

## ARTICLE

## Covariance Analyses of Self-Shielding Factor and Its Temperature Gradient for Uranium-238 Neutron Capture Reaction

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Covariances of the self-shielding factor and its temperature gradient for the uranium-238 neutron capture reaction have been evaluated from the resonance parameter covariance matrix and the sensitivity of the self-shielding factor and its temperature gradient to the resonance parameters. The resonance parameters and their covariance matrix for uranium-238 were taken from JENDL-3.3, while the sensitivity coefficients were calculated by varying resonance parameters and temperature. A set of computer code modules has been developed for the calculation of the sensitivity coefficients at numerous resonance levels. The present result shows that the correlation among resonance parameters yields a substantial contribution to the standard deviations of the self-shielding factor and its temperature gradient. In addition to the standard deviations of these quantities, their correlation matrices in the JFS-3 70 group structure are also obtained.

**KEYWORDS:** Doppler reactivity, self-shielding factor, temperature gradient, uranium-238, neutron capture, JENDL-3.3, covariance, resolved resonance parameter, sensitivity coefficient, ERRORF

### I. Introduction

Doppler reactivity has been recognized as one of the most important safety parameters among the self-regulation characteristics of reactors, and a high accuracy in the prediction of the reactivity has been vigorously sought in reactor design. To improve the prediction accuracy in fast reactor systems, Doppler reactivities at various critical assemblies have been measured<sup>1–6)</sup> and analyzed.<sup>7–9)</sup>

In standard sensitivity analyses of nuclear characteristics, the relative sensitivity of a nuclear characteristic  $R$  to the infinite dilution cross section  $\hat{\sigma}_\infty$ ,  $S_{R,\sigma} = (\hat{\sigma}_\infty/R)(\partial R/\partial \hat{\sigma}_\infty)$  has been used. The sensitivity analysis system SAGEP<sup>10)</sup> has used this relative sensitivity coefficient for improving the adjusted reactor constants with fixed self-shielding factors. This formalism is not applicable to temperature-related nuclear characteristics such as Doppler reactivity, however, because such characteristics depend on the self-shielding factor as well as the infinite dilution cross section. Regarding the temperature gradient of the self-shielding factor as a “pseu-

do cross section,” the relative sensitivity of the temperature-related nuclear characteristic  $R$  to the temperature gradient of the self-shielding factor  $\alpha$ ,  $S_{R,\alpha} = (\alpha/R)(\partial R/\partial \alpha)$ , can be introduced. If the temperature gradient is defined using the logarithmic derivative of the self-shielding factor with respect to temperature,  $\alpha = (1/f)(df/dT)$ , the coefficients  $S_{R,\alpha}$  can be obtained from the sensitivity coefficients of effective neutron multiplication factor  $k_{\text{eff}}$  to the infinite dilution cross section  $S_{k_{\text{eff}},\sigma}$ .<sup>11)</sup> In this background, the SAGEP system was extended to temperature-related nuclear characteristics, and an adjusted reactor constant ADJ2000 was obtained by using the coefficients  $S_{R,\alpha}$  for the Doppler reactivities measured in ZPPR-9 and FCAXVII-1 experiments.<sup>11,12)</sup>

The sensitivity coefficient  $S_{R,\alpha}$  can also be used to evaluate the uncertainty in the Doppler reactivity arising from the uncertainties in resonance parameters if the uncertainty in the temperature gradient of the self-shielding factor  $\delta\alpha/\alpha$  is obtained. In practical discussion of the Doppler reactivity in fast reactor systems, the self-shielding factor of the <sup>238</sup>U neutron capture reaction is of paramount importance. It is difficult to calculate the uncertainty in the temperature gradient of the self-shielding factor, however, because there are more than one thousand resonance parameters in <sup>238</sup>U, forcing, consequently, a huge amount of the flux calculations to be done for the change of each parameter. A study of the uncertainty in the Doppler reactivity was made by the direct

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$k_{\text{eff}}$ -difference method and an analytic expression of sensitivity coefficients of Doppler reactivity to the resonance parameters.<sup>13,14)</sup> They discussed the sensitivity of self-shielding factors and Doppler reactivity to resonance parameters as well as the analytic properties of the Doppler broadening function ( $\phi$  and  $\chi$ ). The uncertainty in Doppler reactivity due to uncertainties in resonance parameters was then obtained by changing resonance parameters of interest on the basis of standard deviations in the resolved resonance parameter sets<sup>15)</sup> accompanying JENDL-3.2 (Japanese Evaluated Nuclear Data Library Ver.3.2).<sup>16)</sup> However, the correlation among resonance parameters was not taken into account because the covariance matrix of resonance parameters was not available at the time.

For two data libraries of JENDL-3.2 and JENDL-3.3 (Japanese Evaluated Nuclear Data Library Ver.3.3),<sup>17)</sup> much effort has been devoted to evaluating nuclear data covariance,<sup>18–21)</sup> and the resonance parameter covariance matrix of  $^{238}\text{U}$  is also available for the present study. Therefore, a more precise evaluation of the uncertainty in Doppler reactivity is now possible and should be done on the basis of recent progress in nuclear data evaluation.

In this article, we discuss an evaluation of the covariances in the self-shielding factor  $f$  and its temperature gradient  $\alpha$  in relation to the  $^{238}\text{U}$  neutron capture reaction on the basis of microscopic nuclear data and newly developed computer code modules taking into account the correlation among resonance parameters.

This paper is organized as follows: Section II reviews the source of uncertainty in Doppler reactivity in terms of nuclear data. Section III derives the uncertainties in self-shielding factor and its temperature gradient from the resonance parameter covariance matrix. Code modules developed in this work are also introduced in this section. Section IV contains results and discussion. A conclusion is given in Section V.

## II. Source of Uncertainty in Doppler Reactivity

In order to place the current covariance evaluation of self-shielding factor and its temperature gradient in the uncertainty evaluation of Doppler reactivity, error propagation of these quantities to Doppler reactivity is conceptually reviewed in this section. Here, we consider a homogeneous system, for which the macroscopic cross section of reaction channel  $c$  ( $c = \gamma$  for capture and  $f$  for fission) for incoming neutrons with energy  $E$  at temperature  $T$  is

$$\Sigma_c(E, T) = \sum_i N_i \sigma_{i,c}(E, T), \quad (1)$$

where  $N_i$  is the number density of the  $i$ -th isotope and  $\sigma_{i,c}$  is the cross section of the  $i$ -th isotope for the neutron-induced reaction channel  $c$ . The Doppler reactivity  $R$  for the change in temperature from  $T_0$  to  $T = T_0 + \Delta T$  is defined as

$$R = \frac{1}{k_{\text{eff}}(T_0)} - \frac{1}{k_{\text{eff}}(T)} \quad (2)$$

with the effective neutron multiplication factor  $k_{\text{eff}}(T)$ ,

$$k_{\text{eff}}(T) = \frac{\langle \nu(E) \Sigma_f(E, T) \phi(E, T) \rangle_E}{\langle [\Sigma_\gamma(E, T) + \Sigma_f(E, T)] \phi(E, T) \rangle_E + L(T)}, \quad (3)$$

where

$\langle \dots \rangle_E$ : abbreviation of integration with respect to energy  $E$ ,

$\nu(E)$ : fission neutron multiplicity,

$\phi(E, T)$ : neutron flux,

$L(T)$ : leakage from the system per volume.

The variable  $E$  in  $\nu(E)$ ,  $\Sigma_c(E, T)$ , and  $\phi(E, T)$  is omitted hereafter for simplicity.

By using the expression of  $k_{\text{eff}}$ , the Doppler reactivity in Eq. (2) can be written as

$$R \approx \frac{\langle [\Sigma_\gamma(T_0) - \Sigma_\gamma(T)] \phi(T) \rangle_E + \langle [\Sigma_f(T_0) - \Sigma_f(T)] \phi(T) \rangle_E + [L(T_0) - L(T)]}{\langle \nu \Sigma_f(T) \phi(T) \rangle_E}, \quad (4)$$

on the assumption that the reactivity perturbation due to the Doppler effect is sufficiently small that  $\langle \nu \Sigma_f(T) \phi(T) \rangle_E \approx \langle \nu \Sigma_f(T_0) \phi(T_0) \rangle_E$ . The contribution of the  $i$ -th isotope to the reactivity  $R$  is then

$$\begin{aligned} R_i &= \frac{N_i}{\langle \nu \Sigma_f(T) \phi(T) \rangle_E} \langle [\sigma_{i,\gamma}(T_0) - \sigma_{i,\gamma}(T)] \phi(T) + [\sigma_{i,f}(T_0) - \sigma_{i,f}(T)] \phi(T) \rangle_E \\ &= \frac{N_i}{\langle \nu \Sigma_f(T) \phi(T) \rangle_E} \sum_g \sum_{c=\gamma,f} (\hat{\sigma}_{i,c}^g(T_0) - \hat{\sigma}_{i,c}^g(T)) \langle \phi(T) \rangle_E^g. \end{aligned} \quad (5)$$

Here,  $\hat{\sigma}_{i,c}^g(T) = \hat{\sigma}_{i,c}^g(T, \sigma_b)$  is the effective cross section for the channel  $c$  at the  $g$ -th energy group,

$$\hat{\sigma}_{i,c}^g(T, \sigma_b) = \frac{\langle \sigma_{i,c}(E, T) \phi(E, T, \sigma_b) \rangle_E^g}{\langle \phi(E, T, \sigma_b) \rangle_E^g} \quad (6)$$

with the background cross section of the system  $\sigma_b$ . The symbol  $\langle \dots \rangle_E^g$  expresses the energy integration over the  $g$ -th group.

