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Report on INL Activities for Uncertainty Reduction Analysis of FY12

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SUMMARY

This report presents the status of activities performed at INL under the ARC Work Package on "Uncertainty Reduction Analyses" that has as a main goal the reduction of uncertainties associated with nuclear data on neutronic integral parameters of interest for the design of advanced fast reactors under consideration by the ARC (Advanced Reactor Concepts)program.

First, the theory behind the adjustment methodology is presented. New insights are introduced by proposing χ^2 filtering, a promising technique that can be adopted in the future for better exploiting the available amount of experimental results.

Then the adopted procedure for evaluating sensitivity coefficients, and selecting both experiments and nuclear data to be adjusted is illustrated. Among the achievement related to this step we list: new capabilities to calculate sensitivity coefficients for fission spectrum and anisotropic scattering (elastic and inelastic), evaluation of correlation for experimental and calculational uncertainties for a significant number of integral parameters, a complete data set of sensitivity coefficients for ~150 experiments, codes for retrieving sensitivity coefficients and edit the data set.

Finally the results of the adjustment using ENDF/B-VII.0 data files applied to a set of 87 selected experiments in conjunction with the COMMARA 2.0 covariance matrix in a 33 energy multigroup structure are presented. The adjustment is quite satisfactory; however, some problems are highlighted for the current estimate of cross section uncertainties. These problems are related not only to underestimation of minor isotopes (Pu-238, Am-241, and Cm-242), but also for major isotopes as U238 (fission, capture, and inelastic), Pu-239 (fission, capture, and (n,2n)), Fe-56 and Na-23. In order to obtain satisfying C/E, one needs to have significant changes of the central values of captures of Pu-238, Cm-242 and Cm-244, and for fission products Pd-105, Cs-133, Sm-151, and Eu-153. In terms of reduced uncertainties, U-235 capture, U-238 and Pu-239 inelastic, Np-237 fission, and captures of some fission products are the most promising for having some impact in future studies.

Finally a list of the future activities, if sufficient funding is available, for next fiscal year is provided.

CONTENTS

1. INTRODUCTION

The work scope of this project related to the Work Packages of "Uncertainty Reduction Analyses" with the goal of reducing nuclear data uncertainties is to produce a set of improved nuclear data to be used both for a wide range of validated advanced fast reactor design calculations, and for providing guidelines for further improvements of the ENDF/B files (i.e. ENDF/B-VII, and future releases).

Recent extensive sensitivity/uncertainty studies, performed within an international OECD-NEA initiative, have quantified for the first time the impact of current nuclear data uncertainties on design parameters of the major FCR&D and GEN-IV systems, and in particular on Na-cooled fast reactors with different fuels (oxide or metal), fuel composition (e.g. different Pu/TRU ratios) and different conversion ratios. These studies have pointed out that present uncertainties on the nuclear data should be significantly reduced, in order to get full benefit from the advanced modeling and simulation initiatives.

Nuclear data plays a fundamental role in performance calculations of advanced reactor concepts. Uncertainties in the nuclear data propagate into uncertainties in calculated integral quantities, driving margins and costs in advanced system design, operation and safeguards. This package contributes to the resolution of technical, cost, safety, security and proliferation concerns in a multi-pronged, systematic, science-based R&D approach. The Nuclear Data effort identifies and develops small scale, phenomenon-specific experiments informed by theory and engineering to reduce the number of large, expensive integral experiments. The Nuclear Data activities are leveraged by effective collaborations between experiment and theory, between DOE programs and offices, at national laboratories and universities, both domestic and international.

The primary objective is to develop reactor core sensitivity and uncertainty analyses that identify the improvement needs of key nuclear data which would facilitate fast spectrum system optimization and assure safety performance. The inclusion of fast spectrum integral experiment data is key to minimizing the impact of nuclear data uncertainties on reactor core performance calculations, thus providing the best nuclear data needs assessment.

This report presents the status of activities performed at INL under the ARC Work Package previously mentioned. As major achievement this year a comprehensive adjustment, including 87 experiments, was carried out. The results of this adjustment provide useful insights and helpful feedback to both nuclear data evaluation and measurer communities. In the following, we will document first the theory that underlines the adjustment methodology, and then we will illustrate the sensitivity coefficient computation and the nuclear data and experiment selection. Subsequently, the adjustment results will be shown, and, finally, conclusions, including future work, will be provided.

2. ADJUSTMENT METHODOLOGY

2.1 Problem formulation

Given a set of M integral quantities (true values):

$$I_i = Q_i(\sigma_1, \sigma_2, \ldots, \sigma_N), \qquad (i = 1 \ldots M) \tag{1}$$

And given a set "σ_j^0" (with $j = 1 \ldots$N) of nuclear parameters close enough to the true values "σ_j", by expanding to first order the Eq. (1) becomes:

$$I_i = Q_i\left(\sigma_1^0, \sigma_1^0, \ldots \sigma_N^0\right) + \sum_{j=1}^{N} \left(\frac{\partial Q_i}{\partial \sigma_j}\right)_{\sigma_j = \sigma_j^0} \cdot \left(\sigma_j - \sigma_j^0\right), \qquad (i = 1 \ldots M) \tag{2}$$

By defining:

$$\begin{cases} y_j = \sigma_j - \sigma_j^0 & (j = 1 \ldots N) \\ y_{N+i} = \dfrac{I_i - Q_i^{calc}}{Q_i^{calc}} & (i = 1 \ldots M) \end{cases} \tag{3}$$

where:

$$Q_i^{calc} = Q_i\left(\sigma_1^0, \sigma_2^0, \ldots \sigma_N^0\right) \tag{4}$$

and introducing the variables:

$$\begin{cases} A_{i,j} = \dfrac{1}{Q_i^{calc}} \left(\dfrac{\partial Q_i}{\partial \sigma_j}\right)_{\sigma_j - \sigma_j^0} & (j = 1, \ldots, N) \\ A_{i,N+k} = -\delta_{ik} & (k = 1, \ldots, M) \end{cases}, \qquad (i = 1, \ldots, M) \tag{5}$$

and:

$$s_i^o = 0 \qquad (i = 1, \ldots, M) \tag{6}$$

the relationship expressed by Eq. (2) may be written:

$$s_i^o + \sum_{j=1}^{N} A_{ij} y_j + \sum_{j=1}^{M} A_{i,N+j} \delta_{ij} = 0 \qquad (i = 1, \ldots, M) \tag{7}$$

i.e.:

$$s_i^o + \sum_{j=1}^{N+M} A_{ij} y_j = 0 \qquad (i = 1, \ldots, M) \tag{8}$$

In this equation, for a generalisation, further relationships relative to the nuclear data may be included.

If it is assumed that the number of these is H, the index "i" runs from 1 to ($M + H$).

In these last "H" equations the elements "s_i^o" have generally non-zeros values.

The range of the index "j" which appears in the Eq. (8) does not change. In this more general case the Eq. (8) becomes:

$$s_i^o + \sum_{j=1}^{N+M} A_{ij} y_j = 0 \qquad i = 1,\ldots,(M+H) \tag{9}$$

which, by adopting a matrix notation, can be written:

$$s^o + Ay = 0 \tag{10}$$

where:

$$s^0 = \begin{vmatrix} s_1^0 \\ s_2^0 \\ \vdots \\ s_q^0 \end{vmatrix} \tag{11}$$

$$y = \begin{vmatrix} y_1 \\ y_2 \\ \vdots \\ y_r \end{vmatrix} \tag{12}$$

$$A = \begin{vmatrix} A_{11} & A_{12} & \ldots\ldots & A_{1r} \\ A_{21} & A_{22} & \ldots\ldots & A_{2r} \\ \vdots & \vdots & & \vdots \\ A_{q1} & A_{q2} & \ldots\ldots & A_{qr} \end{vmatrix} \tag{13}$$

where "q" and "r" represent the values ($M + H$) and ($N + M$) respectively. The true values of the integral data cannot be known, therefore in Eq. (3) the true values are replaced by their available experimental value E_i. In this way it is defined:

$$\begin{cases} y_i^{ex} = \sigma_j^{ex} - \sigma_j^0 & (j = 1, \ldots, N) \\ y_{N+i}^{ex} = \dfrac{E_i - Q_i^{cal}}{Q_i^{cal}} & (i = 1, \ldots, M) \end{cases} \tag{14}$$

and, hence:

$$y^{ex} = \begin{vmatrix} y_1^{ex} \\ y_2^{ex} \\ \vdots \\ y_r^{ex} \end{vmatrix} \tag{15}$$

The solution of problem may now be obtained by the method of statistics.

