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Consistent Data Assimilation of Isotopes: ^{242}Pu and ^{105}Pd

G. Palmiotti
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Idaho National Laboratory
Idaho Falls, Idaho 83415

http://www.inl.gov

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SUMMARY

In this annual report we illustrate the methodology of the consistent data assimilation that allows to use the information coming from integral experiments for improving the basic nuclear parameters used in cross section evaluation.

A series of integral experiments are analyzed using the EMPIRE evaluated files for ^{242}Pu and ^{105}Pd. In particular irradiation experiments (PROFIL-1 and -2, TRAPU-1, -2 and -3) provide information about capture cross sections, and a critical configuration, COSMO, where fission spectral indexes were measured, provides information about fission cross section.

The observed discrepancies between calculated and experimental results are used in conjunction with the computed sensitivity coefficients and covariance matrix for nuclear parameters in a consistent data assimilation.

The results obtained by the consistent data assimilation indicate that not so large modifications on some key identified nuclear parameters allow to obtain reasonable C/E. However, for some parameters such variations are outside the range of 1 σ of their initial standard deviation. This can indicate a possible conflict between differential measurements (used to calculate the initial standard deviations) and the integral measurements used in the statistical data adjustment. Moreover, an inconsistency between the C/E of two sets of irradiation experiments (PROFIL and TRAPU) is observed for ^{242}Pu.

This is the end of this project funded by the Nuclear Physics Program of the DOE Office of Science. We can indicate that a proof of principle has been demonstrated for a few isotopes for this innovative methodology. However, we are still far from having explored all the possibilities and made this methodology to be considered proved and robust. In particular many issues are worth further investigation:

- Non-linear effects
- Flexibility of nuclear parameters in describing cross sections
- Multi-isotope consistent assimilation
- Consistency between differential and integral experiments

CONTENTS

1. INTRODUCTION

The major drawback of the classical adjustment method is the potential limitation of the domain of application of the adjusted data since adjustments are made on multigroup data, and the multigroup structure, the neutron spectrum used as weighting function and the code used to process the basic data file are significant constraints.

A new approach has been developed in order to adjust physical parameters and not multigroup nuclear data, the objective being now to correlate the uncertainties of some basic parameters that characterize the neutron cross section description, to the discrepancy between calculation and experimental value for a large number of clean, high accuracy integral experiments.

This new approach is the first attempt to build up a link between the wealth of precise integral experiments and basic theory of nuclear reactions. A large amount of exceptionally precise integral measurements has been accumulated over last 50 years. These experiments were driven by the necessities of nuclear applications but were never fully exploited for improving predictive power of nuclear reaction theory. Recent advances in nuclear reaction modeling and neutron transport calculations, combined with sensitivity analyses methods offer a reasonable possibility of de-convoluting results of the integral experiments in a way to obtain feedback on parameters entering nuclear reaction models. Essential ingredients of such a procedure will be covariances for model parameters and sensitivity matrices. The latter will provide direct link between reaction theory and integral experiments. By using integral reactor physics experiments (meter scale), information is propagated back to the nuclear level (femtometers) covering a range of more than 13 orders of magnitude.

The assimilation procedure results in more accurate and more reliable evaluated data files that will be of universal validity rather than tailored to a particular application. These files will naturally come with cross section covariances incorporating both microscopic an integral measurements as well as constrains imposed by the physics of nuclear reactions. Thus, these covariances will encompass the entire relevant knowledge available at the time of evaluation.

On the physics side, the assimilation improves knowledge of model parameters, increasing the predictive power of nuclear reaction theory and it would bring a new quality into nuclear data evaluation as well as refinements in nuclear reaction theory.

In this FY2012 report we deal with the minor plutonium isotope ^{242}Pu and the fission product ^{105}Pd. First, we illustrate, again for clarity, the theoretical basis of the new approach. Then, we show the analysis of selected experiments that are relevant to the three isotopes that were the object of this year work. Next, we present a preliminary data assimilation for ^{242}Pu, and ^{105}Pd. For these two isotopes we used only a limited number of experimental results for which the sensitivities are dominated by the isotope in question. Finally, we present some conclusions and directions for future work.

2. THEORY

The classical "statistical adjustment" techniques [1,2,3] provide adjusted multigroup nuclear data for applications, together with new, improved covariance data and reduced uncertainties for the required design parameters, in order to meet target accuracies.

One should, however, set up a strategy to cope with the drawbacks of the methodology, which are related to the energy group structure and energy weighting functions adopted in the adjustment.

In fact, the classical statistical adjustment method can be improved by "adjusting" reaction model parameters rather than multigroup nuclear data. The objective is to associate uncertainties of certain model parameters (such as those determining neutron resonances, optical model potentials, level densities, strength functions, etc.) and the uncertainties of theoretical nuclear reaction models themselves (such as optical model, compound nucleus, pre-equilibrium and fission models) with observed discrepancies between calculations and experimental values for a large number of integral experiments. The experiments should be clean (i.e., well documented with high QA standards) and high accuracy (i.e., with as low as possible experimental uncertainties and systematic errors), and carefully selected to provide complementary information on different features and phenomena, e.g., different average neutron spectrum energy, different adjoint flux shapes, different leakage components in the neutron balance, different isotopic mixtures and structural materials etc.