Let us introduce the self-shielding factor  $f_{i,c}^g(T, \sigma_b)$  and its temperature gradient  $\alpha_{i,c}^g(T, \sigma_b)$ ,<sup>11)</sup>

$$f_{i,c}^g(T, \sigma_b) = \frac{\hat{\sigma}_{i,c}^g(T, \sigma_b)}{\hat{\sigma}_{i,c}^g(T_{\text{ref}}, \sigma_b = \infty)}, \quad (7)$$

$$\alpha_{i,c}^g(T, \sigma_b) = \frac{1}{f_{i,c}^g(T, \sigma_b)} \frac{\partial f_{i,c}^g(T, \sigma_b)}{\partial T}, \quad (8)$$

where

$$\hat{\sigma}_{i,c,\infty}^g = \hat{\sigma}_{i,c}^g(T_{\text{ref}}, \sigma_b = \infty) \quad (9)$$

is the infinite dilution cross section calculated at a reference temperature  $T_{\text{ref}}$ .<sup>a</sup> Hereafter, we omit  $\sigma_b$  for simplicity. Then  $\hat{\sigma}_{i,c}^g(T_0)$  can be related to  $\hat{\sigma}_{i,c}^g(T)$

$$\hat{\sigma}_{i,c}^g(T_0) = (1 - \alpha_{i,c}^g(T) \Delta T) \hat{\sigma}_{i,c}^g(T), \quad (10)$$

and  $R_i$  in Eq. (5) is consequently expressed in terms of the product of  $\alpha_{i,c}^g$ ,  $f_{i,c}^g$ ,  $\hat{\sigma}_{i,c,\infty}^g$ , and  $\langle \phi \rangle_E^g$ :

$$R_i = - \frac{N_i \Delta T}{\langle \nu \Sigma_f(T) \phi(T) \rangle_E} \sum_g \sum_{c=\gamma,f} [\alpha_{i,c}^g(T) f_{i,c}^g(T) \hat{\sigma}_{i,c,\infty}^g(T_{\text{ref}})] \langle \phi(T) \rangle_E^g. \quad (11)$$

The variation of Eq. (11) corresponding to the variation of the temperature gradient of the  $g$ -th group  $\delta\alpha_{i,c}^g$  is

$$\begin{aligned} \delta R_i &= -\delta \left[ \frac{N_i \Delta T}{\langle \nu \Sigma_f(T) \phi(T) \rangle_E} \sum_g \sum_{c=\gamma,f} [\alpha_{i,c}^g(T) f_{i,c}^g(T) \hat{\sigma}_{i,c,\infty}^g(T_{\text{ref}})] \langle \phi(T) \rangle_E^g \right] \\ &= R_i w_g \frac{\delta\alpha_{i,c}^g(T)}{\alpha_{i,c}^g(T)} \end{aligned} \quad (12)$$

with the weight  $w_g$ ,

$$w_g = \frac{\sum_{c=\gamma,f} \alpha_{i,c}^g(T) f_{i,c}^g(T) \hat{\sigma}_{i,c,\infty}^g(T_{\text{ref}}) \langle \phi(T) \rangle_E^g}{\sum_g \sum_{c=\gamma,f} \alpha_{i,c}^g(T) f_{i,c}^g(T) \hat{\sigma}_{i,c,\infty}^g(T_{\text{ref}}) \langle \phi(T) \rangle_E^g}. \quad (13)$$

The variation  $\delta R_i/R_i$  for simultaneous change of all  $\alpha_{i,c}^g$ ,  $f_{i,c}^g$ ,  $\hat{\sigma}_{i,c,\infty}^g$ , and  $\langle \phi \rangle_E^g$  becomes

$$\left( \frac{\delta R_i}{R_i} \right)^2 = \sum_{g,g'} w_g w_{g'} \sum_{X,Y} \sum_{c,c'=\gamma,f} \rho_{X^g Y^{g'}} \frac{\delta X^g}{X^g} \frac{\delta Y^{g'}}{Y^{g'}}, \quad (14)$$

where  $X$  and  $Y$  denote  $\alpha_{i,c}^g$ ,  $f_{i,c}^g$ ,  $\hat{\sigma}_{i,c,\infty}^g$  or  $\langle \phi \rangle_E^g$ , and  $\rho_{X^g Y^{g'}}$  is the correlation coefficient between two quantities  $X^g$  and  $Y^{g'}$ . This expression tends toward a simpler form

$$\left( \frac{\delta R_i}{R_i} \right)^2 = \sum_g w_g^2 \sum_{c=\gamma,f} \left[ \left( \frac{\delta\alpha_{i,c}^g(T)}{\alpha_{i,c}^g(T)} \right)^2 + \left( \frac{\delta f_{i,c}^g(T)}{f_{i,c}^g(T)} \right)^2 + \left( \frac{\delta\hat{\sigma}_{i,c,\infty}^g(T_{\text{ref}})}{\hat{\sigma}_{i,c,\infty}^g(T_{\text{ref}})} \right)^2 + \left( \frac{\delta\langle \phi(T) \rangle_E^g}{\langle \phi(T) \rangle_E^g} \right)^2 \right] \quad (15)$$

if the correlation among all quantities is neglected. As shown in Eqs. (14) and (15), the uncertainty in the Doppler reactivity  $\delta R_i/R_i$  is related to the uncertainty in the temperature gradient  $\alpha_{i,c}^g$ , self-shielding factor  $f_{i,c}^g$ , infinite dilution cross section  $\hat{\sigma}_{i,c,\infty}^g$ , and group-averaged flux  $\langle \phi \rangle_E^g$ .

In the following sections, we evaluate the first term  $\delta\alpha_{i,c}^g/\alpha_{i,c}^g$  and the second term  $\delta f_{i,c}^g/f_{i,c}^g$  regarding these uncertainties as propagated from uncertainties in the  $^{238}\text{U}$  resonance parameters via the self-shielding factor of  $^{238}\text{U}$  neutron capture reaction. An example of the self-shielding factor  $f$  and its temperature gradient  $\alpha$  for the neutron capture of  $^{238}\text{U}$  are shown in **Fig. 1**.

### III. Evaluation of Covariances of the Self-Shielding Factor and its Temperature Gradient

We evaluate the covariances of the self-shielding factor  $\delta f_{i,c}^g(T)/f_{i,c}^g(T)$  and its temperature gradient  $\delta\alpha_{i,c}^g(T)/\alpha_{i,c}^g(T)$  in the first and second terms of Eq. (15) for the  $^{238}\text{U}$  neutron capture reaction. Hereafter, we omit the suffix  $i$  for isotope

and  $c$  for reaction channel. Error propagation from resonance parameters to the self-shielding factor and its temperature gradients are

$$\begin{aligned} \theta_{gg'} \frac{\delta f^g}{f^g} \frac{\delta f^{g'}}{f^{g'}} &= \sum_{i,j} \frac{x_i}{f^g} \frac{\partial f^g}{\partial x_i} \frac{x_j}{f^{g'}} \frac{\partial f^{g'}}{\partial x_j} \rho_{ij} \frac{\delta x_i}{x_i} \frac{\delta x_j}{x_j} \\ &= \sum_{i,j} s_i^g s_j^{g'} \rho_{ij} \frac{\delta x_i}{x_i} \frac{\delta x_j}{x_j}, \end{aligned} \quad (16)$$

$$\begin{aligned} \tau_{gg'} \frac{\delta\alpha^g}{\alpha^g} \frac{\delta\alpha^{g'}}{\alpha^{g'}} &= \sum_{i,j} \frac{x_i}{\alpha^g} \frac{\partial\alpha^g}{\partial x_i} \frac{x_j}{\alpha^{g'}} \frac{\partial\alpha^{g'}}{\partial x_j} \rho_{ij} \frac{\delta x_i}{x_i} \frac{\delta x_j}{x_j} \\ &= \sum_{i,j} S_i^g S_j^{g'} \rho_{ij} \frac{\delta x_i}{x_i} \frac{\delta x_j}{x_j}, \end{aligned} \quad (17)$$

where

$\theta_{gg'}$ : Correlation matrix of self-shielding factor  $\{f^g\}$

$\tau_{gg'}$ : Correlation matrix of temperature gradient  $\{\alpha^g\}$

$x_i$ : Resonance parameter  $\mathbf{x} = \{x_i\} = (E_{r,1}, \Gamma_{n,1}, \Gamma_{\gamma,1}, \dots)$

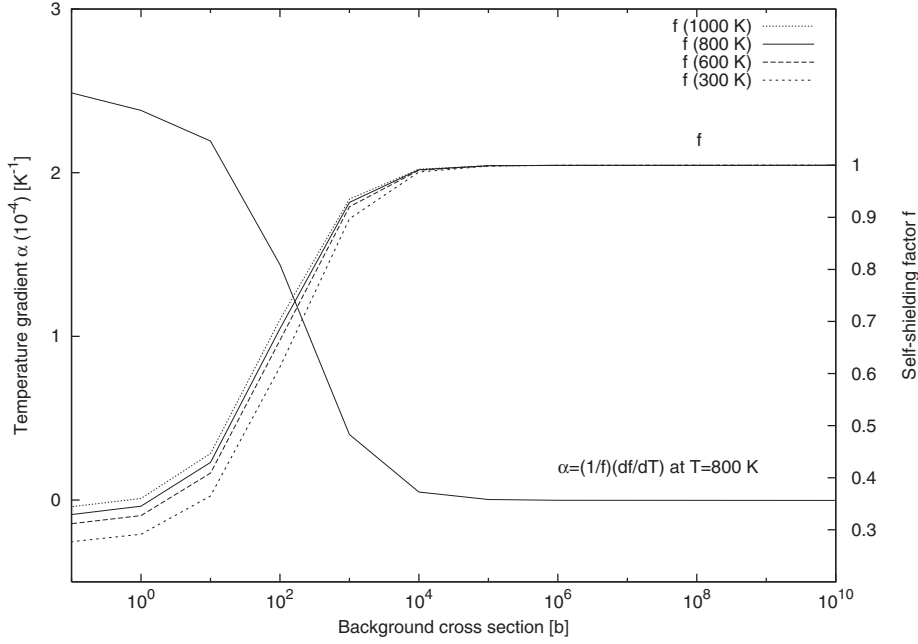
$\rho_{ij}$ : Correlation matrix of resonance parameter  $\mathbf{x}$

$\delta x_i$ : Absolute standard deviation of resonance parameter  $x_i$

$s_i^g$ : Relative sensitivity coefficient of self-shielding factor  $f^g$  to resonance parameter  $x_i$

$S_i^g$ : Relative sensitivity coefficient of temperature gradient  $\alpha^g$  to resonance parameter  $x_i$

<sup>a</sup> We can set any temperature to  $T_{\text{ref}}$ . In this work, the lowest temperature in the central difference formula (600 K) is chosen as  $T_{\text{ref}}$  as explained in the description of ERRORF in Section III.3.



**Fig. 1** Dependence of self-shielding factor  $f$  and its temperature gradient  $\alpha = 1/f(df/dT)$  on background cross section ( $\sigma_b$ ) for  $^{238}\text{U}$  neutron capture reaction at the energy interval of 1 to 2 keV calculated from JENDL-3.3. Values at four temperatures ( $T = 300, 600, 800,$  and  $1000\text{ K}$ ) and at one temperature ( $T = 800\text{ K}$ ) are shown for  $f$  and  $\alpha$ , respectively.

