M&C 2017 - International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering, Jeju, Korea, April 16-20, 2017, on USB (2017)

PIA and REWIND: Two New Methodologies for Cross Section Adjustment

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Abstract - *This paper presents two new improvements to cross section adjustment methodologies intended for coping with the problem of compensations. The first one PIA, Progressive Incremental Adjustment, gives priority to the utilization of experiments of elemental type (those sensitive to a specific cross section), following a definite hierarchy on which type of experiment to use. Once an adjustment step is performed, both the new adjusted data and the new covariance matrix are kept. The second methodology is called REWIND (Ranking Experiments by Weighting for Improved Nuclear Data). This new proposed approach tries to establish a methodology for ranking experiments by looking at the potential gain they can produce in an adjustment. Practical applications for different adjustments illustrate the results of the two methodologies against the current one and show the potential improvement for reducing uncertainties in target reactors parameters.*

I. INTRODUCTION

The problem of compensations in cross section adjustments was illustrated in /1/. In fact, in many cases the adjustment can produce untrustworthy results in terms of adjusted cross sections, when possible a-priori forms of compensation exist. Examples, among others, of source of compensations are:

- Variations of different reactions of the same isotope can compensate each other (e. g. ^{239}Pu fission spectrum χ and inelastic cross section)
- Different isotope cross section variations have opposite and compensating effects (e.g. ^{238}U capture increase associated to ^{239}Pu fission increase)

These potential sources of compensations can produce unreliable adjustments if there is lack of specific reactions and of cross correlations in the covariance matrix or if there are inadequate values in the covariance matrix that in an adjustment lead adjusting certain cross sections more than others, e.g. due to unjustified very small uncertainty values.

A major improvement in order to cope with the problem of compensations, regarding the availability of integral experiments, is to use more integral experiments of the elemental type that allow to discriminate among the parameters (cross sections), and, therefore, to insure the reliability of the adjustment. In particular there is a need for specific (preferably of elemental type) integral experiments:

- irradiation experiments (for capture, (n,2n))
- spectral indices (mainly capture and fission and, at a lesser extent, inelastic)
- "flat" or "steep" adjoint flux reactivity experiments (to separate inelastic from absorption cross section and, partly, from fission spectrum reactivity effects)
- oscillation experiments to get the reactivity of single isotope samples in different spectra
- neutron transmission or leakage experiments (mostly for inelastic and elastic cross sections and for angular scattering effects)
- reaction rate spatial distribution slopes (elastic, and inelastic, including, partly, angular scattering effects)

Along this line we define, in the following, an adjustment strategy that takes advantage of an ampler availability of integral experiments of the elemental type in order to limit the effect of compensations.

II. PIA (PROGRESSIVE INCREMENTAL ADJUSTMENT)

In the proposed adjustment strategy, PIA (Progressive Incremental Adjustment), the starting point is giving priority to the utilization of experiments of elemental type (those sensitive to a specific cross section), following a definite hierarchy on which type of experiment to use. Once an adjustment step is performed, both the new adjusted data and the new covariance matrix are kept. This limits the range of variability of the adjusted cross sections. In the final steps integral experiments that are sensitive to a large variety of cross sections (global type like critical mass) are added.

The following PIA experiment hierarchy is adopted:

- For actinides:

1. Fission spectral indices: sensitive to fission cross sections (but also to inelastic and fission spectrum, in the case of threshold fission cross sections)
2. Irradiation experiments: sensitive to capture cross sections (and second order to fission) and (n,2n)

3. Sample oscillation experiments and other experiment sensitive to inelastic (e. g. transmission, flat/steep adjoint, etc.)
4. Critical masses
5. Reactivity variations (both reactivity coefficients and reactivities associated to fissile isotope variations in the same core geometry)

- For structural materials:

1. Propagation experiments (inelastic and elastic)
2. Sample oscillations (add ? capture and scattering)
3. Critical masses
4. Reactivity variations (e.g. sodium void, control rods worth).

1. Application to ENDF/B-VII.0 Cross Section Adjustment

PIA then has been applied to the large adjustment of cross sections that is described in /2/, which uses a total of 91 experiments (see table II), ENDF/B-VII.0 starting cross sections, and COMMARA 2.0 covariance matrix /3/.

