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PROCEEDINGS OF THE SPECIALISTS' MEETING ON COVARIANCE DATA

July 15~16, 1993, Tokai, Japan

March 1994

Ed. Yutaka NAKAJIMA

日本原子力研究所
Japan Atomic Energy Research Institute

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Proceedings of the Specialists' Meeting on Covariance Data July 15 ∿ 16, 1993, Tokai, Japan

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Japanese Nuclear Data Committee
Tokai Research Establishment
Japan Atomic Energy Research Institute
Tokai-mura, Naka-gun, Ibaraki-ken

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This report consists of the Proceedings of the Specialists' Meeting on Covariance Data organized by the Japanese Nuclear Data Committee and the Nuclear Data Center, Japan Atomic Energy Research Institute. The meeting was held on July 15 - 16, 1993, at the Tokai Research Establishment, Japan Atomic Energy Research Institute with the participants of twenty six specialists, who were the evaluators of the nuclear data or users of the covariance data. The main object of this meeting was to review the methodology of the eveluation of the covariance data and to promote the evaluation of the covariance data in Japan through the discussions and conclusions of the meeting. After the general review of the evaluation of the covariance, different evaluation methods and applications of the covariance data were presented, which were followed by the lively discussions among evaluators and users.

Keywords : Proceedings, Nuclear Data, Covariance, Evaluation

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共分散評価専門家会議報文集

1993年7月15～16日，東海村

日本原子力研究所東海研究所
シグマ研究委員会
（編）中島　豊

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本報文集は，シグマ研究委員会と原研核データセンターの共催で開催された共分散評価専門家会議の報文を収録したものである。この専門家会議は，1993年7月15日と16日の両日，日本原子力研究所東海研究所において26名の専門家の出席の下に開催された。出席者は，核データの評価者と共分散データの利用者であった。この会議の主要な目的は共分散の評価方法をレビューするとともに，評価法を検討し，わが国における共分散の評価活動の活性化に図ることにあった。会議では共分散評価法の全体的なレビューの後，共分散の各種の評価法およびその利用法が紹介され，さらに共分散の評価を進める上での問題点について活発な討論が行われた。この会議は共分散の評価活動を今後一層活発に行うための契機になると思われる。

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1. Meaning of Covariance

1.1 Covariance of the Nuclear Data

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There is an introductory review on the present status of covariance for evaluated nuclear data. The following articles are briefly discussed : Necessity of covariance for evaluated data, basic assumption of covariance production, dependency of produced covariance on methods, consistency of evaluated value and covariance, confirming of produced covariance and methods of comparing covariance matrices.

1. Introduction

It has been a long time since an idea of covariance matrices for evaluated nuclear data is introduced to express uncertainties inevitably associated with evaluating physical quantities on the basis of measurement and model calculation which, the both, are not so reliable to result in accurate values. There have been many works discussed about the covariance. Therefore, understanding on it is widely spread in nuclear data community including not only evaluators but also users of evaluated values. Nevertheless, there are scarce evaluated covariance matrices enough to use for calculations in nuclear reactor physics in spite of earnest requirement from the users. The causes for the standstill of producing the covariance estimations demanded for available evaluated data files are primarily lack of suitable methods which can be applied with confidence by evaluators while few covariance estimations for major cross sections in fission and fusion reactors are tried to estimate with some methods.

At this time, we should confirm the status about the covariances in the nuclear data field in order to develop the methodologies and then produce more confidential results.

2. Necessity of covariance for Evaluated Data

Both evaluators and users of nuclear data necessitate the covariances associated with evaluated nuclear data. The former represents uncertainties of the values of the evaluated results with the diagonal components in the covariance matrix and the shape of the evaluated curve with the non-diagonal components in it. The uncertainties have two kinds of significance for an evaluator. The one is that they give quantitative reliability on the basis of comprehensive knowledge for him of nuclear data. He should apply his abilities to estimate them from available experimental, theoretical and methodological information. Therefore, they are a confidential region given by the evaluator. The other is that they give quantitative tolerance : The evaluator allows users to choice the value different from the evaluated one in the limit given with the uncertainty. The user can adjust the evaluated value by his own convenience to the extent that he needs it to obtain reasonable consistency with the information which is not used in the evaluation. This is the important point for the user of the evaluated value. Reactor physicists use the evaluated values and associated covariances to obtain adjusted reactor constants which can reproduce integral experiments through reactor physics calculation.

3. Basic Assumption of Covariance Production

The covariance of the nuclear data is primarily experimental uncertainty. Its components are cumulatively estimated from the uncertainties associated with the data base used in the evaluation applying the law of error propagation. Under the procedure it is assumed as an unspoken agreement that an error distribution is random and then the Gauss statistics can be applied. This provides us most developed mathematical formulae in quantitative calculation of uncertainties. The assumption is, however, not always rigorously correct for experimental uncertainty. There are statistical and systematic errors in measurements. The former can be considers as random and treated as a Gauss distribution. The latter depends on the condition of individual experiments and can result in biased values. Although corrections in a experimental data procedure are conducted to exclude the bias come from the experimental conditions it is difficult to succeed completely the object of the correction.

These consideration is not proper on the covariance estimation but valid for the evaluated values. This point must be always understood when we

produce or use them. At this time we can not clarify the effect resulted from a discrepancy between the methodology in data procedures based on the assumption of the Gauss statistics and the practical situation in data base possibly biased with systematic errors which can not treated with the Gauss statistics. A way to improve it is to develop the methods adapted to available experiments because new measurements with high quality will not be expected in the nuclear data field.

4. Dependency of Produced Covariance on Methods

There are significant discrepancies among the covariances produced by individual evaluators because they have adopted in their estimations the methods developed on their proper ideas for estimating and processing the uncertainties in measurements and calculations. They show that the covariance depends strongly on the method or, we must say, the idea. This means that there is no confidential methodology agreed in the nuclear data field.

5. Consistency of Evaluated Value and Covariance

Evaluated nuclear data are produced from experimental data bases. Even if they are calculated with nuclear reaction models, the root of the parameters used in the calculation are primarily experimental data. Therefore, every evaluated value must be naturally accompanied with its covariance since they intrinsically have the uncertainty originated from available measurements. Besides, they are not unique in the condition of the same data base because of using distinct methods in the evaluations. This is similar in the covariance production. Accordingly, both evaluated value and covariance are indivisible and they must be consistently and simultaneously estimated in the same evaluation. The cause which it has not been performed is that valid methods have not been developed and evaluators have not time to spare for covariance evaluation. In order to compile additively the covariance consistent with the evaluated value in the files already issued we have to study to attain the consistency and overcome many various difficulties.

6. Confirming of Produced Covariance

We have no measure to confirm the validity of the produced covariance. Although the evaluated values can be compared with available experiments the

covariance has no counterparts to be compared to make sure whether the result is reasonable or not. Evaluator hesitates to present his outcome because he does not have any ways to be convinced that it is quantitatively acceptable. The diagonal components only as standard deviations can be compared with experimental data such as error bars and distribution of measured values. These are a part of the covariance matrix. There is not such an effective way to compare the non-diagonal components with experimental information. We should always accept the covariance given together with those evaluated results by the evaluator which can be confirmed with experimental information.

7. Methods of Comparing Covariance Matrices

There is a difficulty to compare quantitatively individual covariance matrices obtained by different evaluators. Evaluated values can be schematically compared on a two-dimensional graph. Usually a covariance matrix is schematically drawn with a bird's-eye view of a three-dimensional graph. The evaluated curve can be shown on a graph even if there are several curves corresponding different evaluations. They can be compared directly on the same graph and in addition if available experiments are also plotted on the one it is possible which evaluated curve is more agreeable with the measurements. The quantitative comparison of three-dimensional graphs is difficult. This is one of the reasons that evaluators are not encourage to challenge covariance estimation.

8. Conclusion

The necessity of the evaluated covarian has been understood by evaluators as well as users. While the formers are trying to produce covariances there are several difficulties to be solved by them. They have different problems from evaluation of values themselves and demand to develop appropriate methodologies to estimate the covariances. It will be achieved it through solving the problems step by step.

1.2 Some comments on Peelle's Pertinent Puzzle

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Abstract

Peelle's Pertinent Puzzle is introduced as an anomaly which appears in obtaining a least-squares average of two strongly correlated data. Reason of this anomaly is explained to be the inconsistency in transforming the data covariance and sensitivity matrices. Effects of data truncations give an explanation on another aspect of Peelle's Puzzle.

1. Introduction

The least-squares method (LSM) is commonly used as a tool of parameter estimation and curve fitting in many fields of science and technology[1,2]. However, the LSM sometimes yields strange results which are not correct intuitively. For example, a solution of the least-squares method (Least-squares solution, LSS) for the average of a set of two discrepant and strongly correlated data can be a value lower than both of the data. Furthermore, a LSS, obtained after three data values are transformed by a set of simple non-linear functions, is sometimes significantly different from the answer obtained before the transformation is applied. These anomalies are known as "Peelle's Pertinent Puzzle (often abbreviated as PPP)[3]" in the field of nuclear data. Some people have claimed that these anomalies result from the discrepant nature of the underlying data, or from consideration of a small number of data which is not consistent with the concept of the statistical methods. There have been a lot of arguments of how to avoid such fallacious results[4-9], e.g., by introducing informative prior, by combining data in different ways, by transforming the data into logarithmic scale, use of the law of error propagation with averaged values, etc. Some of them seem to be successful to some extent (however mostly to more restricted problems[7,8]), but no clear explanation was given on the reason why LSM yields such a strange result.

The two types of PPP are described in this paper, and answers to these problems are explained as 1) inconsistent transformation of covariance and sensitivity matrices and 2) improper truncation of the data space.

2. Peelle's Pertinent Puzzle - as originally introduced

The following statement summarizes the problem known as PPP which was originally introduced by Peelle[3].

"Suppose we are required to obtain the weighted average of two experimental results for the same physical quantity. The first result is 1.5, and the second result 1.0. The full covariance matrix of these data is believed to be the sum of three components. The first component is fully correlated with standard error 20% of each respective value. The second and third components are independent of the first and of each other, and correspond to 10% random uncertainties in each experimental result.

The weighted average obtained from the least-squares method is 0.88 ± 0.22, a value outside the range of the input values! Under what conditions is this the reasonable result that we sought to achieve by use of an advanced data reduction technique?

One's first reaction is to blame the non-intuitive result on the discrepant nature of the input data. This is not the reason, because the whole input data covariance matrix can be scaled up without changing its 'shape' until the data are consistent. The input data are indeed strange, but a similar if muted effect would occur if a less-odd example of this type were offered."

We will give our interpretation of his words here because the above statement has a certain ambiguity; There are three uncorrelated raw data values, two measurements 1.5 and 1.0 (with 10% uncertainty) of the same quantity which is a product of physical quantities X and C, and another data 1.0 (with 20% uncertainty) providing the normalization (C) of the former two data. Then, by dividing the former two data by the third one, we have now "two" correlated data, which directly correspond to the physical quantity X which we are supposed to be interested in. Now, let these two correlated data be the two components of a vector $\mathbf{d}$, i.e., $\mathbf{d}=(d_1, d_2)^t = (1.5, 1.0)^t$ where the superscript t denotes a transpose of a vector or a matrix which in turn is indicated by a bold character. The covariance matrix $\mathbf{V_d}$ associated with $\mathbf{d}$ is calculated from the above information according to the "law of error propagation" as

$$\mathbf{V_d} = \begin{pmatrix} 1.5^2\cdot(0.1^2 + 0.2^2) & (1.5\cdot0.2)\cdot(1.0\cdot0.2) \\ (1.5\cdot0.2)\cdot(1.0\cdot0.2) & 1.0^2\cdot(0.1^2 + 0.2^2) \end{pmatrix} = \begin{pmatrix} 0.1125 & 0.06 \\ 0.06 & 0.05 \end{pmatrix} \qquad (1)$$

The observation equation which relates the data and the parameter X is written as;

$$\boldsymbol{d} = \begin{pmatrix} d_1 \\ d_2 \end{pmatrix} = \begin{pmatrix} 1.5 \\ 1.0 \end{pmatrix} - \begin{pmatrix} X \\ X \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}\cdot X \equiv \boldsymbol{G}\cdot X. \qquad (2)$$

Therefore, the sensitivity matrix "G" (which is referred to as "design matrix" as well) is determined to be $\mathbf{G} = (1, 1)^t$. The LSS for X and its covariance matrix $\mathbf{V_x}$ are obtained as[1,2];

$$X = (\boldsymbol{G}^t\boldsymbol{V}_d^{-1}\boldsymbol{G})^{-1}\boldsymbol{G}^t\boldsymbol{V}_d^{-1}\boldsymbol{d} = 0.88, \qquad (3)$$

$$V_X = (\boldsymbol{G}^t\boldsymbol{V}_d^{-1}\boldsymbol{G})^{-1} = 0.22^2 \qquad (4)$$

We can therefore successfully reproduce the result given by Peelle. The value of chi-square is calculated to be 5.88, indicating that the input data are statistically discrepant. This point, however, does not alter the significance of this problem because the chi-square becomes 0.98 without changing the solution if the whole covariance matrix is multiplied by a factor of six

as Peelle correctly pointed out. In this definition, the PPP is defined as such an anomaly as **"getting a LSS outside the range of the input data."** This is the original definition of PPP.

Before giving our interpretation of this problem, it will be worthwhile to present the second definition of PPP which was proposed by Zhao[4,7] to understand the origin and significance contained in this puzzle in more detail.

