EPJ Web of Conferences **281**, 00009 (2023) https://doi.org/10.1051/epjconf/202328100009
CW2022

Evaluation of covariance data in JENDL

Osamu Iwamoto[1]*

[1]Nuclear Data Center, Japan Atomic Energy Agency, 2-4 Shirakata, Tokai-mura, Naka-gun, Ibaraki 319-1195, Japan

Abstract. Evaluation of covariance for JENDL was virtually started after the release of JENDL-3.2. The covariance data were obtained for 16 nuclides and compiled to the JENDL-3.2 Covariance File. At the time of the JENDL-4.0 development, covariances were much enhanced especially for actinides; covariance data were given for 99 nuclides in total. The latest version JENDL-5 includes covariance data for 105 nuclides by adding new evaluations for light nuclides and structure materials. An overview of the covariance evaluation for JENDL is presented.

1 Introduction

Covariance of evaluated nuclear data libraries provides information about the uncertainties of the evaluated data including correlations. The covariance data enable users to estimate uncertainties originated from nuclear data. Therefore, it is important to provide the covariance data in the evaluated nuclear data libraries for nuclear data applications.

Concerning the covariance of JENDL, discussions were started as a next scope of JENDL-2 [1]. Those discussions were performed from both development and application points of view, including topics of evaluation methods on theoretical calculations, uncertainty in measurement, covariances in least square fitting, sensitivity analyses for reactivity analyses, decay heat estimations, and dosimetry utilizations. The first covariance data were provided in JENDL-3 released in 1989. However, the covariance data were given only for ^{55}Mn. To provide enough covariance data for applications, the Covariance Evaluation WG was established in 1993 under the Sigma Committee [2] and covariance data for 16 nuclides were evaluated for JENDL-3.2. The evaluation of covariance data has been continued for JENDL-3.3, JENDL-4.0 and JENDL-5 to increase both of the amounts and qualities.

At the beginning, major targets of the covariance data of JENDL were about fast reactors [3]. The covariance was used to increase the accuracy of the calculation for the fast reactors by means of nuclear data adjustment methods [4, 5]. Recently, the covariance data were also utilized to estimate the uncertainties for an innovative reactor, e.g., for accelerator-driven system [6]. In addition, to promote the use of the covariance data, a couple of working groups: Covariance Utilization WG (2011-2017), and Covariance Data Utilization and Promotion WG (2018-2020) were organized under the JENDL Committee (one of successors of the former Sigma Committee).

An overview of the evaluation and current status of covariance data in JENDL is presented, mainly for actinides.

2 Progress of covariance evaluation for JENDL

Figure 1 shows the number of nuclides with covariance data in the released libraries as JENDL so far. As shown in the figure, the evaluation of the covariance data was virtually started after the release of JENDL-3.2. For JENDL-3.2, the covariance data for 16 nuclides were evaluated and compiled as the JENDL-3.2 Covariance File. This covariance evaluation was performed with a motivation to give data for the nuclear data adjustment for fast reactor applications. The library included the data for the isotopes of H, B, O, Na, U and Pu as well as some of structural materials. Most of them were taken over to JENDL-3.3 with some new evaluations; the number of nuclides with covariance increased to 20 for JENDL-3.3. At the time of the JENDL-4.0 development, much efforts were made for covariance evaluation especially for actinides. Finally, the covariances of JENDL-4.0 were provided for the cross sections in the resonance to fast neutron energy regions, angular distributions of elastic scattering, and fission neutron related data. The number of nuclides with covariance increased to 99 (24% of all nuclides) in the updated file JENDL-4.0u. The latest version JENDL-5 provides covariance data for 105 nuclides by adding new evaluations for light nuclides and structure materials. However, due to the large increase of the total number of nuclides in JENDL-5, the percentage of isotopes with covariance data was down to 13% as shown in Fig. 1.