In the past, a few attempts were made [4,5,6] to apply a consistent approach for improving basic nuclear data, in particular to inelastic discrete levels and evaporation temperatures data of ^{56}Fe for shielding applications, and to resolved resonance parameters of actinides (e.g., Γ and total widths, peak positions etc.). This effort indicated the validity of the approach but also challenges to be overcome for its practical application. This was mainly related to the way of getting the sensitivity coefficients and to the need of reliable covariance information.

2.1 Consistent Data Assimilation Approach

The Consistent Data Assimilation methodology allows overcoming both difficulties, using the approach that involves the following steps:

- Selection of the appropriate reaction mechanisms along with the respective model parameters to reproduce adopted microscopic cross section measurements with the EMPIRE [7] code calculations. Use of coupled channels, quantum-mechanical pre-equilibrium theories, and advanced statistical model accounting for width fluctuations and full gamma cascade ensure state of the art modelling of all relevant reaction mechanisms.
- Determination of covariances matrices for the set of nuclear reaction model parameters obtained in the previous step. This is achieved by combining initial estimates of parameter uncertainties, with uncertainties/covariances for the adopted experimental data through the KALMAN [8] code. This way, the resulting parameter covariances will contain constraints imposed by nuclear reaction theory and microscopic experiments. Several parameters have been considered, including resonance parameters for a few dominating resonances, optical model parameters for neutrons, level density parameters for all nuclei involved in the reaction, parameters entering pre-equilibrium models, and parameters determining gamma-strength functions.
- Sensitivity of cross sections to the perturbation of the above mentioned reaction model parameters are calculated with the EMPIRE code.
- Use of the adjoint technique to evaluate sensitivity coefficients of integral reactor parameters to the cross section variations, as described in the previous step. To perform this task, the ERANOS code system [9] that computes sensitivity coefficients based on generalized perturbation theory is employed.
- Performing analysis of selected experiments using the best calculation tools available (in general Monte Carlo codes like MCNP).
- Performing consistent data assimilation on basic nuclear parameters using integral experiment analysis with best methodology available to provide discrepancies between calculation and measured quantities. After the C/E's are available, they are used together with the sensitivity coefficients coming from the previous step in a data assimilation code.
- Constructing new ENDF/B type data files based on modified reaction theory parameters for use by neutronic designers.

2.2 Evaluation of Nuclear Physics Parameter Covariances

As indicated in the outline of the methodology, the first step is to provide estimated range of variation of nuclear physics parameters, including their covariance data. To this end the code EMPIRE [7] coupled to the KALMAN [8] code is employed.

KALMAN code is an implementation of the Kalman filter technique based on minimum variance estimation. It naturally combines covariances of model parameters, of experimental data and of cross sections. This universality is a major advantage of the method. KALMAN uses measurements along with their uncertainties to constrain covariances of the model parameters via the sensitivity matrix. Then, the final cross section covariances can be calculated from the updated covariances for model parameters. This procedure consistently accounts for the experimental uncertainties and the uncertainties of the nuclear physics parameters. We emphasize that under the term `reaction model' we mean also the resonance region described by models such as the Multi-Level Breit-Wigner formalism.

2.3 Evaluation Sensitivity Coefficients for Integral Experiments

In order to evaluate the sensitivity coefficients of the nuclear parameters to the integral parameters measured in a reactor physics experiment, a folding procedure is applied, where the sensitivity calculated by EMPIRE, are folded with those calculated by ERANOS (i.e multigroup cross section sensitivity coefficient to integral parameters).

Following this procedure, the sensitivities of integral experiments to nuclear parameters p_k are defined as:

$$\frac{\Delta R}{\Delta p_k} = \sum_j \frac{\Delta R}{\Delta \sigma_j} \times \frac{\Delta \sigma_j}{\Delta p_k} \qquad (1)$$

where R is an integral reactor physics parameter (e. g. K_{eff}, reaction rates, reactivity coefficient, etc.), and σ_j a multigroup cross section (the j index accounts for isotope, cross section type and energy group).

In general to compute σ_j one can use a) EMPIRE with an appropriate set of parameters $\boldsymbol{p_k}$ to generate first b) an ENDF/B file for that specific isotope and successively, c) to use NJOY, to obtain multi-group cross sections.

As specified in the previous section, one can compute the variation of the cross sections $\boldsymbol{\Delta\sigma_j}$ resulting from a variation of each parameter p_k variation.

Specifically, the procedure would consist in the generation of the $\Delta\sigma_j$ corresponding to fixed, well chosen variations of each p_k taken separately and therefore generating the $\frac{\Delta\sigma_j}{\Delta p_k}$. Following each EMPIRE calculation, an ENDF/B file for the isotope under consideration is generated and a subsequent run of NJOY on this file generates multigroup cross sections in the same energy structure used for the computation of the reactor physics integral parameters. The multigroup cross section variations associated to the individual fundamental parameter that has been varied in the corresponding EMPIRE calculation are readily computed by difference with the reference NJOY calculation for the isotope under consideration.

In parallel, the cross section sensitivity coefficients to integral parameter R:

$$\frac{\Delta R}{\Delta \sigma_j}$$

are provided, using the standard Generalized Perturbation Theory in the ERANOS code system [9].

Folding the two contributions (from EMPIRE and ERANOS) one obtains the sensitivity coefficients of the nuclear physics parameters to the integral measured parameters, see Eq. (1).