3. Second Definition of PPP proposed by Zhao

This definition also utilizes the three uncorrelated data appeared in the above interpretation, but retains the number of data points. Let us suppose that a 3-dimensional vector **d** and its covariance matrix $\mathbf{V_d}$ are related with the physical quantities X and C by the following observation equation;

$$\boldsymbol{d} = \begin{pmatrix} d_1 \\ d_2 \\ d_3 \end{pmatrix} = \begin{pmatrix} 1.5 \\ 1.0 \\ 1.0 \end{pmatrix} - \begin{pmatrix} X \cdot C \\ X \cdot C \\ C \end{pmatrix} \equiv \begin{pmatrix} t_1(p) \\ t_2(p) \\ t_3(p) \end{pmatrix} \equiv \boldsymbol{t}(\boldsymbol{p}),$$

$$\boldsymbol{V_d} = \begin{pmatrix} 0.15^2 & 0 & 0 \\ 0 & 0.1^2 & 0 \\ 0 & 0 & 0.2^2 \end{pmatrix}, \tag{5}$$

where $\mathbf{p} = (X,C)^t$ denotes the parameter vector to be sought, and **t** is the model (theory) vector containing the parameters to be estimated, e.g., $t_1(p) = X \cdot C$. The elements of sensitivity matrix **G** of this problem is calculated from its definition to be

$$G_{ij} = \frac{\partial t_i}{\partial p_j}, \quad \therefore \; \boldsymbol{G} = \begin{pmatrix} C & X \\ C & X \\ 0 & 1 \end{pmatrix}. \tag{6}$$

The LSS for this non-linear problem is written down as

$$\boldsymbol{p} = \boldsymbol{p}_0 + (\boldsymbol{G}^t \boldsymbol{V}_d^{-1} \boldsymbol{G})^{-1} \boldsymbol{G}^t \boldsymbol{V}_d^{-1} [\boldsymbol{d} - \boldsymbol{t}(\boldsymbol{p}_0)], \tag{7}$$

where $\mathbf{p_0}$ denotes an initial estimate of the parameter vector **p**. Because of the non-linearity of the problem, iterations are required. The covariance matrix for **p**, $\mathbf{V_p}$, is given by the same expression as given in Eq. (4), i.e., $(\mathbf{G}^t \cdot \mathbf{V_d}^{-1} \mathbf{G})^{-1}$. The LSS is obtained after a few iterations to be

$$\boldsymbol{p} = \begin{pmatrix} X \\ C \end{pmatrix} = \begin{pmatrix} 1.15 \\ 1.0 \end{pmatrix}, \; \boldsymbol{V_p} = \begin{pmatrix} 0.06 & -0.046 \\ -0.046 & 0.04 \end{pmatrix}. \tag{8}$$

which we presume is the correct answer.

Now let us transform the data and the covariance matrix according to the following vector transformation $\mathbf{f} = (f_1,f_2,f_3)^t$

$$
\begin{aligned}
d_1 \rightarrow d'_1 &= f_1(d_1,d_2,d_3) = d_1/d_3 = 1.5 \\
d_2 \rightarrow d'_2 &= f_2(d_1,d_2,d_3) = d_2/d_3 = 1.5 \\
d_3 \rightarrow d'_3 &= f_3(d_1,d_2,d_3) = d_3 = 1.0
\end{aligned}
\tag{9}
$$

$$
(V_{d'_{ij}}) = \left(\frac{\partial d'_i}{\partial d_k} (V_d)_{k,m} \frac{\partial d'_j}{\partial d_m} \right) = \begin{pmatrix} 0.1125 & 0.06 & -0.06 \\ 0.06 & 0.05 & -0.04 \\ -0.06 & -0.04 & 0.04 \end{pmatrix}.
$$

This transformation may be written in a vector form as $\mathbf{d} \rightarrow \mathbf{d}' = \mathbf{f}(\mathbf{d})$. The quantities corresponding to the transformed data are denoted with a prime. Einstein's summation rule is adopted above and throughout this paper which indicates that the occurrence of repeated subscripts signifies a summation over the labels unless otherwise stated.

If this transformation is to be applied to the data, the "model" should be also transformed by using the same functional form in order to keep the physical meanings of the two parameters X and C to be unchanged. Therefore, the model should now be transformed in the following way.

$$
t(p) \rightarrow t'(p) = f(t) = \begin{pmatrix} \frac{t_1}{t_3} \\ \frac{t_2}{t_3} \\ t_3 \end{pmatrix} = \begin{pmatrix} \frac{XC}{C} \\ \frac{XC}{C} \\ C \end{pmatrix} = \begin{pmatrix} X \\ X \\ C \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} X \\ C \end{pmatrix} = G' p,
\tag{10}
$$

$$
G' = \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix},
$$

where the matrix G' is the sensitivity matrix corresponding to the transformed data. Therefore, the model is linearized as is done in many applications by means of such a transformation. By putting these (primed) quantities into Eqs. (3) and (4), the results now become

$$
p' = \begin{pmatrix} X \\ C \end{pmatrix} = \begin{pmatrix} 0.88 \\ 1.24 \end{pmatrix}, \quad V_{p'} = \begin{pmatrix} 0.22^2 & -0.035 \\ -0.035 & 0.031 \end{pmatrix}.
\tag{11}
$$

Therefore, the least-squares solution for the same physical quantity became completely different from that obtained before the transformation, i.e., Eq. (8), showing another paradox of the least-squares method. Zhao and Perey[4,7] argued that we should call this **"difference of LSSs before and after a transformation"** as PPP. **This is the second definition of PPP.**

These two definitions of PPP seem to be strongly correlated because the data vector **d**, covariance matrix $\mathbf{V_d}$ and design matrix **G** which appeared in the original definition of PPP (Eqs. (1) and (2)) can be regarded as sub-matrices of the corresponding quantities in Eqs. (9) and (10).

4. "Our" Interpretations

4.1 Invariant LSS under Isomorphic Transformations

Here, the term "isomorphic transformation **f**" is defined as a set of transformations ($\mathbf{f}=(f_1,...,f_n)^t$) of a vector $\mathbf{d}$ ($=(d_1,d_2,...,d_n)^t$) into another as $\mathbf{d}' = \mathbf{f}(\mathbf{d}) = (f_1(\mathbf{d}),f_2(\mathbf{d}),...,f_n(\mathbf{d}))^t$ without changing the number of data points, i.e., [dimension of $\mathbf{d}'$] = [dimension of $\mathbf{d}$][5,9]. Furthermore, the isomorphic transformation must have its inverse $\mathbf{f}^{-1}$ which satisfies $\mathbf{f}^{-1}(\mathbf{d}') = \mathbf{d}$. This condition eliminates such a spurious transformation as $\mathbf{f}(d_1,d_2) = (d_1,d_1^2)^t$ where information on d_2 is lost by the transformation. The transformation which appeared in the second definition of PPP falls into the category of isomorphic transformations. On the contrary, if the dimension of $\mathbf{d}'$ is less than that of $\mathbf{d}$, the transformation is referred to as "truncation of a data space". This is responsible for the original definition of PPP as will be shown later.

Let us suggest a general problem in which a data vector $\mathbf{d} = (d_1,d_2,..,d_n)^t$ having covariance matrix $\mathbf{V_d}$ is to be fitted with a set of theoretical values $\mathbf{t}$ ($=(t_1(\mathbf{p}),...,t_n(\mathbf{p}))^t$), where $\mathbf{p}=(p_1,...,p_q)^t$ denote a parameter vector to be estimated ($q < n$). The observation equation of this problem is therefore written down as;

$$\boldsymbol{\varepsilon} = \begin{pmatrix} d_1 \\ d_2 \\ \cdots \\ d_n \end{pmatrix} - \begin{pmatrix} t_1(p_1,\cdots,p_q) \\ t_2(p_1,\cdots,p_q) \\ \cdots \\ t_n(p_1,\cdots,p_q) \end{pmatrix} = \mathbf{t}(\mathbf{p}). \tag{12}$$

The "sensitivity matrix **G**" which contains the essence of this "model" $\mathbf{t}$ is defined as follows,

$$\mathbf{G} = (G_{ij}) = \left(\frac{\partial t_i}{\partial p_j}\right) \equiv \left(\left(\frac{\partial \mathbf{t}}{\partial \mathbf{p}}\right)_{ij}\right), \tag{13}$$

where the matrix $(\partial \mathbf{t}/\partial \mathbf{p})$ is defined by this relation. Then, the least-squares solution vector $\mathbf{p}$ is obtained by Eq. (7). The sensitivity matrix **G** should be calculated using $\mathbf{p}_0$. If the theoretical model t_i's are not linear in $\mathbf{p}$, iterations are needed by replacing $\mathbf{p}_0$ and **G** by means of the updated parameters until certain convergence criteria are satisfied. The quantity

$$\Delta \boldsymbol{\varepsilon} = \mathbf{d} - \mathbf{t}(\mathbf{p}) \tag{14}$$

is referred to as the residual vector.

Let us now transform the data vector $\mathbf{d}$ into another $\mathbf{d}'$ denoted by $d'_i = f_i(d_1,d_2,..,d_n)$, where f_i (i=1,..n) are elements of a set of isomorphic transformations denoted by a vector $\mathbf{f}$. Then, the model vector $\mathbf{t}$ should be also transformed in the same way as $t'_i(p_1,...,p_q) = f_i[t_1(p_1,..,p_q),..,t_n(p_1,...,p_q)]$ in order to keep the physical significance of the parameters unchanged.

Let us define matrices $\mathbf{c}^{(+)}$, $\mathbf{c}^{(-)}$ and $\mathbf{c}^{(0)}$ as below;

$$c_{ij}^{(+)} \equiv \frac{\partial f_i}{\partial t_j} \equiv \frac{\partial f_i(t_1,\ldots,t_n)}{\partial t_j},$$

$$c_{ij}^{(-)} \equiv \frac{\partial f_i}{\partial d_j} \equiv \frac{\partial f_i(d_1,\ldots,d_n)}{\partial d_j}, \tag{15}$$

$$c^{(0)} \equiv \frac{1}{2}(c^{(+)} + c^{(-)}).$$

The various quantities after transformation are expressed by using the original ones as[5,9];

$$\begin{aligned} d' - t'(p) &= c\,[d - t(p)] \\ V_{d'} &= c\,V_d\,c^t \\ G' &= c\,G \end{aligned} \tag{16}$$

where c can be either one of $c^{(+)}$, $c^{(-)}$ or $c^{(0)}$ independently as long as the first order Taylor series expansion is involved. The p' is written down using the quantities in the original data space;

$$\begin{aligned} p' &= p_0 + (G'^t V_{d'}^{-1} G')^{-1} G'^t V_{d'}^{-1} [d' - t'(p_0))] \\ &= p_0 + \left[(G^t c^t)(c^t)^{-1} V_d^{-1} c^{-1}(c\,G)\right]^{-1} (G^t c^t)(c^t)^{-1} V_d^{-1} c^{-1} c[d - t(p_0)] \end{aligned} \tag{17}$$

If the data vector d is close to the theoretical values t, the three c matrices become identical. In that case, the above expression reduces to the original answer, Eq. (7) because each pair of the form $c^t(c^t)^{-1}$ or $c^{-1}c$ cancels out. In actual data analyses, however, these three matrices are rarely equal because of imperfections in the data and/or the theory. Therefore, if p' is to be equal to p, each c should be replaced by $c^{(-)}$, $c^{(+)}$ or $c^{(0)}$ simultaneously. This statement claims that the sensitivity matrix G and the covariance matrix V_d must be "covariant" under the isomorphic transformation f. Usually, the covariance matrix of the transformed data is calculated as $c^{(-)}V_d c^{(-)t}$. On the contrary, the sensitivity matrix is usually calculated in the transformed data space by its definition which is equal to $c^{(+)}G$. Because of this inconsistency, the least-squares solution p' is quite generally different from the original solution p, and this is the very origin of the second definition of PPP.

If the transformation f is linear, i.e., let F be a square matrix so that d' = f(d) = F·d, then t'(p) = f[t(p)] = F·t(p). Therefore, the expression $(\partial f/\partial d) = c^{(-)} = (\partial f/\partial t) = c^{(+)} = F$ is always valid. By introducing this result in Eq. (17), the equality p' = p is always guaranteed; the LSS is invariant under the linear isomorphic transformations.

It is an easy task to show that the LSS is invariant under the transformation achieved in the second definition of PPP if each c is replaced simultaneously[5,9]. If, however, us transform the covariance and sensitivity matrices by neglecting this condition, for example,

$$V_{d'} = c^{(-)} V_d c^{(-)t} = \begin{pmatrix} 0.1125 & 0.06 & -0.06 \\ 0.06 & 0.05 & -0.04 \\ -0.06 & -0.04 & 0.04 \end{pmatrix} \tag{18}$$

$$G' = e^{(\cdot)} G = \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{19}$$

the LSS becomes (X,C) = (0.88,1.24). It must be recognized that the covariance and sensitivity matrix used in this solution are exactly the same as given in Eqs. (9) and (10) which leaded to the wrong answer of Eq. (11). Therefore, the anomaly which appeared in Section 3 is completely understood to be the result of an improper combination of transformed covariance matrix and sensitivity matrix.

4.2 Impact of Truncation of a Data Space

A "truncation" is defined as a transformation which does not conserve the dimensions of the data vector, its covariance matrix and/or the design matrix. By defining the operators α_i and β_i which delete the i-th row and column of a matrix, respectively, the truncation is schematically written as[5,9]

$$d' = \alpha_i d, \quad V_{d'} = \alpha_i \beta_i V_d \tag{20}$$

It was shown that the least-squares solutions before and after this type of transformation are generally not equivalent and sometimes cause serious disagreements which correspond to the original definition of PPP[5,9].

In PPP, as originally introduced, the off-diagonal term of the 2×2 covariance matrix is not zero. This fact indicates the existence of the third data value which introduces correlation between the two data. Therefore, the minimum dimension of this problem must be identified to be 3, and the correct solution must be sought in the 3-dimensional parent space. Once this is recognized, the correct answer is obtained as described in section 4.1. This is the answer to the original definition of PPP.