Regarding the evaluation methods, eye-estimation with experimental data was used to obtain the first covariance data for ^{55}Mn in JENDL-3.1. After that, for the JENDL-3.2 development, a covariance evaluation system KALMAN was developed [7]. KALMAN can be

---

* Corresponding author: iwamoto.osamu@jaea.go.jp

applied to various data to which nuclear model calculations were applied. In other case, the evaluation was sometimes performed with the least square method, which provided the most probable value with uncertainty and the covariance could be adopted to the libraries. The simultaneous evaluation of fission cross sections was one of those examples, the least square code SOK [8] was developed and applied to the simultaneous evaluations. It also provided the cross correlations between different nuclides. A new resonance analysis code AMUR [9] based on the R-matrix theory was developed for JENDL-5. It was mainly used for the evaluation of the light nuclides; the covariance of the cross sections of ^{16}O and ^{15}N were given based on the AMUR analyses in JENDL-5.

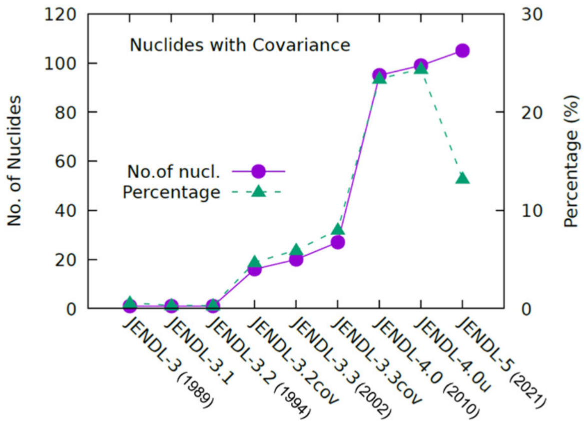

Fig. 1. The number of nuclides with covariance in JENDL

3 Covariance evaluation

The covariance evaluation was essentially based on the least square method with available experimental data. The KALMAN code developed for JENDL-3.2 was widely applied to the covariance evaluations in combination with the nuclear model codes used in the cross-section evaluations. By using the model codes depending on the evaluated data, the sensitivities of model parameters to the cross sections were calculated and applied to the least square fitting to obtain the model parameter covariance. While the nuclear reaction modelling codes were changed from the JENDL-3.2 evaluation to those of JENDL-4.0 or JENDL-5, the KALMAN code has been continuously used.

For non-model evaluations such as for fission cross sections, the values at certain energy grid points were estimated by the least square fitting with interpolation to the given energy grid; for those evaluations, the SOK [8] and GMA [10, 11] codes were applied. Both codes have similar capabilities, but SOK is better in use for the simultaneous evaluation. Covariance data obtained at the same time were adopted in JENDL with or without modifications. The least square method with a large number of data points would often give unrealistically small uncertainties which might be due to ignoring correlations and averaging the data points with a simplified model. In this case, the obtained covariance was sometimes modified to become more reasonable uncertainties by comparing with experimental data using expert judgement.

3.1 Resonance region

The resonance parameters of JENDL were sometimes taken from the published literatures, which usually gave only the resonance parameter uncertainties without correlations. The covariance data of those resonance parameters have been adopted for JENDL. However, the uncertainty of spectrum averaged cross-sections would be underestimated if the correlations were not given. To mitigate this underestimation, the background covariance was given as cross-section uncertainty.

The newly developed R-matrix resonance analysis code AMUR gives the cross sections with covariance data. For JENDL-5, AMUR was used for the evaluation of the resonance cross sections for the light nuclides of ^{16}O and ^{15}N, and the covariance data were also adopted.

Regarding the major actinides whose resonance parameters were taken from the other libraries, the covariance data of resonance region for $^{235,\ 238}$U and ^{239}Pu were also taken from the same library as the resonance parameter i.e., ENDF/B-VIII.0.