2.4 Data Assimilation

Finally as far as data adjustment (or data “assimilation”) the methodology makes use of:
quantified uncertainties and associated variance-covariance data;
well documented, high accuracy and “representative” integral experiments;
sensitivity coefficients for a variety of integral parameters.
A statistical adjustment is performed using these quantities. Formulation is given in reference [1].

3. INTEGRAL EXPERIMENT ANALYSIS

The files containing the evaluation by BNL of ^{242}Pu and ^{105}Pd using the EMPIRE code were used to analyze a set of experiments intended for a future consistent data assimilation. The selected experiments include: the irradiation experiments of PROFIL 1 and 2, TRAPU 1, 2 , and 3, and the mock up experiment COSMO.

3.1 Irradiation Experiments: PROFIL and TRAPU

Experimental data from the PROFIL and TRAPU irradiation experiments [10], performed at the CEA PHENIX fast reactor, provide clean and precise information on both cross section data and transmutation rates of actinides and fission products. These data are essential for the validation of the methods and data to be used in advanced fuel cycles where transmutation systems will be used to reduce the existing inventory of nuclear waste.

During the PROFIL-1 experiment (see Figure. 5), performed in 1974, a pin containing 46 samples, including fission products plus major and minor actinides (Uranium, Plutonium, and Americium isotopes) was irradiated in the PHENIX reactor for the first three cycles, corresponding to a total of 189.2 full-power days. The experimental pin was located in the central subassembly of the core, and in the third row of pins inside the subassembly. This location is far away from neutronic perturbations allowing clear irradiation conditions. Following the reactor irradiation, mass spectroscopy was then used, with simple or double isotopic dilution and well-characterized tracers to measure isotopic concentrations. The experimental uncertainty obtained with this method is relatively small.

The second part of the PROFIL irradiation campaign (PROFIL-2, Figure 6) took place in 1979. During this experiment two standard pins, each containing 42 separated capsules of fission products plus major and minor actinides (Uranium, Plutonium, Americium and Neptunium isotopes), were irradiated for four cycles (the 17th through 20th) in the PHENIX reactor. As for PROFIL-1, chemical and mass spectrometry analyses have been subsequently performed to determine the post-irradiation isotopic concentrations.

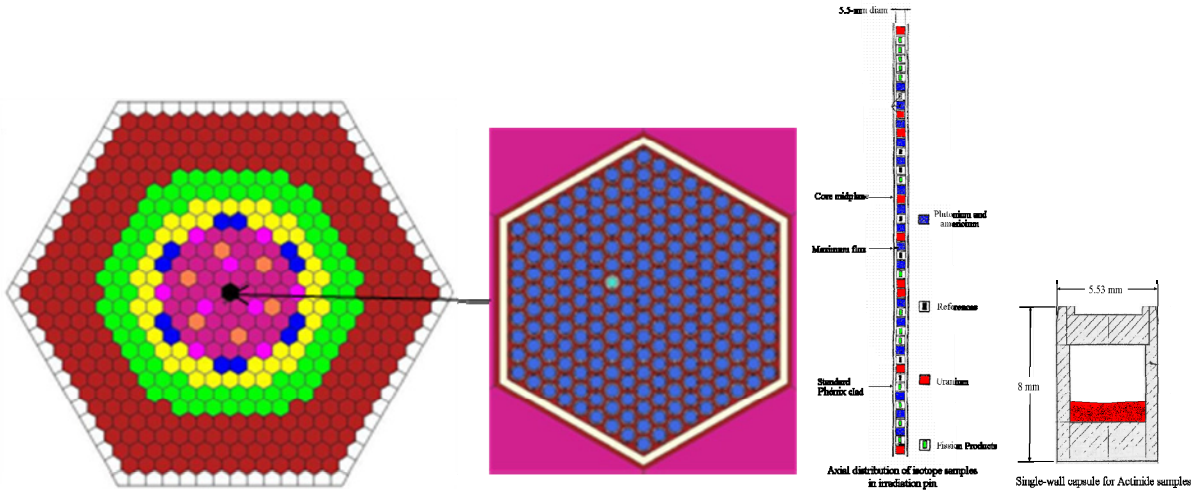
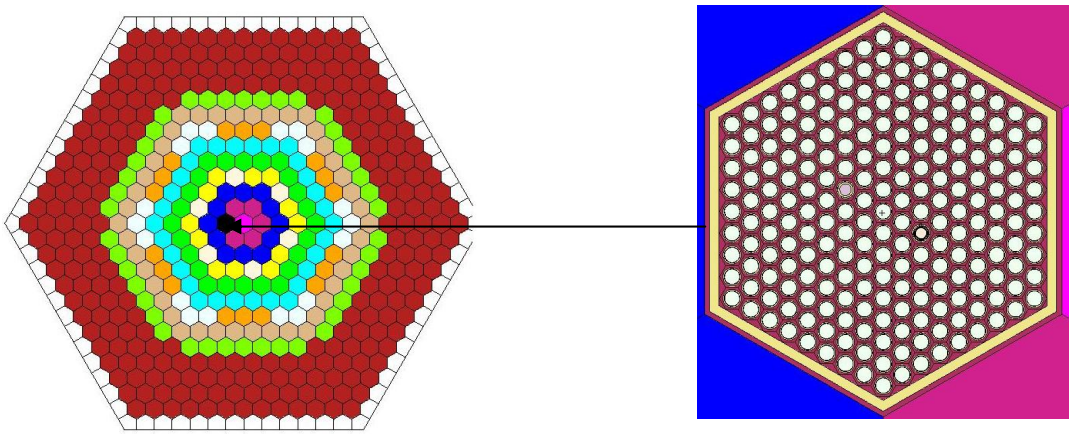
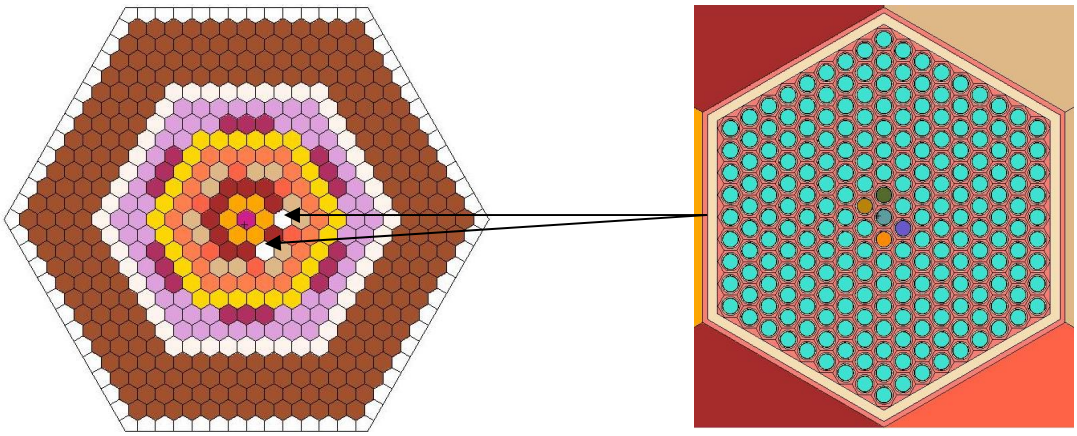