5. Conclusions

Two types of anomalies in the least-squares problem, known as Peelle's Pertinent Puzzle, are explained. The origins of these anomalies were accounted for by 1) improper combination of transformed covariance and sensitivity matrices, and 2) truncation of the data space. These two issues impact significantly on very wide range of topics in science and technology because the least-squares method is the most commonly used procedure of curve fitting and parameter estimation. If these two issues are resolved, the least-squares method can give a correct answer even if the data are discrepant, strongly correlated, and the number of data value is small. In other words, the least-squares method, in its simplest form, is completely valid if all input information is prepared correctly, i.e., if the covariance matrix is correct, the sensitivity matrix is correct, the combination of these is correct, and if the dimensionality of the problem is correct. In the practical applications, however, it is very likely that there will be deficiencies in these quantities. If so, it can be expected that anomalous results will be obtained. However, such "odd" answers might be correct in a certain problem[6,9]. Before deciding on this question and selecting an appropriate LSM approach, it is important to firmly

comprehend the history of how the data were derived.

A complete description of this problem and more details of our interpretation will be given in Ref. 9.

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2. Processing of Covariance Data and their Format

2.1 ENDF Format for Covariance Matrices

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In the ENDF-6 format[1] cov riance matrices for the following quantities can be stored:

Average number of neutrons per fission (ν) (MF=31),

Resolved resonance parameters (MF=32),

Neutron cross sections (MF=33),

Angular distributions (MF=34),

Energy distributions (MF=35).

The covariances obtained from parameter covariances and sensitivities are stored in MF=30. The most important covariance matrices among them are those for cross-section data. Therefore, the format of MF=33 was explained by showing some examples. The contents of this talk are the same as those of Ref. (1).

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2.2 Processing of Covariance File and Related Problems

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Abstract

Processing methods for generating broad group covariance data from ENDF/B format data are described briefly. Outline of covariance file, FORMAT, available processing codes, and processed data generally available are also described. Encountered problems from the processing of ENDF/B files are reviewed. Comments on the compilation strategy for JENDL covariance file, which is in scheduled, are made.

Contents

1. Introduction

Recently much attentions are made for the covariance data of JENDL, where no covariance data are existing at the moment. Officially no definite work assignments are made for the compilation work by JNDC(Japanese Nuclear Data Committee). Several advanced users are requesting these data for their accurate estimate of the design margins of advanced type reactor plant. In this paper, processing methods for generating broad group covariance data from ENDF/B format data are described briefly. Outline of covariance file, FORMAT, available processing codes, and processed data generally available through data centers are also described. Encountered problems from the processing of ENDF/B files are reviewed. Comments on the compilation strategy for JENDL covariance file in future are made.

2. Covariance and Covariance File

General properties of covariance are described below[1];

X: value to be evaluated for item 1,
f(X): normalized density function for item 1,
Y: value to be evaluated for item 2,
f(Y): normalized density function for item 2,

the mean of X can be defined as

$$\langle X \rangle = \int X \, f(X) \, dX \tag{1}$$

the covariance between X and Y can be defined as

$$COV(X, Y) = \int \int (X - \langle X \rangle) \, (Y - \langle Y \rangle) \, f(X, Y) \, dX \, dY \tag{2}$$

and the variance is expressed as

$$VAR(X) = COV(X, X) = \langle (X - \langle X \rangle)^2 \rangle \tag{3}$$

the standard deviation in <x> is defined

$$s(X) = (VAR(X))^{\frac{1}{2}} \tag{4}$$

the correlation between X and Y are written as

$$COR(X, Y) = \frac{COV(X, Y)}{s(X) \; s(Y)} \tag{5}$$

Thus defined covariance matrices have following characteristics. Symmetric behavior comes from by definition and positive definite nature of each element is the consequence of physical quantity involved. Further, this imply that the transformation to diagonal form of the covariance matrices yields non zero eigenvalues. And the correlation having more than 100% indicates that the covariance matrices are completely inconsistent. We cannot trust such data. Because the limit value of covariance is expressed as,

$$\begin{aligned} &COV(X, Y) < VAR(X) \\ &\quad and \\ &COV(X, Y) < VAR(Y) \end{aligned} \tag{6}$$

If 100 % correlation,

$$COV(X, Y) = s(X) * s(Y) \tag{7}$$

Covariance data are used due to the fact that the uncertainties in the various data tend to be highly correlated through the measurement processes and also that the different corrections should be made to the observable quantities to obtain the microscopic cross sections. In many applications when one is interested in estimating the uncertainties in calculated results based on the cross sections, the correlations in the uncertainties of the different data play a crucial role. In principle the uncertainties in the results of a calculation due to the data uncertainties can be calculated provided all of the covariances of the data are given. To assist the request for these users, covariance data file is supplied.

An evaluation and it's covariance correspond one to one, therefore they cannot be used

separately. There are no meaning if you use ENDF/B-VI covariance data for JENDL-3 evaluation unless the same evaluation method is used for both evaluations, i.e., the same results. Thus mixed use of covariances between different evaluations always destroy the consistency of covariances. If mixed use are made, data are combined which have not been evaluated together and which are originate from completely different experimental/theoretical data bases[1].

3. FORMAT and Outline of Processing

As stated before, an evaluation and it's covariance correspond one to one, therefore they cannot be used separately. Covariance data reflect the evaluation method directly used. Correlations between reactions are common features for nuclear cross-section evaluations. Because in nuclear cross-section measurements, absolute measurements are very difficult, relative measurements are frequently made i.e., relative to standard / reference data. Thus many reactions are involved implied or unimplied in the evaluation process. Covariance to other reactions are common feature in the evaluations for cross-section data.

Correlations are divided into several categories according to the nature of the quantity involved. For example, statistical uncertainty, energy resolution, detector efficiency, sample used, measured facility, etc. Usually they are divided to three categories, long-range(the last two example), medium-range (the third one) and short-range (the former two) components[6]. Typical examples are shown in Table 3.1.

For example, File32(for resolved resonance parameters) are only given for short-range components and it is only intended to provide information concerning the rapid variations of the covariance matrices of the different partial cross-sections over the resonances. Other long range covariances should be given in File 33. In the unresolved resonance region the covariances of the cross sections must be given entirely in File 33.

According to the ENDF/B documentation[6], File 33 is used to give a measure of the "accuracies and their correlations" of the data in File 33 and does not indicate the precision with which the data are entered in the File 33. Since ENDF/B represents the current knowledge of the microscopic data, the File 33 is used to give the covariances of the microscopic data. The data presentation is more or less broad group basis, because the main target of users of these files are designers and/or shielders of reactors, who are working with group constants. Generally File 33 is produced to give adequate data for the following items; (1) the variance of group cross sections, (2) the correlations of the uncertainties between the several adjacent groups, (3) the long-range correlations of the uncertainties over many groups. File structure of File 33 is summarized in Fig. 3.1.

File 31 is used to give the uncertainty of average total number of neutrons per fission including delayed and prompt neutrons. Format and processing specifications are the same as File 33.

For processing, following procedure are used to generate broad group covariance matrices from ENDF/B File 33 data.

If weighting function is uncorrelated to the cross section of interest

$COV(X_G,Y_H)$	: multi group covariance between reaction x for group G and reaction Y for group H;
Φ_G	: weight for group G;
$X_{G,K}$	: multi group cross-section for reaction X for a supergrid (i,k)
$\Phi_{G,K}$	: the weight for this group
F	: components of covariance taken directly from the uncertainty file
LB	: a flag whose numerical value determines the meaning of the numbers given in the arrays $\{E_k, F_k\}$ $\{E_l, F_l\}$ of ENDF

LB=0 Absolute components only correlated within each E_k interval

$$COV(X_G, Y_H) = \frac{\sum_{k \in G,H} F_{XY,k}\Phi_{G,k}\Phi_{H,k}}{\Phi_G\Phi_H} \tag{8}$$

LB=1 Fractional components only correlated within each E_k interval

$$COV(X_G, Y_H) = \frac{\sum_{k \in G,H} F_{XY,k}\Phi_{G,k}X_{G,k}\Phi_{H,k}Y_{H,k}}{\Phi_G\Phi_H} \tag{9}$$

LB=2 Fractional components correlated over all E_k interval

$$COV(X_G, Y_H) = \frac{(\sum_{k \in G} F_{XY,k}\Phi_{G,k}X_{H,k})\ (\sum_{k' \in H} F_{XY,k}\Phi_{H,k'}Y_{H,k'})}{\Phi_G\Phi_H} \tag{10}$$

LB=3 Fractional components correlated over E_k and E_l interval

$$COV(X_G, Y_H) = \frac{(\sum_{k \in G} F_{X,k}\Phi_{G,k}X_{G,k})\ (\sum_{l \in H} F_{Y,l}\Phi_{H,l}Y_{H,l})}{\Phi_G\Phi_H} \tag{11}$$

LB=4 Fractional components correlated over all E_l intervals within each E_k interval

$$COV(X_G, Y_H) = \frac{\sum_{k\in G} F_k \left(\sum_{l\in G} F_{xy,l}\Phi_{G,l}X_{G,l}\right)\left(\sum_{l'\in H} F_{xy,l}\Phi_{H,l'}Y_{H,l'}\right)}{\Phi_G\Phi_H} \quad (12)$$

LB=5 Relative covariance matrix components

$$COV(X_G, Y_H) = \frac{\sum_{k\in G,\, k'\in H} F_{xy;k,k'}\Phi_{G,k}X_{G,k}\Phi_{H,k'}Y_{H,k'}}{\Phi_G\Phi_H} \quad (13)$$

4. Processing Codes Available in the world

In Table 4.1 currently available processing code for ENDF/B are given[2].
In JAERI we developed our processing system[5] for ENDF/B-5 format data, adopting PUFF-2[8] code and ERROR[9] module in NJOY system. We adopted working format of covariance data for broad group is COVERX[7]. Processing outline is shown in Fig. 4.1 and a sample of processed output is shown in Fig. 4.2.

In Table 4.2 group averaged covariance data generally are available from data centers[2]. These ready made data sets are completely application oriented, for examples fusion blanket / shielding studies, PWR dosimetry, oil well logging and FBR reactor benchmarks. And these data are rather old, you must pay attention when you use.

5. Problem of ENDF/B-5 and -6 Format

For ENDF/B-5 format, following drawbacks are pointed out from several users[1-5];

1. no data given for File-4 (Angular distribution) and File-5 (Energy Distribution), i.e., secondary angular / energy distribution,
2. incapable of including the correlation between ν at 2200 m/s and fission cross-section,
3. processing was unnecessarily complex.

In ENDF/B (including B-5 and B-6 format) data specification, no covariance information in the file does not mean no existing correlations. In applications, this indication is very important to distinguish the two situations. Explicit indication is required for no correlation to some particular reactions.

For ENDF/B-6 format, following problems are reported[1-4];

1. LB=6 sub sub-section in file 33

There is no easy way to find out whether one specific reaction is used in some sub-section unless whole file search is applied. If information on covariances between reactions is created/modified, the data have to be stored/updated always in the files of both reactions.

2. NC type sub-subsection in File 33

In some case, where accurate cross-section measurements were made such as total(MT=1), usage of NI type sub-subsection is recommended, i.e., independent from summed up one.

Mixed use of NI and NC should be permitted for particular MT case. Candidates are given in Table 5.1. Updating the existing covariance matrices it is necessary not to miss any implicitly existing correlations.

6. Comments on Covariance File Compilation of JENDL

Now we are just the point to make our decision whether to develop a covariance file for JENDL, in which we have no data up to now. One of the main reasons of this meeting is to get a consensus to make a JENDL covariance file. As seen from the nature of the uncertainty file and the characteristics of the covariance file, the covariance file directly reflects the evaluation process of JENDL. Then, if covariance information is treated once, all existing correlation have to be taken into account and updated to keep the integrity of the whole system. This means, once covariance matrices introduced in the evaluated nuclear data file, update to any one data should be made on this system to keep the consistency between data. Such a system must be very complicated. But if the system maintained correctly, all information can be manipulated mechanically. These task should be very expensive one, in some case it takes much time than the original evaluation efforts if all the evaluation process retraced again. But users needs are very keen. If the decision is "go" then evaluators should know well the problem of covariance file stated in the previous section.

For the practical compilation of covariance data, following advises are raised according to the fundamental requirements of evaluated data file[3-4];

1. Use File1 comment section to identify what covariances are involved explicitly,
2. To limit the propagation of interrelation of covariances, correlation below the negligible amount (ex. lower than 10%) should be neglected.
3. Identification and minimization of correlated uncertainties should be made.
4. Decreasing statistical uncertainties much below the level of correlated uncertainties is no good strategy.

7. Summary

Processing methods for broad group covariance data in ENDF/B format were described briefly. Outline of covariance file, FORMAT, available processing codes, and processed data generally available were also described. Encountered problems from the processing of ENDF/B files were reviewed. Comments on the strategy for the compilation of JENDL covariance file in future were made.

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Table 3.1 Analogies Between File 33 Covariances Within One Section and Experimental Uncertainties

File 33	Experimental	Energy Dependence
short-range	statistical	Rapid variation
medium-range	Detector Efficiency Multiple Scattering In/Out Scattering	Slowly varying
long-range	Geometry Flux Background Normalization	More or less constant

Table 4.1 Processing code for covariance data of ENDF-B

code	comments
NJOY91:	most widely used code for processing evaluated covariance data into a multigroup form
	ERROR module: multi group processing
	COVR module: format transformation and data compression to the compact BOXR format.
PUFF-2:	B-5 FORMAT (COVERX FORMAT output)
UNC 32/33:	B-5 FORMAT (Resonance parameter uncertainties)

Table 4.2 Group Averaged Covariance Data

data	comment
COVERX format:	FORSS system with service module very compact and convenient for users
COVERX:	multigroup covariance library for reactor applications.
COVFIL:	neutron cross-section & covariances for sensitivity analysis.
DOSCOV:	24 group covariance data library from B/V for dosimetry.
SENPRO/45C:	multigroup sensitivity library for fast & thermal reactors.
VITAMIN J/COVA:	covariance matrix data library for uncertainty analysis.
GRESS:	the general purpose tool for perturbation. FORTRAN precompiler with differentiation enhancement. automatic sensitivity study can be made. specify sensitivity to be requested. Applied to: neutron transport, nuclear model code

Table 5.1 Redundant reactions

MT	reaction
1	total
3	nonelastic
4	inelastic
18	total fission
103	p (600-649)
104	d (650-699)
105	t (700-749)
106	He-3 (750-799)
107	alpha (800-849)

Those MT reactions are defined by sum-up of relevant reactions.