The relative sensitivity coefficients  $s_i^g$  and  $S_i^g$  are defined as

$$s_i^g(\mathbf{x}, T) = \frac{x_i}{f^g(\mathbf{x}, T)} \frac{\partial f^g(\mathbf{x}, T)}{\partial x_i}, \quad (18)$$

$$S_i^g(\mathbf{x}, T) = \frac{x_i}{\alpha^g(\mathbf{x}, T)} \frac{\partial \alpha^g(\mathbf{x}, T)}{\partial x_i}. \quad (19)$$

The summations in Eqs. (16) and (17) are taken over all resolved resonance parameters. By equating  $g$  and  $g'$  in Eqs. (16) and (17), we obtain the relative variance of the self-shielding factor and its temperature gradient in the  $g$ -th group,

$$\left(\frac{\delta f^g}{f^g}\right)_{\text{tot}}^2 = \sum_{i,j} s_i^g s_j^g \rho_{ij} \frac{\delta x_i}{x_i} \frac{\delta x_j}{x_j}, \quad (20)$$

$$\left(\frac{\delta \alpha^g}{\alpha^g}\right)_{\text{tot}}^2 = \sum_{i,j} S_i^g S_j^g \rho_{ij} \frac{\delta x_i}{x_i} \frac{\delta x_j}{x_j}. \quad (21)$$

From Eqs. (16) and (17), the correlation matrices  $\theta_{gg'}$  and  $\tau_{gg'}$  can be expressed as

$$\theta_{gg'} = \left( \sum_{i,j} s_i^g s_j^{g'} \rho_{ij} \frac{\delta x_i}{x_i} \frac{\delta x_j}{x_j} \right) / \left( \frac{\delta f^g}{f^g} \frac{\delta f^{g'}}{f^{g'}} \right), \quad (22)$$

$$\tau_{gg'} = \left( \sum_{i,j} S_i^g S_j^{g'} \rho_{ij} \frac{\delta x_i}{x_i} \frac{\delta x_j}{x_j} \right) / \left( \frac{\delta \alpha^g}{\alpha^g} \frac{\delta \alpha^{g'}}{\alpha^{g'}} \right). \quad (23)$$

In the present work, the resonance parameter set  $\mathbf{x} = \{x_i\}$  and its covariance matrix  $V$  ( $V_{ij} = \rho_{ij} \delta x_i \delta x_j$ ) are taken from the evaluated nuclear data library JENDL-3.3, while the sensitivity coefficients  $s_i^g$  and  $S_i^g$  are obtained using a newly developed code system ERRORF described in Section III.3.

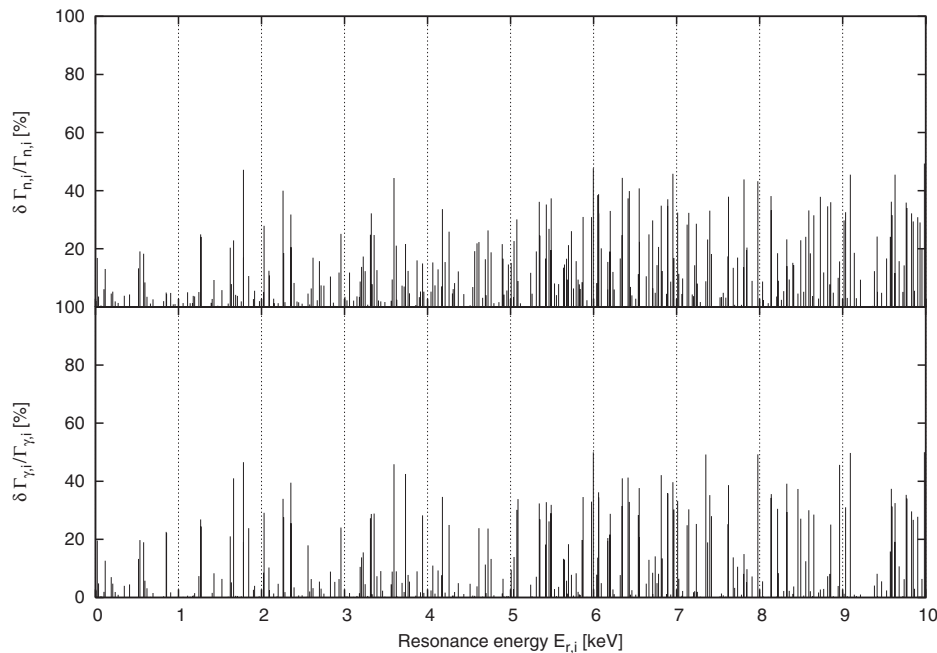
## 1. Resonance Parameter $\mathbf{x}$ and Covariance Matrix $V$

In the current evaluation, we take the resonance parameter set  $\mathbf{x}$  and its covariance matrix  $V$  from evaluated nuclear data files compiled in the ENDF-6 format.<sup>22)</sup> Among the major evaluated nuclear data libraries, JENDL-3.3 is the unique solution in the present study because the other libraries do not include the resonance parameter covariance matrix in their  $^{238}\text{U}$  data evaluation.<sup>b</sup>

In the evaluation of  $^{238}\text{U}$  data for JENDL-3.3, the resonance parameters of 561  $s$ -wave resonance levels and 1129  $p$ -wave resonance levels are compiled in the resolved resonance region (up to 10 keV) with the Reich-Moore formalism. The fission cross section is several orders of magnitude smaller than the elastic and capture cross sections in the resolved resonance region and not compiled in JENDL-3.3. Thus, we ignore the fission widths  $\Gamma_{f,i}$  in the discussion.

The  $^{238}\text{U}$  resonance parameters compiled in JENDL-3.3 are originally taken from the JEF-2 evaluation;<sup>23)</sup> however, the resolved resonance region was divided into 10 energy intervals in JENDL-3.3, and in each energy interval, the cross section is calculated from resonance parameters of levels in the interval (*inside levels*) as well as certain important levels outside the interval (*outside levels*). For example, the 6.67 eV resonance level ( $\Gamma_n = 1.493\text{ meV}$  and  $\Gamma_\gamma = 23\text{ meV}$  in JENDL-3.3) is compiled in all 10 intervals so that the tail effect of this resonance is taken into account in the intervals above 1 keV. This level is an inside level for cross section in the first interval ( $10^{-5}$ –1 keV) and an outside level for cross sections in the intervals above 1 keV (1–2, 2–3, ..., 9–10 keV).

<sup>b</sup> The resonance parameter set and its covariance matrix of  $^{238}\text{U}$  evaluated for JENDL-3.2 is adopted in JENDL-3.3



**Fig. 2** Relative standard deviations ( $1\sigma$ ) in neutron width  $\delta\Gamma_{n,i}/\Gamma_{n,i}$  (upper) and capture width  $\delta\Gamma_{\gamma,i}/\Gamma_{\gamma,i}$  (lower) compiled in JENDL-3.3<sup>19)</sup> for neutron-induced  $^{238}\text{U}$  reaction. Vertical dashed lines show the boundaries of energy intervals.

The  $^{238}\text{U}$  resolved resonance parameter covariance matrix in JENDL-3.3<sup>19)</sup> was evaluated using the KALMAN system,<sup>24)</sup> where the uncertainties in resonance parameters were estimated so that the uncertainties in the cross sections give constant uncertainties (3% for the total and 5% for the capture, in general) in the cross sections averaged over an appropriate energy range. The resonance parameters of  $p$ -wave resonance levels are excluded in the evaluation of the covariance matrix because of their small contribution to the cross section.

The resonance energies of all levels and widths of outside levels are assumed to be not uncertain in the JENDL-3.3 evaluation. In other words, the cross section in an interval should be regarded as not sensitive to resonance parameters of outside levels when we study error propagation with the covariance matrix. For example, cross sections above 1 keV are regarded as not sensitive to the change in the resonance parameter of the 6.67 eV level even though we use the tail of this resonance when we calculate cross sections above 1 keV, because the JENDL-3.3 resonance parameter covariance does not give uncertainty of the 6.67 eV level parameters for neutrons with energies higher than 1 keV. The covariance matrix then becomes

$$V = \begin{pmatrix} V^1 & 0 & 0 \\ 0 & V^2 & 0 \\ & & \ddots & 0 \\ 0 & 0 & 0 & V^{10} \end{pmatrix}, \quad (24)$$

where  $V^1, V^2, \dots, V^{10}$  are resonance parameter covariance submatrices for cross sections in the 10 energy intervals. A similar submatrix structure can also be introduced to the correlation matrix,  $\rho_{ij}^l = V_{ij}^l / (\delta x_i \delta x_j)$ . In the JENDL-3.3  $^{238}\text{U}$  evaluation, the neutron and capture widths of approxi-

mately 30  $s$ -wave resonance levels are chosen from levels in each interval, and their covariance matrix  $V^l$  in each energy interval was evaluated for  $\Gamma_n$  and  $\Gamma_\gamma$ .

The right-hand sides of Eqs. (20) and (21) are accordingly decomposed to the sum of 10 quadratic forms  $\rho^l[S^g \delta x/x]$  and  $\rho^l[S^g \delta x/x]$ ,

$$\left(\frac{\delta f^g}{f^g}\right)_{\text{tot}}^2 = \sum_{l \in L_g} \sum_{i,j \in M_l} s_i^g s_j^g \rho_{ij}^l \frac{\delta x_i}{x_i} \frac{\delta x_j}{x_j} \equiv \sum_{l \in L_g} \rho^l[S^g \delta x/x], \quad (25)$$

$$\left(\frac{\delta \alpha^g}{\alpha^g}\right)_{\text{tot}}^2 = \sum_{l \in L_g} \sum_{i,j \in M_l} S_i^g S_j^g \rho_{ij}^l \frac{\delta x_i}{x_i} \frac{\delta x_j}{x_j} \equiv \sum_{l \in L_g} \rho^l[S^g \delta x/x], \quad (26)$$

where  $L_g$  means the set of energy intervals overlapping with the  $g$ -th group, and  $M_l$  means the set of all resonance parameters of the levels in the  $l$ -th interval. Note that  $s_i^g$  and  $S_i^g$  are zero if  $i \in M_l$  and  $l \notin L_g$  because we assume that the cross section in an energy interval in  $L_g$  is not sensitive to the change in the  $i$ -th resonance parameter.

