	2.24	4.82	1.84	0.55
11	ZPR6-7	F49/F25	0.979	0.979	2.1	1.43	1.15	0.81	0.75
12	ZPR6-7	C28/F25	1.017	1.011	2.4	1.22	2.00	1.12	0.50
13	ZPR6-7 240	$k_{\rm eff}$	1.0033	1.0009	0.22	0.03	0.81	0.12	0.39
14	ZPPR-9	$k_{\rm eff}$	1.0021	1.0002	0.117	0.02	0.90	0.11	0.23
15	ZPPR-9	F28/F25	0.983	0.979	2.7	2.09	5.28	2.01	0.27
16	ZPPR-9	F49/F25	0.999	0.999	2.0	1.21	1.15	0.82	0.03
17	ZPPR-9	C28/F25	1.019	1.013	1.9	1.39	2.03	1.12	0.60
18	ZPPR-9	Na Void Step 3	1.068	1.046	1.9	5.26	5.95	3.29	0.84
19	ZPPR-9	Na Void Step 5	1.052	1.019	1.9	4.96	7.31	4.03	0.58
20	JOYO MK-I	$k_{\rm eff}$	0.9982	0.9984	0.18	0.03	0.58	0.16	0.29
21	ZPR-9/34	$k_{\rm eff}$	1.0142	1.0012	0.11	0.24	1.15	0.25	1.21

[a] Ratio of $\lvert C/E-1\rvert$ to prior total-uncertainty: $\lvert C/E-1\rvert/\sqrt{SM_\sigma S^t + V_e + V_m}$.

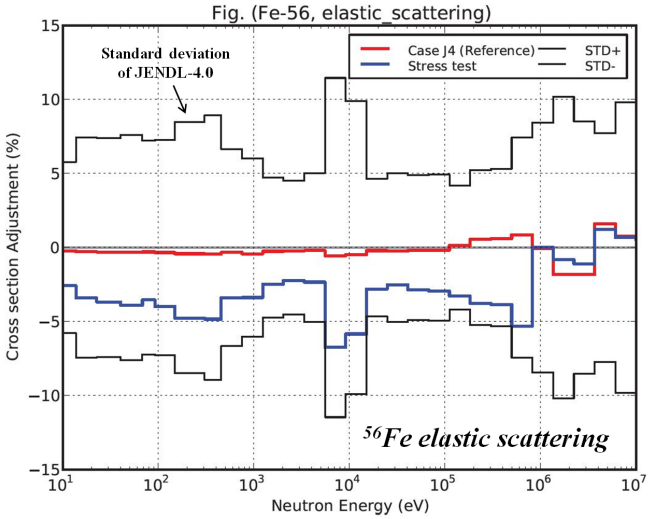

FIG. 28. Change of cross sections by adjustment: ^{56}Fe(n,n).

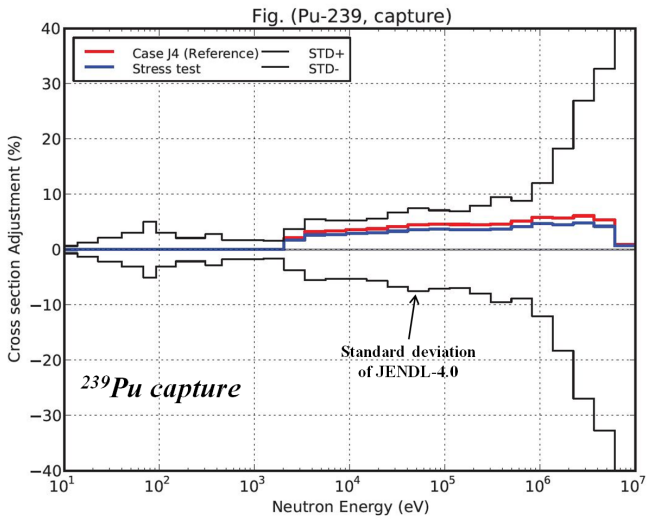

FIG. 29. Change of cross sections by adjustment: ^{239}Pu(n,γ).

quantified, because they drive the weight in the adjustment process (see Cook distance). In other words, a mis-estimated experimental uncertainty can lead to biased trends on cross sections and overestimation of the uncertainty reduction.

- Final calculated uncertainties on benchmarks do not seem to depend on chosen a priori cross section covariance; uncertainty reduction through integral experiment is driven by integral experiment uncertainties.

- A posteriori cross section covariances are only driven by the competition between a priori covariance matrix and initial experimental matrix with deterministic adjustments procedure.

VII. CONCLUSIONS

Subgroup 33 has succeeded in providing a deeper understanding of nuclear data adjustment methods and of their application.

The findings of the Subgroup 33 have pointed out that the statistical adjustments methodologies in use worldwide for different reactor analysis and design purposes are well understood and that they are essentially equivalent.

The results of the adjustments indicate, for some important data, common trends for modification even if starting from different basic nuclear data and different covariance matrices. The results obtained show also some degree of robustness in the sense that the observed trends can "survive" rather severe "stress tests".

In this respect, these methodologies can provide a powerful tool for nuclear data (and associated uncertainties) improvement if used in an appropriate manner. In fact, it has been indicated that the associated sensitivity analysis requires careful use of existing methods and that the choice of specific integral experiments of different types (critical masses but also reaction rates, reactivity coefficients and irradiation experiments) and sensitive to different energy neutron spectra, is of high relevance to avoid as much as possible compensating effects in the adjustments.

Finally, it has been pointed out the crucial role of the covariance data used, both those associated to the nuclear data and those associated to the integral experiments. The a posteriori correlations are mainly responsible for the uncertainty reduction of parameters of reference design systems. Their physics meaning and appropriate utilization will need further study.

The deeper understanding of the methodologies and of their applications implies that the role for cross section adjustment is more and more perceived as that of providing useful feedback to evaluators and differential measurement experimentalists in order to improve the knowledge of neutron cross sections to be used in a wider range of applications.

This new role for cross section adjustment requires tackling and solving a new series of issues: definition of criteria to assess the reliability and robustness of an adjustment; requisites to assure the quantitative validity of the covariance data; criteria to alert for inconsistency between differential and integral data; definition of consistent approaches to use both adjusted data and a posteriori covariance data to improve quantitatively nuclear data files; provide methods and define conditions to generalize the results of an adjustment in order to evaluate the "extrapolability" of the results of an adjustment to a different range of applications (*e.g.*, different reactor systems) for which the adjustment was not initially intended; suggest guidelines to enlarge the experimental data base in order to meet needs that were identified by the cross section adjustment.

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