Impact of the treatment procedure of recently available nuclear data covariance matrices on nuclear reactor uncertainty analysis

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Abstract

Large effort is being invested recently in the preparation of covariance matrices for the new generation evaluated nuclear data. In the Resolved Resonance Range (RRR), new evaluation procedure provides the uncertainties on the resonance parameter uncertainties. This new data is associated with new programs which propagate the uncertainties trough the cross section processing.

The covariance matrices can now be self-shielded in the same way as the cross section. The impact of this treatment on the obtained covariance matrices and their dependence on parameters like energy group structure is presented in this paper.

KEYWORDS: Nuclear data uncertainties, covariance matrices, sensitivity analysis, uncertainty analysis, self-shielding

1. Introduction

An increased demand for nuclear data uncertainty studies can currently be observed, driven by the needs for applications like innovative reactors (generation IV or ADS) [1, 2, 3] that will use materials for which nuclear data are less well known, fusion reactor and criticality safety. For the estimation of confidence level to be assigned to the numerical simulations of nuclear applications, new evaluation tools [4, 5] able to provide nuclear data uncertainties together with the classical nuclear data, are being developed.

This paper presents some applications of the recent nuclear data covariance matrices. Experience with the impact of the treatment procedure (self-shielding and energy group collapsing) of the resolved resonance range uncertainty data is shown in details. Numerical examples are based on ^{233}U and ^{232}Th made in the framework of the IAEA-CRP on Evaluated Nuclear Data for Thorium-Uranium Fuel.

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Recent development of the treatment of uncertainties in Resolved Resonance Range allows the propagation of the uncertainty on resonance parameter down to the averaged cross sections [6]. The uncertainty can be self-shielded using Bodarenko factors, in the same way as the cross sections are processed in the NJOY [7] module GROUPR. The impact of self shielding on the total uncertainty of the k_{eff} for some reactors is studied, using the sensitivity and uncertainty code package available from OECD/NEA.

2. Presentation of the new data

2.1 Evaluation procedure

Nuclear data in the resonance range are now based on the R-matrix theory. The resonances are described by Reich-Moore formalism. The new fitting procedure [5] gives the uncertainty on the resonance parameters together with these parameters. It is even possible to reevaluate the uncertainty on these parameters subsequently [8].

JENDL3.3 was the first library containing such nuclear data uncertainties for 6 nuclei. This paper presents results based on more recent evaluation of ^{233}U and ^{232}Th. The ^{233}U data are a "working" version provided by L. Leal, limited to the Resonance Region, the one of interest in this paper. The ^{232}Th data were provided by A. Trkov [9] and correspond to the close to the final version of the file. Updates of some modules of NJOY were found to be needed to be consistent with the new format and were also provided by A. Trkov.

2.2 Treatment in ERRORJ

2.2.1 Calculation principle

The evaluation files contain the information on the basic nuclear data such as resonance parameters. All deterministic and some stochastic transport programs need group-averaged cross sections. The module ERRORR of NJOY [7] was developed to process covariance matrix data but is not able to treat some new formats. An extension of the code, called ERRORJ [6], was therefore prepared at JAERI, Japan.

ERRORJ calculates the sensitivity of the average group cross section to one resonance parameter by recalculating this cross section after a 1% change of this parameter. At present the processing of the covariances by ERRORJ is limited to one temperature (1K).

