Fundamentals of sensitivity analyses of neutron multiplication factor to nuclear data[1]

Go CHIBA
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1 Integral test of nuclear data

A particle interacts with a nucleus under a probability that depends on the particle's own incident energy. This interaction probability is defined as a *cross section* and is generally written as $\sigma_{n,x}(E)$ for nuclide n, reaction x, and particle incident energy E. Some cross sections also take into account the dependence of the energy of the secondary particles emitted as a result of the interaction. An example of this is a scattering reaction, in which the cross section can be written as $\sigma_{n,x}(E \rightarrow E')$ using the energy E' of the secondary emitted particle. Such a tabular cross section is called a *differential cross section* to distinguish it from the cross section $\sigma(E)$, which considers dependence on incident energy only. When the energy dependence of the secondary emitted particles is considered, it is called an energy differential cross section and written as $\sigma_{n,x}(E \rightarrow E')$, and when angular dependence is considered, an angular differential cross section is defined and it is referred to as the angular differential cross section. In addition, there is a cross section written as $\sigma_{n,x}(E \rightarrow E', \mu)$ which takes into account the dependence on both the energy E' of the secondary particles and the cosine of the scattering angle μ, and such a cross section is called a *double-differential cross section*[2].

The cross sections, energies/angular differential cross sections, and double differential cross sections described above, the average number of neutrons produced per fission $\nu(E)$, the fission spectrum $\chi(E)$ and others are collectively called *nuclear data*.

Since it is impossible to theoretically derive the true value of nuclear data, the most likely value is estimated from measured data and nuclear model calculations. This process is called *nuclear data evaluation*. The measured data used in this nuclear data evaluation is the data for nuclear data. On the other hand, by using the evaluated nuclear data, it is possible to numerically evaluate various characteristics of a nuclear reactor. If we can measure the characteristics data of a nuclear reactor, we can discuss whether the employed nuclear data are good or bad by comparing them with the results of numerical calculations of reactor characteristics using the nuclear data. In general, it is customary to refer to the measured data for nuclear data as *differential data* and the measured data for reactor characteristics as *integral data*. Differential data correspond to individual nuclear data while integral data are determined by multiple nuclear data.

In general, nuclear data will be made available for use as *evaluated nuclear data files*, and as indicated above, integral data will be very useful for their verification. The verification of nuclear data files using integral data is called an integral test of nuclear data, a benchmark test, and so on.

Here is an example of an integral test of nuclear data files: the ratio of calculated to experimental values (C/E values) for criticality data of ultra-small fast critical assemblies using four evaluated nuclear data files (JENDL-3.3, JEFF-3.1, ENDF/B-VII.1, and JENDL-3.2). **Figure 1** shows the ratio of calculated to experimental values (C/E values) for the criticality data of these critical assemblies. The error bars in this figure indicate the uncertainty of the measured values.

The U.S. Evaluated Nuclear Data File ENDF/B-VII reproduces experimental values within 0.4% for all criticality data, which is the best reproducibility for the criticality data covered here. On the other hand, the Japanese nuclear data file JENDL-3.3 does not show as good reproducibility as ENDF/B-VII, since the C/E value varies depending on the criticality data.

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[2] When neutron traveling directions before and after the reaction are denoted to as $\vec{\Omega}$ and $\vec{\Omega}'$, a probability of neutron traveling direction change from $\vec{\Omega}$ to $\vec{\Omega}'$ depends on the angle formed by these two vectors (called as the scattering angle), and the reaction probability is defined for its cosine.