Standard deviations in  $\Gamma_n$  and  $\Gamma_\gamma$  compiled in the covariance matrix of JENDL-3.3 are shown in **Fig. 2**, with the boundaries of the 10 energy intervals. We can see that the deviation is approximately 50% at maximum for both  $\Gamma_n$  and  $\Gamma_\gamma$ .

In JENDL-3.3, the covariance matrix in the unresolved resonance region (10 to 150 keV) was evaluated in one group expression because of the limitation of the data file format, and we exclude the region from the present evaluation.

## 2. Sensitivity Coefficients $s_i^g$ and $S_i^g$

Sensitivity coefficients of the self-shielding factor  $f^g$  and its temperature gradient  $\alpha^g$  with respect to the  $i$ -th resonance parameter,  $s_i^g$  and  $S_i^g$  are calculated according to their definition in Eqs. (18) and (19). We modify Eq. (18) for numerical calculation of  $S_i^g$ ,

$$S_i^g(\mathbf{x}, T) = \frac{x_i}{\alpha^g(\mathbf{x}, T)} \frac{\partial \alpha^g(\mathbf{x}, T)}{\partial x_i} = \frac{1}{\alpha^g(\mathbf{x}, T)} \frac{\partial s_i^g(\mathbf{x}, T)}{\partial T}. \quad (27)$$

The self-shielding factor  $f^g(\mathbf{x}, T)$  is obtained from the resonance parameter set  $\mathbf{x}$  according to Eq. (7) using NJOY.<sup>25</sup> The neutron flux  $\phi(E, T, \sigma_b)$  is calculated according to the Bondarenko model,

$$\phi(E, T, \sigma_b) = \frac{C(E)}{\sigma(\mathbf{x}, E, T) + \sigma_b}, \quad (28)$$

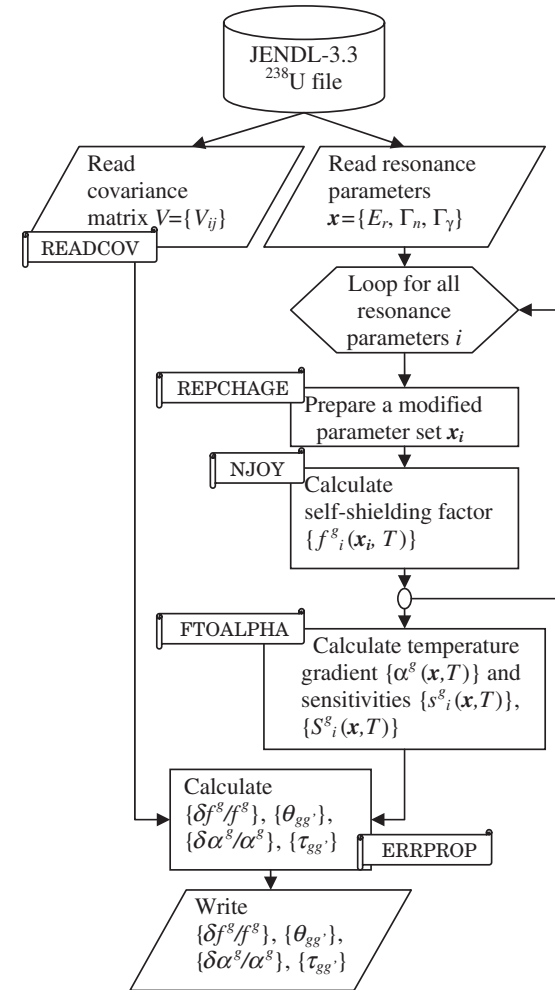
where  $C(E)$  is a weighting function (a priori flux) for which we take an analytic form of the Maxwell distribution +  $(1/E)$  + fission neutron distribution.

### 3. Code Modules-ERRORF

We have developed a new set of code modules to prepare a modified resonance parameter set  $\mathbf{x}_i$ , and to calculate the self-shielding factor  $f^g$ , sensitivity coefficients  $s_i^g$  and  $S_i^g$  in Eqs. (18) and (27), and the correlation matrices  $\theta_{gg'}$  and  $\tau_{gg'}$  in Eqs. (22) and (23). This code system—ERRORF<sup>26</sup>—consists of NJOY and certain newly developed code modules (READCOV, REPCHANGE, FTOALPHA, and ERRPROP). The flow of calculation in the ERRORF system is summarized in **Fig. 3**.

The function of each module in the ERRORF is as follows:

- (1) **READCOV**: To read nuclear data file in the ENDF-6 format and output resonance parameter covariance matrix.
- (2) **REPCHANGE**: To read nuclear data file in the ENDF-6 format and to change the  $i$ -th resonance parameter  $x_i$  in  $\mathbf{x}$  to obtain a modified parameter set  $\mathbf{x}_i$ , where the  $i$ -th parameter is changed from  $x_i$  to  $(1 + \epsilon)x_i$ . We set  $\epsilon$  to 0.05 in the present work.  
Note that the parameters in outside levels are unchanged. Concerning the resonance parameters of the 6.67 eV resonance level in all 10 intervals, the parameters given in the first interval ( $10^{-5}$ –1 keV) are changed while the parameters in the intervals above 1 keV (1–2, 2–3, . . . 9–10 keV) are not changed, because the parameters of outside levels are assumed to be certain in the covariance in JENDL-3.3.
- (3) **NJOY**: To construct cross section  $\sigma(\mathbf{x}_i, E, T)$  from the modified resonance parameter set  $\mathbf{x}_i$ , and to calculate self-shielding factor  $f^g(\mathbf{x}_i, T)$  from effective cross sections  $\hat{\sigma}^g(\mathbf{x}_i, T, \sigma_b)$  and infinite dilution cross sections  $\hat{\sigma}^g(\mathbf{x}_i, T_{\text{ref}}, \sigma_b = \infty)$  according to Eqs. (6), (7), and (28). We calculate  $\sigma(\mathbf{x}_i, E, T)$  at three temperature points (600, 800, and 1000 K) so that we obtain temperature gradient  $\alpha^g$  at 800 K (a typical condition of sodium-cooled first breeder reactor-FBR) in step  $\Delta T = 200$  K by the central difference formula. In the calculation of self-shielding factor  $f^g(\mathbf{x}_i, T)$ , we use a background cross section  $\sigma_b = 37$  barn as a typical value in FBR.<sup>c</sup>
- (4) **FTOALPHA**: To obtain temperature gradient  $\alpha^g(\mathbf{x}_i, T)$  and sensitivity coefficients  $s_i^g(\mathbf{x}_i, T)$  and  $S_i^g(\mathbf{x}_i, T)$  from partial derivatives of  $f^g(\mathbf{x}_i, T)$  with respect to the resonance parameter and temperature according to Eqs. (8), (18), and (27). The partial derivative with respect to resonance parameters was obtained using the forward difference formula, while the partial derivative with respect to temperature was obtained using the central difference formula for numerical accuracy; namely,  $\alpha^g(\mathbf{x}_i, T)$ ,  $s_i^g(\mathbf{x}_i, T)$ , and  $S_i^g(\mathbf{x}_i, T)$  are obtained using



**Fig. 3** Flow of calculation in the ERRORF system. Self-shielding factors are calculated using NJOY.<sup>25</sup>

NJOY sets  $T_{\text{ref}}$  in Eq. (8) to 600 K. Calculation is done from the upper boundary of the thermal region ( $\sim 3$  eV) to the upper boundary of the resolved resonance region (10 keV) in the 70 group structure defined in the JFS-3 (JAERI-Fast Set Ver.3) format.<sup>7,27</sup> Energies of upper boundaries in the 70 group structure are tabulated in **Table 1** for fast reactors.

- (4) **FTOALPHA**: To obtain temperature gradient  $\alpha^g(\mathbf{x}_i, T)$  and sensitivity coefficients  $s_i^g(\mathbf{x}_i, T)$  and  $S_i^g(\mathbf{x}_i, T)$  from partial derivatives of  $f^g(\mathbf{x}_i, T)$  with respect to the resonance parameter and temperature according to Eqs. (8), (18), and (27). The partial derivative with respect to resonance parameters was obtained using the forward difference formula, while the partial derivative with respect to temperature was obtained using the central difference formula for numerical accuracy; namely,  $\alpha^g(\mathbf{x}_i, T)$ ,  $s_i^g(\mathbf{x}_i, T)$ , and  $S_i^g(\mathbf{x}_i, T)$  are obtained using

$$\alpha^g(\mathbf{x}_i, T) = \frac{1}{f^g(\mathbf{x}_i, T)} \frac{f^g(\mathbf{x}_i, T + \Delta T) - f^g(\mathbf{x}_i, T - \Delta T)}{2\Delta T}, \quad (29)$$

$$s_i^g(\mathbf{x}_i, T) = \frac{x_i}{f^g(\mathbf{x}_i, T)} \frac{f^g(\mathbf{x}_i, T) - f^g(\mathbf{x}, T)}{\Delta x_i}, \quad (30)$$

<sup>c</sup> Obtained by potential scattering cross sections of 3.7 barn (<sup>16</sup>O), 3.2 barn (Na), 11.5 barn (Fe), 4.4 barn (Cr), and 17.7 barn (Ni), and the core composition of a typical large fast reactor, 0.00173 (<sup>16</sup>O), 0.00967 (Na), 0.0113 (Fe), 0.00328 (Cr), 0.00224 (Ni), and 0.00764 (<sup>238</sup>U).