Figure 5: PROFIL-1 irradiation experiment in the French fast reactor PHENIX.



(a) Radial configuration during PROFIL-2 experiment (b) Subassembly containing irradiated samples

Figure 6: Radial cross sectional view of the PROFIL-2 model by MCNP5.



(a) Radial configuration during TRAPU experiment (b) Subassembly containing irradiated samples

Figure 1: Radial cross sectional view of the TRAPU model by MCNP5.

The TRAPU experiment (Figure 1) consisted of a six-cycle irradiation (10th to 15th) of mixed-oxide pins containing plutonium of different isotopic compositions but heavily loaded in the higher isotopes (^{240,241,242}Pu) compared to typical PHENIX fuel. In the third assembly ring there are two subassemblies having total of 10 irradiated fuel pins (5 each). Unlike other two experiments, each irradiated fuel pin has only one sample which has the same size as that of ordinal fuel pin.

After irradiation, 20 mm tall samples were cut from the pins (both fuel and clad) and put into a solution in order to determine the fuel composition by nuclide. ^{148}Nd was used as a burn-up indicator as it is a stable fission product with a small capture cross section, thereby enabling accurate determination of the number of fission reactions that took place in the sample. Again, isotopic data were obtained using mass spectrometry techniques, with simple or double isotopic dilution and well-characterized tracers.

3.1.1 Evaluation of One-Group Cross Sections by Monte Carlo Method

In order to perform three-dimensional burn-up Monte Carlo calculations, it is important to obtain accurate and statistically reliable one-group cross sections for each irradiated sample that are to be used for solving the Bateman equations. Unlike other PROFIL-1&2 experiments, each irradiated fuel pin for TRAPU experiment has only one sample which has the same size as that of ordinal fuel pin. The large volume of irradiated samples makes Monte Carlo calculations much easier to obtain statistically reliable tallies. However, it is extremely difficult to obtain statistically reliable results for PROFIL-1&2 since the size of each sample is very small (~0.06 cm^3), and some of reactions (e.g., (n,2n), (n,3n)) are caused by very fast neutrons (5 MeV ~) which are usually not well populated. Moreover, it is not straightforward to perform variance reduction in criticality calculations. Thus, we came up with a calculation procedure that uses MCNP's surface source capability (Figure 2). In this approach, first, a full-core criticality calculation is performed with the surface source write (SSW) card in order to generate the binary source file containing the surface and fission volume sources around and in the irradiated fuel samples, respectively. This source file is used to perform the fixed source calculation with the reduced geometry modeling only the irradiated fuel pin. The fixed source calculation can be performed with only the recorded particles from the full-core criticality calculation. If the number of recorded source particles is small, then it is not feasible to obtain statistically reliable solutions even with variance reduction techniques. In order to resolve this problem, we wrote a program that duplicates the recorded information of source particles. However, the number of duplications is limited because adding additional source particles enlarges the size of the source file. To address this issue, we performed several fixed source calculations by skipping random numbers corresponding to the number of histories for each run. After finishing all fixed source calculations, the solutions were collected, and then the batch statistics was taken.