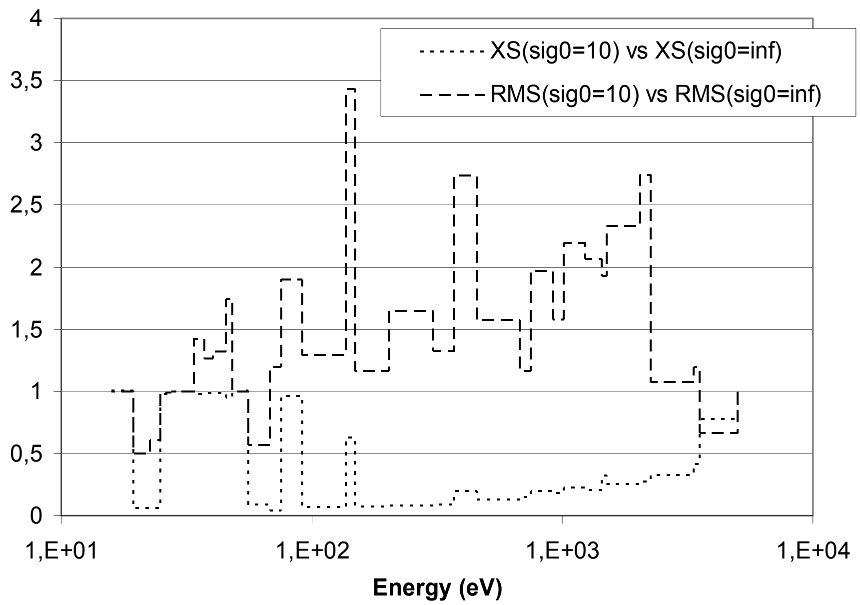
2.2.2 Self-shielding

Self-shielding tends to reduce the effective cross-section in the resonance range when compared to the unshielded one. This means that the impact of resonances on the effective cross section is not as high as one can expected. Hence, if the uncertainties on the resonance parameters are the biggest contribution to the total one, the global uncertainty should tend to decrease with self-shielding., as it used to be with the first evaluation of ^{238}U using these techniques [6] in JENDL3.3 library. As shown on Fig. 1 this is the case with the latest ^{232}Th evaluation only in groups containing the main resonances around 22 eV and 69 eV.

The cross section sensitivity/uncertainty (S/U) program SUSD3D [10] by OECD/NEA Data Bank uses self-shielded cross sections for the sensitivity calculation. The value of the dilution cross section is representative of the values given by the cell-code in the region of maximum sensitivity. Even if unique for all groups, this solution has proven to be reliable. The same value of the dilution cross section is used in ERRORJ to self-shield the uncertainties in a consistent approach. The values used are 10 barns for the ^{232}Th and 100 barns for the ^{233}U.

Fig. 2 presents the older ENDF/B-V covariance matrices of ^{232}Th. Fig 3 a and b show the new covariance matrices, respectively unshielded and shielded. The quantity of information contained in the new matrices appears clearly in the resonance structure of the uncertainty.

Figure 1: Comparison of the uncertainty on the ^{232}Th capture cross section in function of the dilution cross section in the resonance region.



2.4 Mathematic properties of the matrices

2.4.1 ANGELO program

The user is strongly recommended to check that the matrix processing does not affect the mathematical properties (positiveness, number of positive eigenvalues) of the matrices. The LAMBDA [11] program can be used for this purpose. Tab. 1 shows the number of positive eigenvalues of some matrices processed using various options. All the matrices are positive. Some cross correlations between different reactions were found to be inconsistent, i.e. their correlations were larger than one.

The reduction of number of groups from 172 to 26 reduces considerably the quantity of information contained in the covariance matrices. One should keep in mind that even with 172 groups, this quantity has already been reduced as compared to the large size of the original covariance matrices. Each resonance is represented by many parameters (resonance energy, resonance width, partial widths…) and more than 700 resonances are resolved in the new thorium evaluation file!

Table 1: Total number of positive eigenvalues of the covariance matrices for some reactions of ^{233}U and ^{232}Th

	^{233}U		^{232}Th	
Reaction	172 G	26 G	172 G	26 G
Total	29	10	55	17
Diffusion	29	12	47	15
Fission	33	11	12	3
Capture	50	15	40	14

Figure 2: Covariance matrix of ^{232}Th capture cross section available in the ENDF/B-V evaluation.