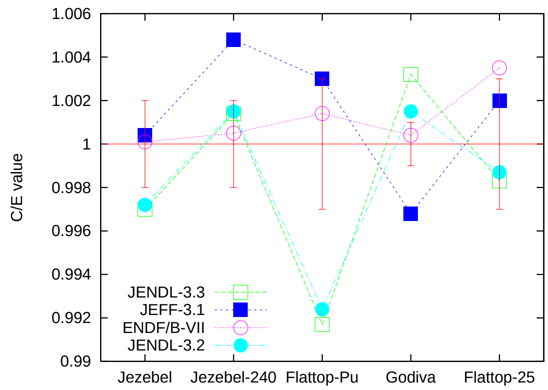

Fig. 1: C/E values of criticality data of the ultra-small fast critical assemblies

So, let us consider what information can we take from these results from the standpoint of improving JENDL-3.3?

The following is a summary of the five criticality data listed here.

- Jezebel: Bare spherical core consisting of 95% Pu-239 and 5% Pu-240
- Jezebel-240: Bare spherical core consisting of 77% Pu-239 and 20% Pu-240
- Flattop-Pu: Bare spherical fuel used in Jezebel surronded by the depleted uranium (DU) reflector
- Godiva: Bare spherical core consisting mostly of U-235
- Flattop-25: Bare spherical fuel used in Godiva surrounded by the DU reflector

Below are examples of answers to the questions posed above.

First, it may be pointed out that JENDL-3.3 underestimates the reactivity of Jezebel. Since Jezebel is a system consisting almost exclusively of Pu-239, the nuclear data of Pu-239 in JENDL-3.3 underestimates the reactivity.

Whereas it is important to discuss the "absolute" C/E values, it should be noted that there are uncertainties in the measured values. On the other hand, there is a high possibility that there is a strong relationship (correlation) between the uncertainties of measured values, for example, in integral data measured with the same facility/material/equipment, as in the case of Jezebel and Jezebel-240. In such cases, it is effective to focus on the "difference" of C/E values for these two critical data since the uncertainties of the measured values are expected to appear in the same direction and to the same extent.

Considering this point, we can first focus on the difference in C/E values between Jezebel and Jezebel-240. The fact that the C/E value of Jezebel-240, which contains a larger amount of Pu-240, is larger than that of Jezebel may indicate that the contribution of Pu-240 to the reactivity is overestimated or that the contribution of Pu-239 to the reactivity is underestimated. The possibility that the contribution of Pu-240 to reactivity is overestimated or the contribution of Pu-239 is underestimated can be pointed out.

The difference in C/E values between Jezebel and Flattop-Pu and that between Godiva and Flattop-25 can also be noted. The C/E value of the core with the DU reflector is smaller than that of the core without the DU reflector in the JENDL-3.3 result. This indicates that the neutron reflection effect of U-238 contained in the depleted uranium may be underestimated when JENDL-3.3 is used.

As described above, the results of the integral test (C/E values) allow us to raise various possibilities regarding the accuracy of the nuclear data files, and we may ask "Why is the C/E value better for ENDF/B-VII? What is the difference between JENDL-3.3 and ENDF/B-VII?" Sensitivity analysis of nuclear data can provide the answer to such questions.

2 Sensitivity analysis of the effective multiplication factor to nuclear data

The effective multiplication factor k_{eff} is obtained by numerically solving the neutron transport (diffusion) equation. Since nuclear data such as reaction cross sections between neutrons and nuclei are used for each term of the neutron transport equation, the effective multiplication factor obtained will change when the nuclear data change.

Here let us introduce the sensitivity coefficient S as an index to quantify the impact of each of nuclear data on the calculated neutron multiplication factor. The sensitivity coefficient S is defined as follows:

$$S = \frac{\partial k_{\text{eff}}}{\partial \sigma} \cdot \frac{\sigma}{k_{\text{eff}}}, \tag{1}$$

where σ is nuclear data. In this case, S is called the sensitivity coefficient of k_{eff} to σ.