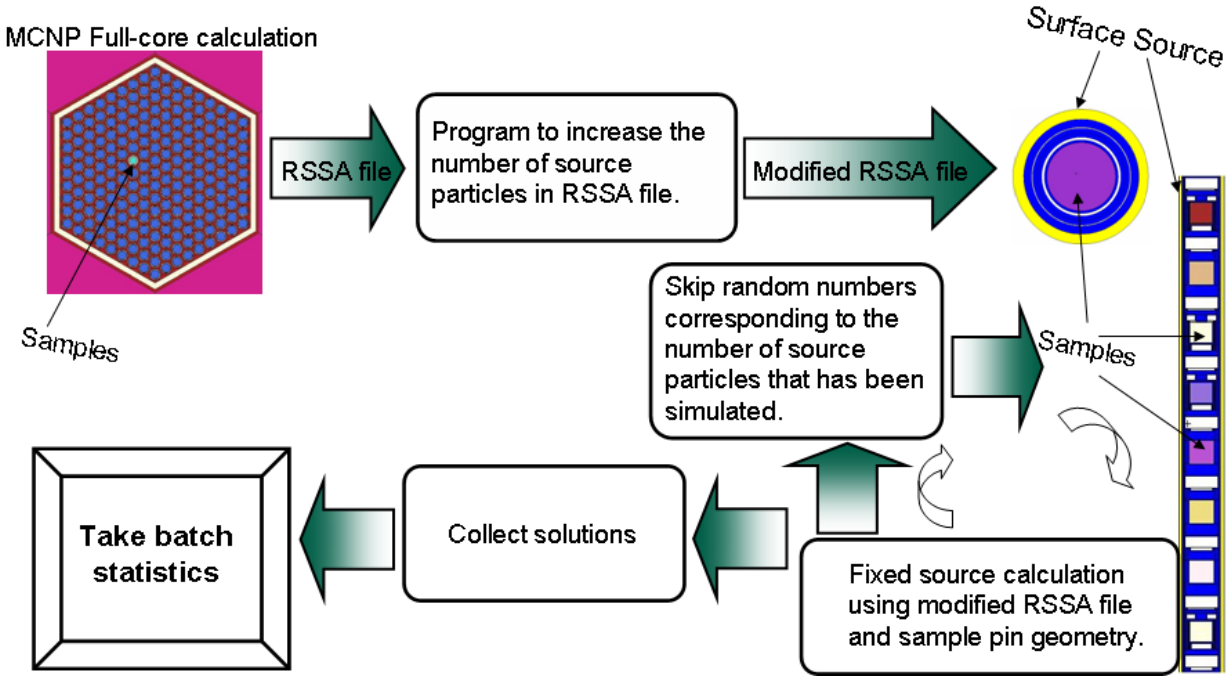


Figure 2: Procedure for calculating one-group cross sections for PROFIL-1 & 2 by MCNP.

3.1.2 Depletion analysis with MCNP cross sections

The "experimental" axial flux distribution has been provided by the French reports and has been derived by measurements of reaction rates at different places and times. Because of the differences between the experimental and calculated axial flux distributions, a comparison on the Neodymium production for the samples of ^{235}U was performed using the two distributions. The results indicated that the experimental distribution provides a consistent (almost constant) set of C/E's, while the calculated one shows a drift in the bottom part. Based on this observation, it was decided that in the analysis we would use the experimental axial distribution. The likely reason for the observed discrepancy has to be attributed to the lack of information on the control rod movement during the cycles, and the actual flux calculations were performed with a fixed average control rod position.

For what regards PROFIL-2 no clear "experimental" information was provided by the French documentation; therefore, it was decided to use the calculated axial distribution. For TRAPU the value (there is no axial distribution in this case, as we are talking of a 2 cm piece at the midplane of the reactor) provided by the French documentation was used.

Next step was to correctly normalize the isotope build up results to the actual values of the fluence (and hence eliminate the uncertainty in the irradiation history). To this latter purpose the neodymium production in the ^{235}U samples has been calculated and compared with the correspondent experimental values. The corrective factor, by which the experimental fluxes are divided, has been subsequently derived. The normalization values used in the successive analysis are: 1.047 for PROFIL-1, 1.021 for PROFIL-2, and 1.1436 for TRAPU.

Depletion calculations have been carried out using the NUTS [11] code in order to evaluate the isotope build up. The one group cross sections from the MCNP calculations and normalized fluxes were provided as inputs for the depletion calculations. The information that can be gathered from the post-irradiation analysis is related to the evaluation of the reaction rates (mainly capture and (n,2n) rates) for a given isotope. In particular, the analysis of the experiment is based on the relation existing between the burn-up dependent variations of the atom number densities and the microscopic cross-sections. For isotopes for which the descendant, obtained via neutron capture, is stable or has a long radioactive period, the most accurate experimental technique for obtaining information on the integral capture cross section is to determine the variation in composition that results from high-flux irradiation of a pure sample. Capture and (n,2n) reaction rates for an isotope of mass A, which has received a total fluence of τ, can be evaluated by the measurement of ratios of concentrations using Equations (2) and (3) respectively:

$$\sigma_{(c),A} \cdot \tau \cdot f(\tau) \cong \frac{\Delta N_{A+1}}{N_A} = \frac{N_{A+1}(\tau)}{N_A(\tau)} - \frac{N_{A+1}(0)}{N_A(0)} \qquad (2)$$

$$\sigma_{(n,2n),A} \cdot \tau \cdot f(\tau) \cong \frac{\Delta N_{A-1}}{N_A} = \frac{N_{A-1}(\tau)}{N_A(\tau)} - \frac{N_{A-1}(0)}{N_A(0)} \qquad (3)$$

where $f(\tau)$ is a correcting factor which takes into account the physical phenomena different from capture (or (n,2n) reactions) that the considered isotope A can experience during the irradiation. Because of its definition $f(\tau)$ is a measure of the fertile or fissile properties of a given isotope, being lower and

higher than one for fertile and fissile isotopes respectively. It can be evaluated by a time dependent calculation, as follows:

$$f(\tau)=\left[\frac{N_{A+1}^{(\tau)}}{N_{A}^{(\tau)}}-\frac{N_{A+1}^{(0)}}{N_{A}^{(0)}}\right]\times\frac{1}{\sigma_{CA}\cdot\tau_{calc.}} \qquad (4)$$

In Equation (4), σ_{CA} and τ_{calc} represent the one-group capture cross section for the isotope A and the calculated fluence, respectively.

