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Application of an iterative methodology for cross-section and variance/covariance data adjustment to the analysis of fast spectrum systems accounting for non-linearity

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ABSTRACT

The data assimilation benchmark launched by the "Subgroup 33" on "Methods and issues for the combined use of integral experiments and covariance data" of the Working Party on Evaluation Cooperation (WPEC) of the OECD Nuclear Energy Agency Nuclear Science Committee is recalculated by means of a multistep adjustment procedure using the deterministic code system ERANOS in conjunction with a dedicated Generalized Linear Least-Squares approach based on the Bayesian parameter estimation method. Nuclear data in terms of multi-group cross-sections as well as their variances and covariances, are adjusted for 11 nuclides, namely ^{10}B, ^{16}O, ^{23}Na, ^{56}Fe, ^{52}Cr, ^{58}Ni, ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu and ^{241}Pu and 6 nuclear reactions which are elastic and inelastic scattering, lumped (n,2n) and (n,3n), capture, fission and $\bar{\nu}$. The adjustment is carried out by making use of experimental data for 19 integral parameters obtained in 7 different fast spectrum systems. In the determination of a posteriori values for these integral parameters including effective multiplication factors, spectral indices and void effects, along with their nuclear data uncertainty, the required adjusted data for these nuclides and reactions are generated in conjunction with pre-computed sensitivity coefficients of the analytical integral parameters to the nuclear data to adjust. The suggested multistep scheme aims at accounting for non-linear effects. Correspondingly, the sensitivity coefficients are recalculated within an iterative procedure on the basis of the a posteriori analytical values and adjusted cross-sections. The adjustment is thus repeated several times until convergence is reached for the analytical values and their uncertainties.

An important result of the study is that the asymptotic analytical values of the integral parameters are closer to the experimental values as compared to the standard first adjustment results. Moreover, the asymptotic analytical values seem rather independent of the specific a priori variance/covariance data used in the analysis, namely COMMARA-2.0 or BOLNA, despite different a priori analytical values respectively obtained with JEFF-3.1 or ENDF/B-VI.8 data. The asymptotic uncertainties obtained on the basis of the two libraries are also similar.

1. Introduction

The international "Subgroup 33" on "Methods and issues for the combined use of integral experiments and covariance data" of the Working Party on Evaluation Cooperation (WPEC) of the OECD Nuclear Energy Agency Nuclear Science Committee has investigated methods and issues of the combined use of integral experiments and covariance data, in order to give directions for finally recommending a set of best and consistent practices to improve evaluated libraries (Salvatores et al., 2014). In particular, a benchmark exercise has been launched in order to test the reliability of the current nuclear data adjustment methodologies which are based on data assimilation methods (Rearden et al., 2011).

In this study, the re-calculated benchmark focuses on the French deterministic code system ERANOS and the associated data libraries (Rimpault et al., 2002) used in conjunction with recent variance/covariance libraries, namely COMMARA-2.0 (Herman et al., 2011) and BOLNA (Salvatores et al., 2008).

In the analysis, standard ERANOS options for sodium-cooled configurations are employed in conjunction with a Generalized Linear Least-Squares (GLLS) approach based on the Bayesian parameter estimation method in order to carry out the adjustment. More precisely, nuclear data in terms of multi-group cross-sections as well as their variances and covariances, are adjusted for 11 nuclides, namely ^{10}B, ^{16}O, ^{23}Na, ^{56}Fe, ^{52}Cr, ^{58}Ni, ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu

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and ^{241}Pu and 6 nuclear reactions which are elastic and inelastic scattering, lumped (n,2n) and (n,3n), capture, fission and $\bar{\nu}$. The selection criteria for this set of nuclides limiting the calculation effort but at the same time emphasizing important trends are described in Section 2. The adjustment is carried out by making use of experimental data (*E*-values) for integral parameters obtained in 7 different fast spectrum systems also described in Section 2. In the determination of a posteriori values for these integral parameters including effective multiplication factors, spectral indices and void effects, along with their nuclear data uncertainty, the required adjusted data for these nuclides and reactions are generated in conjunction with pre-computed sensitivity coefficients of the analytical integral parameters (*C*-values) to the nuclear data to adjust. The suggested multistep scheme aims at accounting for non-linear effects. Correspondingly, the sensitivity coefficients are recalculated within an iterative procedure on the basis of the a posteriori *C*-values and adjusted cross-sections. About 5 iterations were found in general sufficient to reach convergence. A similar approach was originally proposed in the eighties (D'Angelo et al., 1988; Muir, 1989) and revisited later on (Latten and Cacuci, 2012,) to cope with non-linear effects by using higher order sensitivity coefficients in conjunction with a Gauss–Newton iteration scheme.

Nuclear data assimilation techniques get nowadays more relevance, since the number of facilities in operation and consequently the amount of dedicated high-quality measurements in specific energy ranges are steadily decreasing. To improve the overall core characterization in design studies of advanced reactors, it is clearly of primary importance to reduce the uncertainty of performance parameters due to nuclear data uncertainties below limits which normally cannot be reached by using unadjusted data.