In order to consider the physical meaning of the sensitivity coefficient, Eq. (1) is transformed as follows

$$S = \frac{\Delta k_{\text{eff}}/k_{\text{eff}}}{\Delta\sigma/\sigma}, \tag{2}$$

where Δk_{eff} is the variation of k_{eff} when the nuclear data σ varies by $\Delta\sigma$. From this, it can be seen that the sensitivity coefficient S means the ratio of the relative variation of k_{eff} to the relative variation of σ. If the sensitivity coefficient S is 0.5, then a 100% change in σ results in a 50% change in k_{eff}.

Let us assume that there are two nuclear data files, and let us denote them as σ^A and σ^B. If the effective multiplication factor is calculated using each nuclear data file, the resulting k^A_{eff} and k^B_{eff} will be obtained. Here, the difference between k^A and k^B (the subscript $_{\text{eff}}$ is omitted hereafter), Δk, can be calculated from the following equation:

$$\Delta k = \left(\frac{\Delta k}{\Delta\sigma}\right)(\sigma^A - \sigma^B). \tag{3}$$

The relative variation of k, $\Delta k/k^B$, can be written as follows using the sensitivity coefficient defined in Eq. (1).

$$\frac{\Delta k}{k^B} = \frac{k^A - k^B}{k^B} = \left(\frac{\partial k^B}{\partial \sigma^B} \cdot \frac{\sigma^B}{k^B}\right)\frac{\Delta\sigma}{\sigma^B} = S^B \cdot \frac{\sigma^A - \sigma^B}{\sigma^B} \tag{4}$$

In other words, the relative variation of k can be obtained by the product of the relative variation of σ and the sensitivity coefficient.

Now, suppose that σ^B is given and k^B is calculated based on it; if the calculation of k takes an enormous amount of time (say, one month), it would be very tedious to calculate k^A corresponding to a different nuclear data file σ^A. However, if the sensitivity coefficient S is known in advance, k^A does not need to be calculated directly and can be calculated using the above equation[3]. The sensitivity coefficient S^B is calculated using the nuclear data file σ^B. If there is no significant difference between the nuclear data files σ^A and σ^B, we can consider $S^A \approx S^B$.

[3]Strictly speaking, this calculation is only an approximation. The exact writing of Eq. (3) is

$$\Delta k = \left(\frac{\partial k}{\partial \sigma}\right)\Delta\sigma + \frac{1}{2}\left(\frac{\partial^2 k}{\partial \sigma^2}\right)(\Delta\sigma)^2 + \frac{1}{3!}\left(\frac{\partial^3 k}{\partial \sigma^3}\right)(\Delta\sigma)^3 + ... \tag{5}$$

and it can be seen that Eq. (3) is only a drop of terms above the second order. When $\Delta\sigma$ is small, the effect of terms above the second order can be considered negligible, but otherwise these terms will also have an effect.

The nuclear data depends on the nuclide, the type of reaction, and the energy group. If we write $\sigma_{n,x,g}$ for nuclear data of nuclide n, reaction x, and energy group g, and write $S_{n,x,g}$ for the sensitivity to $\sigma_{n,x,g}$, Eq. (4) can be written as follows:

$$\frac{k^A - k^B}{k^B} = \sum_n \sum_x \sum_g S^B_{n,x,g} \frac{\sigma^A_{n,x,g} - \sigma^B_{n,x,g}}{\sigma^B_{n,x,g}} = \sum_n \sum_x \sum_g (\Delta k/k)_{n,x,g} \tag{6}$$

where $(\Delta k/k)_{n,x,g}$ is the (relative) effect on k of differences in nuclear data for nuclide n, reaction x, and energy group g.

To know quantitatively how much the difference in nuclear data files σ^A and σ^B affects k, we can obtain k^A and k^B by neutron transport calculations and take the difference. However, such an evaluation can only tell us $(k^A - k^B)$, and it cannot tell us specifically which nuclide, which reaction, and which energy group have significances on $k^A - k^B$. On the other hand, by obtaining $(\Delta k/k)_{n,x,g}$ using sensitivity based on Eq. (6), it is possible to quantitatively evaluate what differences in $\sigma_{n,x,g}$ causes difference between k^A and k^B.