This approach works very well when we are considering a reaction rate that is dominant in the formation of the measured resulting isotope (i. e., capture cross section) but it will attribute the same C/E also when the reaction rate is not dominant like in the case of an (n,2n) cross section. In order to avoid this problem a slightly different approach was adopted. We correct the experimental density variation by a calculated quantity that takes out the variation due to all the phenomena other than the reaction rate that we are considering:

$$\sigma_{(c),A}\cdot\tau\cdot\cong\frac{^{corr}\Delta N_{A+1}}{N_A}=\frac{^{exp}\Delta N_{A+1}(\tau)-(^{calc}\Delta N_{A+1}-N_A^{(0)}e^{-\sigma\tau})}{N_A} \qquad (5)$$

where $^{exp}\Delta N_{A+1}(\tau)$ is the experimental measured density variation, and $^{calc}\Delta N_{A+1}$ is the calculated one.

In the end, Eq. 5 was used to derive an initial guess for the unknown experimental cross section and then this latter is computed by changing its value until the final measured experimental densities were matched. Using this approach C/E's were calculated for the sample isotope build up.

3.2 COSMO Configuration in MUSE-4 Benchmark

The PROFIL and TRAPU experiments can also provide information on fission cross sections. In the case of PROFIL the experimental results provide the Nd isotope build-up in the actinide samples. If the fission product yield is well known, an estimate can be made for the fission cross section. Nevertheless, the knowledge of the fission yields is based on the fission cross sections, so this can be a tautological situation. In the case of TRAPU, the fission information comes through the sensitivity to this cross section to the buildup of the isotopes.

A more accurate way to gather information on fission cross sections from elemental experiments is through the analysis of fission spectral indices. In this case, fission reaction rates of actinides are measured against a standard, in particular ^{235}U fission. If the measurements are done in the center of a reactor in a well characterized spectrum, indirect effects are minimal and the result can be directly related to the actinide fission cross section. This is the situation for the COSMO experimental campaign, part of the MUSE-4 benchmark project [12] performed at the French zero power fast spectrum facility MASURCA, where different actinide fission spectral indices were measured.

The MUSE-4 benchmark project, organized by OECD/NEA, was performed for studying the physics of accelerator-driven subcritical systems (ADS). The benchmark model was oriented to compare simulation predictions based on available codes and nuclear data libraries with experimental data related to TRU transmutation, criticality constants and time evolution of the neutronic flux following source variation, within liquid metal fast subcritical systems.

A set of experiments were performed in MASURCA reactor which can be configured as critical or subcritical by loading a different number of fuel tubes. The benchmark consists of three configurations.

One of configurations is called COSMO (Figure 3), which is a very simple and symmetric critical configuration and has no external source, vacuum tube nor lead buffer.

The experiment was analyzed based upon the benchmark specifications provided in Ref. [12].

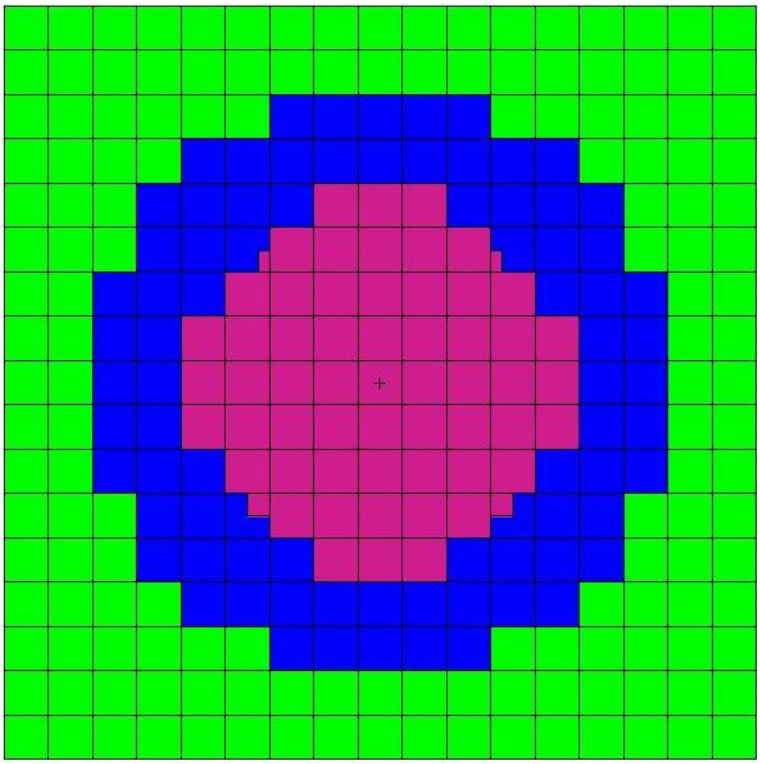


Figure 3: Radial view of COSMO configuration modeled by MCNP5

4. ^{242}Pu DATA ASSIMILATION

For this case we have six experimental results for the associated integral parameters: the ^{243}Am build up in the irradiation experiments of PROFIL1, PROFIL2, TRAPU1, TRAPU2, and TRAPU3 and the fission spectral index od ^{242}Pu in COSMO. The first 5 experimental results provide information on the capture cross section of ^{242}Pu, while the last one provides information on the fission cross section. A total of 50 nuclear parameters were used in EMPIRE for characterizing the evaluation of the ^{239}Pu cross sections.

