**DRAFT**

**(21 October 2010)**

2010 Oct. 20 MS Update of section II and V (main conclusions)

2010 Oct. 13 GP Update of Section IV with a summary of answers to the assessment questionnaires plus editorial changes.

2010 Oct. 1 ED Addition of references to the main part of the document and editorial changes.

2010 Sept. 24 MI Update of Section III with ANL and ORNL adjustment methodologies,

 Editorial changes.

2010 Sept. 14 ED Addition of Appendix B (ANL, ORNL, CEA),
Replacement of Appendix A (NRG) with Word translation.

2010 Sept. 1 ED Addition of Appendix A (ORNL) and Appendix B (IPPE, IJS),
Replacement of Appendix A (IJS, CEA) with original Word document.

2010 Aug. 4 ED Addition of Appendices A, B on the methodology used by the participants.

2010 July 28 CdSJ Addition of Section II on the “Identification of Merit and Drawbacks of Existing Methodologies”.

2010 July 6 MI Addition of Section III on the “Comparison of Mathematical Formulations and Specific Features”.

2010 July 5 GP First version

**OECD/NEA WPEC Subgroup 33 First Deliverable: Assessment of Existing Cross Sections Adjustment Methodologies**

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# I. Introduction

The Working Party on Evaluation Cooperation (WPEC) of the OECD Nuclear Energy Agency Nuclear Science Committee has established an International 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 first request, which this document is fulfilling, is about a deliverable assessing 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 it has been asked to the participants to provide a documentation of the used adjustment methodologies. The following organizations have provided the requested documentation: ANL, CEA, INL, IPPE, JAEA, JSI, NRG, ORNL. These documents are reported, for the different organizations, in Appendices A.

The rest of this document includes a first section on the identification of merit and drawbacks of the existing adjustment methodologies, a section on comparison of mathematical formulation and specific features, a section on criteria used for assessing the different methodologies, and finally some conclusions drawn from the assessment.

# II. Identification of Merit and Drawbacks of Existing Methodologies

Since the early 60’s, physicists, involved in the design of fast reactors, proposed to use integral experiments to improve multigroup cross sections by using integral experiments. This approach was justified by the limited knowledge at the time of the very large number of nuclear data needed in a wide energy range both for design and for experiment analysis. Early proposals were presented and discussed at the UN Conference on Peaceful Uses of Nuclear Energy in Geneva in 1964(Ref.1) G. Cecchini, U. Farinelli, A. Gandini and M. Salvatores: "Analysis of integral data for few-group parameter evaluation of fast reactors," Proc. 3rd Int. Conf. Peaceful Uses Atomic Energy, Geneva, P/627, p.388 (1964), (Ref.2) M. Humi, J. J. Wagschal and Y Yeivin: ”Multi-group constants from integral data,” ibid., P/668, p.398 (1964)).

**II.1 General description**

Let  () denote some new experimentally measured variables, and let  denote the parameters defining the model used to simulate theoretically these variables and  the associated calculated values to be compared with .

After several mathematical equations and additional approximations (beyond the scope of this chapter : see dedicated chapter), if the expectation and covariance matrix are  and M, the evaluation of posterior expectation and covariances are done by finding the minimum of the following cost function (a generalized least-square):

 

In this framework of traditional multigroup cross section adjustment,  parameters are indeed the multigroup cross sections themselves.

With the following change in notations :

*  : vector of size N= Number of Isotopes  Number of Reactions  Number of energy groups
*  is the a priori covariance matrix on multigroup cross sections.
*  : vector of size N = Number of Integral Experiments
*  is the experimental covariance matrix, including the analytical modeling covairance matrix, in principle.
*  : vector of size N = Number of Integral Experiments

 is a set of measurements which is related to cross sections (k, ...) and  its associated set of calculated values.

The generalized least-square may be written as follows:

 

Information related to integral experiments simulation are condensed in the  values as well as in their derivatives with respect to cross sections.