3 Calculation of sensitivity coefficients

There are several methods for calculating the sensitivity coefficient of the effective multiplication factor to nuclear data. The simplest method is to slightly vary the nuclear data of interest and calculate the sensitivity from the corresponding variation in the effective multiplication factor. This can be expressed in the following equation:

$$\frac{\partial k}{\partial \sigma_i} = \frac{\Delta k}{\Delta \sigma_i} = \frac{k' - k}{\Delta \sigma_i}, \tag{7}$$

where k' denotes the effective multiplication factor obtained when the variation $\Delta\sigma_i$ is given for nuclear data σ_i. In principle, the sensitivity to any nuclear data can be calculated in this way, but the nuclear data depend on nuclides, reactions, and energy groups. When the numbers of nuclides, reactions, and energy groups to be treated are N, X, and G, the number of sensitivity coefficients to be calculated is $(N \times X \times G)$. In order to calculate sensitivity coefficients for all of these nuclear data, k' calculations must be performed many times, which requires a large amount of calculation time.

In contrast to the direct method described above, there is a method to calculate sensitivity using the solution of the adjoint neutron transport equation. This is referred to as the method based on the perturbation theory.

In the perturbation theory (first-order perturbation), the reactivity (or change in the multiplication factor) due to a perturbation (small variation) of a system can be easily obtained from the neutron flux of the system before the perturbation and the adjoint neutron flux. k sensitivity coefficient can be calculated from the variation of k with the variation of cross section as shown in Eq. (7), so the variation of cross section is regarded as a perturbation and the reactivity due to the perturbation can be calculated by the perturbation theory-based calculation. Since it is not necessary to calculate the neutron flux of the system after the change in cross section in the first-order perturbation theory, the sensitivity of k to arbitrary nuclear data can be obtained by the perturbation theory-based calculation if the neutron flux of the system before the perturbation (reference system) and the adjoint neutron flux are calculated beforehand.

Almost all CBZ neutron transport (diffusion) solvers implement methods for solving the adjoint equations, neutron flux distributions, and methods for calculating sensitivity coefficients using the adjoint neutron flux distributions.

4 Example of sensitivity analysis

In this section, as an example of the implementation of the sensitivity analysis, we show the example of the ultra-small fast critical assemblies mentioned at the beginning of this document.

The difference between the calculated values of JENDL-3.3 and ENDF/B-VII for Jezebel and Jezebel-240 can be decomposed into the differences for each nuclear data using sensitivity coefficients as shown in **Table 1**.

Table 1: Sensitivity analysis results of Jezebel and Jezebel-240 (Nuclear data-wise difference of the ENDF/B-VII result from the JENDL-3.3 result with the unit of $\%\Delta k/kk'$)

Nuclide	Reaction	Jezebel	Jezebel-240
Pu-239	(n,f)	-0.20	-0.15
	(n,γ)	+0.18	+0.16
	ν	+0.29	+0.24
	$\bar{\mu}$	-0.18	-0.15
	(n,n')	+0.40	+0.35
Pu-240	ν		+0.11
	$\bar{\mu}$		-0.36
	χ		-0.15
	(n,n)		+0.12
	(n,n')		-0.16
Total		+0.44	+0.11

In Figure. 1, the C/E value of ENDF/B-VII is about $0.3\%dk/kk'$ larger than that of JENDL-3.3 for Jezebel, which can be considered to contain only Pu-239, mainly because of the difference in the inelastic scattering cross section of Pu-239 and the difference in the average number of neutrons produced per fission. In terms of the fission cross section of Pu-239 and the average cosine of the scattering angle, JENDL-3.3 contributes to a larger evaluation of k_{eff}. On the other hand, for Jezebel-240, which has a smaller Pu-239 content, the effect of the difference in Pu-239 nuclear data between ENDF/B-VII and JENDL-3.3 is smaller than that of Jezebel. Nevertheless, in Jezebel-240, the difference in Pu-239 nuclear data contributes to a larger k_{eff} evaluation by ENDF/B-VII, whereas the difference in Pu-240 nuclear data has a compensating effect, resulting in a smaller net nuclear data difference.