3.2 Simultaneous evaluation of fission cross section

The simultaneous evaluation was developed to estimate the fission cross sections of major actinides by taking into account the absolute and ratio measurements simultaneously for JENDL-3 for the first time. The covariance data deduced by the simultaneous evaluation were included in the JENDL-3.2 Covariance File. A new simultaneous evaluation code SOK was developed and applied to the evaluations for JENDL-3.3, JENDL-4.0 and JENDL-5. Figure 2 shows the uncertainties of the fission cross sections based on the simultaneous evaluation and the other evaluations in the IAEA Neutron Data Standards 2017 (IAEA-2017), ENDF/B-VIII.0 and JEFF-3.3. In general, those evaluated uncertainties have a relatively large differences each other, excepting between IAEA-2017 and ENDF/B-VIII.0 that adopts the IAEA data. Even for the JENDL evaluations that are derived by almost the same method,

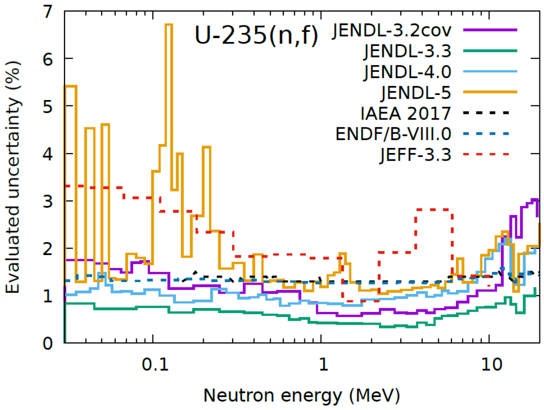

Fig. 2. Uncertainty of ^{235}U fission cross sections in JENDL and other evaluations

the differences are significant. The newest version JENDL-5 provides the largest uncertainties in spite of the accumulation of the experimental data. This situation may indicate difficulty of the evaluation of covariance. The evaluated results highly depend not only on the selection of the experimental data but also on the treatment of the experimental uncertainties. In addition, the least square method often gives unrealistically small uncertainties for fitting with a large number of the data points; to avoid this, the deduced uncertainty by the simultaneous evaluation was multiplied by a factor of 2 in the JENDL-4.0 case, where the factor was determined by the comparison with the experimental data by the evaluator.

3.3 Fission cross sections of minor actinides

The fission cross sections of minor actinides for fast neutrons were evaluated by GMA for JENDL-4.0 and most of them were carried over to JENDL-5. In the evaluation, statistical and systematic experimental uncertainties were carefully taken into account. Figure 3 shows the uncertainty and correlation of the ^{241}Am fission cross section deduced by GMA. Strong positive correlations are observed in a wide energy range; these correlations reflect the systematic uncertainties of the experimental data used for the evaluation.

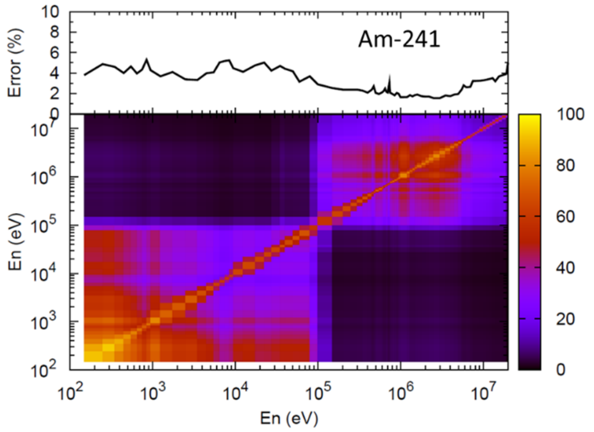

Fig. 3. Uncertainty and correlation of ^{241}Am fission cross section for fast neutrons

3.4 Capture cross section

A large part of the capture cross sections of the actinides of JENDL-4.0 was evaluated by CCONE and were taken over to JENDL-5. The KALMAN code system was applied to the evaluation of the covariance for them. The KALMAN calculation needed the sensitivities of the cross section to the model parameters. About 50 parameters such as optical model potential, level density, gamma-ray strength function and fission barrier were used.