2.2 Lagrange's multipliers method

If the experimental integral quantities E_i and the experimental nuclear data σ_j^{ex} are supposed normally distributed, the same can be said for the vector y^{ex} defined by Eq. (14).

Therefore, if B_y is the correlation matrix, the likelihood function is given by the expression:

$$p(y/y^{ex}) = \frac{1}{(2\pi)^{1/2} B_y^{\ 1/2}} e^{-1/2\left(y^{ex} - y^T\right)B_y^{-1}\left(y^{ex} - y\right)} \tag{16}$$

and the best estimator of "y" results to be that vector "$\tilde{y}$" for which this function assumes the maximum value.

This condition is equivalent to the minimum condition:

$$\left(y^{ex} - \tilde{y}\right)^{T} B_y^{+} \left(y^{ex} - \tilde{y}\right) = min \tag{17}$$

with the constraints:

$$s_0 + A\tilde{y} = 0 \tag{18}$$

By defining the vectors:

$$v = y - y^{ex} \tag{19}$$

$$\tilde{v} = \tilde{y} - y^{ex} \tag{20}$$

$$m = s_0 + Ay^{ex} \tag{21}$$

Eqs. (17) and (18) may be written:

$$\tilde{v}^T B_y^{-1} \tilde{v} = min \tag{22}$$

and:

$$m + A\tilde{v} = 0 \tag{23}$$

The vector $\tilde{v}$ can be calculated introducing the Lagrange multipliers: $k_1, k_2, \ldots, k_q$.

Defining the vector:

$$k = \begin{vmatrix} k_1 \\ k_2 \\ \vdots \\ k_q \end{vmatrix} \tag{24}$$

The Lagrange function now results to be:

$$\psi = \tilde{v}^T B_y^{-1} \tilde{v} - k(m + A\tilde{v}) \tag{25}$$

The differentiation of the first and second term at the right hand side of Eq. (25) gives:

$$d(\tilde{v}^T B_y^{-1} \tilde{v}) = 2\tilde{v}^T B_y^{-1} d\tilde{v} \tag{26}$$

and:

$$d\{k(m + A\tilde{v})\} = kAd\tilde{v} \tag{27}$$

The Eq. (26) is obtained considering that B_y, and therefore B_y^{-1}, is a symmetrical matrix.

Now, since it has to be:

$$d\psi = 2\left(\tilde{v}^T B_y^{-1} - \frac{1}{2}kA\right)d\tilde{v} = 0 \tag{28}$$

the following equation is obtained:

$$\tilde{v}^T B_y^{-1} - \frac{1}{2} kA = 0 \tag{29}$$

which has to be satisfied together with the constraints:

$$m + A\tilde{v} = 0 \tag{30}$$

Both Eqs. (29) and (30) allow to calculate the estimate "$\tilde{v}$" and, if requested, the vector "k" of Lagrange's multipliers.

From Eq. (29) it results:

$$\tilde{v} = \frac{1}{2} B_y kA = \frac{1}{2} B_y A^T k \tag{31}$$

and, by substituting Eq. (31) in Eq. (30):

$$m = -\frac{1}{2} A B_y A^T k \tag{32}$$

which gives:

$$k = -2G^{-1} m \tag{33}$$

where:

$$G = AB_y A^T \tag{34}$$

The substitution of Eq. (33) in Eq. (32) gives the solution expression:

$$\tilde{v} = -B_y A^T G^{-1} m \tag{35}$$

It may be seen that this calculation method requires the inversion of a matrix of dimensions $q \times q$. Since generally the number of integral data is considerably smaller than that of nuclear data to be corrected, this method should be preferable with respect to those requiring the inversion of matrices of dimensions "$N \times N$" or "$r \times N$". As far as it is concerning with the calculation of the correlation matrix By, this is defined as:

$$B_{\tilde{y}} = \left[(\tilde{y} - y)(\tilde{y} - y)^T \right] \tag{36}$$

and:

$$E(\tilde{y}) = y \tag{37}$$

From Eq. (19) and Eq. (20) it results to be:

$$\begin{aligned}\tilde{y} - y &= \tilde{v} - v = \\ &= -B_y A^T G^{-1} m - v = \\ &= -B_y A^T G^{-1}\left(-Av\right) - v = \\ &= \ B_y A^T G^{-1} A v - v = \\ &= -\left(I - B_y A^T G^{-1} A\right)v\end{aligned} \tag{38}$$

where I is identity matrix.

With the assumption:

$$X = -\left(I - B_y A^T G^{-1} A\right) \tag{39}$$

the Eq. (38) becomes:

$$\tilde{y} - y = -Xv \tag{40}$$

Therefore [3]:

$$B_{(\tilde{y}-y)} = XB_v X^T \tag{41}$$

Since "y" represents an exact vector, its correlation matrix is equal to zero, whence:

$$B_{(\tilde{y}-y)} = B_{\tilde{y}} \tag{42}$$

Moreover, as easily may be seen from Eq. (19):

$$B_v = B_y \tag{43}$$

and the Eq. (41) may be written:

$$\begin{aligned}B_{\tilde{y}} &= XB_y X^T = \\ &= \left(I - B_y A^T G^{-1} A\right) B_y \left(I - B_y A^T G^{-1} A\right)^T\end{aligned} \tag{44}$$

Setting:

$$R = B_y A^T G^{-1} A \tag{45}$$

it results to be:

$$R^T = A^T G^{-1} A B_y = B_y^{-1} R B_y \tag{46}$$

and:

$$R^2 = R \cdot R = R \tag{47}$$

whence:

$$
\begin{aligned}
B_{\tilde{y}} &= B_y - R^2 B_y = \\
&= \left(I - R^2\right) B_y = \\
&= \left(I - R\right) B_y
\end{aligned}
\tag{48}
$$

i.e.:

$$
B_{\tilde{y}} = \left(I - B_y A^T G^{-1} A\right) B_y
\tag{49}
$$

Assuming, as it occurs in practical cases:

$$
\sigma^0 = \sigma^{ex}
\tag{50}
$$

it results:

$$
Q_i^{cal} = C_i
\tag{51}
$$

where C_i represents the value of the integral data as obtained by calculations with nuclear libraries available, that is with σ^{ex}.

With this notation consistent with that used in Ref. [2], Eq. (5) may be written:

$$
\begin{cases}
A_{ij} = \dfrac{1}{C_i}\dfrac{\partial C_i}{\partial \sigma_j} = S_{ij} & \begin{matrix}(i = 1,\dots,M)\\(j = 1,\dots,N)\end{matrix} \\
A_{i,N+j} = -\delta_{ij} & \begin{matrix}(i = 1,\dots,M)\\(j = 1,\dots,M)\end{matrix}
\end{cases}
\tag{52}
$$

while Eq. (3) becomes:

$$
\begin{cases}
y_j = \sigma_j - \sigma_j^{ex} & (j = 1,\dots,) \\
y_{N+i} = \dfrac{I_i - C_i}{C_i} & (i = 1,\dots, M)
\end{cases}
\tag{53}
$$

and, analogously, Eq. (14) results:

$$
\begin{cases}
y_j^{ex} = 0 & (j = 1,\dots, N) \\
y_{N+i}^{ex} = \dfrac{E_i - C_i}{C_i} = \varepsilon_i & (i = 1,\dots, M)
\end{cases}
\tag{54}
$$

Consequently with notation used in Ref. [2], Eq. (19) may be written:

$$
\begin{cases}
\boldsymbol{v}_j = \boldsymbol{\sigma}_j - \boldsymbol{\sigma}_j^{ex} = \boldsymbol{f}_j & (j = 1....N) \\
\boldsymbol{v}_{N+i} = \dfrac{\boldsymbol{I}_i - \boldsymbol{E}_i}{\boldsymbol{C}_i} = -\boldsymbol{\Delta}_i & (i = 1......M)
\end{cases}
\tag{55}
$$

where "f" is a vector representing the true absolute corrections requested to the set "σ^{ex}" of nuclear data, while Δ represents the true relative error vector of the integral experiments.

Moreover, as obtained by Eq. (21) where "s^0" is assumed to be zero, it simply results:

$$\begin{cases} m_i = -\dfrac{E_i - C_i}{C_i} & (i = 1, \ldots, M) \\ m_{M+j} = s_j & (j = 1, \ldots, H) \end{cases} \qquad (56)$$

With these definitions Eq. (35) is solved in the AMARA code with respect to the random variable "$\tilde{v}$" which, for the first "N" elements, represents the vector "f" of the required correction of nuclear data.