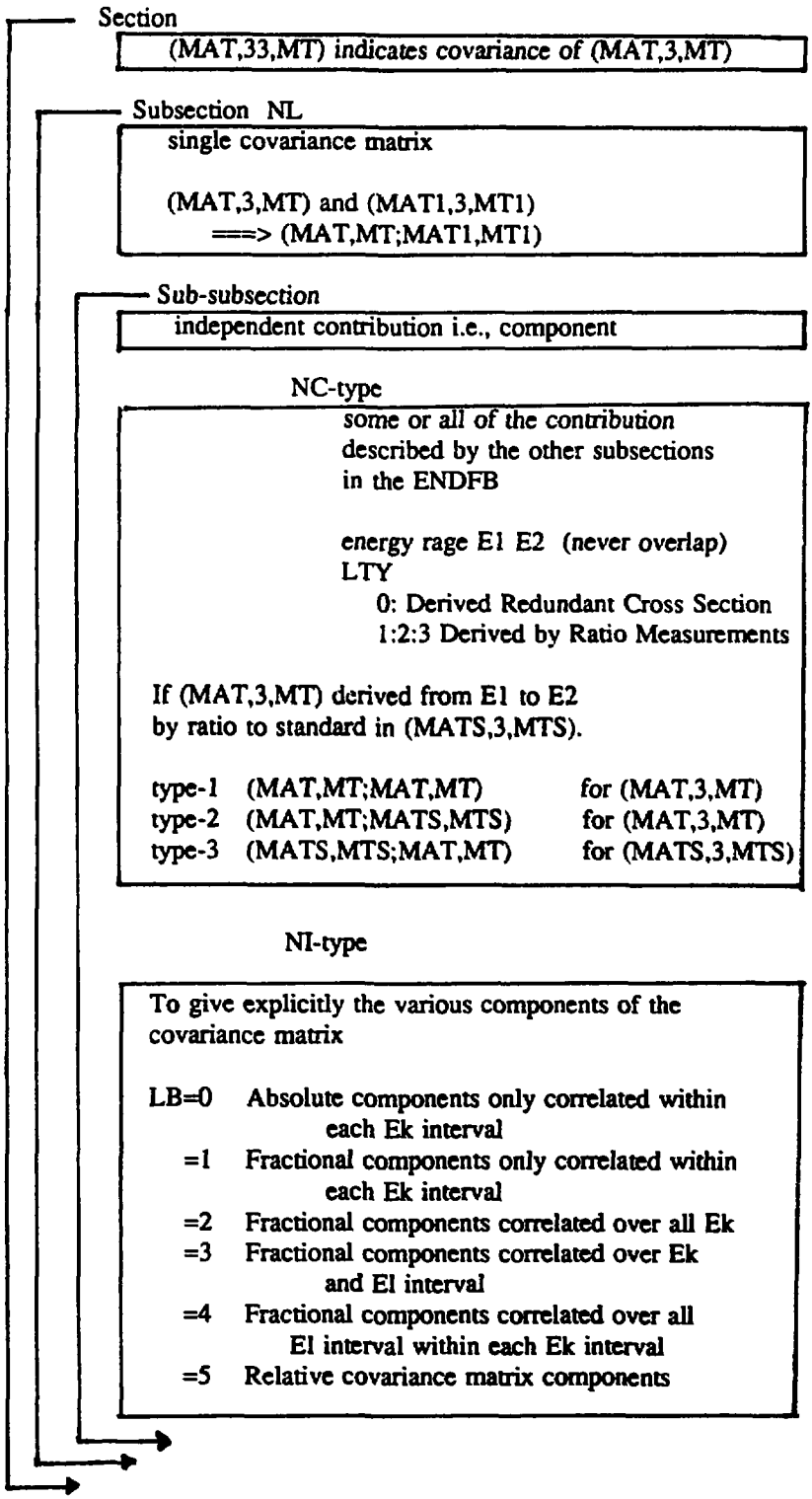

Fig. 3.1 FILE 33 (Covariance for Cross-sections) structure

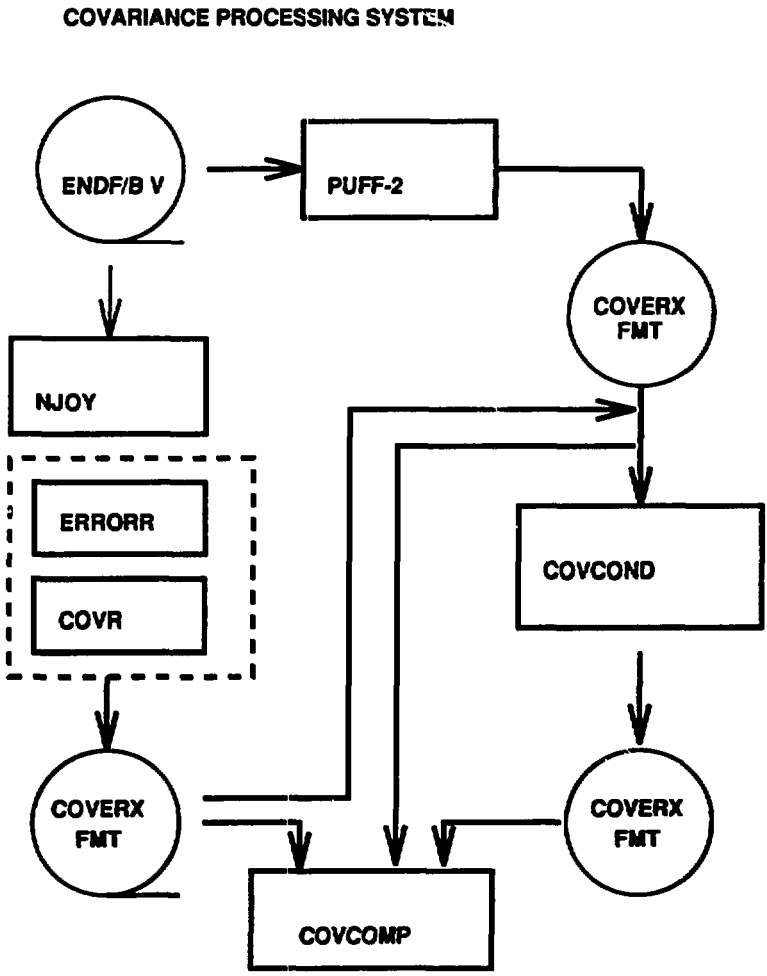

Fig. 4.1 Covariance processing system of JAERI

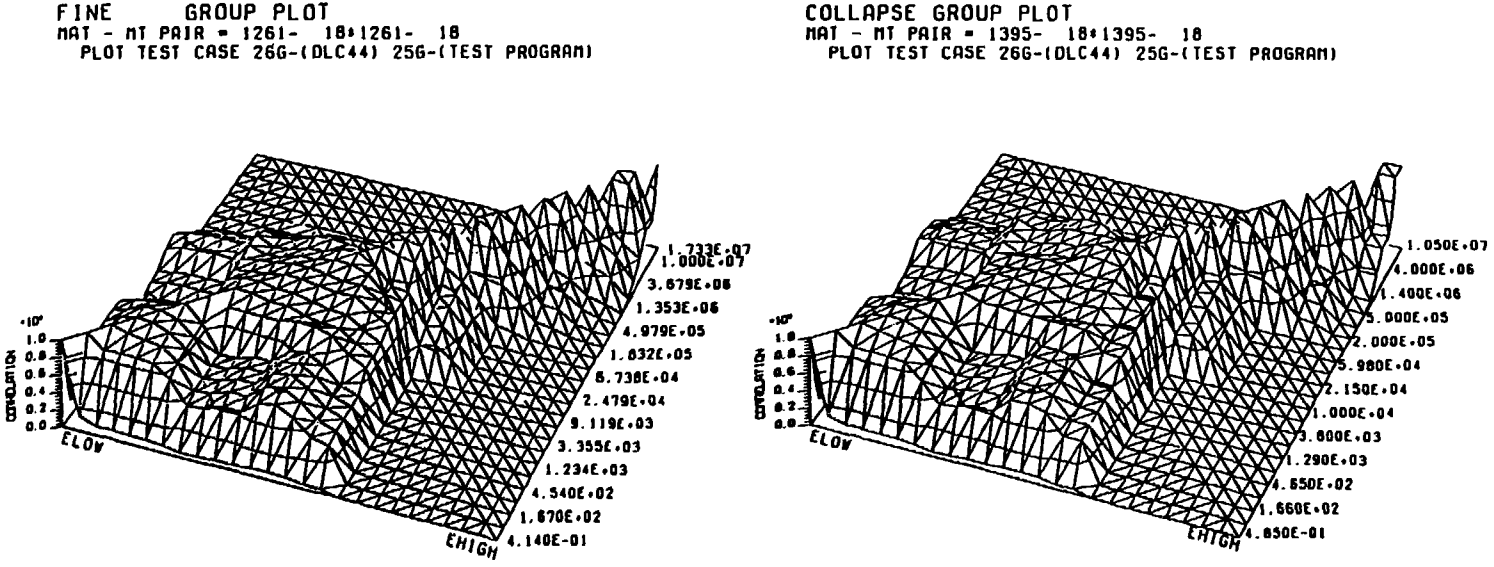

Fig. 4.2 Output example of covariance processing system of JAERI Comparison of covariance matrices between collapsed and calculated by PUFF-2 code. (left : PUFF-2 calculated right : collapsed)

2.3 Experience on Preparation of a Covariance Library for the NEUPAC Code

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Some comments are given for making group averaged covariance matrices through an experience of preparation of a dosimetry cross section and covariance library for the spectrum adjustment code, 'NEUPAC'.

1. Introduction

Neutron dosimetry using activation detectors is often used to measure neutron fluence, neutron energy spectrum and related nuclear transmutation rates in heavy neutron irradiation environments. This method utilizing several kinds of activation reactions with different energy responses needs a well-evaluated activation cross sections, that is, 'Dosimetry File'. In particular, their covariance data are indispensable to spectrum adjustment (or unfolding) techniques based on probabilistic statistics, which are the most preferable in the activation method.

Here are given some comments through a work experience of making group averaged covariance matrices for one of the spectrum adjustment code, 'NEUPAC'[1].

2. Methods for making group averaged covariance matrices

When the evaluated covariance files, such as ENDF/B-V, IRDF etc., are available, two kinds of methods are adopted to make group averaged covariance matrices; one is called 'COVRX,' or revised 'COVSIG', which uses a transformation matrix $\mathbf{T}$ from i group covariance matrix $\mathbf{C_i}$ to m group $\mathbf{C_m}$ ($=^t\mathbf{T}\mathbf{C_i}\mathbf{T}$), keeping reaction rate unchanged[2]. The other is 'ERRORR', which is one of the modules in NJOY system[3]. Using the group flux ϕ_i and covariance data $\mathbf{Z_i}$ on the union energy grid synthesizing the user's grid with the original file's one, the covariance matrix is made in an arbitrary energy group structure.

In a very rare case that there is no covariance data in the files, the diagonal elements in a covariance matrix, that is, the variance of cross section curves was roughly estimated by eyesight on some figure and the gaussian correlation was assumed as follows;
$Cov(\sigma_i,\sigma_j) = \Delta\sigma_{sys}^2 + P_{ij}\Delta\sigma_i\Delta\sigma_j$, $P_{ij} = (1-\theta)\,\delta_{ij} + \theta \exp[-(i-j)^2/2\gamma^2]$,
where $\Delta\sigma_{sys}$: Systematic uncertainty component
$\Delta\sigma_i$, $\Delta\sigma_j$: Estimated diagonal uncertainty components of i and j group cross sections, respectively
P_{ij} : Gaussian correlation matrix function
θ, γ : Index parameters giving group correlations.

3. Validity check on prepared covariance matrices

The experimental data of reaction rates in standard neutron fields, that is, the measured spectrum averaged cross sections are very useful to check the validity of the prepared covariance matrices. The statistical testing such as χ^2 test and 3σ test are preferably used, in which the following quantity is evaluated;

$$\chi 2 = \frac{1}{n}\sum_{i=1}^{N} (R_i^{exp} - R_i^{cal})2/[(\Delta R_i^{exp})2 + (\Delta R_i^{cal})2]$$

and

$$\left|R_i^{exp} - R_i^{cal}\right| \le 3[(\Delta R_i^{exp})2 + (\Delta R_i^{cal})2]^{1/2}$$

Another advanced approach is the adjustment of the original covariance matrix by using a set of the spectrum averaged cross sections R_i of the same reaction type in different kinds of standard neutron fields ϕ_{ij}, of which relation is expressed as;

$$R_i^{exp} \pm \Delta R_i^{exp} = \sum_j [\phi_{ij} \pm \Delta\phi_{ij}]\sigma_j$$

i: the suffix for different neutron fields,
j: the suffix for energy group

The solutions after adjustment of the original cross section data σ_0 and its covariance matrix $\mathbf{M_0}$ are formally given by;

$$\sigma_{adj} = \sigma_0 + \mathbf{M_0}^t\mathbf{A}(\mathbf{A}\mathbf{M_0}^t\mathbf{A} + \mathbf{M_R})^{-1}(\mathbf{R} - \mathbf{A}\sigma_0)$$

$$\mathbf{M_{adj}} = \mathbf{M_0} - \mathbf{M_0}^t\mathbf{A}(\mathbf{A}\mathbf{M_0}^t\mathbf{A} + \mathbf{M_R})^{-1}\mathbf{A}\mathbf{M_0},$$

where $(M_0)_{gk} = \Delta\sigma_{go}\Delta\sigma_{go}$, $(M_R)_{ij} = \Delta R_i\Delta R_j$ and $(A)_{ij} = \phi_{ij}$.