The χ^2 value of the fitting can be a measure of the adequacy of the fitted results and the reduced chi-square may become close to 1 in an ideal case. However, in an actual case, due to unknown uncertainties of the experimental data and deficits of the nuclear modelling, large χ^2 values often come out. For the capture cross section, to compensate those deficiencies, the uncertainties of the experimental data were modified so as to become χ^2 =1 via fitting to each experimental data independently.

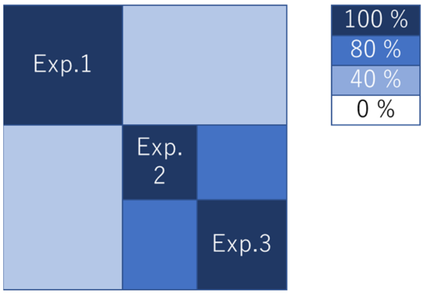

Fig. 4. Assumed correlation between experimental data sets

A generalized least square method used in KALMAN is usually applied to each experimental data by sequentially updating the covariances. However, this sequential update neglects the correlations between the experimental data sets. Because there are similarities between the experimental methods and analysis among the data sets, neglected correlations might exist. For the JENDL-4.0 evaluation, the correlations between the experimental data sets were introduced. Due to the difficulty for estimating the correlations, those correlations were assumed to be 0.8 for the data sets (e.g., Exp.2 and Exp. 3) by the same author, and 0.4 for different authors (e.g., Exp. 1 and Exp.2) with expert judgement as shown in Fig. 4.

Because the posterior cross section estimated by KALMAN would be changed from the original evaluated data, the covariance matrix was deduced as

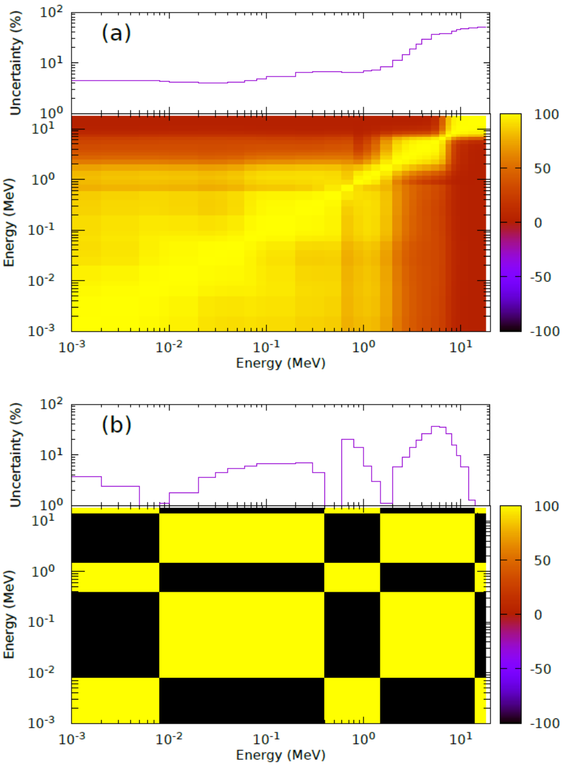

Fig. 5. Covariances of (a) KALMAN and (b) difference between posterior and original value for ^{237}Np capture cross section

covariance with respect to the original evaluated value σ_0^i, i.e.

$$C^{i,j} = \langle(\sigma^i - \sigma_0^i)(\sigma^j - \sigma_0^j)\rangle$$
$$= C_K^{i,j} + \Delta^i\Delta^j,$$

where i and j indicate the energy indexes, $C_K^{i,j}$ is a covariance deduced by KALMAN, Δ^i is difference between the posterior cross section and original value. Figure 5 shows covariance data for neutron capture cross section for ^{237}Np. Strong positive correlations are observed for covariance deduced by KALMAN, while the strong positive and negative correlations alternately appear in the component of the cross-section difference.