BNL provided the covariance matrix of these parameters as well the sensitivity of them in terms of multigroup cross sections. The classical 33 group structure, used mostly for fast reactors and reported in Table I, was adopted. The ERANOS code [9] was used to calculate the multigroup sensitivity coefficients to the six integral parameters previously indicated.

With these two sets the sensitivity of the nuclear parameters to the measured quantities was calculated following Eq. (1). Subsequently, this set of sensitivity coefficients was used together with the calculated C/E for performing a statistical adjustment. Table II shows the C/E before and after adjustment with related uncertainties.

Table I. Multigroup energy 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**	**$1.00\ 10^{-1}$**

Table II. Old and new C/E before and after adjustment for JEZEBEL experiments

Experiment	old C/E ± σ	new C/E ± σ
^{243}Am buildup PROFIL1	**1.107 ± 0.035**	**1.047± 0.018**
^{243}Am buildup PROFIL2	**1.116 ± 0.046**	**1.057 ± 0.017**
^{243}Am buildup TRAPU1	**1.020 ± 0.045**	**0.962 ± 0.018**
^{243}Am buildup TRAPU2	**0.998 ± 0.048**	**0.942 ± 0.018**
^{243}Am buildup TRAPU3	**1.047 ± 0.036**	**0.987 ± 0.018**
Fis.^{242}Pu/Fis.^{235}U COSMO	**0.890 ± 0.023**	**0.988± 0.022**

In general C/Es look are better for the PROFIL experiments while for the TRAPU experiments only TRAPU3 show a definite amelioration. The COSMO C/E shows a spectacular improvement; however the uncertainty after adjustment stays about the same, which is an indication of the presence of some problem.

Table III shows the obtained parameter variations and the related standard deviations before and after the data

assimilation for the parameters that mostly affect the assimilation.

Table III ^{242}Pu parameter variations and standard deviations obtained by data assimilation.

Parameter	Variation (%)	Init. Stand. Dev. (%)	Final Stand. Dev. (%)
TUNE00000 [a)]	4.841	12.875	8.077
FUSRED00000 [b)]	0.432	2.500	2.310
FISVF10000 [c)]	-1.601	1.000	0.430
TOTRED00000 [d)]	-0.898	1.000	0.849
LDSHIF0000 [e)]	-0.883	3.067	2.951
FISVF20000 [f)]	-0.869	1.000	0.878
FISVE20000 [g)]	2.208	5.537	5.407
ATILNO0001 [h)]	0.513	1.755	1.732

[a)] Scaling of the gammas - compound, [b)] Scaling of the fusion cross section, [c)] Height of the 1st barrier - compound , [d)] Scaling of the total cross section, [e)] Level density shift - compound, [f)] Height of the 2nd barrier - compound, [g)] Level Vibrational enhancement (saddle) of 2nd barrier - compound, [h)] Scaling of the level density (parameter "a") - target

One can notice that only the FISVF10000 parameter variation indicated by the data assimilation exceeds the 1 σ initial uncertainty, while the other variations stay within that range. The In Table 11 we report the contribution of the parameter variations of Table 10 to the relative change of the C/Es of the PROFIL1, TRAPU2, and COSMO (The contributions for the pROFIL2 experiment are very similar to those of PROFIL1, and those of TRAPU1 and TRAPU3 are very similar to those of TRAPU2).

The χ^2 test after adjustment provided a normalized (to the number of degrees of freedom) value of 1.40; however, most of the contributions to this value are coming from the two PROFIL experiments and the COSMO one as shown in table V. This is mainly due to the fact that two PROFIL experiments and the three TRAPU ones have very similar sensitivities but their C/Es are contradictory (large discrepancies for PROFIL and acceptable ones for TRAPU). For COSMO the large contribution is due to the fact that in order to achieve a reasonable C/E the variation on the FISVF10000 (by large the main contributor) has to exceed in a significant amount the1 σ uncertainty.

An attempt was done using only the two PROFIL and the COSMO experiments. The χ^2 Stay essentially the same with the major contribution now coming from the COSMO experiment (~0.999), but for the PROFIL experiments the new C/E after adjustment are very close to (~1.01).

Table IV Contribution of the parameter variation to the relative change of the C/E of selected experiments.