Following the PIA experiment hierarchy, previously indicate, four adjustment steps are carried out. Specifically:

1. Fission step. Fission spectral indices mostly oriented to fission cross section: 24 experiments.
2. Capture step. Added capture spectral indices and irradiation experiments for capture and (n,2n): 42 experiments.
3. K_{eff} step. Added critical masses: 18 experiments.
4. Reactivity step. Added reactivity variations: 7 experiments.

At each step the following calculations are performed:

- Cross sections variations are calculated and used for next step.
- New C/E (relative to cross section variations) are calculated and used for successive adjustment step
- New covariance matrix calculated and used for successive adjustment step.

Table I. List and type of experiments used in the PIA adjustment.

	keff	Reactivity Coefficients	Spectral index	Irradiation	total # cases
Jezebel	2		3		5
Flattop	1		2		3
ZPR-3,6,9	6		3		9
JOYO	1				1
Godiva	1		3		4
BigTen	1		3		4
Np Sphere	1				1
ZPPR-9,10,15	3	7	3		13
COSMO			9		9
PROFIL				25	25
TRAPU				15	15
CIRANO	2				2
Total	18	7	26	40	91

It has to be noticed that nonlinear effects are neglected as sensitivity coefficients are kept the same during all process and the new C/E are calculated using sensitivity coefficients folded with cross section variations. Moreover, this strategy will produce different results from a standard adjustment only when correlation (both types: experimental or calculation) exist among experiments /4,5/.

Table II shows the PIA steps C/E for the K_{eff} of some of the critical mass experiments. The initial C/E's with ENDF/B-VII.0 are all very close to one, but in the two first PIA steps we can observe several hundred pcm swings. This indicates that compensations exist, if we give priority to the elemental experiments. At this moment there is no experimental reason to give priority to one experiment with respect to another, but it is just an expert judgment and the adopted strategy that defines the step sequences in the adjustment. In general we observe that the final C/E's after adjustment tend to be essentially the same (i.e. within the final post adjustment uncertainty), as those obtained in the traditional adjustment that is using all the experiments in one step (and called from now on: Global Adjustment).

Table II. PIA steps influence on C/E of some K_{eff} experiments.

Experiment	ENDF/B-VII.0	Fission step	Capture Step	K_{eff} step	Reactivity step
JEZEBEL ^{239}Pu	0.99986	1.00294	1.00210	1.00061	1.00059
FLATTOP ^{239}Pu	1.00097	1.00376	1.00346	0.99959	0.99994
ZPR6 7	1.00043	1.00494	0.99859	0.99880	0.99927
GODIVA	0.99983	0.99382	1.00324	1.00084	1.00036
BIGTEN	1.00002	1.00336	1.00665	1.00075	1.00004

We will not report all the results of the PIA adjustment, but we will focus on the difference obtained on five isotopes of interest (U^{235}, U^{238}, Pu^{239}, Fe^{56}, and Na^{23}) between PIA and the Global Adjustment.

We will start by providing some general observation and then provide some specific comparison.

For cross section changes of the five isotopes of interest:

- Fission, nubar, and fission spectra do not change significantly for both the Global Adjustment and PIA. This is due to the fact that the initial standard deviations in COMMARA 2.0 are very small.
- Some significant changes (even different behavior) can be observed for inelastic cross sections (^{23}Na, ^{238}U, ^{239}Pu) and capture cross sections (^{235}U, ^{239}Pu).

For standard deviation changes of the five isotopes of interest:

- In general they follow the same behavior of cross sections and tend to be lower in PIA than the corresponding ones of the Global Adjustment
- In some cases they can be higher than those of the Global Adjustment, but that occurs for cross sections that are less or not adjusted at all in PIA.

The changes observed respectively on cross section and standard deviation of ^{56}Fe inelastic during the 4 PIA steps

compared against the initial ENDF/B-VII.0 values and the Global Adjustment ones show that there is no PIA significant impact on final central cross section values, whereas some noticeable difference are present for the standard deviations of the 2 to 800 keV energy range. Figures 1 and 2 show the related comparisons.