3.5 Other nuclear data evaluated with CCONE

For the nuclear data evaluated with CCONE, the covariances other than of the capture cross sections were deduced by a rather simple way. The KALMAN fitting was applied with the representative data that was evaluated to have the original value with the uncertainties to be consistent with the uncertainty and/or scatter of the experimental data points. With this method, posterior cross sections have the same values with the priors. Therefore, it was not needed to consider the change of the cross sections unlike for the capture cross section.

Regarding the angular distribution of elastic scattering of ^{238}U, the uncertainty of P$_1$ component at around 144 keV, where the P1 dominated the distribution, was estimated by comparing the experimental data. Figure 6 shows the uncertainties of the angular distributions calculated by assuming 5, 10 and 20 % uncertainties for P$_1$ coefficient. From the comparison the P$_1$ coefficient uncertainty was evaluated to be about 10 % and applied to KALMAN as a representative data to obtain the energy dependent covariances.

In the case of the nuclear data for which the experimental data were not available, the covariance was estimated with the global parameter uncertainties that were deduced by comparing the calculated results with the default model parameters and the experimental data for non-actinide nuclides, due to the difficulty in the prediction for fission cross sections with default parameters.

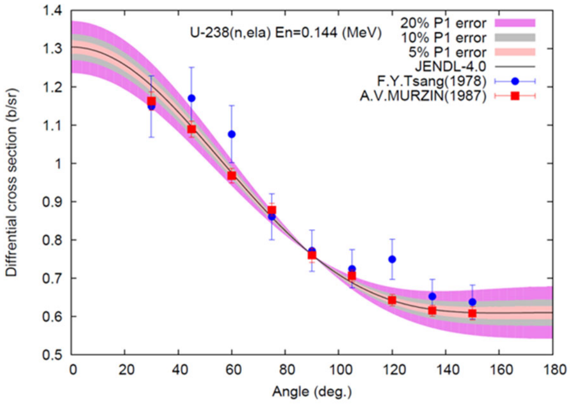

Fig. 6. Angular distribution of elastic scattering for ^{238}U. The shaged areas show uncertainties by assuming the uncertainties of the P$_1$ coefficient.

4 Conclusions

Overview of the covariance evaluation for JENDL was described. The covariance evaluation was started after JENDL-3. The latest version JENDL-5 provides the covariance data for 105 nuclides including a large part of the actinides that are needed for reactor applications. Evaluation methods and results for the covariance evaluation were briefly shown. Because the covariance data of JENDL are still limited in amount and quality in a viewpoint of utilization for various applications, they will be revised and enhanced in future JENDL releases.

The author acknowledges all of the contributors for JENDL covariance developments.

References

1. Sigma Committee, Proc. 1980 Seminar on Nuclear Data, JAERI-M 9523 (1981)
2. Y. Kanda, Nuclear Data News, **49**, 111 (1994), in Japanese
3. M. Ishikawa, Nuclear Data Sheets, **109**, 2778 (2008)
4. M. Ishikawa et al., J. Nucl. Sci. Technol., **39**: sup2, 1073 (2002)
5. K. Yokoyama et al., JAEA-Research 2018-011 (2019)
6. H. Iwamoto et al., J. Nucl. Sci. Technol., **50**, 856 (2013)
7. T. Kawano, K. Shibata, JAERI-Data/Code 97-037 (1997)
8. T. Kawano et al., J. Nucl. Sci. Technol., **37**, 327 (2000)
9. S. Kunieda et al, Nucl. Data Sheets, **118**, 250 (2014)
10. W. P. Poenitz, Proc. Conf. Nuclear Data Evaluation Methodsand Procedures, BNL-NCS-51363, Vol. I, 249 (1981)
11. S. Chiba, D. L. Smith, ANL/NDM-121 (1991)