Finally, it may be noted that the "B" matrix containing weight factor for the present calculation is related to those resulting in the other mathematical method described in Refs. [1,2] by relationship:

$$B_y = P^{-1} = \left(\pi^T \pi\right)^{-1} \qquad (57)$$

where "P" is the matrix which appears in the "classical least squares method" [1,4] and "π" is used for the "generalised least squares method" [2].

In the AMARA code the residual quantity:

$$\tilde{R} = \tilde{v}^T B_y^{-1} \tilde{v} \qquad (58)$$

which, by substituting Eq. (20), results to be:

$$\tilde{R} = m^T G^{-1} m \qquad (59)$$

is also evaluated. To be noticed that the use of the last expression does not imply a further matrix inversion, since the elements of G^{-1} have been already evaluated.

2.3 χ^2 filtering

Equation (17) is the initial χ^2 and the $\chi^2_{\min}$ value (i.e. after adjustment) can also be written as:

$$\chi^2_{\min} = m^T \left(A B_y A^T\right)^{-1} m \qquad (60)$$

$$\chi^2_{\min} = m^T G^{-1} m. \qquad (61)$$

From equation (59) it follows that

$$\chi^2_{\min} = \tilde{R} \qquad (62)$$

The expression for $\chi^{é}_{\min}$ given in (61) is exactly equivalent to what is found in other similar derivations. As an example, in the ORNL derivation (Ref. 5):

$$\chi^2_{\min} = d^T C_{dd}^{-1} d \qquad (63)$$

The equivalence of the vectors m and d and of the matrices G and C_{dd} is easily shown.

Following Ref. 5, we recall that the most rigorous way to "filter" the $\chi^2_{\min}$ in order to evaluate the contribution of each individual experiment "i" is given by the following algorithm:

$$\Delta\chi_i^2 = m^T G^{-1} m - m_{\neq i}^T G_{\neq i}^{-1} m_{\neq i} \quad (64)$$

where $m_{\neq i}$ and $G_{\neq i}^{-1}$ are, respectively, the m vector and the G^{-1} matrix "without" the contribution of experiment "i".

3. SENSITIVITY COEFFICIENTS, EXPERIMENT AND NUCLEAR DATA SELECTION AND ASSOCIATED CORRELATIONS

The methodology adopted (and previously) described for the cross section adjustment makes use of the following input quantities:

- C/E for the measured integral parameters
- Associated experimental and calculational uncertainties on integral parameters, and, if available, correlations among them
- "A priori" covariance data on cross sections
- Sensitivities of cross sections to integral parameters

The C/E for 148 experiments and associated calculational and experimental uncertainties have been provided and documented in the last fiscal year deliverable [5]. The analysis of the experiments has been carried out using ENDF/B-VII data files and the best calculational tools (in general Monte Carlo) in order to minimize their uncertainties.

Some correlations have been evaluated. In general the formula used for both experimental and calculational correlation is the following one for integral parameters *a* and *b*:

$$\alpha^{a,b} = \frac{\sigma_{sh}^{a}+\sigma_{sh}^{b}}{\sigma_{tot}^{a}+\sigma_{tot}^{b}} \qquad (65)$$

Where $\alpha^{a,b}$ is the correlation between the two integral parameters, σ_{sh}^{a} is the uncertainty of experiment *a* that is the common (shared) to experiment *b*, and σ_{tot}^{a} is the total uncertainty of experiment *a*.

In particular, for the 20 experiments used in the OECD/NEA Subgroup 33 exercise [5] the correlations proposed by Dr. Ishikawa have been adopted, while for the irradiation experiments (PROFIL-1, PROFIL-2, and TRAPU) and COSMO experiments Eq. (65) has been used. At ANL currently there is an evaluation for further experimental correlations associated to the ZPPR experiments that will be available next fiscal year.

The cross section covariance data used in the adjustment are those of the COMMARA 2.0 matrix [6] provided by BNL.

Sensitivity coefficients have been calculated for almost all experiments using the ERANOS code system [7] and the best calculational tools available (in general generalized perturbation theory in two-dimensional transport discrete ordinate approximation) in the 33 energy multigroup structure shown in Table I. We have introduced new coding and formulation in ERANOS in order to add the capability for calculating fission spectrum, and anisotropic scattering (both elastic and inelastic) sensitivity coefficients that were not present in the current distribution version of the code system. The irradiation experiment sensitivity coefficients have been computed by ANL using the DPT (Depletion Perturbation Theory) and are documented separately. A file containing all the sensitivity coefficients has been created and codes for retrieving and editing them have been written.

As said before, the original number of analyzed experiments is 148; however, the actual number used in the adjustment is 87 (listed in next chapter). The reduction in the number of experiments is due to several different reasons. First experiments that were duplicate in nature (i. e. with very similar sensitivity coefficients with respect to the same cross sections) were eliminated. This regards the samples in the PROFIL-2 irradiation experiment that were already measured in PROFIL-1, and the TRAPU-1 and TRAPU-3 isotope build-up (only the TRAPU-2 data were retained).The duplicate results will be used as cross-check for the adjusted data. For some isotopes no covariance data were available. That has been the case for the Nd-144 and Sm-147 samples of the PROFIL-2 irradiation experiments. For some configurations (ZPPR-15 sodium void and central control rod) no reliable sensitivity coefficient calculational model was available. For certain integral parameters (control rod rings of ZPPR-10) generalized perturbation three-dimensional transport capability is necessary and at present not available. Finally, all the configurations relevant to reflector effects (and therefore Fe-56) have been excluded (ZPR3-53 and 54, CIRANO configurations, and their associate reaction rate distributions). This is a long standing issue that will be the focus of next fiscal year activity in nuclear uncertainty reduction.

In order to limit the number of parameters to be adjusted, the multigroup cross sections have been preselected based on their contribution to the total uncertainty of each measured integral parameters taken into account in the adjustment. In practice the following formula is used:

$$\left|\Delta \mathbf{R}_{ip}^{2}\right| = \left|\mathbf{S}_{R}^{+}\mathbf{D}\mathbf{S}_{R}\right| \geq \boldsymbol{\varepsilon}^{2} \qquad (66)$$

where $\mathbf{\Delta R_{ip}}$ is the uncertainty for the measured integral parameter **p** induced by the uncertainty on cross section **i**, $\mathbf{S_R}$ is the sensitivity array, **D** the covariance matrix, and $\boldsymbol{\varepsilon}$ a user input parameter that is used as relative contribution to the total uncertainty (i. e., if $\boldsymbol{\varepsilon}$=0.001, all cross sections that contribute more than one thousandth of the total uncertainty are taken into consideration for adjustment). In particular for K_{eff} integral parameters an $\boldsymbol{\varepsilon}$=0.0001 has been used, and for spectral indices, reactivity coefficients (sodium void, control rod worth), and isotope build up an $\boldsymbol{\varepsilon}$=0.001 has been used.

Table I. 33 energy group structure (eV).

Group	Up Ener.	Group	Up Ener.	Group	Up Ener.
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	$1.00\ 10^{-1}$

4. ADJUSTMENT RESULTS

The list of the 34 isotopes included in the adjustment is the following: B-10, O-16, Na-23, Cr-52, Fe56, Ni-58, Mo-95, Mo-97, Ru-101, Pd-105, Pd-106, Cs-133, Nd-143, Nd-145, Sm-149, Sm-151, Eu-153, U-234, U-235, U-236, U-238, Np-237, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Am-241, Am-242m, Am-243, Cm-242, Cm-243, Cm-244, Cm-245.

The list of the 8 reactions considered is the following: capture, fission, nu-bar, elastic scattering, inelastic scattering, (n, 2n), fission spectrum, P_1 elastic anisotropic scattering. This list is consistent with that available in the COMMARA 2.0 covariance matrix, even though very few isotopes have covariance data for fission spectrum (only 3) and P_1 elastic anisotropic scattering (only 2).

When the selection criteria, indicated in the previous chapter, using Eq. (66) has been applied to the set of the selected 87experiments, the resulting set of selected cross sections to be adjusted amounts to 1126 against a theoretical initial number of 8976 (this does not take into account the zero cross sections of threshold reactions).

The selected cross sections present 8133 nonzero elements in their correlation terms of the covariance matrix. The COMMARA 2.0 dataset mostly contains energy correlation terms with few inter-reaction terms, and practically none inter-isotope terms.