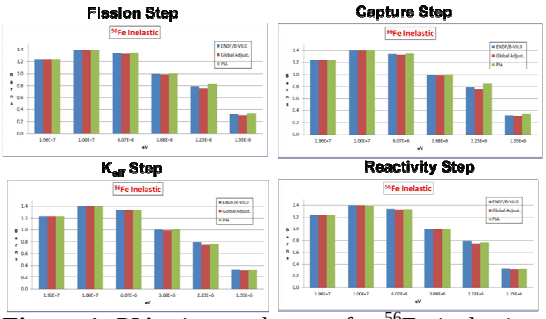

Figure 1. PIA: 4 step changes for ^{56}Fe inelastic cross section

The same comparisons for the ^{23}Na inelastic cross sections (for the standard deviation only the PIA final step is shown) indicate that PIA obtains in general higher (than Global Adjustment) cross sections whereas the standard deviations are substantially the same.

Similar comparisons for the ^{235}U capture exhibit an opposite behavior for the cross section change between PIA and the Global Adjustment: PIA decreases in the range of 5 keV to 2 keV while the Global Adjustment increases, while the opposite happens in the range from 200 KeV to 800 eV. Concerning the standard deviation PIA obtains lower values except in the 5 keV to 3 keV energy group.

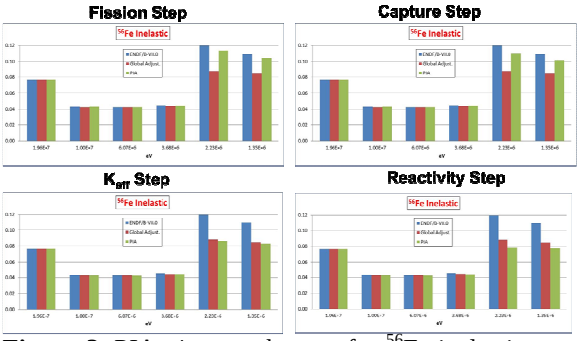

Figure 2. PIA: 4 step changes for ^{56}Fe inelastic cross section standard deviations.

A similar behavior can be noticed for the ^{238}U inelastic cross section and ^{239}Pu inelastic cross sections with some opposite trends for the cross section changes, and general decrease of the PIA standard deviations. Figure 3 and 4 illustrate this type of comparison for the case of ^{238}U inelastic.

The comparisons shown up to now, regarding the new covariance matrix, have illustrated only the effects on the diagonal element (i. e. the standard deviations); however, significant effects can be obtained on the off diagonal terms, but this is not easy to be shown in a graphical manner. One way to evaluate the impact is to look at the total uncertainty reduction obtained on a target reactor. More negative correlation is obtained by the adjustment more uncertainty reduction will be observed. Tables III through V show the uncertainty evaluation on the K_{eff} of the ABR /6/ with oxide fuel using respectively: the reference covariance matrix COMMARA 2.0, the one obtained with the Global Adjustment, and that with the PIA adjustment.

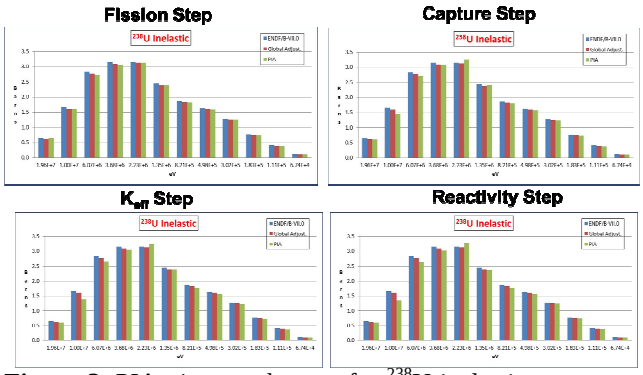

Figure 3. PIA: 4 step changes for ^{238}U inelastic cross section.

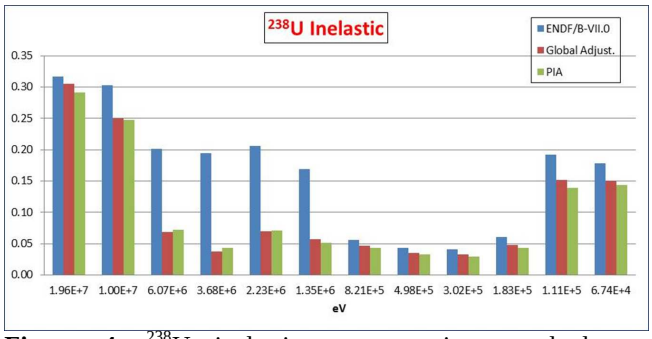

Figure 4. ^{238}U inelastic cross section standard deviations comparison (PIA final step).