To make good use of this procedure, the data base of the measured spectrum averaged cross sections in as many different neutron fields as possible should be systematically constructed.

4. Summary

The dosimetry cross section and covariance libraries for the NEUPAC code has been so far prepared in 103 and 135 energy group structures mainly from the ENDF-B/V and IRDF-82 dosimetry files, and a new version of the library is now being made from the JENDL dosimetry file[4]. It seems, however, that the following problems still remain unclear;

(1) Theoretical backgrounds in transformation of energy group structure of covariance matrices, in particular for the uncertainty estimation when the transformed group width becomes smaller than the original one,

(2) Evaluation of cross section uncertainty in resonance region, such as the validity of fitting with the Breit-Wigner formula, correlation between different resonances etc.,

(3) Treatment of correlations between cross sections obtained from relative measurement to a common standard, which should be clearly distinguished in uncertainty propagation when making covariance files,

(4) Uncertainty estimation due to group averaging of cross section data with weighting spectrum $\phi(u)$, where a large correlation may occur between group averaged cross sections through the uncertainty of the weighting spectrum $\Delta\phi(u_1)\Delta\phi(u_2)$.

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3. Evaluation Methods of Covariance Data

3.1 An Experience of Preparation of Covariance Matrices for the Simultaneous Evaluation of Heavy Nuclide Cross Sections

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Preparation of covariance matrices for experimental data is described briefly,and the standard deviation and covariance matrix of the simultaneous evaluation are presented.

The simultaneous evaluation of neutron fission cross sections of U-235,U-238,Pu-239,Pu-240 and Pu-241, and neutron capture cross sections of U-238 and Au-197 were performed in 1984-85 as a preliminary evaluation for JENDL-3 /1/. Covariance matrices of the experimental data were required and were estimated by the evaluators of each elements on the same procedures which were discussed and determined by the working group members (*). Details of the estimation procedure were already reported at the 1984 Seminar on Nuclear Data and described in reference /2/.

In short, partial errors of the measured data of the cross sections, fission ratios and so on were classified into three groups; strong, medium and weak correlation between different incident neutron energies. These groups were assumed to have correlation of 100 %, 50 % and 0 %,repectively. In case of no partial errors were given in the experimental papers, estimation of the partial errors was made by dividing the total errors of the experimental data, considering the adopted techniques of the measurement .

Thus obtained correlation matrices of the each experiments were utilized to process the cross section and ratio data with the least squares computer program developed by Uenohara and Kanda /3/. About 75 data sets and several thousands data points were manipulated simultaneously. The evaluated cross sections and their standard deviations are shown in Fig.1 for some reactions. Figure 2 displays the parts of the evaluated covariance correlation matrices which correspond to the cross sections shown in Fig.1. The total correlation matrix has size of 245 x 245, and has correlation more than 50 %, in some energy regions, between different quantities such as fission cross sections of U-235 and Pu-239.

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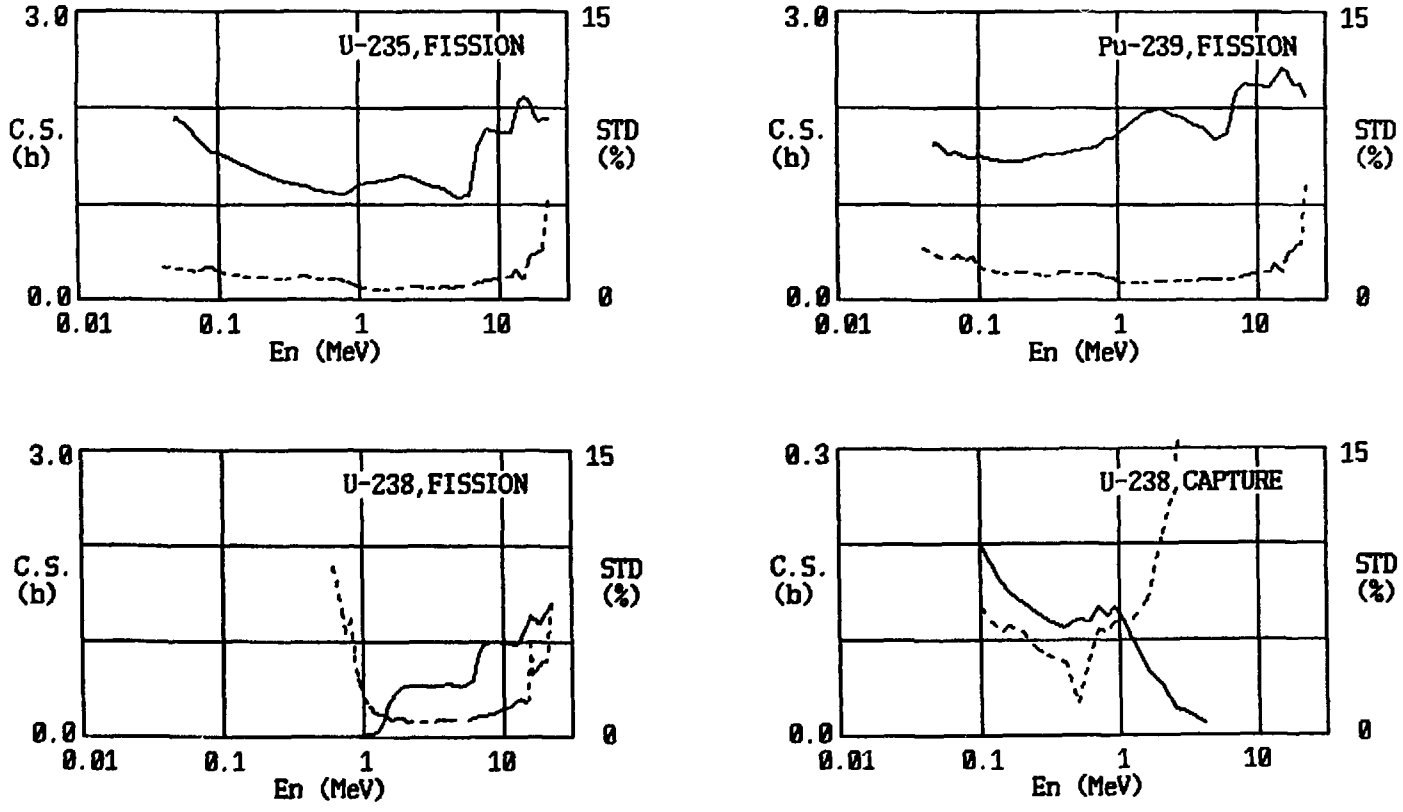

Fig.1 Examples of the simultaneously evaluated cross sections (solid lines) and their standard deviations (dashed lines).

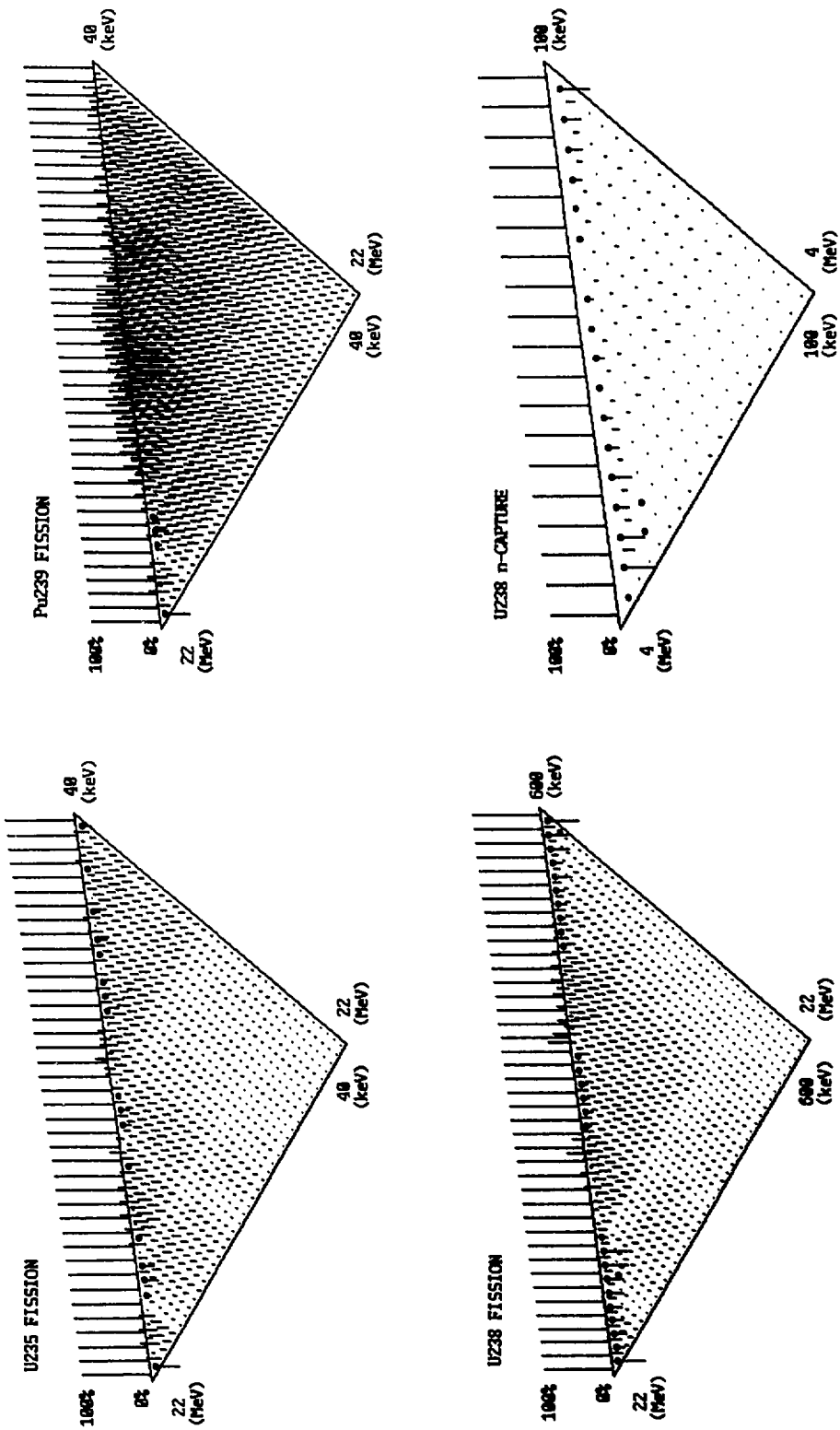

Fig.2 Partial covariance (correlation) matrices of the simultaneous evaluation. Negative correlation values are indicated by small circles at zero-points of the bars.

3.2 Covariance Matrix Calculated from Nuclear Models

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Abstract : A production method of a covariance matrix from a nuclear model calculation is described. An optical model is used to estimate the covariance matrix of the ^{54}Fe total cross section, and a Hauser-Feshbach and a precompound models are used for the covariance matrices of ^{54,56}Fe(n,p) reaction cross sections. These matrices are calculated from the uncertainties of level density parameters, a precompound parameter, and the optical potential parameters for neutron, proton, and α-particle. The neutron optical potential parameters and their uncertainties are evaluated from the experimental total and elastic scattering data, while the other parameters and their uncertainties are evaluated from the experimental ^{54,56}Fe(n,p), (n,α), $(n,2n)$, (n,Xp) and $(n,X\alpha)$ reaction cross sections.

1.INTRODUCTION

A covariance matrix accompanied with an evaluated nuclear data depends on a nuclear data evaluation method. In a case of a curve-fitting method, one must search the best values of parameters which characterize the fitting curve. Once the parameters and their uncertainties are obtained, one can estimate the covariance matrix accompanied with the evaluated curve by means of the principle of error propagation. The derived covariance strongly depends on the character of the fitting curve, and it usually gives strong correlations among the evaluated data even though there are no correlations among the used experimental data.

Since the fitting function is a nuclear model calculation in the nuclear data evaluation, the estimation of the evaluated data and their covariance is equivalent to the search of the proper model parameters which characterize the nuclear model calculation. The

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nuclear model parameters are physical quantities and they usually are not free. However, we can regard the parameters as adjustable within a certain acceptable limit. The acceptable limit to variation of the parameters is given by *a priori* knowledge, theoretical consideration and/or experimental information about the parameters, and it can be expressed as the prior covariance matrix of the parameters. When the nuclear model calculation is fitted to the experimental data, an uncertainty of the model parameters are determined according to the prior covariance of the parameters and the covariance of the experimental data. This uncertainty of the model parameters brings some uncertainties to the evaluated nuclear data, and the covariance matrix of the evaluated values can be generated. The uncertainty of a certain model parameter propagates into the different calculations, then the uncertainties in the evaluated data are correlated each other.

In this paper, we show the derivation method of the covariance matrix from the nuclear model calculation. An optical model, a Hauser-Feshbach model, and a precompound model are used to the nuclear data evaluation of neutron induced reaction cross sections of ^{54,56}Fe. The parameters and their uncertainties of the nuclear models are estimated from *a priori* knowledge about the parameters and the experimental data concerned.

2. Calculation Method

In order to make a covariance matrix, one must search suitable parameters to the experimental data, and also evaluate uncertainties of these parameters. This is achieved with a parameter estimation method based on a Bayes theorem[1].