Using a first order approximation, one can write :

 

S is a matrix (size N  N) of calculated derivatives supposed to be constant (when the cross-sections slightly change):

 

Most of the time, S is referred to sensitivities :

 

**II.2 Merits of the methodology**

During the 70’s and 80’s the continuous improvement of the analytical tools, the reduction of approximations in the solution of the Boltzmann equation and in the multigroup generation algorithms coupled to the increase of computing capabilities, suggested that the major source of uncertainty in the assessment of the total neutron balance and of its components had to be found in the nuclear cross sections data. At the same time a very large number of high accuracy integral experiments were performed in several critical facilities all over the world (see, for example, International Handbook of Evaluated Reactor Physics Benchmark Experiments (IRPhe), OECD, VEA/NSC/DOC(2006)1, supplied as DVD, Mar. 2010), providing evidence of potential significant uncertainties if extrapolation to design was attempted. Only very accurate mock-up experiments, if feasible, could possibly overcome that difficulty. The mock-up approach was mainly followed in the US, while more analytical experimental programs were performed in France, UK, Japan and Russia (former USSR). (MS: if needed, references can be added)

While in the mock-up approach one would attempt to apply directly the observed calculation-to-experiment discrepancies to the calculation of the reference design configuration (with an appropriate use of the integral experiment uncertainties and an appropriate evaluation of possible calculation approximation effects differences between experimental and design configurations), the adjustment methodology outlined above was applied when a set of appropriately designed experiments were available. As it will be seen in the Appendixes, different variants have been developed and used in the different laboratories. Major requirements for the integral experiments were, from one side, to be as “clean” (e.g. easy to analyse) as possible and, from another side, to provide complementary information on specific nuclear data (e.g. structural material capture, Pu vs. U fission etc.) in specific energy ranges (e.g. tailoring the neutron spectrum or the neutron leakage component of the core etc.).

As indicated in the previous paragraph, common ingredients are the sensitivity coefficients (generally calculated at first order, using the so-called adjoint methods, e.g. the Generalized Perturbation Theory, originally developed by L. Usachev (Ref. L. N. Usachev: "Perturbation Theory for the Breeding Ratio and for Other Number Rations Pertaining to Various Reactor Processes," Journal of Nuclear Energy parts A/B, Vol.18, p.571 (1964))) and uncertainty values. While robust methods and tools were developed for sensitivity calculations, the uncertainty (covariance data) on multigroup nuclear parameters were mostly the result of expert judgement, in absence of systematic evaluation work. It is worth noting that taken as such, these covariances give rise to unacceptable level of uncertainties on the design integral parameters (for example, between 1000 and 2000 pcm for initial reactivity of fresh cores).(Ref. M. Salvatores, et al.: "Uncertainty and Target Accuracy Assessment for Innovative Systems Using Recent Covariance Data Evaluations", OECD, NEA/WPEC-26, International Evaluation Co-operation, Vol.26 (2008))

To reduce these uncertainties, the use of ad-hoc conceived integral experiments has been a pragmatic and mathematically-based solution [1] (several references). By having a large number of these experiments, related to specific design parameters, covering a defined domain of application, one can expect a reduction of the major uncertainties via a reduction of the observed calculation-to-experiment discrepancies, in the hypothesis that those observed discrepancies were to be attributed mostly to nuclear data. As an example of the performance of adjusted data, the use of the CANAVAL-IV adjusted library did allow to predict the critical mass of SUPERPHENIX with accuracy of the order of 300 pcm(Ref. J. C. Cabrillat, G. Palmiotti, M. Salvatores, et al.: "Methods and Data Development from the Super-Phenix Start-up Experiments Analysis", Proc. International Reactor Physics Conference, Jackson Hole, Vol.2, p.II-13 (1988)).

More recently, the multigroup cross section library ERALIB1 (obtained also with this methodology) used with the ERANOS system has a very good predictive power on fast reactor systems such as Super-Phénix and Phénix in France [2].