Section 2 briefly recalls the benchmark specifications and the experimental data base used in the adjustment. Section 3 describes the principles and gives the main equations of the adjustment methodology; Section 4 presents the main results which are obtained using unadjusted (or a priori) as well as adjusted (or a posteriori) nuclear data, in addition to those generated with the same data, but for integral parameters measured in other configurations which are not part of the benchmark. Finally, the concluding Section 5 gives besides the summary, recommendations for future work.

2. Benchmark exercise and current customization

The basis of this study is the benchmark exercise defined in the framework of the International "Subgroup 33" on "Methods and issues for the combined use of integral experiments and covariance data" of the Working Party on Evaluation Cooperation (WPEC) of the OECD Nuclear Energy Agency Nuclear Science Committee (Salvatores et al., 2014). The selection of 20 fast neutron spectrum integral parameters, including the effective multiplication factor k_{eff}, spectral indices in terms of reaction rates relative to ^{235}U fission near the core center, and sodium void reactivity effects, has been decided based upon the availability of well documented specifications and experimental uncertainties covering a wide range of fast neutron energy spectra.

With the abbreviations *F28*, *F25*, *F49*, and *F37* respectively used for ^{238}U, ^{235}U, ^{239}Pu, and ^{237}Np microscopic fission reaction rate per atom; *C28* denoting the ^{238}U capture reaction rate per ^{238}U atom expressed as the former reaction rates in s^{-1}, these parameters, which were obtained in 7 different experimental configurations, are

1. k_{eff}, *F28/F25*, *F49/F25*, *F37/F25* which were measured in Jezebel (^{239}Pu configuration), named Jezebel-Pu239.
2. k_{eff} which was measured in Jezebel (^{240}Pu configuration), named Jezebel-Pu240.
3. k_{eff}, *F28/F25*, *F37/F25* which were measured in Flattop (Pu configuration), named Flattop-Pu.
4. k_{eff}, *F28/F25*, *F49/F25*, *C28/F25* which were measured in ZPR6-7.
5. k_{eff} which was measured in ZPR6-7 (High ^{240}Pu content), named ZPR6-7 Pu240.
6. k_{eff}, *F28/F25*, *F49/F25*, *C28/F25*, as well as reactivity effects for two sodium void configurations, which were measured in ZPPR9. The two sodium void configurations include a small voided configuration situated near the core center and a larger, leakage dominated configuration, respectively named "Na Void Step 3" and "Na Void Step 5".
7. k_{eff} which was measured in JOYO.

The current adjustment was carried out by assimilating, i.e. taking into account and integrating into the approach useful information provided by the integral parameters, and this essentially in terms of experimental values along with their uncertainties, whence the general terminology "data assimilation" (Rearden et al., 2011). When calculating a priori and a posteriori analytical values of these integral parameters along with their nuclear data uncertainties, unadjusted, respectively adjusted multi-group cross-sections and associated variance/covariance data for 11 nuclides were considered (Salvatores et al., 2014).

On the one hand, for non-fuel materials, ^{10}B, which is a major absorbing material, has been primarily chosen for cross correlation testing. Cross correlations may include, besides covariance data of different energy groups for the same nuclide and reaction, also covariance data of different reactions for the same nuclide and additionally for different nuclides. As it is well-known (Salvatores et al., 2014) cross correlations do largely originate from the adjustment of the variance/covariance data itself. ^{16}O has been envisaged as an important slowing down material which is part of the oxide fuel. ^{23}Na has been selected as the coolant material in view of analyses of sodium-cooled systems. ^{56}Fe, ^{52}Cr and ^{58}Ni are major structural materials.

As regards fuel nuclides, on the other hand, the selection was directed towards the main actinides. In addition, ^{235}U and ^{239}Pu may also be important for cross correlation testing, ^{238}U for indirect spectral effects due to its large inelastic scattering cross-section, and last but not least, ^{240}Pu and ^{241}Pu as important constituents of Pu based fuels.

In the analysis,

1. The deterministic code system ERANOS (Edition 2.2-N) is thoroughly used. The simulations make use of standard options for typical sodium-cooled configurations with blankets (Rimpault et al., 2002), including cell calculations carried out with 1968 fine groups in conjunction with probability tables used within the subgroup method. More specifically, the one- and two-dimensional, finite-difference, discrete-ordinates transport-theory code BISTRO is used for direct and adjoint flux calculations in spherical or cylindrical geometry depending on the experimental configuration to investigate. In these calculations performed with the standard 33 neutron group structure in conjunction with P_1S_{16} approximations, since higher order anisotropic cross-sections are not provided in 1968 groups, the angular fluxes are approximated on the basis of the built-in symmetric level weights and directions (Stacey, 2007). These angular fluxes allow determining, besides the targeted ratios (*C/E*s) of analytical (*C*) to experimental (*E*) values, sensitivity coefficients of the integral parameters to the data to adjust, using standard perturbation-theory methods. These sensitivity coefficients are then used both in the adjustment of the cross-sections and variance/covariance data (Section 3) and in related