The parameter estimation is carried out by the following equations,

$$\begin{aligned} \boldsymbol{x}_1 &= \boldsymbol{x}_0 + \mathbf{P}\mathbf{C}^t\mathbf{V}^{-1}(\boldsymbol{y} - \boldsymbol{f}(\boldsymbol{x}_0)) \\ &= \boldsymbol{x}_0 + \mathbf{X}\mathbf{C}^t(\mathbf{C}\mathbf{X}\mathbf{C}^t + \mathbf{V})^{-1}(\boldsymbol{y} - \boldsymbol{f}(\boldsymbol{x}_0)), \qquad (1) \\ \mathbf{P} &= (\mathbf{X}^{-1} + \mathbf{C}^t\mathbf{V}^{-1}\mathbf{C})^{-1} \\ &= \mathbf{X} - \mathbf{X}\mathbf{C}^t(\mathbf{C}\mathbf{X}\mathbf{C}^t + \mathbf{V})^{-1}\mathbf{C}\mathbf{X}, \qquad (2) \end{aligned}$$

where $\boldsymbol{x} = (x_1, x_2, \ldots, x_m)^t$ is a model parameter vector, $\boldsymbol{y} = (y_1, y_2, \ldots, y_n)^t$ is an experimental data vector, $\mathbf{V}$ is a covariance matrix of the experimental data, and matrix $\mathbf{C}$ is a sensitivity matrix which is obtained by numerical derivatives of the model calculations around the parameters. We assume that distribution of the vector $\boldsymbol{x}$ is a m−dimensional normal distribution with $\langle \boldsymbol{x} \rangle = \boldsymbol{x}_0$, and $\langle (\boldsymbol{x} - \boldsymbol{x}_0), (\boldsymbol{x} - \boldsymbol{x}_0)^t \rangle = \mathbf{X}$, where $\boldsymbol{x}_0$ is a prior parameter vector.

Equations (1) and (2) give a posterior parameter vector $\boldsymbol{x}_1$ and its covariance $\mathbf{P}$. The covariance $\mathbf{P}$ contains the information of the experimental data and *a priori* knowledge about the model parameters. A covariance matrix of evaluated nuclear data $\mathbf{M}$ is calculated with the posterior covariance $\mathbf{P}$ by a principal of error propagation,

$$\mathbf{M} = \mathbf{C}\mathbf{P}\mathbf{C}^t. \tag{3}$$

3. Results and Discussions

3.1. Optical Model

The optical model gives a total cross section, an elastic scattering cross section and its angular distribution. The covariance matrices of these cross sections can be estimated with uncertainties of the optical potential parameters.

In the energy range $1 \leq E_n \leq 20$ MeV, calculated cross sections — total, and the angular distribution of the elastically scattered neutrons — with a geometry-fixed optical potential are sometimes insufficient to reproduce the experimental data. Then we estimated the optical potential parameters for ^{54,56}Fe with an energy-dependent-geometry from the experimental data of the elastic scattering cross sections[2,3,4,5], and the total cross sections[5,6,7]. The estimated optical potential parameters are expressed by volume integrals per nucleon J_v and J_w where $J_{v,w} = (\frac{4\pi}{A})\int_0^\infty \{V(r), W(r)\}r^2dr$, and they are shown in Fig. 1. In this figure, the symbols are derived values from the experimental data. We fitted a linear function of the neutron energy E_n to the estimated parameters. The solid line in Fig. 1 is J_v for ^{54}Fe, the dotted line is J_v for ^{56}Fe. The strength of the imaginary potential J_w is identical to ^{54}Fe and ^{56}Fe. Comparisons of the calculated angular distribution of the elastic scattering with these J_v and J_w at E_n =9.94 and 20 MeV are shown in Fig. 2.

The covariance matrix of the total cross sections is produced from the uncertainties of J_v, J_w, and the geometrical parameters (radius and diffuseness). The calculated covariance matrix of the ^{54}Fe total cross section is depicted in Fig. 3. In this figure, x- and y-axis are neutron energy, z-axis for the left portion is a correlation coefficient, and the right portion is a relative uncertainty(%) of the cross section. The calculated total cross section with the optical model is characterized by the optical potential parameters, and these parameters are used for over a wide energy range. Then the uncertainties of the parameters propagate to the wide energy range of calculations. As seen in Fig. 3, the correlation exists between the different energies though the difference of these energy is wide.

3.2.Hauser-Feshbach Model

Particle-emission-reaction cross section such as (n,p), (n,α), and $(n,2n)$ reaction is calculated with the Hauser-Feshbach and the precompound models. The important quantities in these models are, optical potential parameters for neutron, proton, and α-particle which generate a transmission coefficient, a level density parameter, and a precompound parameter. These parameters are estimated from experimental ^{54,56}Fe(n,p), (n,α), and $(n,2n)$ reaction cross section data including additional (n,Xp) and $(n,X\alpha)$ data. The cross sections are calculated from 5 MeV to 20 MeV at intervals of 1 MeV, and we use a linear interpolation between the calculation points.

The optical potential parameters for neutron were determined from the experimental data described in the last section. We take the global optical potential parameters of Perey's[8] for proton and Lemos'[9] for α-particle. The prior level density parameters are taken from Gilbert-Cameron[10].

First, we fix the optical potential parameters and the precompound parameter, and we estimate the level density parameters only. The prior covariance matrix $\mathbf{X}$ is prepared with the assumption that the uncertainties of the level density parameters are 5 %, and there are no correlation among the parameters. The estimated level density parameters are indicated as "Posterior 1" and they are shown in Fig. 4. The calculated ^{54,56}Fe(n,p) reaction cross sections with the prior and the posterior parameters are shown in Fig. 5. As shown in the drawing of ^{56}Fe(n,p) reaction, the calculated cross sections with the posterior parameters above 15 MeV disagree with the experimental data. In these energy range, two particles emission can be possible, however an excitation energy of a residual nucleus after two particles emission is low. Then a transition from a continuum to a discrete level is dominant after the first proton is emitted, and the level density of the residual nucleus is insensitive to this probability. In order to solve discrepancies between the calculation and the experimental data above 15 MeV, it is required to include the other parameters that have influence upon the cross section calculation.

We regard the real and imaginary potential depths of the global parameters for the charged particles (Perey and Lemos) as prior parameters to be estimated. The potential depths are expressed by a first order polynomial function, $V = V_0 - V_1 E, W = W_0 + W_1 E$. We include the V_0 and W_0 in the parameter estimation. In addition, the precompound parameter K' in Ref. 11 with the value of 120 is included in the estimation. We give the uncertainty of 5 % for these parameters, while the uncertainties of the level density parameter are 30 %.

The deviations of the potential depths and the precompound parameter between the prior and the posterior values were less than 1 % except for the real depth of proton, that was reduced 9.1 %. The estimated level density parameters are also depicted in Fig. 4 (Posterior 2). The calculated cross sections with these parameters are shown in

Fig. 5. The reproducibility of the experimental data is improved in comparison with the calculated cross sections with "Posterior 1" parameters, as seen in Fig. 5.

The covariance matrix is calculated from the covariance matrix of the posterior parameters (posterior 2) as well as contribution of the uncertainties of the neutron optical potential parameters. The final covariance matrices for ^{54,56}Fe(n,p) reaction are plotted in Fig. 6.

4. Conclusion

A production method of a covariance matrix from a nuclear model calculation was summarized.

Uncertainties of neutron optical potential parameters were estimated from the experimental total and elastic scattering cross section data. The covariance matrix of ^{54}Fe total cross section was calculated from the uncertainties of the neutron optical potential parameters. The covariance matrices of ^{54,56}Fe(n,p) reaction cross sections were calculated from the uncertainties of the level density parameters, the precompound parameter, and the optical potential parameters for charged particles and neutron.

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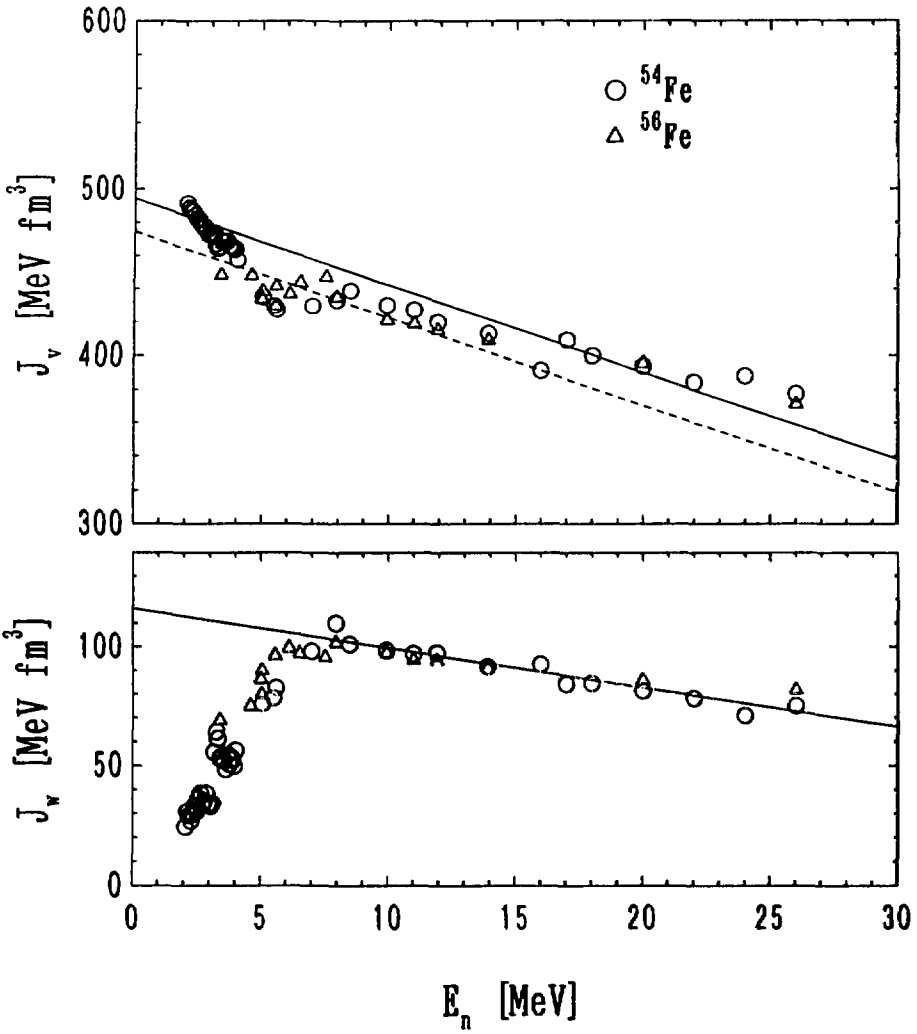

Fig. 1 Volume integrals per nucleon for real and imaginary potentials. The symbols are derived values from experimental data (○ for ^{54}Fe, △ for ^{56}Fe). The lines are obtained with the least square fitting. The solid lines are J_U for ^{54}Fe, and the dotted line is J_U for ^{56}Fe. The J_ω is identical to ^{54}Fe and ^{56}Fe.

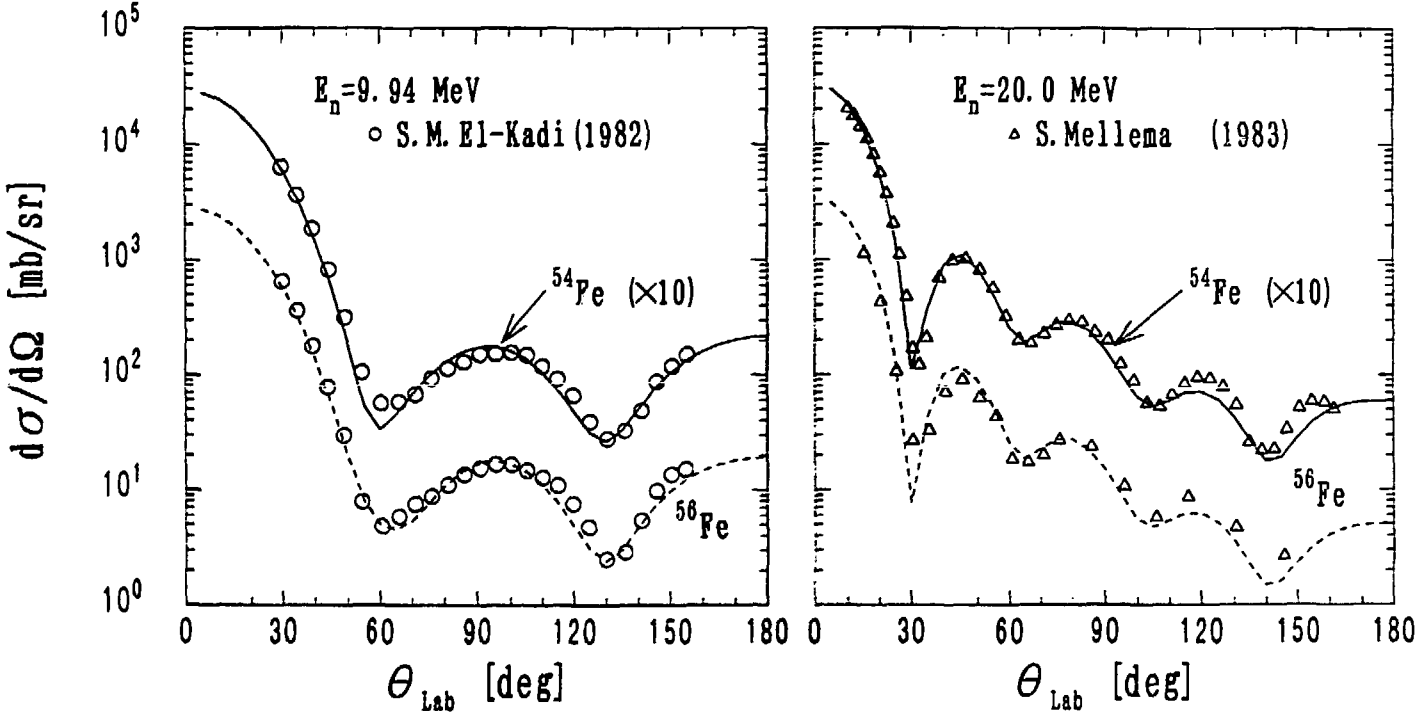

Fig. 2 Comparisons of the calculated angular distribution of elastic scattering cross section with the estimated neutron optical potential parameters.