**Table 1** Upper energy boundaries in the JFS-3 70 group structure.<sup>27)</sup> “1.00000E+07” means “1.00000 × 10<sup>7</sup> eV”

Group	Energy	Group	Energy	Group	Energy	Group	Energy
1	1.00000E+07	21	6.73795E+04	41	4.53999E+02	61	3.05902E+00
2	7.78801E+06	22	5.24752E+04	42	3.53575E+02	62	2.38237E+00
3	6.06531E+06	23	4.08677E+04	43	2.75365E+02	63	1.85539E+00
4	4.72367E+06	24	3.18278E+04	44	2.14454E+02	64	1.44498E+00
5	3.67879E+06	25	2.47875E+04	45	1.67017E+02	65	1.12535E+00
6	2.86505E+06	26	1.93045E+04	46	1.30073E+02	66	8.76425E-01
7	2.23130E+06	27	1.50344E+04	47	1.01301E+02	67	6.82560E-01
8	1.73774E+06	28	1.17088E+04	48	7.88932E+01	68	5.31579E-01
9	1.35335E+06	29	9.11882E+03	49	6.14421E+01	69	4.13994E-01
11	8.20850E+05	30	7.10174E+03	50	4.78512E+01	70	3.22419E-01
12	6.39279E+05	31	5.53084E+03	51	3.72665E+01		
13	4.97871E+05	32	4.30743E+03	52	2.90232E+01		
14	3.87742E+05	33	3.35463E+03	53	2.26033E+01		
15	3.01974E+05	34	2.61259E+03	54	1.76035E+01		
16	2.35177E+05	35	2.03468E+03	55	1.37096E+01		
10	1.05399E+06	36	1.58461E+03	56	1.06770E+01		
17	1.83156E+05	37	1.23410E+03	57	8.31529E+00		
18	1.42642E+05	38	9.61117E+02	58	6.47595E+00		
19	1.11090E+05	39	7.48518E+02	59	5.04348E+00		
20	8.65170E+04	40	5.82947E+02	60	3.92786E+00		

$$S_i^g(\mathbf{x}, T) = \frac{1}{\alpha^g(\mathbf{x}, T)} \frac{s_i^g(\mathbf{x}, T + \Delta T) - s_i^g(\mathbf{x}, T - \Delta T)}{2\Delta T}, \quad (31)$$

where  $\Delta x_i = 0.05x_i$  and  $\Delta T = 200$  K are chosen as mentioned above.

Self-shielding factors  $f^g$  listed in the output of NJOY have 6 digits, and therefore, the values have a numerical error of an order of  $1.0 \times 10^{-5}$ . To minimize truncation error, we introduce a cut-off parameter  $c = 1.0 \times 10^{-5}$  and set  $\partial f^g / \partial x_i = 0$  if  $|f^g(\mathbf{x}_i, T) - f^g(\mathbf{x}, T)| \leq c$ . We use the same parameter  $c = 1.0 \times 10^{-5}$  for the change in infinite dilution cross section; namely,  $\partial f^g / \partial x_i = 0$  if  $|\hat{\sigma}^g(\mathbf{x}_i, T_{\text{ref}}, \sigma_b = \infty) - \hat{\sigma}^g(\mathbf{x}, T_{\text{ref}}, \sigma_b = \infty)| \leq c$ .

- (5) **ERRPROP**: To calculate standard deviations  $\delta f^g / f^g$  and  $\delta \alpha^g / \alpha^g$ , and correlation matrices  $\theta_{gg'}$  and  $\tau_{gg'}$  according to Eqs. (20)–(23).

A typical CPU time for the NJOY calculation is approximately 4 min for a given resonance parameter set  $\mathbf{x}_i$  at the three temperatures ( $T = 600, 800,$  and  $1000$  K) on a 2.8 GHz Pentium 4 processor. Total CPU time for NJOY calculation is consequently about 3 d when we change two parameters ( $\Gamma_n$  and  $\Gamma_\gamma$ ) of the 561  $s$ -wave levels in JENDL-3.3.

Calculation time depends on the structure of resolved resonance parameters as well as the total number of resonance parameters in the adopted nuclear data library. The 10-energy interval structure employed in JENDL-3.3 shortens the calculation time required to generate cross sections  $\sigma(\mathbf{x}_i, E, T)$  from  $\mathbf{x}_i$  because the number of levels considered is limited to those in one energy interval. CPU time for the NJOY calculation increases to 20 min for a resonance parameter set at the three temperatures if we use the  $^{238}\text{U}$  resonance parameters in the ENDF/B-VII.0 library,<sup>28)</sup> where all resonance parameters in the resolved resonance region

(up to 20 keV) are compiled into one energy interval. Note that the ENDF/B-VII.0 library does not provide the covariance matrix of  $^{238}\text{U}$  resonance parameters, and therefore, cannot be used in the present work.

## IV. Results and Discussions

### 1. Self-Shielding Factor and Temperature Gradient

The self-shielding factor  $f^g$  and its temperature gradient  $\alpha^g$  for  $^{238}\text{U}$  neutron capture reaction are shown in **Table 2** and **Fig. 4**. The neutron capture cross section of  $^{238}\text{U}$  at 300 K in JENDL-3.3 is also plotted in Fig. 4. In the figure, the correlation between the position of the resonance level and the self-shielding factor is clearly seen below 200 eV, where level spacing is wider than the energy widths of groups. Then  $f^g$  takes unity if there is no resonance level in the group except a small resonance tail effect. On the other hand, level spacing is narrower than the energy widths of groups above 200 eV, and number of levels per group gradually increases with neutron energy. The self-shielding factor then increases monotonically with neutron energy and approaches unity. Temperature gradient  $\alpha^g$  is in the order of  $10^{-4}$  if resonance levels exist in the  $g$ -th energy group. Below 200 eV, the temperature gradient is enhanced around positions of the resonance levels although the self-shielding factor  $f^g$  shrinks due to neutron absorption by resonance. However, the trend is masked by many resonance levels above 200 eV.

### 2. Sensitivity Coefficient

The sensitivity coefficients of the temperature gradient to resonance parameters  $S_i^g$  for  $\Gamma_{n,i}$  and  $\Gamma_{\gamma,i}$  are shown in **Fig. 5**. Here, we consider the sensitivity to resonance parameters that are included in the evaluation of the covariance matrix in JENDL-3.3.

**Table 2** Self-shielding factor  $f^g$  and its temperature gradient  $\alpha^g$  with their relative standard deviations ( $1\sigma$ ) for  $^{238}\text{U}$  neutron capture reaction in the JFS-3 group structure ( $T = 800\text{ K}$ ,  $\sigma_b = 37\text{ barn}$ ). Two cases are considered for relative standard deviations: “tot” gives the contribution of both variances and covariances of all resonance parameters. “var” is the same as “tot,” except that covariances are not considered

Grp	$E_{\max}$ [eV]	$f$	$\delta f^g/f^g$ [%]		$\alpha$ [ $10^{-4}/\text{K}$ ]	$\delta\alpha^g/\alpha^g$ [%]		
			tot	var		tot	var	
...	...		Unresolved resonance region					
27	1.5034E+04							
28	1.1709E+04	0.9444	0.0289	0.0437	0.3813	1.0054	1.0776	
29	9.1188E+03	0.9258	0.1017	0.1490	0.4481	1.4260	1.6756	
30	7.1017E+03	0.8792	0.1488	0.3142	0.7400	1.2854	1.7108	
31	5.5308E+03	0.8913	0.1080	0.2258	0.6509	1.0125	1.3370	
32	4.3074E+03	0.7721	0.3064	0.4182	1.1065	1.4537	1.6364	
33	3.3546E+03	0.7877	0.2242	0.3687	1.2258	1.0435	1.3294	
34	2.6126E+03	0.6534	0.6841	0.9353	1.4786	1.5242	1.6700	
35	2.0347E+03	0.5290	1.3905	1.9059	1.8930	1.6642	1.6645	
36	1.5846E+03	0.5724	0.6365	1.0292	1.7635	0.9159	2.2293	
37	1.2341E+03	0.5227	0.1913	0.2321	1.9270	0.2856	0.2994	
38	9.6112E+02	0.4546	0.5194	0.9475	2.3185	0.1997	0.9847	
39	7.4852E+02	0.4065	0.5080	0.8958	2.4933	0.6442	0.5627	
40	5.8295E+02	0.4154	1.7276	3.7449	2.5972	0.4129	1.0545	
41	4.5400E+02	0.5179	0.7790	1.0278	2.5550	0.2084	0.3675	
42	3.5357E+02	0.2607	0.5723	0.9962	2.7972	0.6127	0.6709	
43	2.7537E+02	0.2310	0.6997	0.7048	3.1906	0.1280	0.1655	
44	2.1445E+02	0.0991	1.3409	1.3037	1.7293	3.2950	3.6340	
45	1.6702E+02	0.5395	0.0461	0.1249	2.5092	0.0758	0.1155	
46	1.3007E+02	0.0768	3.3638	3.1617	2.1981	3.4535	5.2937	
47	1.0130E+02	0.4179	0.3395	0.4751	2.5724	0.7534	0.9883	
48	7.8893E+01	0.0663	0.2503	0.1981	1.8597	0.3075	0.4401	
49	6.1442E+01	1.0049	0.0161	0.0287	0.0304	0.9149	0.9469	
50	4.7851E+01	0.6032	1.1246	1.4205	0.5384	2.5131	3.0564	
51	3.7267E+01	0.0308	1.8899	1.4225	0.4830	5.0272	5.9589	
52	2.9023E+01	0.9712	0.3320	0.7178	0.0661	5.4800	4.3853	
53	2.2603E+01	0.0447	12.2758	8.8289	1.1948	5.8284	17.4631	
54	1.7604E+01	1.0038	0.0475	0.0388	0.0346	7.7558	26.0629	
55	1.3710E+01	0.9981	0.0133	0.0277	0.0261	3.6872	7.6771	
56	1.0677E+01	0.9907	0.0099	0.0253	0.0984	0.7534	2.3966	
57	8.3153E+00	0.0481	0.2168	1.3814	1.2504	2.7591	2.0000	
58	6.4760E+00	0.7456	0.9495	0.6619	1.0289	3.3961	2.4171	
59	5.0435E+00	1.0002	0.0006	0.0011	0.0423	0.5157	0.3673	
60	3.9279E+00	1.0005	0.0004	0.0004	0.0220	1.5629	1.1944	
61	3.0590E+00							
...	...		Thermal region					