14 correlations were used among experiment uncertainties and 357 among calculational uncertainties on the integral parameters. Adjustment was run with and without these two sets of correlations. The impact is relatively negligible as the most visible effect was a slight increase of the normalized χ^2 (going from 1.43 to 1.63). The difference in the two χ^2 is essentially due just to one experiment: the buildup of Pu-239 in the sample of Pu-238. The results that are presented in the following are those that take into account the correlations.

Table II show the results in terms of previous observed C/E (calculational results over experimental one) and the associated uncertainties. In general the agreement is satisfactory as the new C/E after adjustments stay close to 1 within two σ of the uncertainties with some notable exceptions (among others: Pu-239 fission spectral index in ZPR6/7 and ZPPR9, Step2 sodium void and central rod worth in ZPPR10, Pu238 and Am241 fission spectral indices in COSMO, Pu-239 buildup in the U238 sample of PROFIL-1, Pu-238 buildup in Am241 sample of PROFIL-1, and Pu-238 build up in TRAPU2) . Table III show the experiments ranked (ordered) following the relative change of the uncertainties before and after adjustment. This ranking gives a first evaluation of the gain obtained at the level of the uncertainties due to the adjustment.

More significant is the ranking shown in Table IV, where experiments are ordered following the magnitude of their contribution to the χ^2. This is a negative ranking as a large contribution indicates some problem with the experiment that produces it. An ideal adjustment would have a normalized χ^2 of 1 or less. As it can be seen, the largest contributor, the buildup of Pu-239 in the sample of Pu-238, gives almost all the difference with respect to χ^2=1. Other notable contributors, but in a lesser magnitude, are the Am-241 fission spectral index in COSMO, Pd-106 buildup in Pd-105 sample of PROFIL-1, the U-238 fission spectral index in Godiva, the Pu-238 fission spectral index in COSMO, the central control rod worth in ZPPR-10, the Pu-239 fission spectral index in JEZEBEL and BIGTEN, the Cm-243 buildup in TRAPU2, and Pu-240 buildup in Pu-239 sample of PROFIL-1.

For these experiments we have taken a look to both the sensitivity coefficients and the major contributors to the change of C/E. The first indication, if we trust the integral experimental data, is that the current estimate for uncertainties of the following reactions in specific energy range consistent with the spectrum of the experiment, are likely underestimated:

- Pu-238 capture

- Am-241 fission
- Pd-105 capture
- U-238 fission
- Pu-238 fission
- Pu-239 fission
- Cm-242 capture
- Pu-239 (n,2n)

In other words the existing covariance data do not provide enough room to perform a robust adjustment. To this list, and using the same approach (sensitivity coefficients and contributions to the adjusted C/E) applied to the experiments previously indicated in which the new C/E are outside the 2 σ margins, we can add the following reactions, where uncertainties are likely underestimated:

- U-238 capture
- Pu-239 capture
- U-238 inelastic
- Na-23 elastic
- Na-23 inelastic
- Fe-56 elastic
- O-16 elastic
- Pu-239 fission spectrum

More complex is to give the adjustment impact on the individual cross sections given the large amount of data used (1126 cross sections). A preliminary overview is given by Table V where we ranked the first 100 cross sections based on the magnitude of the change induced by the adjustment. One will notice the large change for captures of specific groups of actinide Pu-238, Cm-242 (notoriously wrong in ENDF/B-VII.0), and Cm-244, and for fission products Pd-105, Cs-133, Sm-151, and Eu-153. Notable are also the changes needed in the (n,2n) of Pu-239 and Pu-240 in order to improve the C/E of the corresponding samples in PROFIL-1.

Table V is a measure of the change in the central value; however, in an adjustment more important is the gain in terms of reduced uncertainty associated with the cross sections, because of the potential gain in reducing uncertainties on integral parameters of the targeted reactor designs. Table VI ranks the first 100 cross sections based on the relative change of their uncertainty after adjustment. Among others we observe impressive improvements in uncertainties of U-235 capture, U-238 and Pu-239 inelastic, Np-237 fission, and captures of some fission products. In any case, the final verdict will be out when the new covariance matrix after adjustment will be used to evaluate uncertainties on target reactor design parameters, but this is part of next fiscal year activity.

TABLE II. Old and new C/E with associated uncertainties.

#	Experiment	Old C/E	Old C/E Unc. (%)	New C/E	New C/E Unc. (%)
1	JEZ_PU239 KEFF	0.99986	0.20	1.00083	0.16
2	JEZ_PU239 U238/U235	0.97700	1.42	0.99065	1.03
3	JEZ_PU239 NP237/U235	0.98700	1.43	0.99426	0.86
4	JEZ_PU239 PU239/U235	0.97530	0.95	0.98341	0.44
5	JEZ_PU240 KEFF	0.99981	0.20	0.99975	0.18
6	FLATTOP KEFF	1.00097	0.30	1.00048	0.18
7	FLATTOP U238/U235	0.98220	1.86	0.99554	0.87
8	FLATTOP NP237/U235	0.99560	1.43	1.00385	0.80
9	ZPR6/7 KEFF	1.00043	0.23	1.00091	0.08
10	ZPR6/7 F8/F5	1.00450	3.50	1.01843	1.07
11	ZPR6/7 F9/F5	0.96380	2.52	0.96731	0.33
12	ZPR6/7 C8/F5	1.00980	2.68	1.00953	0.60
13	ZPR6/7 PU40 KEFF	0.99937	0.22	0.99974	0.08
14	ZPPR9 KEFF	0.99922	0.12	0.99962	0.07
15	ZPPR9 F8/F5	0.97100	2.92	0.99096	1.03
16	ZPPR9 F9/F5	0.98080	2.12	0.98502	0.33
17	ZPPR9 C8/F5	1.00930	1.99	1.00812	0.60
18	ZPPR9 STEP3	1.01920	7.74	0.99810	2.28
19	ZPPR9 STEP5	0.97320	7.54	0.95484	2.67
20	JOYO KEFF	0.99746	0.18	1.00029	0.14
21	GODIVA KEFF	0.99983	0.20	0.99770	0.16
22	GODIVA F28/F25	0.95500	1.34	0.97720	0.93
23	GODIVA F49/F25	0.98600	1.84	0.99573	0.35
24	GODIVA F37/F25	0.99100	1.65	1.00635	0.89
25	BIGTEN KEFF	1.00002	0.07	1.00012	0.07
26	BIGTEN F28/F25	0.94700	0.92	0.99422	0.84
27	BIGTEN F49/F25	0.97400	0.92	0.98455	0.38
28	BIGTEN F37/F25	0.96700	1.35	0.99466	1.03
29	NP SPHERE KEFF	0.99441	0.36	0.99738	0.29
30	ZPR6-6A KEFF	0.99876	0.10	0.99981	0.09
31	ZPPR-15 KEFF	0.99873	0.01	1.00000	0.01
32	ZPPR-10 KEFF	1.00015	0.11	1.00070	0.07
33	ZPPR-10 STEP2	1.15898	9.69	1.14126	2.11
34	ZPPR-10 STEP3	1.05639	5.68	1.04072	2.14
35	ZPPR-10 STEP6	1.03665	4.54	1.02213	2.22
36	ZPPR-10 STEP9	1.00826	5.46	0.99518	2.49
37	ZPPR-10 CENTER ROD	1.06700	2.20	1.04314	0.73
38	COSMO F28/F25	0.98400	1.80	0.99004	0.89
39	COSMO F37/F25	1.00500	1.58	1.00320	0.89
40	COSMO F48/F25	1.07250	2.53	1.05624	1.75
41	COSMO F49/F25	0.99090	1.30	0.99508	0.33
42	COSMO F40/F25	1.05100	2.30	1.02060	1.62
43	COSMO F41/F25	1.00370	2.03	1.00473	0.39
44	COSMO F42/F25	1.01810	2.31	1.00370	2.03
45	COSMO F51/F25	1.08920	2.30	1.06561	1.27
46	COSMO F53/F25	1.01010	2.32	1.00170	2.24
47	PROFIL1 U236 IN U235 SAMPLE	0.94900	2.31	0.97608	1.01
48	PROFIL1 PU239 IN U238 SAMPLE	0.97200	2.50	0.96082	0.59
49	PROFIL1 PU239 IN PU238 SAMPLE	1.37700	2.43	1.01171	1.47
50	PROFIL1 PU240 IN PU239 SAMPLE	0.90600	2.47	0.97259	1.36

TABLE II. (Cont.)