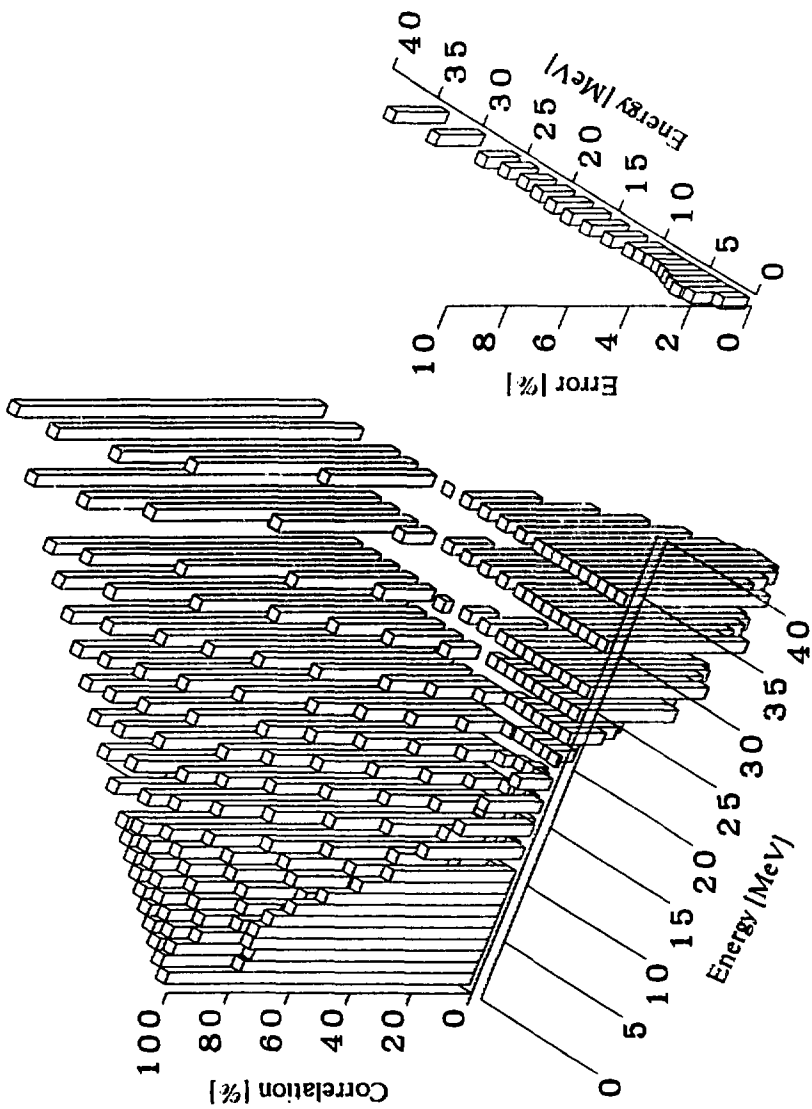

Fig. 3 3D-plot of the covariance matrix of the ^{54}Fe total cross section.

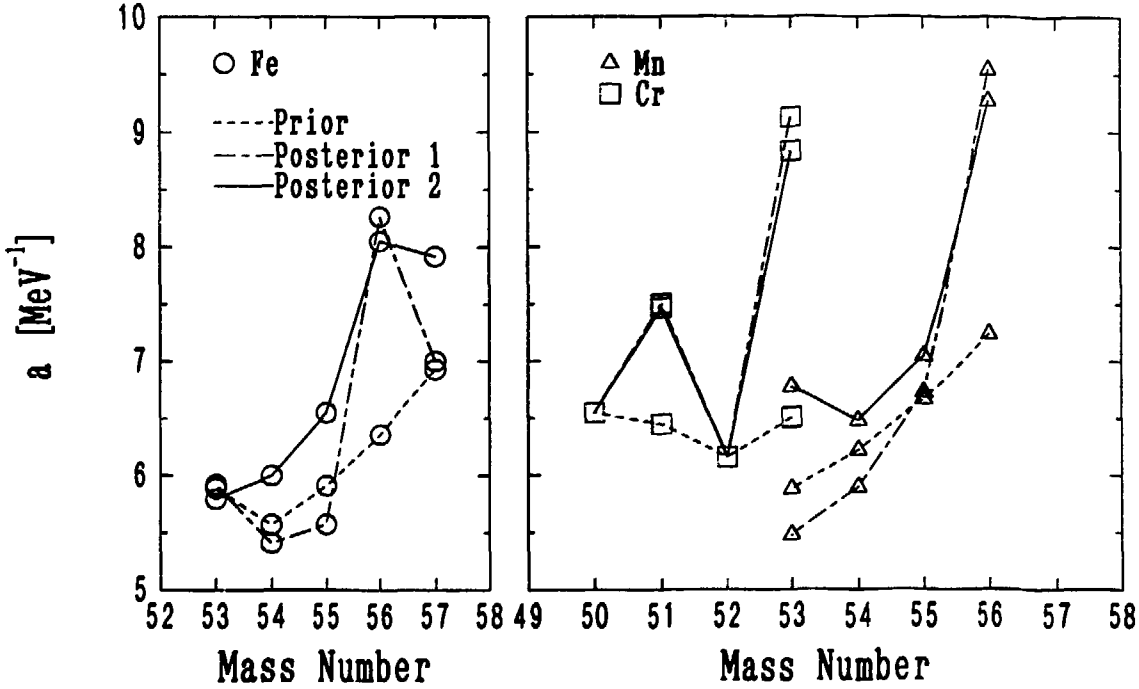

Fig. 4 Level density parameters. The dotted lines are the prior values, the dot-dashed lines are the posterior values when the only level density parameters are included in the parameter estimation. The solid lines are the posterior values when the charged particle optical potential parameters and the precompound parameters are added in the estimation.

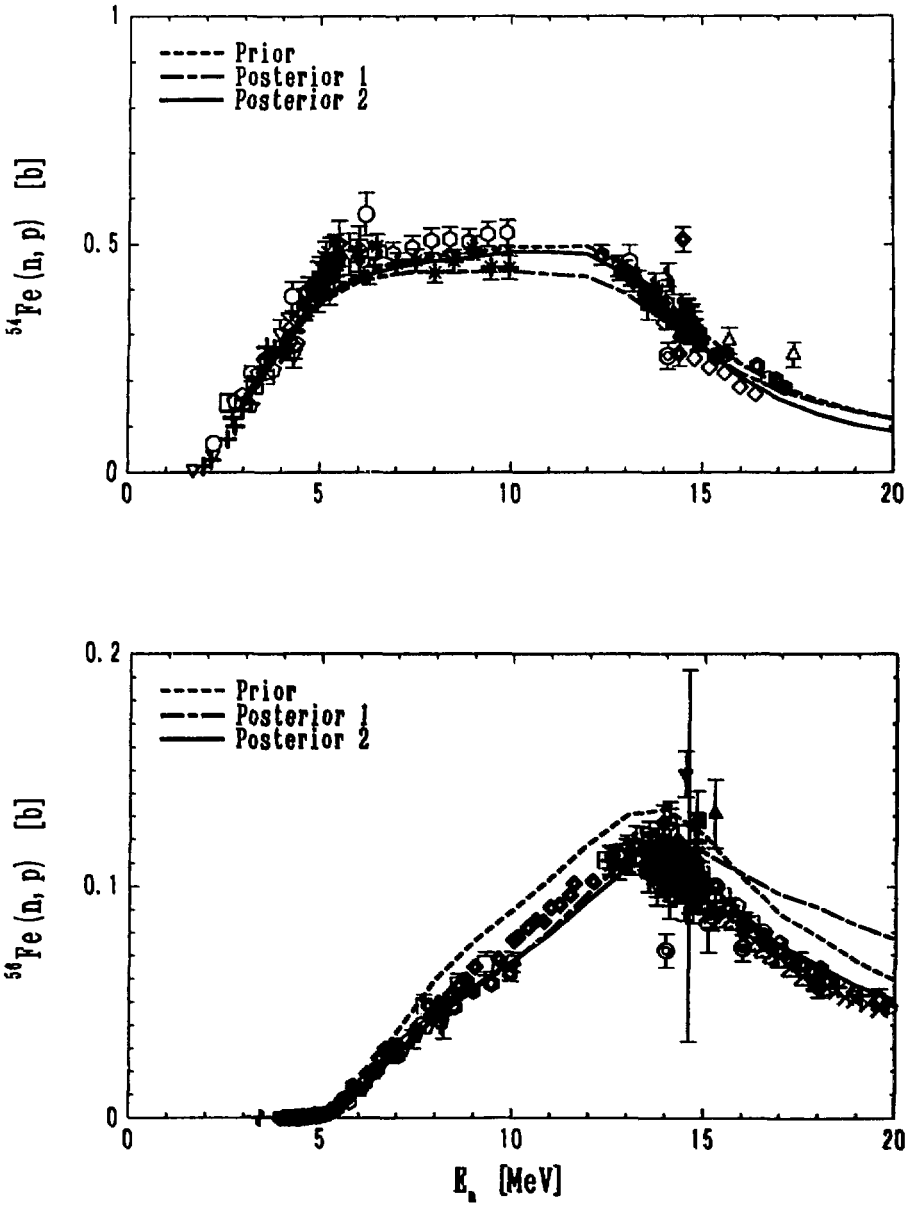

Fig. 5 Calculated $^{54, 56}$Fe (n, p) reaction cross sections.

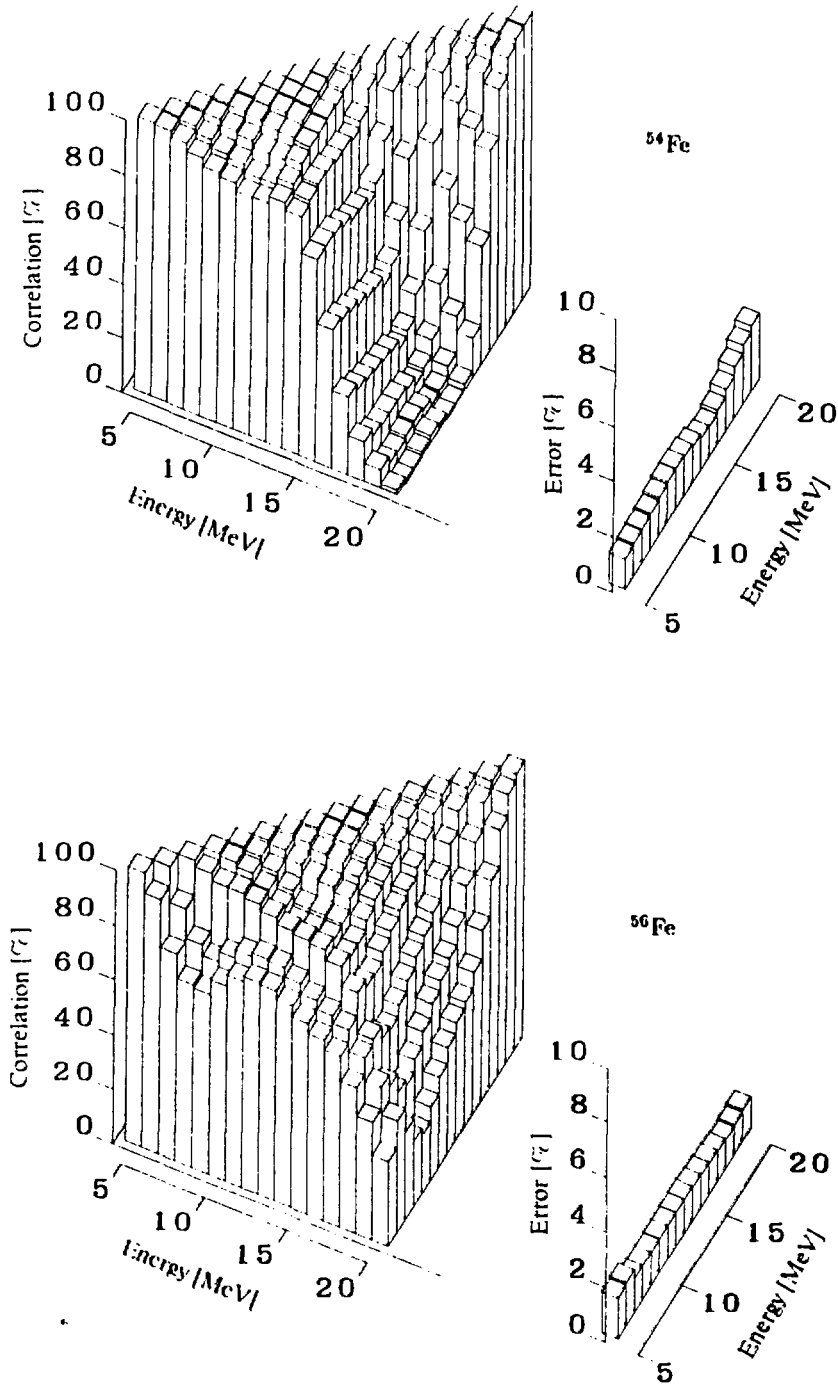

Fig. 6 Covariance matrices of ^{54}, ^{56}Fe (n, p) reaction cross sections.

3.3 Covariance Analysis of Experimental Data

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Abstract: Making use of activation data for the cross section measurements, it has been demonstrated how the covariance matrix of the data can be generated. A procedure for combining the data has been also illustrated using the covariance matrix by means of numerical examples taken from three experimental values to obtain an estimate of the best value.

INTRODUCTION

Although the concept of experimental errors and their propagation is well known, it would seem that the practical treatment of the experimental data is not always enough for the aspect of reactor dosimetry and calculations[1,2], because all of the data information are not often taken into account in the error analyses. In order to propagate the uncertainties in the input data, it is necessary to obtain all of the partial derivations of the experimental results. Until recently, this task has not been carried out, sometimes neglecting the covariance matrix which includes all of the uncertainty information in the experimental data.

The first introduction of the covariance matrix was made aiming at improvement of the reactor dosimetry[1] and neutron spectrum adjustment with activation data[3,4]. In these days, much interest has been paid to the generation of covariance matrix[1,5] and to the evaluated data file with the matrix[6,7].

The purpose of this paper is to demonstrate how to generate a covariance matrix in the experimental data and how experimentalists should show the uncertainties in their measurements for the further evaluation to combine them by using the numerical examples. A procedure to estimate the best value from the experimental data with covariance matrices is also described.