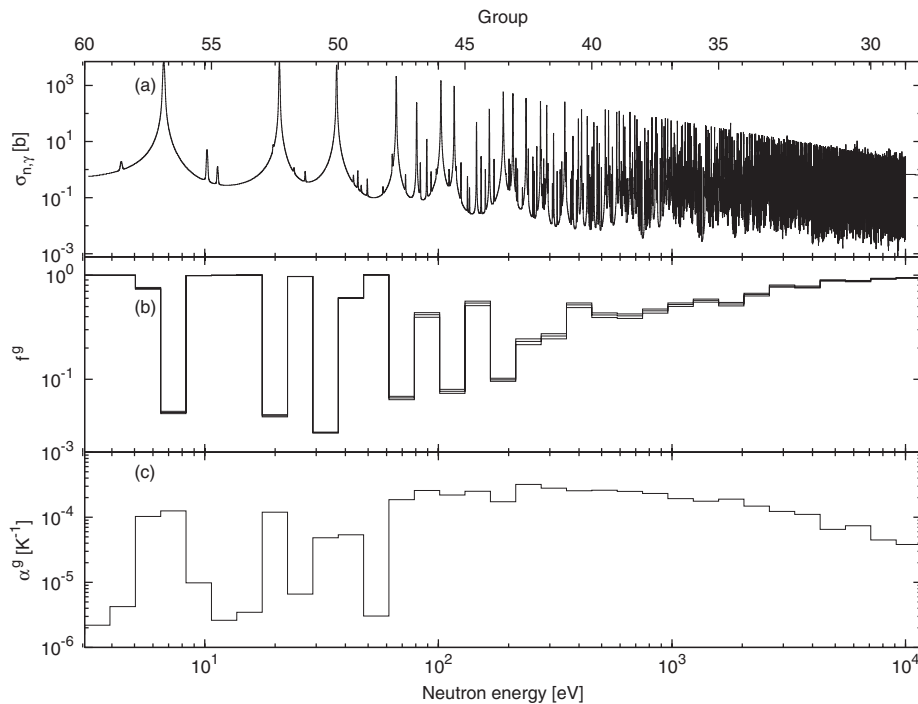
In Fig. 5, we can divide the  $E$ - $g$  plane into two regions at ( $E_{r,i} = 1\text{ keV}$ ,  $g = 37$ ) according to the property of sensitivity coefficients: Coefficients for  $E_{r,i} \geq 1\text{ keV}$  and  $g \leq 37$  take finite values near the diagonal line in the  $E$ - $g$  plane, while some coefficients at ( $E_{r,i}, g$ ) far from the diagonal line are finite in  $E_{r,k} \leq 1\text{ keV}$  and  $g \geq 37$  in the  $E$ - $g$  plane. This structure is from the block diagonal matrix structure of the covariance matrix shown in Eq. (24). For groups with energies higher than the 37th group ( $g \leq 37$ ), energy widths of groups in the JFS-3 70 structure are about 1 keV and comparable to the energy interval in the block diagonal matrix structure ( $=1\text{ keV}$ ). Thus, the sensitivities  $S_i^g$  ( $g \leq 37$ ) are well described using the contribution of resonance levels inside the  $g$ -th group. On the other hand, all groups with energies lower than the 36th group ( $g \geq 36$ ) are in the first interval ( $10^{-5}$  to 1 keV); namely, they are correlated using the sub-

matrix  $V^1$ . Therefore, temperature gradients of more than one group ( $g \geq 36$ ) are sensitive to a change of one resonance parameter below 1 keV.

### 3. Uncertainties in Self-Shielding Factor and Temperature Gradient

The relative standard deviation ( $1\sigma$ ) of self-shielding factor  $\delta f^g/f^g$  and its temperature gradient  $\delta\alpha^g/\alpha^g$  are shown in Table 2 and Fig. 6 (labeled “tot”). The correspondence of the position of resonance level to  $\delta f^g/f^g$  and  $\delta\alpha^g/\alpha^g$  is still visible, as we see in Fig. 4; however,  $\delta f^g/f^g$  and  $\delta\alpha^g/\alpha^g$  are also affected by the resonance levels outside the  $g$ -th group. Above 200 eV, fluctuations in  $\delta f^g/f^g$  and  $\delta\alpha^g/\alpha^g$  are smaller than those at lower energy, and they are less than several percent.

In order to investigate the contributions of diagonal ele-



**Fig. 4** (a) Neutron capture cross section of  $^{238}\text{U}$  in JENDL-3.3 at 300 K. (b) Self-shielding factor  $f^g$  for  $^{238}\text{U}$  neutron capture reaction in the JFS-3 group structure ( $T = 600, 800, 1000$  K,  $\sigma_b = 37$  barn). (c) Same as (b), but for temperature gradient  $\alpha^g$  at 800 K.

ments (variance) and off-diagonal elements (covariance) in matrix  $V$  to  $(\delta f^g/f^g)_{\text{tot}}^2$  and  $(\delta \alpha^g/\alpha^g)_{\text{tot}}^2$ , we decompose them to two terms:

$$\left(\frac{\delta f^g}{f^g}\right)_{\text{tot}}^2 = \left(\frac{\delta f^g}{f^g}\right)_{\text{var}}^2 + \rho_{\text{cov}}[S^g \delta x/x], \quad (32)$$

$$\left(\frac{\delta \alpha^g}{\alpha^g}\right)_{\text{tot}}^2 = \left(\frac{\delta \alpha^g}{\alpha^g}\right)_{\text{var}}^2 + \rho_{\text{cov}}[S^g \delta x/x], \quad (33)$$

where the terms “var” and “cov” for the self-shielding factor  $f^g$  are defined as

$$\begin{aligned} \left(\frac{\delta f^g}{f^g}\right)_{\text{var}}^2 &= \sum_{l \in L_g} \sum_{i,j \in M_l} s_i^g s_j^g \rho_{ij}^l \frac{\delta x_i}{x_i} \frac{\delta x_j}{x_j} \delta_{ij} \\ &= \sum_i (s_i^g)^2 \left(\frac{\delta x_i}{x_i}\right)^2, \end{aligned} \quad (34)$$

$$\rho_{\text{cov}}[S^g \delta x/x] = \sum_{l \in L_g} \sum_{i,j \in M_l} s_i^g s_j^g \rho_{ij}^l \frac{\delta x_i}{x_i} \frac{\delta x_j}{x_j} (1 - \delta_{ij}) \quad (35)$$

( $\delta_{ij}$  is Kronecker’s delta). Note that  $\rho_{ij}^l = 1$  if  $i = j$ . Similar terms can also be defined for the temperature gradient  $\alpha^g$ . The contribution of variance is shown in Table 2 and Fig. 6, labeled “var.” The significant contribution of correlation between resonance parameters is visible in the deviation of “tot” from “var.” This shows that the correlation among resonance parameters should be taken into account in the evaluation of the uncertainties.

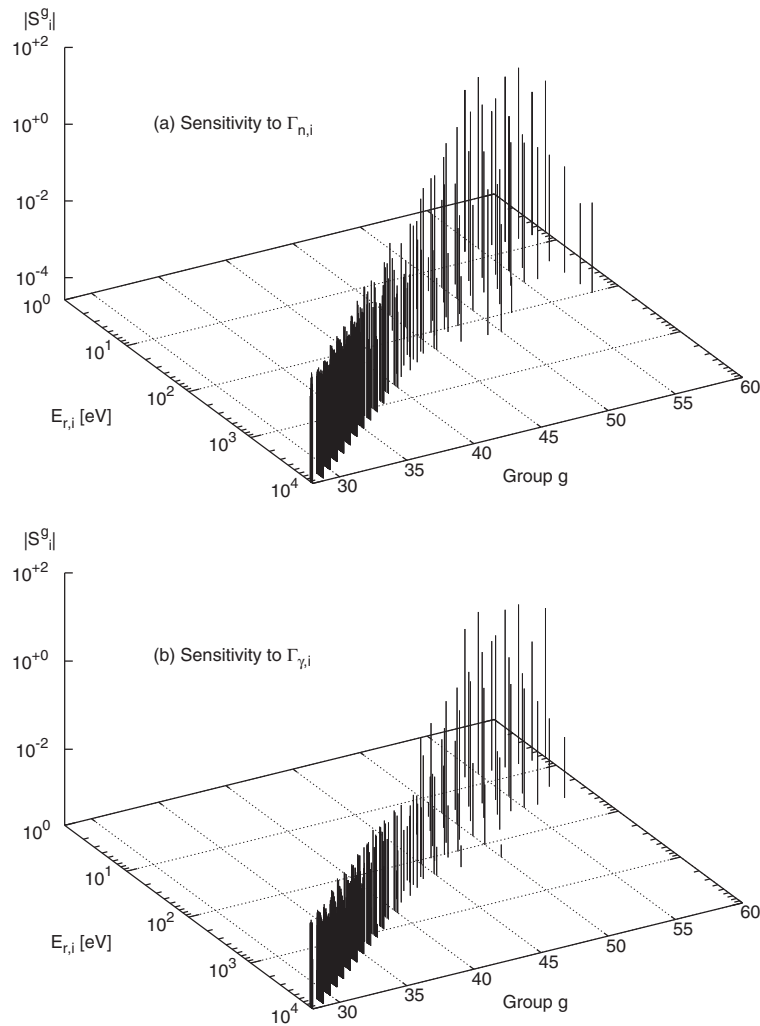
The effect of correlation among resonance parameters is more clearly seen in Fig. 7, where the ratios of “var” to “tot” are plotted for  $\delta f^g/f^g$  and  $\delta \alpha^g/\alpha^g$ . The ratio is nearly

larger than 1, which means that the correlation among resonance parameters suppresses the total standard deviations  $(\delta f^g/f^g)_{\text{tot}}$  and  $(\delta \alpha^g/\alpha^g)_{\text{tot}}$ . The ratios reach approximately 5 at maximum for both  $f^g$  and  $\alpha^g$ . In the practical evaluation of uncertainties in these quantities, it is, therefore, important to take into consideration the correlation among resonance parameters as well as the standard deviations in resonance parameters.

Due to the block diagonal matrix structure of the covariance matrix (Eq. (24)), we can regard the relative standard deviation  $(\delta \alpha^g/\alpha^g)_{\text{tot}}$  as the quadratic summation of the quadratic form  $\sqrt{\rho^l [S^g \delta x/x]}$  over all  $l \in L_g$  (Eq. (26)). Values of quadratic forms  $\sqrt{\rho^l [S^g \delta x/x]}$  are tabulated in Table 3, where cells of energy intervals that overlapped with each group ( $l \in L_g$ ) are shaded. Relative standard deviations  $(\delta \alpha^g/\alpha^g)_{\text{tot}}$  for all groups lower than 1 keV ( $g = 38, 39, \dots$ ) are described by the covariance of the first interval ( $10^{-5}$ –1 keV), and are not affected by levels above 1 keV due to the fact that there is no correlation between levels lower than 1 keV and higher than 1 keV in JENDL-3.3.