#	Experiment	Old C/E	Old C/E Unc. (%)	New C/E	New C/E Unc. (%)
51	PROFIL1 PU238 IN PU239 SAMPLE	0.75300	8.77	0.92935	7.59
52	PROFIL1 PU241 IN PU240 SAMPLE	0.96000	2.51	0.97669	1.52
53	PROFIL1 PU239 IN PU240 SAMPLE	0.77400	14.40	0.93717	12.67
54	PROFIL1 PU242 IN PU241 SAMPLE	0.95800	2.32	0.97964	1.32
55	PROFIL1 AM243 IN PU242 SAMPLE	1.06000	3.47	1.04031	2.21
56	PROFIL1 AM242 IN AM241 SAMPLE	0.98700	3.09	0.98020	1.40
57	PROFIL1 CM244 IN PU242 SAMPLE	0.89500	6.05	0.93942	2.58
58	PROFIL1 MO96 IN MO95 SAMPLE	1.03300	4.52	0.99810	3.18
59	PROFIL1 MO98 IN MO97 SAMPLE	0.98900	4.26	0.98171	3.04
60	PROFIL1 RU102 IN RU101 SAMPLE	1.10400	2.47	0.98563	1.58
61	PROFIL1 PD106 IN PD105 SAMPLE	0.84800	2.75	0.96948	1.81
62	PROFIL1 CS134 IN CS133 SAMPLE	0.87900	3.00	0.97384	2.26
63	PROFIL1 ND146 IN ND145 SAMPLE	0.95200	2.88	0.97345	1.94
64	PROFIL1 SM150 IN SM149 SAMPLE	0.97400	2.45	0.97916	1.60
65	PROFIL1 PU242 IN AM241 SAMPLE	0.97700	3.36	0.97310	1.21
66	PROFIL1 PU238 IN AM241 SAMPLE	0.94900	3.48	0.95218	1.24
67	PROFIL2 CM245 IN CM244 SAMPLE	1.09600	2.50	0.98493	2.16
68	PROFIL2 EU154 IN EU153 SAMPLE	0.91100	2.38	0.98701	2.03
69	PROFIL2 ND144 IN ND143 SAMPLE	0.98000	2.81	0.98438	2.08
70	PROFIL2 PD107 IN PD106 SAMPLE	0.93700	2.85	0.98635	2.55
71	PROFIL2 SM152 IN SM151 SAMPLE	1.11100	2.40	0.98658	2.07
72	PROFIL2 PU238 IN NP237 SAMPLE	0.93700	3.11	0.97713	2.26
73	TRAPU2 U234 BUILD UP	1.02300	3.27	1.01736	1.55
74	TRAPU2 U235 BUILD UP	1.02000	2.41	1.02121	0.19
75	TRAPU2 U236 BUILD UP	0.99500	2.43	1.02314	1.00
76	TRAPU2 NP237 BUILD UP	0.96300	10.53	0.94227	7.12
77	TRAPU2 PU238 BUILD UP	0.99000	2.43	1.06889	0.67
78	TRAPU2 PU239 BUILD UP	1.01200	2.72	1.00272	0.21
79	TRAPU2 PU240 BUILD UP	0.98400	2.62	1.00300	0.41
80	TRAPU2 PU241 BUILD UP	0.99200	3.01	1.00053	0.46
81	TRAPU2 PU242 BUILD UP	1.01000	2.43	1.01980	0.54
82	TRAPU2 AM241 BUILD UP	0.98600	4.33	0.99027	0.43
83	TRAPU2 AM242 BUILD UP	1.03900	4.66	1.02799	2.26
84	TRAPU2 AM243 BUILD UP	0.95900	4.83	0.94249	2.44
85	TRAPU2 CM242 BUILD UP	1.01700	3.75	0.98851	1.51
86	TRAPU2 CM243 BUILD UP	0.48300	4.04	1.00618	3.63
87	TRAPU2 CM244 BUILD UP	0.94600	3.64	1.00297	2.50

TABLE III. Experiments ordered following standard deviations relative change magnitude.

#	Experiment	(E-C)/C Change (%)	Old Stan. Dev. (%)	New Stan. Dev. (%)	Rel. Change (%)
1	TRAPU2 PU239 BUILD UP	-0.92	2.72	0.21	92.09
2	TRAPU2 U235 BUILD UP	0.12	2.41	0.19	91.93
3	TRAPU2 AM241 BUILD UP	0.43	4.33	0.43	90.17
4	ZPR6/7 F9/F5	0.36	2.52	0.33	86.89
5	TRAPU2 PU241 BUILD UP	0.86	3.01	0.46	84.58
6	TRAPU2 PU240 BUILD UP	1.93	2.62	0.41	84.33
7	ZPPR9 F9/F5	0.43	2.12	0.33	84.25
8	GODIVA F49/F25	0.99	1.84	0.35	81.27
9	COSMO F41/F25	0.10	2.03	0.39	80.64
10	ZPPR-10 STEP2	-1.53	9.69	2.11	78.25
11	TRAPU2 PU242 BUILD UP	0.97	2.43	0.54	77.76
12	ZPR6/7 C8/F5	-0.03	2.68	0.60	77.55
13	PROFIL1 PU239 IN U238 SAMPLE	-1.15	2.50	0.59	76.60
14	COSMO F49/F25	0.42	1.30	0.33	74.75
15	TRAPU2 PU238 BUILD UP	7.97	2.43	0.67	72.36
16	ZPPR9 STEP3	-2.07	7.74	2.28	70.59
17	ZPPR9 C8/F5	-0.12	1.99	0.60	69.74
18	ZPR6/7 F8/F5	1.39	3.50	1.07	69.36
19	ZPR6/7 KEFF	0.05	0.23	0.08	67.31
20	ZPPR-10 CENTER ROD	-2.24	2.20	0.73	66.53
21	ZPR6/7 PU40 KEFF	0.04	0.22	0.08	65.20
22	ZPPR9 F8/F5	2.06	2.92	1.03	64.68
23	ZPPR9 STEP5	-1.89	7.54	2.67	64.66
24	PROFIL1 PU238 IN AM241 SAMPLE	0.33	3.48	1.24	64.40
25	PROFIL1 PU242 IN AM241 SAMPLE	-0.40	3.36	1.21	63.97
26	ZPPR-10 STEP3	-1.48	5.68	2.14	62.26
27	TRAPU2 CM242 BUILD UP	-2.80	3.75	1.51	59.67
28	TRAPU2 U236 BUILD UP	2.83	2.43	1.00	58.88
29	BIGTEN F49/F25	1.08	0.92	0.38	58.32
30	PROFIL1 CM244 IN PU242 SAMPLE	4.96	6.05	2.58	57.31
31	PROFIL1 U236 IN U235 SAMPLE	2.85	2.31	1.01	56.20
32	PROFIL1 AM242 IN AM241 SAMPLE	-0.69	3.09	1.40	54.73
33	ZPPR-10 STEP9	-1.30	5.46	2.49	54.42
34	JEZ_PU239 PU239/U235	0.83	0.95	0.44	53.63
35	FLATTOP U238/U235	1.36	1.86	0.87	53.36
36	TRAPU2 U234 BUILD UP	-0.55	3.27	1.55	52.51
37	TRAPU2 AM242 BUILD UP	-1.06	4.66	2.26	51.45
38	ZPPR-10 STEP6	-1.40	4.54	2.22	50.97
39	COSMO F28/F25	0.61	1.80	0.89	50.86
40	TRAPU2 AM243 BUILD UP	-1.72	4.83	2.44	49.40
41	GODIVA F37/F25	1.55	1.65	0.89	45.90
42	COSMO F51/F25	-2.17	2.30	1.27	45.03
43	PROFIL1 PU240 IN PU239 SAMPLE	7.35	2.47	1.36	44.83
44	FLATTOP NP237/U235	0.83	1.43	0.80	44.33
45	COSMO F37/F25	-0.18	1.58	0.89	44.01
46	PROFIL1 PU242 IN PU241 SAMPLE	2.26	2.32	1.32	43.02
47	JEZ_PU239 NP237/U235	0.74	1.43	0.86	40.03
48	PROFIL1 PU239 IN PU238 SAMPLE	-26.53	2.43	1.47	39.59
49	PROFIL1 PU241 IN PU240 SAMPLE	1.74	2.51	1.52	39.55
50	FLATTOP KEFF	-0.05	0.30	0.18	39.15

TABLE III. (Cont.)