Table III. Uncertainty evaluation (pcm) on the ABR (oxide fuel) K_{eff} using the COMMARA 2.0 covariance matrix.

Isotope	σ_{tot}	σ_{fis}	ν	σ_{el}	σ_{inl}	χ	P_1	Tota
U238	278	28	112	105	64	145	24	360
PU239	308	223	71	30	78	181	2	428
FE56	170	0	0	172	14	0	44	287
PU240	61	46	82	6	17	24	0	116
NA23	4	0	0	20	80	0	88	107
CR52	21	0	0	38	18	0	0	47
U16	6	0	0	46	2	0	0	46
PU241	10	7	3	0	2	0	0	13
Total	483	229	156	213	174	216	88	646

In general we can observe a significant reduction from the reference value, but PIA produces a total uncertainty that is almost a factor two less than that of the Global Adjustment. These gains are widespread over all isotopes and reactions with more anti-correlation generated by PIA.

Table IV. Uncertainty evaluation (pcm) on the ABR (oxide fuel) K_{eff} using the Global Adjustment covariance matrix.

Isotope	σ_{cap}	σ_{fis}	ν	σ_{el}	σ_{inel}	χ	P_1^*	Total
U238	-70	-12	-11	-17	-47	6	-14	-58
PU239	36	46	17	6	16	-37	2	52
FE56	86	0	0	-4	01	0	8	111
PU240	14	10	29	2	6	1	0	35
NA23	6	0	0	-12	-11	0	13	-9
CR52	6	0	0	-10	-11	0	0	-14
O16	5	0	0	37	2	0	0	37
PU241	2	6	4	0	2	0	0	8
Total	86	49	32	27	41	-36	0	109

Table V. Uncertainty evaluation (pcm) on the ABR (oxide fuel) K_{eff} using the PIA covariance matrix.

Isotope	σ_{cap}	σ_{fis}	ν	σ_{el}	σ_{inel}	χ	P_1^*	Total
U238	-36	-12	-21	-17	-40	-14	-9	-63
PU239	10	8	20	5	16	-45	2	-35
FE56	72	0	0	-24	48	0	8	84
PU240	9	10	30	3	11	-10	0	34
NA23	5	0	0	-12	-16	0	5	-19
CR52	7	0	0	-13	-6	0	0	-13
O16	5	0	0	33	2	0	0	33
PU241	-1	6	4	0	2	0	0	7
Total	85	6	30	-10	29	-49	5	60

III. REWIND (RANKING EXPERIMENTS BY WEIGHTING FOR IMPROVED NUCLEAR DATA)

In PIA the proposed hierarchy for the progressive use of experiments is based on expert judgment more than a scientific sound basis. We have tried to formulate a more scientifically based way to establish the order in the use of the experiments. Hence, a new approach is proposed that tries to establish a methodology for ranking experiments by looking at the potential gain they can produce in an adjustment. The methodology is called REWIND (Ranking Experiments by Weighting for Improved Nuclear Data).

An attempt is made here to rank experiments by using a technique that has been developed for optimizing portfolios of investment assets /7/.

Let us consider the set of integral experiments we have as a "portfolio" of assets and calculate the optimal weights that maximize the portfolio "Sharpe Ratio" /8/. The asset (experiment) return will be different following the application for which the adjustment is intended.

First, let's define some attributes of the portfolio. The covariance of the portfolio is calculated as:

$$\boldsymbol{D_p = SD\, C_p SD^T} \qquad (1)$$

Where $\boldsymbol{SD}$ is the experiment standard deviation, associated to the cross section covariance $\boldsymbol{M_\sigma}$ and $\boldsymbol{C_p}$ is the correlation among experiments and is calculated using the usual formulation with sensitivity coefficients $\boldsymbol{S_E}$ and cross section covariance:

$$\boldsymbol{C_{E'E} = \frac{(S_{E'} M_\sigma S_E)}{[(S_{E'} M_\sigma S_{E'})(S_E M_\sigma S_E)]^{1/2}}} \qquad (2)$$