Besides the inevitable drawbacks (see next chapter), this methodology is:

* pragmatic and well suited for specific and well defined reactor concepts
* used in fast reactor neutronics code validation as well as in PWR cell codes validation (in this last case the mathematical framework is equivalent, but no cross sections adjustment is done)
* potentially traceable with QA
* mathematically based on least square-type theories
* open for improvement in all its aspects (simulation, hypothesis, etc , …)
* successfully applied in real cases

**II.3 Major drawbacks**

From the mathematical point of view, the approach is quite general and has been extensively used for any kind of inverse problems. The drawbacks encountered are most of the time related to the “way” the mathematical problem is solved or posed, with all the successive approximations. We are listing in this section the major drawbacks:

1. The number of parameters to be adjusted may be very large:

N= Number of Isotopes  Number of Reactions  Number of energy groups

In terms of parameter estimation technique it can create numerical resolution problems as well as purely mathematical ones (ill-conditioned problem).

1.  is conventionally a priori covariance matrix on multigroup cross sections:
	* In the past these covariance matrices were based on expert judgement, however, large efforts to give the scientific basis to the nuclear data covariances are being performeed by the field of the nuclear data study cooperated with the reactor physics in the world-wide spread (see, for example, J. K. Tuli, Editor: "Special Issue on Workshop on Neutron Cross Section Covariances", New York, Nuclear Data Sheets Vol.109, Number 12 (2008)), although the common technical basis to evaluate the nuclear data covariances has not been converged yet.
	* The problem solutions (i.e. the cross section adjustments) are dependent on these initial covariance matrices:
		1. It is logical to some extent: outputs are depending on inputs
		2. On the contrary major changes in the solutions (order of magnitude or changes in signs) can indicate a poor level of confidence in the final results, and statistical tests, such as χ2 should be carefully interpreted.
2. , Integral Experiments

One major problem with experiments can be the loss of information related to experimental descriptions: (however, large efforts are ongoing to improve such conditions, see the IRPhE DVD above mentioned.)

* + Geometry
	+ Compositions
	+ Experimental conditions
	+ Uncertainty estimations:
		1. Statistical uncertainties
		2. Systematic uncertainties (normalisation, use of standard,…)
		3.  is then experimental covariance matrix:

Most of the time no correlations between similar integral experiments are provided.

1. Concerning the calculated values and the related bias:
* In the past, neutronic solvers did imply more approximations than nowadays: at some extent, the adjustment was done on the experimental values and on the calculated values as well. The adjusted library was correlated to the calculation scheme used.
* With new 3D transport solvers used in conjunction with Monte-Carlo, this bias is reduced and can be treated in the adjustment procedure (see next chapter).
1. Dedicated adjusted multigroup libraries obtained with specific integral information:
* There exists no clear definition of the application domain of this dedicated multigroup library: at most “representativity” factors can be used to calculate a “distance” (MS: A better definition is needed here) to this domain.
* When a specific reactor concept is obviously outside this domain, it is difficult to define what is the mathematical/physical extrapolation method for the bias factors obtained using the adjusted multigroup library.
1. Most of the time the adjustment is done on a broad energy group description of cross sections creating a macroscopic change of cross sections (i.e. constant over the energy ranges corresponding to the energy groups). Several problem are thus arising:
* how to perform properly broad to fine energy meshes interpolation?
* how to treat explicitly self-shielding?
1. An outcome of the adjustment procedure is a “posterior” correlation matrix. The correlations among cross sections of various isotopes or among reactions can be unexpected and should be carefully analyzed, to understand their reliability, since one may find some of these correlations not to be physical.

**II.4 Conclusions**

As we have seen several drawbacks can be listed when doing multigroup cross sections fitting (adjustments) with integral experiments. However these drawbacks can be in principle overcome:

* With the use of more precise and un-biased deterministic simulation methods,
* With more precise evaluated covariances as assessed by nuclear physicists,
* By introducing more physics into the adjustment procedure :
	+ nuclear model parameters constraints,
	+ better assessed experimental uncertainties,
	+ using different types of integral experiments by independent facilities :
		- some related to one type of cross section for one isotope (or a few number of isotopes)
		- some involving a large number of isotopes

For the first type of integral experiments, some recent solutions were proposed in the community: to use directly proper clean integral information in the nuclear reaction model framework [11-13]. The mathematical description of one of these methods is described in details in the following paper [10] from which the general mathematical notations/methods are taken.