#	Experiment	(E-C)/C Change (%)	Old Stan. Dev. (%)	New Stan. Dev. (%)	Rel. Change (%)
51	ZPPR9 KEFF	0.04	0.12	0.07	36.97
52	PROFIL1 AM243 IN PU242 SAMPLE	-1.86	3.47	2.21	36.28
53	PROFIL1 RU102 IN RU101 SAMPLE	-10.72	2.47	1.58	36.21
54	ZPPR-10 KEFF	0.06	0.11	0.07	34.81
55	PROFIL1 SM150 IN SM149 SAMPLE	0.53	2.45	1.60	34.65
56	PROFIL1 PD106 IN PD105 SAMPLE	14.33	2.75	1.81	34.39
57	PROFIL1 ND146 IN ND145 SAMPLE	2.25	2.88	1.94	32.60
58	TRAPU2 NP237 BUILD UP	-2.15	10.53	7.12	32.38
59	TRAPU2 CM244 BUILD UP	6.02	3.64	2.50	31.21
60	COSMO F48/F25	-1.52	2.53	1.75	30.85
61	GODIVA F28/F25	2.32	1.34	0.93	30.85
62	PROFIL1 MO96 IN MO95 SAMPLE	-3.38	4.52	3.18	29.70
63	COSMO F40/F25	-2.89	2.30	1.62	29.61
64	PROFIL1 MO98 IN MO97 SAMPLE	-0.74	4.26	3.04	28.69
65	JEZ_PU239 U238/U235	1.40	1.42	1.03	27.62
66	PROFIL2 PU238 IN NP237 SAMPLE	4.28	3.11	2.26	27.50
67	PROFIL2 ND144 IN ND143 SAMPLE	0.45	2.81	2.08	25.78
68	PROFIL1 CS134 IN CS133 SAMPLE	10.79	3.00	2.26	24.47
69	BIGTEN F37/F25	2.86	1.35	1.03	23.50
70	NP SPHERE KEFF	0.30	0.36	0.29	21.66
71	JOYO KEFF	0.28	0.18	0.14	20.99
72	JEZ_PU239 KEFF	0.10	0.20	0.16	18.73
73	GODIVA KEFF	-0.21	0.20	0.16	17.92
74	PROFIL2 EU154 IN EU153 SAMPLE	8.34	2.38	2.03	14.48
75	PROFIL2 SM152 IN SM151 SAMPLE	-11.20	2.40	2.07	13.98
76	PROFIL1 PU238 IN PU239 SAMPLE	23.42	8.77	7.59	13.53
77	PROFIL2 CM245 IN CM244 SAMPLE	-10.13	2.50	2.16	13.51
78	COSMO F42/F25	-1.41	2.31	2.03	12.24
79	JEZ_PU240 KEFF	-0.01	0.20	0.18	12.13
80	PROFIL1 PU239 IN PU240 SAMPLE	21.08	14.40	12.67	12.06
81	PROFIL2 PD107 IN PD106 SAMPLE	5.27	2.85	2.55	10.45
82	TRAPU2 CM243 BUILD UP	108.32	4.04	3.63	9.97
83	BIGTEN F28/F25	4.99	0.92	0.84	9.39
84	ZPR6-6A KEFF	0.11	0.10	0.09	7.35
85	COSMO F53/F25	-0.83	2.32	2.24	3.49
86	BIGTEN KEFF	0.01	0.07	0.07	1.40
87	ZPPR-15 KEFF	0.13	0.01	0.01	0.04

TABLE III. Experiments ordered following contribution to χ^2. (χ^2=**1.6315**).

#	Experiment	(E-C)/C (%)	Contrib. to χ^2
1	PROFIL1 PU239 IN PU238 SAMPLE	-27.38	0.480
2	COSMO F51/F25	-8.19	0.107
3	PROFIL1 PD106 IN PD105 SAMPLE	17.92	0.093
4	GODIVA F28/F25	4.71	0.072
5	COSMO F48/F25	-6.76	0.063
6	ZPPR-10 CENTER ROD	-6.28	0.061
7	BIGTEN F49/F25	2.67	0.057
8	TRAPU2 CM243 BUILD UP	107.04	0.057
9	JEZ_PU239 PU239/U235	2.53	0.054
10	PROFIL1 PU240 IN PU239 SAMPLE	10.38	0.051
11	PROFIL1 AM243 IN PU242 SAMPLE	-5.66	0.048
12	BIGTEN F28/F25	5.60	0.046
13	PROFIL1 RU102 IN RU101 SAMPLE	-9.42	0.041
14	PROFIL1 PU238 IN PU239 SAMPLE	32.80	0.038
15	ZPR6/7 F9/F5	3.76	0.032
16	TRAPU2 PU238 BUILD UP	1.01	-0.031
17	PROFIL1 CS134 IN CS133 SAMPLE	13.77	0.029
18	PROFIL1 PU239 IN U238 SAMPLE	2.88	0.028
19	PROFIL1 PU238 IN AM241 SAMPLE	5.37	0.023
20	ZPPR-10 STEP2	-13.72	0.020
21	TRAPU2 AM243 BUILD UP	4.28	0.020
22	PROFIL1 U236 IN U235 SAMPLE	5.37	0.020
23	COSMO F40/F25	-4.85	0.020
24	PROFIL1 CM244 IN PU242 SAMPLE	11.73	0.019
25	PROFIL2 PU238 IN NP237 SAMPLE	6.72	0.015
26	NP SPHERE KEFF	0.56	0.013
27	BIGTEN F37/F25	3.41	0.012
28	TRAPU2 CM244 BUILD UP	5.71	0.011
29	TRAPU2 PU240 BUILD UP	1.63	0.011
30	PROFIL1 PU239 IN PU240 SAMPLE	29.20	0.010
31	PROFIL1 ND146 IN ND145 SAMPLE	5.04	0.010
32	ZPPR9 F9/F5	1.96	0.010
33	COSMO F28/F25	1.63	0.009
34	PROFIL2 EU154 IN EU153 SAMPLE	9.77	0.008
35	ZPPR-10 STEP3	-5.34	0.007
36	TRAPU2 PU239 BUILD UP	-1.19	-0.007
37	PROFIL2 SM152 IN SM151 SAMPLE	-9.99	0.007
38	TRAPU2 CM242 BUILD UP	-1.67	-0.006
39	ZPPR-15 KEFF	0.13	0.006
40	PROFIL1 PU241 IN PU240 SAMPLE	4.17	0.005
41	JEZ_PU239 U238/U235	2.35	0.004
42	PROFIL1 MO96 IN MO95 SAMPLE	-3.19	0.004
43	ZPPR-10 STEP6	-3.54	0.004
44	ZPPR9 C8/F5	-0.92	0.004
45	COSMO F49/F25	0.92	0.004
46	TRAPU2 PU241 BUILD UP	0.81	0.004
47	ZPPR9 KEFF	0.08	0.004
48	FLATTOP U238/U235	1.81	0.004
49	TRAPU2 U235 BUILD UP	-1.96	0.003
50	TRAPU2 NP237 BUILD UP	3.84	0.003

TABLE IV. (Cont.)

#	Experiment	(E-C)/C (%)	Contrib. to χ^2
51	ZPPR9 STEP5	2.75	0.003
52	ZPPR9 F8/F5	2.99	0.003
53	ZPR6/7 C8/F5	-0.97	0.003
54	TRAPU2 AM241 BUILD UP	1.42	0.003
55	ZPR6-6A KEFF	0.12	0.003
56	PROFIL2 PD107 IN PD106 SAMPLE	6.72	0.003
57	JOYO KEFF	0.25	-0.003
58	PROFIL1 PU242 IN AM241 SAMPLE	2.35	0.003
59	GODIVA F37/F25	0.91	-0.002
60	TRAPU2 AM242 BUILD UP	-3.75	0.002
61	GODIVA F49/F25	1.42	0.002
62	PROFIL2 ND144 IN ND143 SAMPLE	2.04	0.002
63	TRAPU2 U236 BUILD UP	0.50	-0.002
64	TRAPU2 U234 BUILD UP	-2.25	-0.002
65	ZPR6/7 F8/F5	-0.45	0.001
66	FLATTOP NP237/U235	0.44	-0.001
67	ZPR6/7 KEFF	-0.04	0.001
68	GODIVA KEFF	0.02	0.001
69	ZPPR9 STEP3	-1.88	0.001
70	JEZ_PU239 NP237/U235	1.32	-0.001
71	ZPPR-10 KEFF	-0.01	0.001
72	PROFIL1 PU242 IN PU241 SAMPLE	4.38	0.001
73	TRAPU2 PU242 BUILD UP	-0.99	0.001
74	COSMO F42/F25	-1.78	0.001
75	FLATTOP KEFF	-0.10	0.001
76	COSMO F37/F25	-0.50	0.000
77	PROFIL2 CM245 IN CM244 SAMPLE	-8.76	0.000
78	COSMO F41/F25	-0.37	0.000
79	PROFIL1 SM150 IN SM149 SAMPLE	2.67	0.000
80	JEZ_PU239 KEFF	0.01	0.000
81	PROFIL1 MO98 IN MO97 SAMPLE	1.11	0.000
82	PROFIL1 AM242 IN AM241 SAMPLE	1.32	0.000
83	ZPR6/7 PU40 KEFF	0.06	0.000
84	ZPPR-10 STEP9	-0.82	0.000
85	JEZ_PU240 KEFF	0.02	0.000
86	BIGTEN KEFF	0.00	0.000
87	COSMO F53/F25	-1.00	0.000

TABLE V. Cross sections ordered following relative change magnitude due to adjustment.