#### 4. Covariances of Self-Shielding Factor and Temperature Gradient

In the evaluation of uncertainty in Doppler reactivity, the correlation matrices of self-shielding factor and its temperature gradient among groups are required as shown in Eq. (14). The obtained correlation matrices  $\theta_{gg'}$  and  $\rho_{gg'}$  given in Eqs. (22) and (23) are tabulated in Tables 4 and 5, where the diagonal elements are normalized to 100. Correlation is weak among groups with energies higher than the energy region of the 38th group ( $g \leq 38$ ), while it exists among



**Fig. 5** Absolute value of sensitivity coefficients of temperature gradient  $\alpha^g$  to resonance parameter,  $|S_i^g(\mathbf{x}, T)|$  for  $^{238}\text{U}$  neutron capture reaction in the JFS-3 group structure ( $T = 800\text{ K}$ ,  $\sigma_b = 37\text{ barn}$ ). The two plots are for  $\Gamma_{n,i}$  (a) and  $\Gamma_{\gamma,i}$  (b).  $E_{r,i}$  and  $g$  are the level energy of the  $i$ -th resonance level and index of group, respectively. Sensitivity coefficients of levels not considered in the covariance matrix of JENDL-3.3 are omitted. See Table 1 for the boundaries of the JFS-3 group structure.

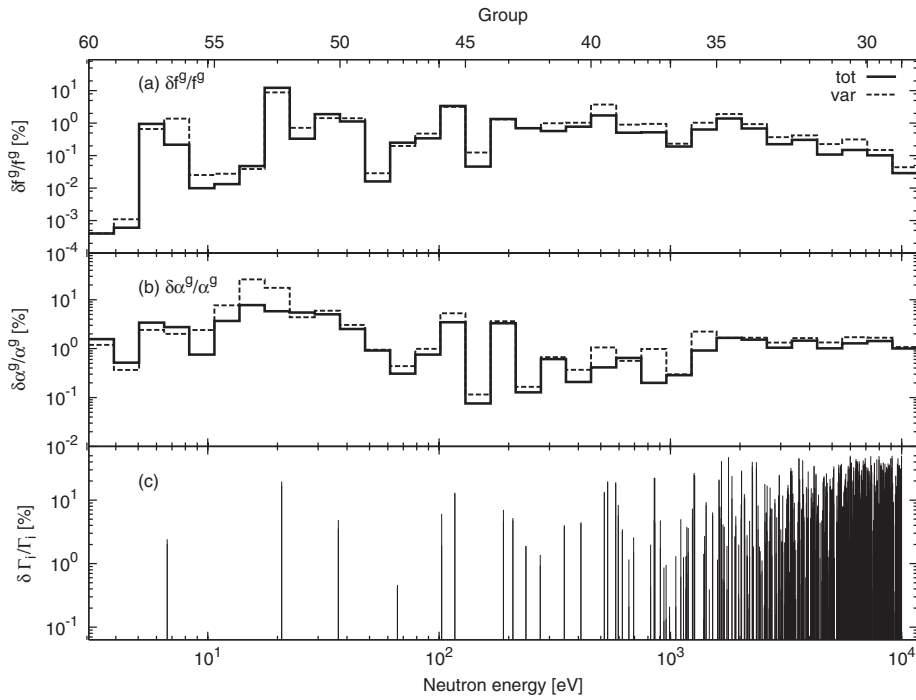
groups with energies lower than the energy region of the 39th group ( $g \geq 39$ ). The strong correlations among groups higher than the 49th group are remarkable.

## V. Conclusions

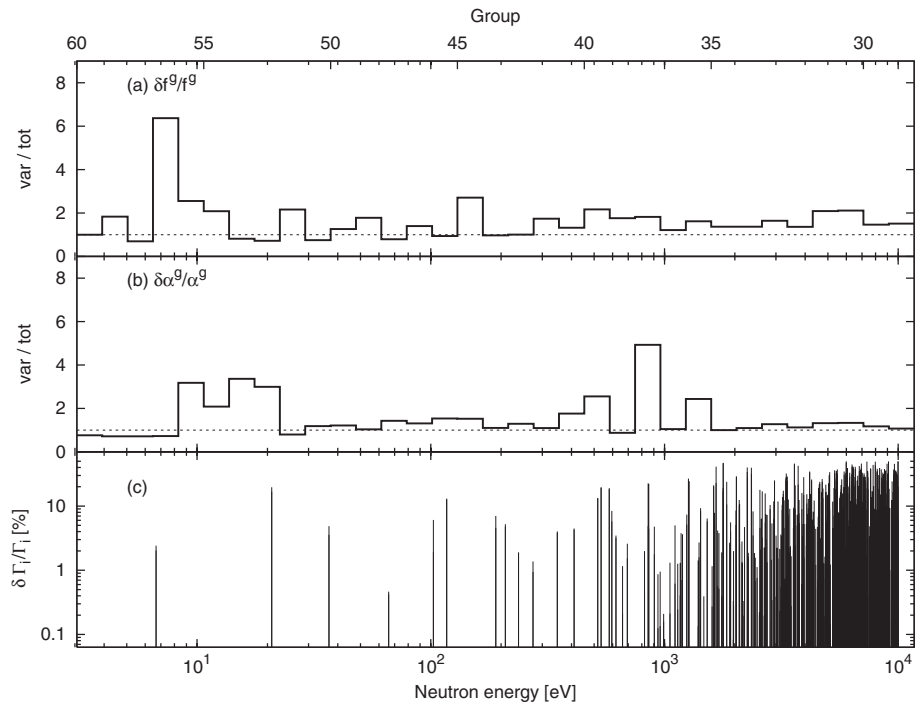
We have derived covariances of self-shielding factors and their temperature gradients from the resonance parameter covariance matrix and the sensitivity coefficients of the self-shielding factor and its temperature gradient with respect to resonance parameters in JENDL-3.3. In order to calculate the sensitivity coefficients for nuclides with numerous resonance levels according to the derived equations, a new system ERRORF has been developed to obtain covariance matrices of self-shielding factor and its temperature gradient. This system was then applied to the evaluation of covariances in the self-shielding factor and its temperature gradient for  $^{238}\text{U}$  neutron capture reaction at  $T = 800\text{ K}$  and background cross section  $\sigma_b = 37\text{ barn}$  in the JFS-3 70 group

structure. We have shown that uncertainties in both the self-shielding factor and temperature gradient are substantially reduced if we include the correlation among resonance parameters. Thus, we can conclude that the correlation among resonance parameters has a crucial role in the precise evaluation of uncertainty in the self-shielding factor and its temperature gradient. The maximum uncertainty of the temperature gradient is 8%, and approximately 2% above 1 keV. Note that these values will not directly influence the uncertainty in Doppler reactivity due to the fact that the uncertainty of each group is weighted using the averaged flux and other quantities of the group.

We have often seen the elimination of long-range correlation, which is introduced using the block diagonal matrix structure of resonance parameter covariance matrix rather than the real nature. Since the covariance matrix in JENDL-3.3 was determined to reproduce uncertainty in the cross section, we believe that the covariance results in reliable uncertainty in the self-shielding factor and its tempera-



**Fig. 6** (a) Relative standard deviation ( $1\sigma$ ) in self-shielding factor  $\delta f^g/f^g$  for  $^{238}\text{U}$  neutron capture reaction in the JFS-3 group structure ( $T = 800\text{ K}$ ,  $\sigma_b = 37\text{ barn}$ ). “tot” gives the contribution of both variances and covariances of all resonance parameters. “var” is the same as “tot,” except that covariances are not considered. (b) Same as (a), but for temperature gradient  $\delta\alpha^g/\alpha^g$ . (c) Same as Fig. 2, although  $\delta\Gamma_n/\Gamma_n$  and  $\delta\Gamma_\gamma/\Gamma_\gamma$  are plotted on the same abscissa.



**Fig. 7** (a) Ratio of  $(\delta f^g/f^g)_{\text{var}}$  (var, contribution of variance) and to the total uncertainty  $(\delta f^g/f^g)_{\text{tot}}$  in self-shielding factor for  $^{238}\text{U}$  neutron capture reaction in the JFS-3 group structure ( $T = 800\text{ K}$ ,  $\sigma_b = 37\text{ barn}$ ). (b) Same as (a) but for temperature gradient  $\alpha^g$ . (c) Same as Fig. 2, although  $\delta\Gamma_n/\Gamma_n$  and  $\delta\Gamma_\gamma/\Gamma_\gamma$  are plotted on the same abscissa.

ture gradient. If another evaluation of the covariance matrix without the block diagonal matrix structure is carried out in the future, we can check the reliability of the use of the block diagonal matrix structure by comparing uncertainties in de-

rived quantities propagated from covariance matrices with and without the structure.

The ERRORF system excludes the unresolved resonance region due to the fact that the ENDF-6 format did not allow

**Table 3** Relative standard deviation ( $1\sigma$ ) in temperature gradient of the self-shielding factor  $(\delta\alpha^g/\alpha^g)_{\text{tot}}$  and the quadratic form of the  $l$ -th energy interval,  $\sqrt{\rho^l[S^g\delta x/x]}$  ( $1 \leq l \leq 10$ ) for  $^{238}\text{U}$  neutron capture reaction in the JFS-3 group structure ( $T = 800\text{ K}$ ,  $\sigma_b = 37\text{ barn}$ ). Note that  $(\delta\alpha^g/\alpha^g)_{\text{tot}}$  is the quadrature sum of  $\sqrt{\rho^l[S^g\delta x/x]}$ . Energy intervals overlapping with the  $g$ -th group ( $l \in L_g$ ) are shaded