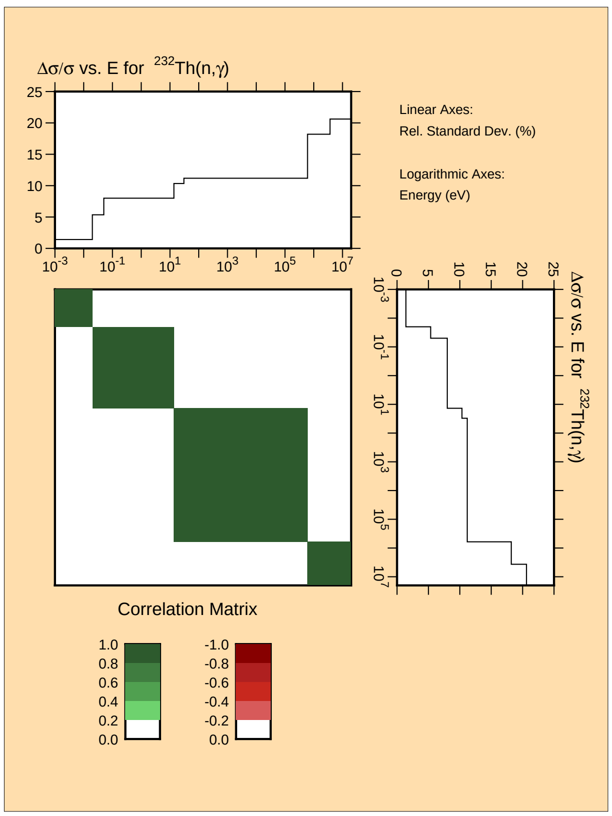
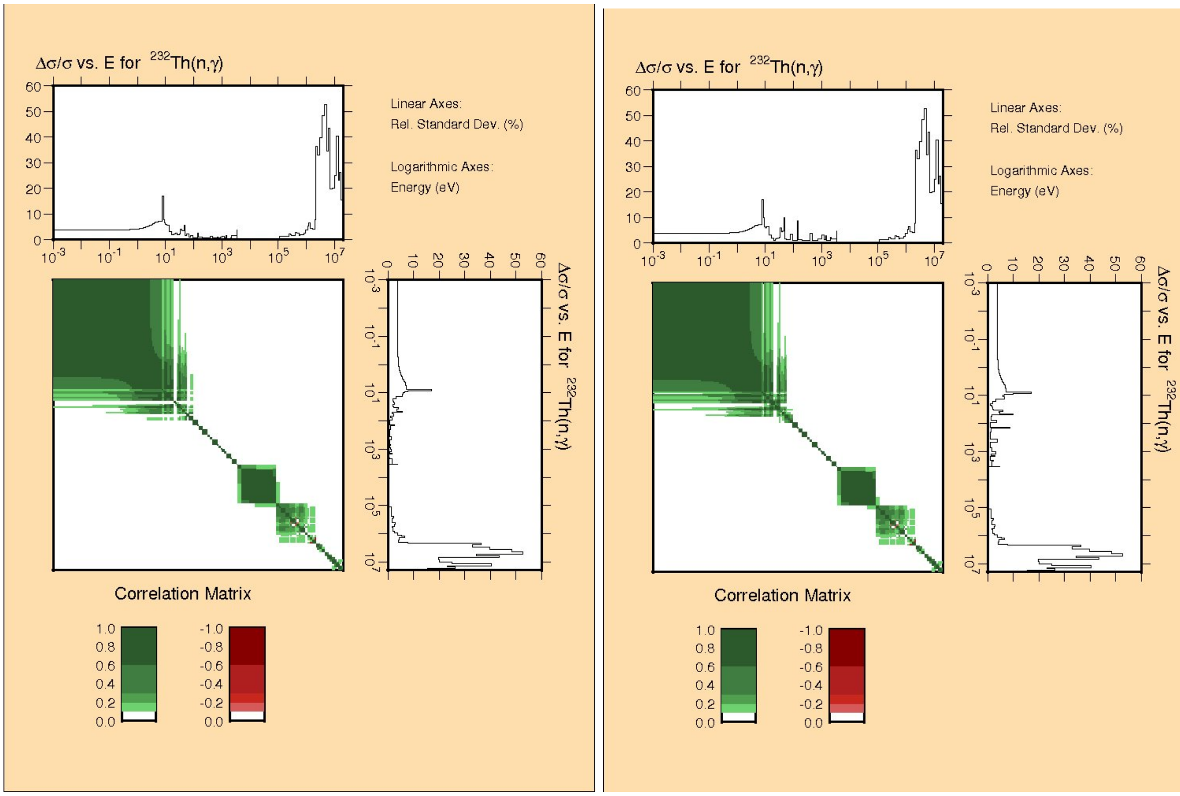


Figure 3 a and b: New covariance matrices of ^{232}Th capture cross section. 3 a is for unshielded and b is shielded case.



3. Applications

3.1 Thorium Molten Salt Reactor

Molten Salt Reactors are one of the six reactor concepts selected as potential GEN IV reactors. In these concepts, the fuel is dissolved in the molten salts, which is used also as coolant. This configuration has proven to be both very efficient and safe in successful experiment done in Oak Ridge during the 60's. Furthermore, the constant circulation of the liquid fuel can be used to assure on-line recycling. This characteristic makes the concept very suitable for Thorium fuelled. In this cycle, the regeneration[1] is limited by the quite low number of neutron available. Thus, the continuous removal of the poisoning fission product makes the regeneration feasible. This concept is being developed [12] in France in the framework of the GEDEPEON research group. The sensitivity and uncertainty analysis of the k_{eff} of one of those concepts has been studied in details [13]. In the configuration chosen, the neutron spectrum is epi-thermal and thus quite sensitive to the nuclear data of the resonance range. The next paragraph presents the comparison of the uncertainty analysis using the new covariance matrices, obtained with various treatment options.