#	σ	σ change (%)
1	CM242 CAPT GR.13	184.42
2	CM242 CAPT GR.14	184.11
3	CM242 CAPT GR.12	183.82
4	CM242 CAPT GR.11	183.11
5	CM242 CAPT GR.10	181.27
6	CM242 CAPT GR. 9	178.63
7	CM242 CAPT GR. 8	174.01
8	CM242 CAPT GR. 7	171.28
9	CM242 CAPT GR. 6	166.70
10	PU238 CAPT GR. 3	-155.78
11	CM242 CAPT GR.15	131.02
12	PU238 CAPT GR.16	-126.51
13	PU238 CAPT GR.17	-111.73
14	PU238 CAPT GR.10	-108.23
15	PU238 CAPT GR.11	-86.92
16	PU238 CAPT GR. 4	-85.11
17	CM242 CAPT GR.17	83.11
18	PU238 CAPT GR.15	-83.04
19	PU238 CAPT GR.18	-78.72
20	PU238 CAPT GR.13	-78.68
21	CM242 CAPT GR. 5	78.13
22	CM242 CAPT GR.16	71.32
23	CM242 CAPT GR.18	70.25
24	PU238 CAPT GR.14	-62.94
25	CM242 CAPT GR.19	62.35
26	PU238 CAPT GR. 9	-61.51
27	PU238 CAPT GR. 5	-60.33
28	PU238 CAPT GR.21	-47.87
29	CM242 CAPT GR. 4	47.24
30	U235 CAPT GR. 3	-47.17
31	PU238 CAPT GR.12	-47.05
32	CM242 CAPT GR.20	46.57
33	CS133 CAPT GR. 3	42.97
34	PU238 CAPT GR.19	-41.43
35	PU238 CAPT GR.20	-40.76
36	PU240 CAPT GR. 4	37.75
37	PU240 CAPT GR. 5	37.33
38	CM242 CAPT GR.21	37.06
39	PU240 CAPT GR. 3	36.31
40	CS133 CAPT GR. 4	36.08
41	PD105 CAPT GR.13	34.72
42	PD105 CAPT GR.12	34.57
43	SM151 CAPT GR.16	-34.46
44	PD105 CAPT GR.14	32.52
45	PD105 CAPT GR.11	32.11
46	SM151 CAPT GR.15	-31.28
47	CM242 CAPT GR.23	31.27
48	CM242 CAPT GR.22	31.27
49	CM242 CAPT GR.24	31.27
50	CM242 CAPT GR.25	31.27

TABLE VI. (Cont.)

#	σ	σ change (%)
51	CM242 CAPT GR.26	31.27
52	CM242 CAPT GR.27	31.27
53	CS133 CAPT GR. 5	31.23
54	PD105 CAPT GR.10	30.89
55	U235 CAPT GR. 4	-29.77
56	PD105 CAPT GR.15	29.60
57	U234 FISS GR.10	29.20
58	PU240 NxN GR. 2	28.87
59	PU241 CAPT GR. 5	28.72
60	SM151 CAPT GR.14	-28.28
61	PD105 CAPT GR. 9	28.07
62	U234 FISS GR. 9	27.90
63	PU240 NxN GR. 1	26.72
64	SM151 CAPT GR. 3	26.70
65	EU153 CAPT GR.16	26.48
66	CS133 CAPT GR. 6	25.85
67	U234 FISS GR. 8	25.75
68	U234 FISS GR. 6	25.74
69	U234 FISS GR. 7	25.74
70	EU153 CAPT GR. 3	-25.71
71	EU153 CAPT GR. 4	-25.46
72	SM151 CAPT GR. 4	25.32
73	PU239 NxN GR. 2	25.30
74	SM151 CAPT GR.13	-25.25
75	EU153 CAPT GR.15	24.25
76	PU241 CAPT GR. 6	24.22
77	PU238 CAPT GR. 6	-23.85
78	PU238 CAPT GR. 8	-23.39
79	CM244 CAPT GR.14	-22.88
80	CM244 CAPT GR.15	-22.88
81	CM244 CAPT GR.16	-22.85
82	PD105 CAPT GR.16	22.63
83	PU241 CAPT GR. 4	22.26
84	EU153 CAPT GR.14	22.12
85	CS133 CAPT GR. 7	22.01
86	PD105 CAPT GR. 8	21.48
87	PU239 CAPT GR.17	20.55
88	PU239 CAPT GR.16	20.43
89	CS133 CAPT GR. 8	20.29
90	CM244 CAPT GR.13	-20.26
91	EU153 CAPT GR.13	20.00
92	EU153 CAPT GR. 5	-19.79
93	SM151 CAPT GR.12	-19.76
94	U235 INEL GR.12	19.74
95	SM151 CAPT GR. 5	19.62
96	CS133 CAPT GR. 9	19.48
97	CS133 CAPT GR.10	19.33
98	CS133 CAPT GR.11	19.02
99	CS133 CAPT GR.12	18.34
100	U235 CAPT GR. 5	-17.90

TABLE VI. Cross sections ordered following standard deviations relative change magnitude.

#	σ	σ change (%)	Old Stand. Dev. (%)	New Stan. Dev. (%)	Rel. Change (%)
1	PU239 INEL GR.15	-9.00	26.65	3.17	88.09
2	U235 CAPT GR.17	1.28	20.00	2.42	87.91
3	U235 CAPT GR.16	2.00	20.00	2.64	86.81
4	U235 CAPT GR.10	9.13	19.97	2.85	85.75
5	U235 CAPT GR.15	3.49	20.00	2.95	85.25
6	U235 CAPT GR.11	7.88	19.99	3.09	84.54
7	U235 CAPT GR.14	4.99	20.00	3.11	84.46
8	U235 CAPT GR.13	6.01	20.00	3.14	84.30
9	U235 CAPT GR. 9	9.21	19.96	3.19	84.04
10	U235 CAPT GR.12	6.85	19.98	3.23	83.84
11	U238 INEL GR. 4	-5.05	19.42	3.33	82.85
12	SM151 CAPT GR.13	-25.25	33.11	6.35	80.82
13	SM151 CAPT GR.12	-19.76	25.91	4.98	80.80
14	PU242 CAPT GR.12	0.79	23.86	4.59	80.77
15	SM151 CAPT GR.14	-28.28	37.09	7.15	80.72
16	PU242 CAPT GR.17	-0.50	15.60	3.03	80.56
17	SM151 CAPT GR.15	-31.28	41.04	8.04	80.40
18	SM151 CAPT GR.16	-34.46	45.26	9.05	80.00
19	PU242 CAPT GR.13	0.61	21.54	4.87	77.37
20	PD106 CAPT GR.12	10.04	22.49	5.20	76.90
21	PU242 CAPT GR.16	0.51	19.35	4.48	76.83
22	SM151 CAPT GR.11	-14.19	18.77	4.35	76.81
23	PU242 CAPT GR.14	0.58	21.17	4.92	76.75
24	PU242 CAPT GR.15	0.52	20.11	4.81	76.06
25	U238 ELAS GR. 4	3.54	15.13	3.63	75.98
26	PU242 CAPT GR.11	1.05	27.28	6.56	75.95
27	PU242 CAPT GR. 8	1.18	29.94	7.31	75.60
28	EU153 CAPT GR.12	16.31	20.49	5.00	75.59
29	EU153 CAPT GR.13	20.00	25.14	6.17	75.45
30	EU153 CAPT GR.14	22.12	27.84	6.96	75.00
31	U235 CAPT GR. 8	6.59	19.62	4.91	74.95
32	EU153 CAPT GR.15	24.25	30.54	7.69	74.80
33	PU242 CAPT GR. 7	1.26	32.54	8.33	74.40
34	EU153 CAPT GR.16	26.48	33.40	8.61	74.22
35	PU242 CAPT GR. 9	1.14	28.69	7.42	74.15
36	PU242 CAPT GR.10	1.09	27.74	7.19	74.10
37	EU153 CAPT GR.11	13.89	17.54	4.58	73.88
38	PU242 CAPT GR. 6	1.40	36.53	9.98	72.69
39	PD106 CAPT GR.11	9.52	21.58	5.94	72.46
40	U235 ELAS GR. 7	0.34	3.25	0.90	72.37
41	SM149 CAPT GR.13	3.35	25.16	7.05	71.99
42	EU153 CAPT GR.10	13.04	16.58	4.72	71.52
43	SM149 CAPT GR.14	3.78	28.43	8.22	71.08
44	PU239 INEL GR.14	-8.07	30.07	8.92	70.34
45	SM149 CAPT GR.15	4.17	31.53	9.45	70.03
46	SM149 CAPT GR.12	2.32	17.54	5.32	69.69
47	U235 INEL GR.10	10.05	14.97	4.55	69.64
48	PD106 CAPT GR.13	9.66	22.10	6.73	69.54
49	PU242 CAPT GR. 5	1.61	40.50	12.41	69.36
50	SM149 CAPT GR.16	4.53	34.32	10.67	68.92

TABLE VI. (Cont.)