The standard portfolio standard deviation is then:

$$\boldsymbol{SD_p = wD_p w^T} \qquad (3)$$

While the internal portfolio correlation is defined as:

$$\boldsymbol{Cor_p = \frac{SD_p - SD_p^{cc}}{SD_p^{cc}}} \qquad (4)$$

Where the complete correlated portfolio standard deviation is defined as:

$$\boldsymbol{SD_p^{cc} = \sum_{i=1}^{N} w_i SD_i} \qquad (5)$$

And the complete uncorrelated portfolio as:

$$\boldsymbol{SD_p^{cu} = \sqrt{\sum_{i=1}^{N} (w_i SD_i)^2}} \qquad (6)$$

The internal portfolio correlation, if one uses an equal weight $\boldsymbol{w_i}$ for each experiment, is a very useful information for determining on how "diversified" is the set of experiments used in the adjustments. Contrary to the analogy of the financial portfolio where a negative internal portfolio correlation is suited, in the adjustment a value close to zero is preferable. In fact, this implies that the portfolio contains experiments that are orthogonal to each other and, therefore, provide a diversified information.

Now let's define the Sharpe Ratio for the case we want to find the optimal experiment weights for improving the information we want on a set of isotopes like those of the WPEC subgroup CIELO /9/. In this case the return of each asset (experiment) is the potential gain an experiment can produce by reducing the uncertainty obtained by the usual sandwich formula limited to the isotopes under consideration. However, to this we have to subtract the experimental uncertainty $\boldsymbol{U_i}$ (both from measurement and calculation). Similarly, the portfolio standard deviation is calculated using only the sensitivity coefficients and covariance data of the isotopes under considerations, so that the Sharpe Ratio $\boldsymbol{SR_p}$ is calculated as:

$$\boldsymbol{SR_p = \frac{\sum_{i=1}^{N} w_i (SD_i - U_i)}{SD_p}} \qquad (7)$$

Note that the Sharpe Ratio for each experiment, defined in this way, is very similar to the Ishikawa factor (Ref. /1/). In fact the Sharpe Ratio equal to zero corresponds to the Ishikawa factor equal to 1. Positive Sharpe ratio is what we want from an experiment (corresponding to the Ishikawa factor, defined in Ref. /1/, greater than one).

The optimization process maximizes this portfolio Sharpe Ratio in order to find the optimal weights, and, therefore we will obtain a ranking of the experiments. Subsequently we can use this ranking to apply a progressive adjustment like in PIA. Note that the optimization process will reward experiments that are not correlated.

If, instead, the adjustment is targeting a specific reactor design, the experiment return (gain) will be defined in the Sharpe Ratio as the reduction of uncertainty obtained using the representativity factor /10/.

1. Application to the adjustment exercise performed by the WPEC NEA Subgroup 33

The REWIND methodology was then applied to the set of experiments used for the adjustment exercise by the WPEC NEA Subgroup 33 /11/. The "portfolio" of the SG33 includes 20 experiments. Eq. (7) was used in the optimization process using the covariance data for 5 isotopes of interest of CIELO: ^{23}Na, ^{56}Fe, ^{235}U, ^{238}U, ^{239}Pu. In our case ^{23}Na has replaced ^{16}O with respect to the CIELO isotopes.

Table VI shows the resulting optimal weights (and some other quantities of interest) coming from the optimization process and successive adjustments. As it can be seen, only 7 experiments have weights different from zero, and the related ranking is determined by the associated weight. Most of the experiments with high weight are of the critical mass type indicating that this type of experiments is the one that provide a large amount of information. Also the experiment portfolio correlation with the optimal weights is very close to zero (i. e. the non-zero weights experiments are almost not correlated).

Table VI. REWIND applied to SG33 set of experiments and 5 Isotopes: ^{23}Na, ^{56}Fe, ^{235}U, ^{238}U, ^{239}Pu. Experiment Portfolio Internal Correlation: -0.02.