Grp	$E_{\text{max}}$ [eV]	$(\delta\alpha^g/\alpha^g)_{\text{tot}}$ [%]	$\sqrt{\rho^l[S^g\delta x/x]}$ [%]										
			0-1keV	1-2keV	2-3keV	3-4keV	4-5keV	5-6keV	6-7keV	7-8keV	8-9keV	9-10keV	
...	...		Unresolved resonance region										
27	1.5E+4		0	0	0	0	0	0	0	0	0	0	1.0054
28	1.2E+4	1.0054	0	0	0	0	0	0	0	0	0	0	0.0955
29	9.1E+3	1.4260	0	0	0	0	0	0	0	1.0376	0.9735	0	
30	7.1E+3	1.2854	0	0	0	0	0	0.7898	0.9997	0.1701	0	0	
31	5.5E+3	1.0125	0	0	0	0	0.7244	0.7074	0	0	0	0	
32	4.3E+3	1.4537	0	0	0	1.3240	0.6001	0	0	0	0	0	
33	3.4E+3	1.0435	0	0	0.7678	0.7066	0	0	0	0	0	0	
34	2.6E+3	1.5242	0	0	1.5242	0	0	0	0	0	0	0	
35	2.0E+3	1.6642	0	1.3691	0.9462	0	0	0	0	0	0	0	
36	1.6E+3	0.9159	0	0.9159	0	0	0	0	0	0	0	0	
37	1.2E+3	0.2856	0.0087	0.2855	0	0	0	0	0	0	0	0	
38	9.6E+2	0.1997	0.1997	0	0	0	0	0	0	0	0	0	
39	7.5E+2	0.6442	0.6442	0	0	0	0	0	0	0	0	0	
40	5.8E+2	0.4129	0.4129	0	0	0	0	0	0	0	0	0	
41	4.5E+2	0.2084	0.2084	0	0	0	0	0	0	0	0	0	
42	3.5E+2	0.6127	0.6127	0	0	0	0	0	0	0	0	0	
43	2.8E+2	0.1280	0.1280	0	0	0	0	0	0	0	0	0	
44	2.1E+2	3.2950	3.2950	0	0	0	0	0	0	0	0	0	
45	1.7E+2	0.0758	0.0758	0	0	0	0	0	0	0	0	0	
46	1.3E+2	3.4535	3.4535	0	0	0	0	0	0	0	0	0	
47	1.0E+2	0.7534	0.7534	0	0	0	0	0	0	0	0	0	
48	7.9E+1	0.3075	0.3075	0	0	0	0	0	0	0	0	0	
49	6.1E+1	0.9149	0.9149	0	0	0	0	0	0	0	0	0	
50	4.8E+1	2.5131	2.5131	0	0	0	0	0	0	0	0	0	
51	3.7E+1	5.0272	5.0272	0	0	0	0	0	0	0	0	0	
52	2.9E+1	5.4800	5.4800	0	0	0	0	0	0	0	0	0	
53	2.3E+1	5.8284	5.8284	0	0	0	0	0	0	0	0	0	
54	1.8E+1	7.7558	7.7558	0	0	0	0	0	0	0	0	0	
55	1.4E+1	3.6872	3.6872	0	0	0	0	0	0	0	0	0	
56	1.1E+1	0.7534	0.7534	0	0	0	0	0	0	0	0	0	
57	8.3E+0	2.7591	2.7591	0	0	0	0	0	0	0	0	0	
58	6.5E+0	3.3961	3.3961	0	0	0	0	0	0	0	0	0	
59	5.0E+0	0.5157	0.5157	0	0	0	0	0	0	0	0	0	
60	3.9E+0	1.5629	1.5629	0	0	0	0	0	0	0	0	0	
61	3.1E+0												
...	...		Thermal region										

**Table 4** Correlation matrix of the self-shielding factor  $\theta_{gg'}$  for  $^{238}\text{U}$  neutron capture reaction in the JFS-3 group structure ( $T = 800\text{ K}$ ,  $\sigma_b = 37\text{ barn}$ ). Diagonal elements are normalized to 100. Matrix elements where correlations are allowed by the block diagonal matrix structure of JENDL-3.3 are shaded

Grp	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60		
28	100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
29	0	100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
30	0	0	100	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
31	0	0	1	100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
32	0	0	0	0	100	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
33	0	0	0	0	3	100	-3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
34	0	0	0	0	0	-3	100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
35	0	0	0	0	0	0	0	100	-1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
36	0	0	0	0	0	0	0	-1	100	-10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37	0	0	0	0	0	0	0	1	-10	100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38	0	0	0	0	0	0	0	0	0	0	100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
39	0	0	0	0	0	0	0	0	0	0	0	100	-57	0	0	1	0	-2	0	0	0	0	0	1	1	0	0	1	0	0	0	0	0	0	0
40	0	0	0	0	0	0	0	0	0	0	0	-57	100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41	0	0	0	0	0	0	0	0	0	0	0	0	0	100	-5	2	0	-3	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0
42	0	0	0	0	0	0	0	0	0	0	0	0	0	-5	100	1	-1	1	1	1	1	0	0	1	1	0	0	0	0	0	0	0	0	0	0
43	0	0	0	0	0	0	0	0	0	0	0	0	1	2	1	100	-12	-30	-2	-3	-3	0	0	0	1	1	0	1	1	0	0	0	0	0	1
44	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	-12	100	-17	3	-1	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0	1
45	0	0	0	0	0	0	0	0	0	0	0	0	-2	-3	1	-30	-17	100	-7	-8	5	-2	-12	-12	14	14	-13	12	-3	6	8	8	8	-7	
46	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	-2	3	-7	100	86	-40	5	0	-2	0	2	-1	5	-2	5	4	5	4	-4	
47	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-3	-1	-8	86	100	-36	2	-3	-5	4	6	-4	7	-2	6	5	6	-5		
48	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	5	-40	-36	100	-16	5	9	-3	-8	8	-9	0	-4	-4	-4	-4	5		
49	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-2	5	2	-16	100	48	-10	-48	6	5	41	15	27	23	22	-22	
50	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	-12	0	-3	5	48	100	81	-99	-83	90	-53	3	-15	-21	-16	17		
51	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	0	0	-12	-2	-5	9	-10	81	100	-79	-99	99	-88	-6	-35	-39	-33	35		
52	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	14	0	4	-3	-48	-99	-79	100	83	-88	52	-3	15	21	16	-15		
53	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	14	2	6	-8	6	-83	-99	83	100	-98	87	6	35	39	33	-33		
54	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	-13	-1	-4	8	5	90	99	-88	-98	100	-82	-3	-31	-35	-30	31
55	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	12	5	7	-9	41	-53	-88	52	87	-82	100	-19	68	70	65	-66	
56	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	-3	-2	-2	0	15	3	-6	-3	6	-3	-19	100	-80	-82	-84	85		
57	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6	5	6	-4	27	-15	-35	15	35	-31	68	-80	100	98	97	-97		
58	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	8	4	5	-4	23	-21	-39	21	39	-35	70	-82	98	100	100	-99		
59	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	8	5	6	-4	22	-16	-33	16	33	-30	65	-84	97	100	100	-99		
60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	-7	-4	-5	5	-22	17	35	-15	-33	31	-66	85	-97	-99	-99	100		

**Table 5** Correlation matrix of the temperature gradient of self-shielding factor  $\tau_{gg'}$  for  $^{238}\text{U}$  neutron capture reaction in the JFS-3 group structure ( $T = 800\text{ K}$ ,  $\sigma_b = 37\text{ barn}$ ). Diagonal elements are normalized to 100. Matrix elements where correlations are allowed by the block diagonal matrix structure of JENDL-3.3 are shaded

Grp	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60		
28	100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
29	0	100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
30	0	0	100	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
31	0	0	1	100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
32	0	0	0	0	100	-13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
33	0	0	0	0	-13	100	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
34	0	0	0	0	0	1	100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
35	0	0	0	0	0	0	0	100	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
36	0	0	0	0	0	0	0	-1	100	-3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37	0	0	0	0	0	0	0	0	-3	100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38	0	0	0	0	0	0	0	0	0	0	100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
39	0	0	0	0	0	0	0	0	0	0	0	100	-92	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
40	0	0	0	0	0	0	0	0	0	0	0	0	-92	100	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100	12	0	1	-3	0	0	0	-3	0	1	0	0	0	0	0	0	0	0	0	0
42	0	0	0	0	0	0	0	0	0	0	0	0	1	12	100	3	0	1	1	0	0	2	1	1	0	0	0	0	1	0	0	0	0	0	0
43	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	100	1	30	0	1	0	22	-1	0	0	1	0	0	0	0	0	0	0	0	1
44	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	1	100	13	5	-3	0	11	0	1	0	0	0	0	0	0	0	-1	-1	-1	2
45	0	0	0	0	0	0	0	0	0	0	0	1	0	-3	1	30	13	100	-29	29	3	71	0	2	-2	-1	-2	-5	-1	-5	-5	-5	-5	6	
46	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	5	-29	100	-97	-22	-9	1	0	3	0	5	2	0	5	4	5	-4		
47	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	-3	29	-97	100	24	11	2	3	-3	-1	-4	-3	1	-4	-3	-4	5	5		
48	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	-22	24	100	5	1	0	1	0	1	0	0	0	0	0	0	0	0	
49	0	0	0	0	0	0	0	0	0	0	0	1	0	-3	2	22	11	71	-9	11	5	100	51	56	-51	-50	-14	-19	33	-18	-20	-18	19		
50	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	-1	0	0	1	2	1	51	100	99	-70	-98	10	-36	42	-15	-18	-15	16		
51	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	2	0	3	0	56	99	100	-78	-96	-2	-34	50	-20	-23	-20	21		
52	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	-2	3	-3	1	-51	-70	-78	100	62	61	16	-71	37	40	37	-36		
53	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	-1	0	-1	0	-50	-98	-96	62	100	-21	39	-33	12	15	12	-11		
54	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-2	5	-4	1	-14	10	-2	61	-21	100	3	-38	54	54	54	-53		
55	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-5	2	-3	0	-19	-36	-34	16	39	3	100	55	85	85	85	-84		
56	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	-1	0	1	0	33	42	50	-71	-33	-38	55	100	33	31	33	-33		
57	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	-5	5	-4	0	-18	-15	-20	37	12	54	85	33	100	100	100	-99	
58	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	-5	4	-3	0	-20	-18	-23	40	15	54	85	31	100	100	100	-99	
59	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1	-5	5	-4	0	-18	-15	-20	37	12	54	85	33	100	100	100	-99	
60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	2	6	-4	5	0	19	16	21	-36	-11	-53	-84	-33	-99	-99	-99	100		

an energy-dependent covariance matrix for unresolved resonance parameters when the JENDL-3.3 evaluation was performed. Extension of the current format of the unresolved resonance parameter covariance to the energy-dependent form is now proposed. Our system should be extended to the unresolved resonance region when the evaluation of the energy-dependent covariance of unresolved resonance parameters becomes feasible.

The present code system can be applied to other nuclides such as  $^{235}\text{U}$ ,  $^{239}\text{Pu}$ , and  $^{240}\text{Pu}$ , for which covariance matrices for JENDL-3.3 are given.<sup>17,29)</sup> Furthermore, a new covariance evaluation of  $^{233}\text{U}$ ,  $^{235}\text{U}$ ,  $^{238}\text{U}$ , and  $^{239}\text{Pu}$  is now ongoing for the ENDF/B-VII library and is expected to be completed in 2007.<sup>28)</sup> Further evaluation of self-shielding factors and their temperature gradients for these other nuclides and libraries is reserved for a future work.

Our final goal is the evaluation of uncertainty in Doppler reactivity and we plan to do it on the basis of the uncertainties in self-shielding factors and their temperature gradients obtained in the present work.

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