# III. Comparison of Mathematical Formulations and Specific Features

The methodology to adjust the differential nuclear data using the integral experimental information, which was adopted by each organization, was reported and compared. Table III.1 summarizes the theory's name and basic mathematical equations the participants submitted. From the table, followings are observed for the basic mathematical equations:

a) five organizations (JSI, IPPE, JAEA, CEA and ANL) apply the identical equations for the adjustment, though the names of theory were different somewhat,

b) ORNL uses almost same equations with the above, except for the factor Fm/k, that is, the E/C ratio, is added to the covariance of integral experimental data.

c) the expression of INL equations seems a little different with others, but it was agreed that they are mathematically identical, and,

d) NRG is developing the total Monte Carlo method to propagate uncertainties. However, this is positioned as an alternative or extensive way for the traditional deterministic method, so the essential results of the adjustment are expected equivalent with others.

From the reporting from participants, several interesting features of individuals are found:

INL: They limit the number of adjusted parameters by the multiplication of sensitivity coefficients and nuclear data covariances. It was agreed that this treatment does not affect the results of adjustment physically, but can alleviate the burden of input preparation or output editing.

IPPE: They check the data consistency of both nuclear data and integral information using the chi-square-value of the data fitting. The selection of criteria, one standard deviation in IPPE case, would be based on some judgement, but not unique.

JSI: At user request, their code will perform a minimally invasive modification of the input covariance matrix to enforce consistency (unit chi-squared). Only the diagonal elements are changed, and an iterative procedure is followed in which only one diagonal element is changed at a time, namely, the one which produces the maximum benefit in lowering chi-squared. This process is repeated until chi-squared reaches unity.

ORNL: They have an option for chi-square filtering to ensure the consistency of a given set of benchmark experiments. In the procedure, they progressively remove individual experiments until the calculated chi-square value is less than an acceptable threshold.

Table III.1 comparison of adjustment methodology by participants



# IV. Criteria for Assessing Methodologies

Criteria for assessing the different methodologies have been defined and agreed among participants. They are separated in two major categories: quantitative (mostly related to computation performance), and qualitative (mostly related to the features of the methodologies). In the following the criteria are formulated.

**1. Quantitative Criteria**

**1.1 Computational effort**:

1. What is the rank of the matrix (or matrices) to be inverted?
2. Does your adjustment use an iterative method?
3. Is there any computational limitation (number of variables, experiments, etc.)?
4. What is a typical running time for a defined number of variables/experiments? Please specify type of machine/CPU used.

**1.2 Input/output burden:**

1. Are all cross sections are taken into account? (If not, please, specify cross section selection strategy).

**2. Qualitative Criteria**

1. Are all reactions taken into accounts?
2. Can self shielding effects be explicitly treated?
3. Can high order effects be taken into account?
4. Can method uncertainties/bias be accounted for?
5. How inelastic matrices and secondary energy distributions are treated?
6. Fission prompt and delayed neutron spectra/data?
7. Is consistency test present?
8. Are cross correlations among nuclear data taken into account?
9. Are correlations among experiments taken into account?
10. Are correlations among nuclear data and experiments taken into accounts?
11. Is a new covariance data set produced?
12. Is the solution unique (local minima)?

These criteria (in form of questions) have been submitted to the participants and their answers are reported in Appendix B.

We can briefly summarize the main characteristics that come out from the answers of the participants, noting that these are consistent with what already observed in the previous chapter. We will also notice that the NRG methodology differs from the others, as not being a classical adjustment one, and therefore the questionnaire is not really applicable to it.

1.1. A: In practice, all methodologies end up inverting a matrix that has the rank of the integral experiments used in the adjustment. This, of course, minimizes the number of operations as the number of cross sections to be adjusted is larger than the used integral experiments.