#	σ	σ change (%)	Old Stand. Dev. (%)	New Stan. Dev. (%)	Rel. Change (%)
51	NP237 FISS GR. 6	0.51	3.17	0.99	68.64
52	SM151 CAPT GR.10	-10.51	14.30	4.66	67.44
53	SM151 CAPT GR.17	-9.08	12.36	4.03	67.40
54	SM149 CAPT GR. 9	2.34	17.83	5.82	67.34
55	U238 INEL GR. 5	-3.35	20.58	6.76	67.14
56	U238 INEL GR. 3	-6.04	20.14	6.62	67.12
57	PD106 CAPT GR.10	9.01	20.79	6.84	67.11
58	SM149 CAPT GR.17	1.28	9.77	3.23	66.97
59	AM243 FISS GR. 5	-0.57	10.00	3.31	66.93
60	CS133 CAPT GR.17	11.72	8.16	2.73	66.60
61	U238 INEL GR. 6	-2.64	16.94	5.68	66.46
62	PD106 CAPT GR. 8	7.89	18.34	6.35	65.38
63	EU153 CAPT GR. 8	12.50	16.26	5.70	64.97
64	PU238 CAPT GR.11	-86.92	20.00	7.02	64.92
65	SM149 CAPT GR. 8	2.18	16.81	5.94	64.65
66	PD106 CAPT GR.14	9.24	21.53	7.64	64.54
67	EU153 CAPT GR. 9	13.52	17.64	6.29	64.34
68	U238 ELAS GR. 3	3.34	13.12	4.71	64.13
69	PD106 CAPT GR. 9	8.04	18.82	6.86	63.55
70	U238 ELAS GR. 5	2.65	18.78	6.85	63.51
71	SM149 CAPT GR.11	1.89	14.62	5.38	63.18
72	PD105 CAPT GR.11	32.11	12.67	4.79	62.16
73	SM149 CAPT GR.10	1.87	14.55	5.53	61.96
74	PD105 CAPT GR.12	34.57	13.66	5.21	61.86
75	PD105 CAPT GR.10	30.89	12.21	4.67	61.78
76	PU239 CAPT GR.15	12.59	7.79	3.05	60.80
77	PD105 CAPT GR.13	34.72	13.79	5.42	60.70
78	PD105 CAPT GR.14	32.52	12.92	5.08	60.68
79	CS133 CAPT GR.12	18.34	13.11	5.19	60.40
80	CS133 CAPT GR.13	16.92	12.10	4.81	60.24
81	PU242 CAPT GR. 4	1.92	46.64	18.55	60.23
82	U235 CAPT GR.18	1.21	18.31	7.30	60.15
83	CS133 CAPT GR.11	19.02	13.63	5.47	59.90
84	U238 ELAS GR. 6	1.43	9.49	3.81	59.88
85	CS133 CAPT GR.10	19.33	13.88	5.63	59.46
86	CS133 CAPT GR. 9	19.48	13.99	5.67	59.45
87	PD105 CAPT GR.15	29.60	11.83	4.80	59.43
88	PD106 CAPT GR.15	8.83	21.05	8.54	59.42
89	CS133 CAPT GR.14	16.17	11.62	4.73	59.33
90	PD105 CAPT GR. 9	28.07	11.23	4.58	59.18
91	CS133 CAPT GR. 8	20.29	14.60	5.99	58.99
92	CS133 CAPT GR.15	15.53	11.24	4.73	57.91
93	CS133 CAPT GR.16	15.53	11.24	4.73	57.90
94	PU238 CAPT GR.12	-47.05	11.00	4.65	57.72
95	NP237 FISS GR. 7	0.91	4.92	2.09	57.61
96	CS133 CAPT GR. 7	22.01	16.00	6.88	56.99
97	EU153 CAPT GR.17	7.39	10.01	4.38	56.25
98	PU239 INEL GR.13	-5.23	31.91	13.98	56.20
99	PD106 CAPT GR.16	8.60	20.86	9.17	56.06
100	NP237 FISS GR. 5	0.25	2.55	1.13	55.59

5. CONCLUSIONS

This report has presented the status of activities performed at INL under the ARC Work Package on "Uncertainty Reduction Analyses" that has as a main goal the reduction of uncertainties associated with nuclear data on neutronic integral parameters of interest for the design of advanced fast reactors under consideration by the ARC program.

First, the theory behind the adjustment methodology has been presented. New insights have been introduced by proposing χ^2 filtering, a promising technique that can be adopted in the future for better exploiting the available amount of experimental results.

Then we have presented the adopted procedure for evaluating sensitivity coefficients, and select both experiments and nuclear data to be adjusted. Among the achievement related to this step we list: new capabilities to calculate sensitivity coefficients for fission spectrum and anisotropic scattering (elastic and inelastic), evaluation of correlation for experimental and calculational uncertainties for a significant number of integral parameters, a complete data set of sensitivity coefficients for ~150 experiments, codes for retrieving sensitivity coefficients and edit the data set.

Finally we have presented the results of the adjustment using ENDF/B-VII.0 data files applied to a set of 87 selected experiments in conjunction with the COMMARA 2.0 covariance matrix in a 33 energy multigroup structure. The adjustment is quite satisfactory, however some problems has been highlighted for the current estimate of cross section uncertainties. These problems are related not only to underestimation of minor isotopes (Pu-238, Am-241, and Cm-242), but also for major isotopes as U238 (fission, capture, and inelastic), Pu-239 (fission, capture, and (n,2n), Fe-56 and Na-23. In order to obtain satisfying C/E, one needs to have significant changes of the central values of captures of Pu-238, Cm-242 and Cm-244, and for fission products Pd-105, Cs-133, Sm-151, and Eu-153. In terms of reduced uncertainties, U-235 capture, U-238 and Pu-239 inelastic, Np-237 fission, and captures of some fission products are the most promising for having some impact in future studies.

For next fiscal years the projected activities at INL, provided that sufficient funding is available, include:

- The coordination and participation in the cross section adjustment exercise of the OECD/NEA WPEC Subgroup 33 will continue, with eventual extension to the subsequent Subgroup that will follow Subgroup 33. This new Subgroup will likely focus on specific issues indicated by the finding of Subgroup 33.
- Evaluation of the impact of the cross sections resulting from the adjustment performed in FY12 on uncertainty reduction in main neutronic parameters of interest for reactor design of target systems will be done. The quantification of the uncertainty reduction will allow to indicate if it is necessary to include specific new existing integral experiments or the need for new experiments.
- Validation of the new evaluated covariance matrix COMMARA 3.0. A beta version of this matrix should be available by the end of 2012. The validation will allow to provide useful feedback to the evaluators and to indicate needed corrections or possible inconsistencies.
- Extension of the formal adjustment to include experiments and data of Fe-56 and isotopes relevant to stainless steel reactor components. Iron has been a long standing issue in nuclear data as many integral experiments devoted to reflectors effects (used in reactors instead of U-238 blankets) have indicated significant discrepancies for this isotope. This will be done by calculating sensitivity coefficients for the experiments, and then performing the nuclear data adjustment. If possible method issues in the experiment analysis will be also explored.
- Support the continuation in collaboration with BNL of the Consistent Data Assimilation effort that was initiated under a project funded by the Office of Science Nuclear Physics Program. Effort should likely focus on preliminary application of the new methodology to U-235 and Pu-239 isotopes

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