Experiment	Optimal weight %	Rank	Exp. Return %	Sharpe Ratio	Ishikawa Factor	Uncert. before adjust. %	Uncert. after adjust. %
JEZ_Pu239 KEFF	27.8	2	0.45	0.69	1.50	0.30	0.15
JEZ_Pu239 F28/F25	3.4	6	2.26	0.61	1.18	1.68	0.90
JEZ_Pu239 F37/F25	5.0	5	0.91	0.39	0.71	1.02	0.64
JEZ_Pu239 F49/F25	0.0	8	-0.13	-0.15	0.85	0.80	0.53
JEZ_Pu240 KEFF	0.0	8	0.29	0.59	2.44	0.49	0.18
FLATTOP KEFF	38.1	1	0.56	0.65	0.92	0.28	0.16
FLATTOP F28/F25	0.0	8	1.22	0.40	0.84	1.56	0.84
FLATTOP F37/F25	0.0	8	0.60	0.30	0.69	0.98	0.63
ZPR6/7 KEFF	0.0	8	0.76	0.77	1.84	0.42	0.12
ZPR6/7 F28/F25	0.0	8	2.97	0.46	0.63	2.19	1.41
ZPR6/7 F49/F25	0.0	8	-1.70	-2.07	0.29	0.72	0.57
ZPR6/7 C28/F25	0.0	8	-1.17	-0.78	0.47	1.26	0.90
ZPR6/7 PU40 KEFF	0.0	8	0.77	0.78	1.92	0.42	0.12
ZPPR9 KEFF	7.5	4	1.10	0.90	3.83	0.45	0.11
ZPPR9 F28/F25	3.3	7	5.10	0.64	0.81	2.37	1.53
ZPPR9 F49/F25	0.0	8	-1.26	-1.47	0.34	0.72	0.56
ZPPR9 C28/F25	0.0	8	-0.45	-0.29	0.64	1.27	0.90
ZPPR9 STEP3	0.0	8	-0.18	-0.02	0.70	5.44	3.93
ZPPR9 STEP5	0.0	8	2.26	0.23	0.91	6.87	4.88
JOYO KEFF	15.0	3	0.70	0.79	1.67	0.30	0.14

The fact that 13 experiments have weight zero seems to indicate that these experiments could be neglected in the adjustment. Therefore, we have performed three adjustments. The first one corresponds to the traditional methodology using all the 20 experiments available at the same time. The second one is the adjustment using the ranking coming from the REWIND methodology. In other words, the adjustment is progressive, like in PIA, starting from the first ranked experiment FLATTOP K_{eff}, then recalculating new C/E with the new adjusted cross sections and related covariance matrices and proceeding to the second step using the second ranked experiment, JEZEBEL K_{eff}, and so on. For the last step, the adjustment is performed using the 13 experiments with zero weights.

Finally a third type of adjustments is done in the traditional way but using at the same time all the 7 experiments with non-zero weights. This is done in order to check if, indeed, the 13 zero weight experiments provide any supplemental information in the adjustment.

Regarding the adjusted cross sections we will remark that, in general, the 20 experiments and REWIND adjustments give quite similar results, with one exception related to the ^{239}Pu inelastic (see figure 5). This should not be a surprise because the REWIND weights have favored the K_{eff} experiments, which contains most of the information and tend to generate compensations. Unfortunately, this goes against the initial purpose of giving priority to the "elemental" type of experiments (e. g. fission spectral indices) like in the PIA adjustment strategy.

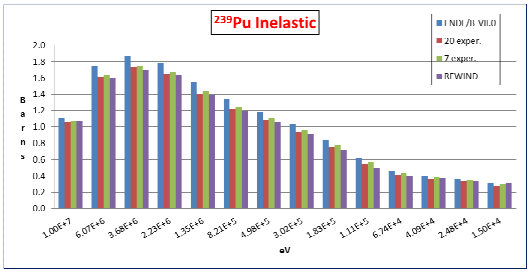

Figure 5. REWIND: Adjusted cross sections comparison for ^{239}Pu inelastic.

Concerning the 7 experiment adjustment we can observe some impact, even though they are not dramatic, when compared against the other two adjustments. Therefore, the first conclusion is that the neglected 13 experiments do indeed provide some further contribution to the adjustment (see again figure 5).

Going to the standard deviations comparisons we can observe some more significant differences. In general, as it was the case for PIA, the REWIND adjustment results, being progressive, tends to show more reduced uncertainties, and this is especially evident for the case of the ^{235}U capture cross section standard deviations (see figure 6). Again for the ^{239}Pu inelastic cross section the standard deviations (see figure 7) show a different behavior, with standard deviations for the REWIND adjustment in the lower energy range larger than those of the 20 experiment adjustment. This corresponds to cross sections that have been "less" adjusted by the REWIND adjustment.