Parameter	^{243}Am buildup PROFIL1 (%)	^{243}Am buildup TRAPU2 (%)	Fis.^{242}Pu/Fis.^{235}U COSMO (%)
TUNE00000 [a)]	-2.53	-2.55	0.20
FUSRED00000 [b)]	-1.33	-1.42	-1.62
FISVF10000 [c)]	-1.15	-1.28	12.15
TOTRED00000 [d)]	-0.79	-0.76	-0.95
LDSHIF0000 [e)]	0.48	0.48	-0.03
FISVF20000 [f)]	-	-	1.02
FISVE20000 [g)]	-	-	0.23
ATILNO0001 [h)]	-	-	-0.18
TOTAL	-5.38	-5.64	10.99

[a)] Scaling of the gammas - compound, [b)] Scaling of the fusion cross section, [c)] Height of the 1st barrier - compound , [d)] Scaling of the total cross section, [e)] Level density shift - compound, [f)] Height of the 2nd barrier - compound, [g)] Level Vibrational enhancement (saddle) of 2nd barrier - compound, [h)] Scaling of the level density (parameter "a") - target

Table V. Contribution by experiment to χ^2

Experiment	Contribution to χ^2
^{243}Am buildup PROFIL1	0.573
^{243}Am buildup PROFIL2	0.419
^{243}Am buildup TRAPU1	-0.060
^{243}Am buildup TRAPU2	0.008
^{243}Am buildup TRAPU3	-0.069
Fis.^{242}Pu/Fis.^{235}U COSMO	0.529
TOTAL	1.402

5. ^{105}Pd DATA ASSIMILATION

In this case we have only one integral parameter the ^{106}Pd build up in the ^{105}Pd sample of PROFIL-1. This parameter provides information on the ^{105}Pd capture cross the section. A total of 24 nuclear parameters were used in EMPIRE for characterizing the evaluation of the ^{23U} cross sections.

BNL provided the covariance matrix of these parameters as well the sensitivity of them in terms of multigroup cross sections, and as before for the ^{242}Pu a statistical adjustment was carried out. Table VI shows the C/E before and after adjustment with related uncertainties.

Table VI. Old and new C/E before and after adjustment for ^{106}Pd build up in the ^{105}Pd sample of PROFIL-1

Experiment	old C/E ± σ	new C/E ± σ
^{106}Pd buildup PROFIL1	**0.835± 0.028**	**0.990± 0.027**

A significant improvement was obtained with respect to the initial discrepancy; however, the χ^2 test after adjustment provided a normalized (to the number of degrees of freedom) value of 3.23which is quite a large value.

Table VI provides the obtained parameter variations and the related standard deviations before and after the data assimilation for the parameters that mostly affect the assimilation (contribution to the relative change of C/E are shown in table VIII).

Table VII ^{105}Pd parameter variations and standard deviations obtained by data assimilation.

Parameter	Variation (%)	Init. Stand. Dev. (%)	Final Stand. Dev. (%)
TUNE000000 [a)]	69.253	40.00	10.77
ATILNO0000 [b)]	-2.573	1.49	0.43
FUSRED00000 [c)]	0.353	2.00	1.99

[a)] equilibrium decay width for ^{106}Pd (compound), [b)] level density parameter for ^{106}Pd (compound), [c)] tuning (scaling factor) for fusion (reaction) cross section

Table VIII Contribution of the parameter variation to the relative change of the C/E for ^{106}Pd build up in the ^{105}Pd sample of PROFIL-1.

Parameter	Contribution (%)
TUNE000000 [a)]	20.46
ATILNO0000 [b)]	-2.14
FUSRED00000 [c)]	0.19
TOTAL	18.52

[a)] equilibrium decay width for ^{106}Pd (compound), [b)] level density parameter for ^{106}Pd (compound), [c)] tuning (scaling factor) for fusion (reaction) cross section

As it can be seen both TUNE00000 and ATILNO0000 require change in their values that exceed significantly the initial standard deviation, and this, therefore, explain the large value of χ^2. The standard deviations of the nuclear parameters are calculated using differential measurements, therefore, it is possible that there is some contradictory information between the differential and integral measurements.

6. CONCLUSIONS

In this annual report we have again illustrated the methodology of the consistent data assimilation that allows to use the information coming from integral experiments for improving the basic nuclear parameters used in cross section evaluation.

A series of integral experiments were analyzed using the EMPIRE evaluated files for ^{242}Pu and ^{105}Pd. In particular irradiation experiments (PROFIL-1 and -2, TRAPU-1, -2 and -3) provide information about capture cross sections, and a critical configuration, COSMO, where fission spectral indexes were measured, provides information about fission cross section.

The observed discrepancies between calculated and experimental results were used in conjunction with the computed sensitivity coefficients and covariance matrix for nuclear parameters in a consistent data assimilation.

The results obtained by the consistent data assimilation indicate that not so large modifications on some key identified nuclear parameters allow to obtain reasonable C/E. However, for some parameters such variations are outside the range of 1 σ of their initial standard deviation. This can indicate a possible conflict between differential measurements (used to calculate the initial standard deviations) and the integral measurements used in the statistical data adjustment. Moreover, an inconsistency between the C/E of two sets of irradiation experiments (PROFIL and TRAPU) was observed for ^{242}Pu.

This is the end of this project funded by the Nuclear Physics Program of the DOE Office of Science. We can indicate that a proof of principle has been demonstrated for a few isotopes for this innovative methodology. However, we are still far from having explored all the possibilities and made this methodology to be considered proved and robust. In particular many issues are worth further investigation:

- Non-linear effects
- Flexibility of nuclear parameters in describing cross sections
- Multi-isotope consistent assimilation
- Consistency between differential and integral experiments

Hopefully, in the future funding will be available to investigate on these issues and make the proposed methodology more powerful and robust. The potential gains in terms of reduced uncertainties attached to nuclear data for the design of advanced nuclear systems are promising and very attractive.

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