In the sensitivity analysis, the difference between JENDL-3.3 and ENDF/B-VII C/E values can be further broken down by energy group. **Figure. 2** shows the factors that contribute to the difference between the ENDF/B-VII calculated values and the JENDL-3.3 calculated values for the k_{eff}. data of Jezebel-240, for each reaction and energy group of the nuclear data of Pu-240. From this figure, it is clear at a glance in which energy region the cross section difference affects the criticality calculation value.

The difference in the average cosine of the scattering angle $\bar{\mu}$ of U-238 has a large influence on the difference between JENDL3.3 and ENDF/B-VII k_{eff} calculations. The cosines are shown in **Fig. 3**, and it can be seen that the evaluated values of JENDL-3.3 are larger in all energy regions. The large value of the average cosine of the scattering angule means the strong forwardness of scattering, which promotes the leakage of neutrons from the system, resulting in smaller critical eigenvalues. Note that this nuclear data has been significantly revised in JENDL-4.0 based on the results of these integral tests and sensitivity analysis.

5 Conclusion

Integral testing and sensitivity analysis are very important because they are essential to ensure the performance of the evaluated nuclear data files and to further improve the performance of the nuclear data files.

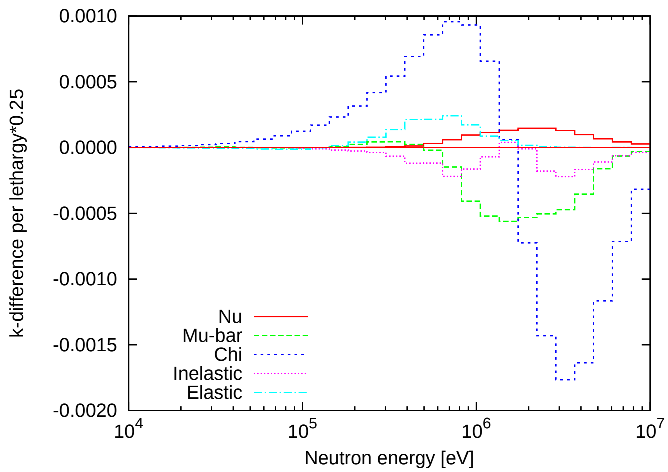

Fig. 2: Sensitivity analysis result of Jezebel-240 (Difference of the ENDF/B-VII result from the JENDL-3.3 result on the Pu-240 nuclear data)

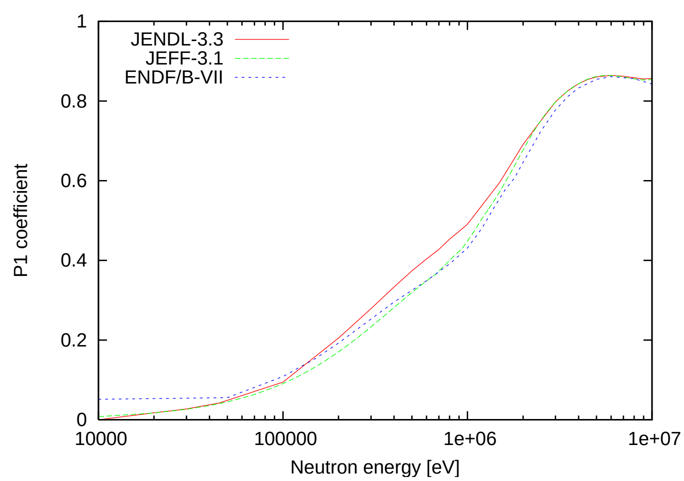

Fig. 3: Average cosine of scattering angle of U-238 elastic scattering reaction