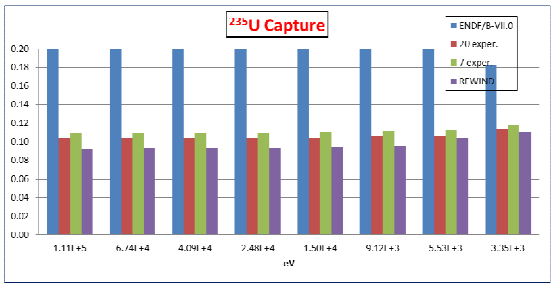

Figure 6. REWIND: Adjusted standard deviation comparison for ^{235}U capture.

Summarizing, we can say that, while the REWIND methodology has been successful in generating a ranking of experiments for a PIA adjustment strategy, the ranking gives more weights to global type of experiments (i. e. K_{eff}), instead of favoring "elemental" type of experiments, which defies the purpose of avoiding compensations.. However, the REWIND approach is flexible and specific more appropriate functionals can be considered in the future for the optimization step in order to give priority to the elemental experiments. Another development that can be foreseen is to directly incorporate the REWIND weights in the adjustment formulation, so that the progressive adjustment procedure would be significantly simplified.

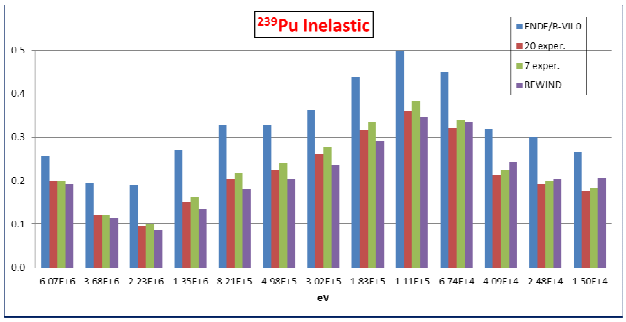

Figure 7. REWIND: Adjusted standard deviation comparison for ^{239}Pu inelastic.

IV. CONCLUSIONS

In this paper we have two new cross section adjustment methodologies intended for coping with the problem of compensations. The first one PIA, Progressive Incremental Adjustment, gives priority to the utilization of experiments of elemental type (those sensitive to a specific cross section), following a definite hierarchy on which type of experiment to use.

An exercise applied to a quite large set of experiments using as starting cross sections those of ENDF/B-VII.0 has shown that, if we trust the elemental experiments, compensations indeed occur in integral type of experiments (e. g. critical masses).

Moreover, PIA indicates some significant impact on both central values and standard deviations. When applied to a target reactor case, the new covariance matrix obtained by PIA produces significantly reduced uncertainty. This result makes the use of PIA preferable to the standard approach used currently in an adjustment (Global Adjustment).

The second methodology is called REWIND (Ranking Experiments by Weighting for Improved Nuclear Data). This new proposed approach tries to establish a methodology for ranking experiments by looking at the potential gain they can produce in an adjustment. REWIND ranks experiments by using a technique that has been developed for optimizing portfolios of investment assets calculating optimal weights to associate to each experiment. In turn the weight determines the experiment rank in a progressive adjustment like that done in PIA.

An application to the SG33 adjustment exercise has shown that the e ranking obtained by REWIND gives more weights to global type of experiments (i. e. K_{eff}), instead of favoring "elemental" type of experiments, which defies the purpose of avoiding compensations.

However, the REWIND approach is flexible, and specific more appropriate functionals can be considered in the future for the optimization step in order to give priority to the elemental experiments. Another development that can be foreseen is to directly incorporate the REWIND weights in the adjustment formulation, so that the progressive adjustment procedure would be significantly simplified.

ACKNOWLEDGMENTS

This submitted manuscript was authored by a contractor of the U.S. Government under DOE Contract No. DE-AC07-05ID14517. Accordingly, the U.S. Government retains and the publisher, by accepting the article for publication, acknowledges that the U.S. Government retains a nonexclusive, paid-up, irrevocable, world-wide license to publish or reproduce the published form of this manuscript, or allow others to do so, for U.S. Government purposes.

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