[1] Regeneration is the first necessary condition of GEN IV concepts: no concepts can be developed on the long term without maintaining, at least, a constant stock of fissile material.

3.1 Results

Tab. 2 summarises the results obtained for the two nuclei of interest.

Table 2: Contribution to the uncertainty on k_{eff} of ^{233}U and ^{232}Th (%)

	^{233}U		^{232}Th	
Dilution (b)	Infinity	100	Infinity	10
172 G	1,4677	1.4783	0,3064	0,3021
26 G	1,5861	1,6254	0,2501	0,2058
Previous data	0.280		3,620	

3.1.1Comparison with older results

The impact of the uncertainties on Thorium cross sections is decreased by more than a factor of 10. This is due to the fact that the new evaluation is based on new measurements [14]. The quality of the new measurements explains most of the reduction of the uncertainties but also of the correlation between energy groups due to their good energy resolution. Nevertheless, the resulting uncertainty on the capture cross section (lower than 2 % in most of the groups above 100 eV) seems surprisingly low when compared to the accuracy achieved experimentally.

No new experimental data were used for the evaluation of ^{233}U. The increase in the uncertainties is explained by the quite different evaluation procedure of the uncertainties used in the JENDL3.3 from which the data were taken for the previous S/U analysis. At this time the uncertainties on the resonance parameters were tuned so as to reproduce the expected uncertainties on a very rough energy grid containing only one group below 100 eV. This used to lead to serious underestimation of the uncertainties in the RR, which were averaged with high uncertainties in the thermal part to give a reasonable average. This compensation between energies is still noticeable in the new nuclear data sets, but this time the new results seem to overestimate the uncertainty on the fission cross section in particular at thermal energy. Even if the nuclear data of the Thorium cycle are not as well known as those of Uranium cycle, many critical experiments and nuclear reactor were fuelled with ^{233}U. Thus an uncertainty of 15% at thermal energies is probably too high, in particular when compared to the proposal of reference [15].

3.1.2Effect of the reduction of the energy grid

Reducing the number of energy groups is needed in deterministic neutron transport programs to keep the calculation time of large simulations reasonable. This reduction of course reduces the information contained in the covariance matrices. This effect was confirmed in the previous part.

The uncertainty on the k_{eff} is a non linear function of covariance matrices and sensitivities. The smallest uncertainties can be quite important once weighted by the sensitivities. So, even if the largest eigenvalues are conserved in the data reduction, the reduction of the group number can still impact the global result.

The combination of these two effects can be seen in Tab. 2. With our tools, the final result can change by 30% when reducing the number of groups from 172 to 26.

3.1.3Effect of self shielding

The effect of the self shielding of the uncertainties seems limited for most of the studied cases except for ^{232}Th in 26 energy group structure. The uncertainties in the cross sections can change by more than a factor of 2 in some groups. The global effect is often weighed by the compensations between different energy groups as well as changes in the correlation matrices. It seems that these compensations do not take place in some cases. Our limited experience, given by the presented tests, show that the self-shielding of the covariance matrices may change the result by ~20%.

5. Conclusion

New evaluation procedures have been developed to extract the uncertainties on the resonance parameters. New computer programs where developed to propagate the uncertainty information down to the user's defined energy groups structure cross sections. Even though the results presented here are based on preliminary evaluated files and processed by programs still in their development and testing phase, the resulting covariance matrices have proven to have both reasonable mathematical properties and physical meaning. Some issues remain to be investigated such as the treatment of the resonance broadening to temperatures different from 1K. Another important point is the study of the tendency of the uncertainty to decrease steadily in the resonance range, in particular in the unresolved part of it.

The new covariance matrices should be considered as a big step forward. They contain considerably more information than the previous data. The information is already sufficiently reliable to prove that the effort made to improve the evaluation of nuclear data needed for Thorium cycle systems has paid off. In particular the capture cross section of ^{232}Th may not be any more the limiting factor of the estimation of the k_{eff}.

The improvement in quality of the new data is linked to an increase in the complexity of the treatment. In this paper, the impact of the tuning of some important parameters on the contributions of the uncertainties of the most important nuclides of the thorium cycle has been studied. Both energy grid reduction and self-shielding were found to change the contribution of some reaction to the uncertainty by about 10%. This is not so important when compared to the confidence that one can have in the uncertainty information. As this confidence will improve with the use of the new evaluation tools and the experience of the evaluators, the details of these impacts should be studied, in particular for applications such as criticality safety.

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