1.1. B: All participants, except JSI, do not use an iterative method. JSI is using an iterative Gauss-Newton method because of explicit treatment of non-linear effects (see 2.C)

1.1. C: No limitations from the computer power are imposed, except those dictated by the coding of the program. JSI has a limitation of 3600 integral experiments.

1.1. D: The computing time, nowadays, are not anymore an issue and have become really negligible. For a reasonable numbers of variables only few seconds are needed.

1.2. A: All participants consider all cross sections, except for INL that has selection criteria for limiting the total number of variable to be adjusted.

2. A: In general, all participants are able to treat all reactions if specified by the user and if associated sensitivity coefficients and covariances are provided.

2. B: JAEA and ORNL can treat explicitly the self-shielding. CEA can do it only for nuclear parameters adjustment, not for multigroup. ANL, INL, and IPPE can treat the self shielding factors has separate variables in the adjustment. JSI cannot treat it.

2. C: Most participants can treat higher order effects only through an iterative, mostly manually, application of the adjustment procedure. This is due to the inherent linear characteristic of the sensitivity coefficients. Only JSI can directly treat non linear effects through the Gauss-Newton method.

2. D: Only JAEA treats directly through explicit inclusion of the calculation uncertainty in the adjustment methodology. The others encompass it in the C/E uncertainty.

2. E: In most cases the total inelastic is adjusted. Secondary energy distribution is adjusted depending on the capability ofpreparing associated covariance matrices.

2. F: Similarly to point 2. E that is related to the individual participant capability of calculating associated sensitivity coefficients.

2. G: All participants have some form of χ2 test.

2. H and 2. I: Yes for all participants when related data are provided.

2. J: Only INL can treat this correlation, but these are quite not common data.

2. K: All participants produce a new covariance data set after adjustment.

2. L: All participants that use non iterative methods in the adjustment produce a unique solution, which should correspond to the minimum. JSI, when applying a non-linear technique can produce local minima.

# V. Conclusions

The present report has provided a summary and an assessment of the different adjustment methodologies, based on formal descriptions of the different mathematical formulations and on answers provided by participants to a questionnaire on detailed defined criteria.

These methodologies have been adopted and widely used in practical applications, the most outstanding having been the design of a power reactor. We have seen that a major drawback is the potential issue of the “domain of applicability” or, in other words the potential risk of error compensations or even systematic errors impact, e.g.; in terms of “artificial” adjustments.

A better understanding the performance of these methodologies is needed in order

1. To improve the confidence of the users on the validity and applicability of the adjustments and of the residual bias factors to be applied to the reference design parameters,
2. To provide a reliable feedback to nuclear data evaluators in order to develop improved versions of evaluated data files.

It has then been decided to have the different organizations to participate to a common benchmark adjustment exercise that allows studying some specific issues. In particular, it was agreed that the main objective of the benchmark is to test different methods of nuclear data adjustment/assimilation and different sets of covariance data, for the purpose of reducing the design uncertainties of a particular type of sodium-cooled fast reactor.

One major expected result of the exercise will be to verify the convergence, if any, of the different adjusted data files produced by the different participants and the impact of the use of different uncertainty data evaluations. The impact of calculation methods approximation bias, of integral experiment uncertainties etc, will also be investigated.

The benchmark will make use of a single, limited set of integral experiments and measurements. The final results will be tested on a model of the Advanced fast Burner Reactor (ABR) with plutonium oxide fuel or/and a model of the JAEA FBR core.

As a byproduct of this exercise, feedback will be sent to the evaluation projects if consistent and unambiguous nuclear data trends can be found.

To facilitate comparisons, a common 33 group structure (available on the subgroup webpage) is adopted for the benchmark input/output. Every participant is responsible for the conversion of its own data into the adopted group structure. The ANGELO code can be used to convert covariance matrices from one group structure to another. For what concerns cross sections, these can be smoothed out (e.g. using lethargy width) on the 33 energy group structure.

All data, especially covariance matrices, should be provided in a “human readable” (ASCII) tabular format. The coordinators and the NEA secretariat will send format specification to the participants. All benchmark input/output will be available on the subgroup webpage.

# Main References

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