COVARIANCES OF EXPERIMENTAL DATA

2.1. Covariances in Ratio Measurement

An unknown cross section is often determined by means of the reaction rate ratio measurement relative to a well-known cross section. This procedure eliminates the measurement of the absolute neutron flux density. The ratio of two cross section values can be generally expressed as

$$R_{ij} = \sigma_i / \sigma_j = P_i / P_j \ , \tag{1}$$

where σ_i is a cross section and P_i is an unnormalized reaction rate given by

$$P_i = \frac{A_i}{N_i \varepsilon_i} \prod_i k_i(l) \ . \tag{2}$$

Here, A_i corresponds to the counting rate, ε_i is the detection efficiency and N_i the number of the nuclei. Each term of $k_i(l)$ is a correction factor corresponding to the measurement. One can obtain the following relations by differentiating Eqs. (1) and (2), respectively;

$$\delta R_{ij} = \delta P_j - \delta P_j \ ,$$
$$\delta P_i = \delta A_i - \delta N_i - \delta \varepsilon_i + \Sigma \delta k_i(l) \ . \tag{3}$$

Since there exists no correlation between the uncertainty elements, covariances of the measured P_i and P_j are as follows, using the respective correlation coefficient r_{ij} ;

$$<\delta P_i \delta P_j> = <\delta A_i \delta A_j> + r_{ij}(\varepsilon) <\delta \varepsilon_i \delta \varepsilon_j> + r_{ij}(N) <\delta N_i \delta N_j> + \Sigma r_{ij}(l) <\delta k_i(l) \delta k_j(l)> \ . \tag{4}$$

The correlation coefficients are derived from common parameters existing in the data or from relations between the data obtained previously[5]. We determine the variances and covariances in the ratio measurements from the following relations;

$$\mathrm{Var}(R_{ij}, R_{ij}) = <\delta R_{ij} \delta R_{ij}> = <\delta P_i \delta P_i> + <\delta P_j \delta P_j> - 2<\delta P_i \delta P_j> \ , \tag{5}$$

$$\mathrm{Cov}(R_{ij}, R_{mn}) = <\delta R_{ij} \delta R_{mn}> = <\delta P_i \delta P_m> + <\delta P_j \delta P_n> - <\delta P_i \delta P_n> - <\delta P_j \delta P_m> \ . \tag{6}$$

2.2. Correlation Matrix

In order to understand how to produce a correlation matrix from the measured data, for example, let us consider the example shown in Table 1, which is based on the experiment for the ^{252}Cf spectrum-averaged cross sections by Kobayashi and Kimura[8]. In the measurements, ^{27}Al(n,α)^{24}Na and ^{115}In(n,n')^{115m}In reactions were taken as reference monitors to the ^{27}Al(n,p)^{27}Mg and ^{24}Mg(n,p)^{24}Na reactions, respectively. The resultant ratio values were

$$\sigma_2\{^{27}\mathrm{Al(n,p)}\}/\sigma_1\{^{27}\mathrm{Al(n,\alpha)}\} = 4.797$$
$$\sigma_4\{^{24}\mathrm{Mg(n,p)}\}/\sigma_3\{^{115}\mathrm{In(n,n')}\} = 0.009651 \ .$$

In the first row of the table, nuclear reactions are shown corresponding to the two irradiations. The error component in each row is independent, and therefore uncorrelated each other. The uncertainties of the A_i are regarded as being independent as the counting statistics. The correlations (a) are from the determination of the detection effi-

ciencies. The correction of the geometrical factor is the same as for all measurements, and so the corresponding uncertainties show full correlation (b). The uncertainties of the back-scattering correction are different, but as the source of the back-scattering (room walls) is the same, the quantities must be assumed to be fully correlated (c). The meas-

Table 1 List of the uncertainty components.

Uncertainties (in %) due to	Symbol	Run-1		Run-2	
		27Al(n,α)	27Al(n,p)	115In(n,n')	24Mg(n,p)
	No.	1	2	3	4
Counting statistics	A_i	1.6	2.0	1.0	3.2
Efficiency	ε_i	1.06[a]	1.39[a]	2.23[a]	1.06[a]
Geometrical factor	kG_i	2.0[b]	2.0[b]	2.0[b]	2.0[b]
Half life	kT_i	0.4[c]	0.5	0.8	0.4[c]
Sample weight	N_i	0.1[d]	0.1[d]	0.1	0.2
Back scattering	kB_i	0.7[e]	1.0[e]	1.0[e]	0.7[e]
Irradiation & cooling t	kH_i	0.3	0.5	0.4	0.3
Gamma-ray attenuation	kS_i	0.5[f]	0.5	1.0	0.5[f]
Gamma-ray intensity	kJ_i	0.1[g]	1.0	1.0	0.1[g]
Others	kR_i	1.0	1.0	1.0	1.0

[a] $Corr(\varepsilon_1,\varepsilon_4)=1.00$,
$Corr(\varepsilon_1,\varepsilon_3)=Corr(\varepsilon_3,\varepsilon_4)=0.80$,
$Corr(\varepsilon_1,\varepsilon_2)=Corr(\varepsilon_2,\varepsilon_4)=0.94$,
$Corr(\varepsilon_2,\varepsilon_3)=0.95$.
b,e : fully correlated,
c,f,g : fully correlated (same product nucleus),
d : fully correlated (same foil).

urements Run-1 and Run-2 are based on the mass determination of a common aluminum foil, therefore the correlation is 100 % (d). The product nucleus, ^{24}Na, is the same for both reactions $^{27}Al(n,\alpha)$ and $^{24}Mg(n,p)$, therefore all uncertainty components depending on the common radioactive decay, half life and mass attenuation must be fully correlated (c,f,g). Table 2 shows detailed calculation procedures with Eq. (4) considering correlation coefficients between the measured data, and the last column gives variance or covariance value for each $<\delta P_i \delta P_j>$.

When we apply the measured data in Table 1 to Eqs. (5) and (6), from Table 2, we obtain

$$Var(\delta R_{12}, \delta R_{12}) = 11.20$$
$$Var(\delta R_{34}, \delta P_{34}) = 19.00$$
$$Cov(\delta R_{12}, \delta R_{34}) = -1.39 \ .$$

Then, the covariance matrix is derived as

$$\begin{pmatrix} 11.20 & -1.39 \\ -1.39 & 19.00 \end{pmatrix}$$

and the correlation coefficients are

$$r_{12} = r_{21} = -1.39 / \{ 11.20 \times 19.00 \}^{0.5} = -0.10 \ .$$

Finally, the result is derived as follows:

	Ration value	Standard deviation	Correlation matrix (x100)	
$\sigma_2\{^{27}Al(n,p)\}/\sigma_1\{^{27}Al(n,\alpha)\}$:	4.797	3.35 %	100	
$\sigma_4\{^{24}Mg(n,p)\}/\sigma_3\{^{115}In(n,n')\}$:	0.009651	4.36 %	-10	100 .

If we do not take into account of the covariance data, cross terms in Eq.(4) will be disappeared, and the results are given as

$$<\delta P_1 \delta P_1> + <\delta P_2 \delta P_2> = 9.69 + 13.69 = 4.86 \ \%$$
$$<\delta P_3 \delta P_3> + <\delta P_4 \delta P_4> = 14.78 + 17.40 = 5.67 \ \% \ .$$

In this case, the experimental uncertainty becomes larger than that treated with the covariance data. This means that all of the information with the measurement have not been properly taken for the data analysis and that some of the important information have been neglected.

LEAST SQUARES AND COVARIANCES

3.1. Least Squares Procedure

In the error analysis taking account of covariances between experimental data, the

Table 2 Calculation procedure of variance or covariance value for each $<\delta P_i \delta P_j>$.

$<\delta P_i \delta P_j>$	$<\delta \varepsilon_i \delta \varepsilon_j>$	$<\delta k_i^G \delta k_j^G>$	$<\delta k_i^B \delta k_j^B>$	$<\delta N_i \delta N_j>$	$<\delta k_i^T \delta k_j^T>$	$<\delta k_i^{IR} \delta k_j^{IR}>$	$<\delta k_i^S \delta k_j^S>$	$<\delta k_i^{IN} \delta k_j^{IN}>$	Σ
$<\delta P_1 \delta P_1>$	(quadratic sum of all uncertainty contributions)								= 9.69
$<\delta P_1 \delta P_2>$	0.94x1.06x1.39 + 2.0x2.0 + 0.7x1.0 + 0.1x0.1								= 6.09
$<\delta P_1 \delta P_3>$	0.80x1.06x2.23 + 2.0x2.0 + 0.7x1.0								= 6.59
$<\delta P_1 \delta P_4>$	1.00x1.06x1.06 + 2.0x2.0 + 0.7x0.7				+ 0.4x0.4 + 0.3x0.3 + 0.5x0.5 + 0.1x0.1				= 6.12
$<\delta P_2 \delta P_2>$									= 13.69
$<\delta P_2 \delta P_3>$	0.95x1.39x2.33 + 2.0x2.0 + 1.0x1.0								= 7.94
$<\delta P_2 \delta P_4>$	0.94x1.39x1.06 + 2.0x2.0 + 1.0x0.7								= 6.08
$<\delta P_3 \delta P_3>$									= 14.78
$<\delta P_3 \delta P_4>$	0.80x2.23x1.06 + 2.0x2.0 + 1.0x0.7								= 6.59
$<\delta P_4 \delta P_4>$									= 17.40

derivation of the best estimate associated with inverse weights of the variance-covariance elements can be based on the Bayes theorem[9]. The method shows how one can combine the vector P for the parameter estimates and covariance matrix M with the data D^o and its covariance matrix V to obtain a result P' which is more consistent with P and the new data D^o. A set of the data is given by the vector $D=(d_i)$, and the elements of which in our case are either $d_i=p_i$ for a direct measurement or $d'_i=p_i/p'_j$ for a ratio measurement. By applying the theorem, we obtain a new value of P and/or M, which we call P' and/or M', which minimizes χ^2 given by [1,2];

$$\chi^2 = (P-P')^t M^{-1} (P-P') + (D^o-D')^t V^{-1} (D^o-D') \ , \qquad (7)$$

where $D' = D + G(P'-P)$.

G is called the sensitivity matrix and the partial derivations are given as $g_{ij}=d_i/p_j$. With the definition $N = GMG^t$, the solution of P' and M' is given by

$$P'-P = MG^t(N+V)^{-1}(D^o-D) \ , \qquad (8)$$

$$M-M' = MG^t(N+V)^{-1}GM \ . \qquad (9)$$

3.2. Data Evaluation by Least Squares

The least squares method is often used for estimating the best value from several measurements with weights inversely proportional to the variance and/or covariance elements. We have selected the numerical examples for three measurements and their covariance matrix, as given in Table 3. The measured data were applied to the relations

Table 3 Numerical examples for three measurements with the covariance matrix

Run No.	Measurement:D^o	Covariance matrix (x 100) :V
1	4.797	11.20
2	4.892	4.64 19.14
3	4.936	4.64 4.64 28.45

of Eqs.(7)-(9), assuming that P and D are equal to (4.87) and that the uncertainties should be rather larger by 8 %, i.e., M=(64).

$$N = GMG^t = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} (64) (1 \ 1 \ 1) = \begin{pmatrix} 64 & 64 & 64 \\ 64 & 64 & 64 \\ 64 & 64 & 64 \end{pmatrix} .$$

Eq.(8) can be written as

$$P'-P = (64)(1\ 1\ 1)(N+V)^{-1}\begin{pmatrix} 4.797-4.87 \\ 4.892-4.87 \\ 4.936-4.87 \end{pmatrix},$$

where,

$$N+V = \begin{pmatrix} 64+11.20 & 64+4.64 & 64+4.64 \\ 64+4.64 & 64+19.14 & 64+4.64 \\ 64+4.64 & 64+4.64 & 64+28.45 \end{pmatrix},$$

$$P'-P = -0.0230\ .$$

Then, P' = 4.847. M' is also derived from Eq.(9) as

$$M-M' = (64)(1\ 1\ 1)(N+V)^{-1}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}(64)$$

M' is easily obtained as 7.4506, and the uncertainty is 2.73 %. One can obtain 4.847$\pm$0.132(2.73 %) as the final result. If we take the simple average value of three measurements, the result is 4.875$\pm$0.215 (4.43 %), which is due to the inappropriate treatment/analysis neglecting the covariance data in the measurements.

SUMMARY

In this paper, it has been demonstrated how the covariance matrix can be generated from the experimental data and used in the least squares method to combine the data to obtain the best value, by showing the numerical examples. We would like to urge experimentalists to report the uncertainties in their measurements in such a way that the covariance matrix of their results can be generated. We also hope that the data compilers will take into consideration of the valuable information for their compilations.

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3.4 Sensitivities of Nuclear Model Calculations and Parameter Covariances

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Abstract

Sensitivities of cross-section calculations have been obtained for the neutron-induced reactions on ^{56}Fe and ^{55}Mn. The optical and statistical models were employed to calculate these cross sections. As for ^{55}Mn, covariances of the model parameters required as input to computer codes were determined from the difference between model calculations and experimental data. A covariance file for ^{55}Mn has been made in the framework of File-30 of the ENDF-6 format.

1. Introduction

Nuclear model calculations have been widely used to evaluate neutron nuclear data. In particular, multi-step Hauser-Feshbach codes enable one to calculate all the necessary cross sections up to an incident energy of 20 MeV. Existing neutron cross-section libraries are to a large extent based on these calculations. Each evaluator makes much effort to determine the values of the parameters required as input to computer codes. It is however difficult to know how the calculated results are sensitive to the parameters, since there are a lot of parameters to be determined such as optical-model parameters, level density parameters, giant-dipole resonance parameters for gamma-ray emission and the parameter for the residual interaction in the preequilibrium mode.

A precompiler named GRESS[1] was developed at ORNL to enhance FORTRAN programs by adding the calculation of derivatives along with the original output. In the present work, a multi-step Hauser-Feshbach code TNG[2] was modified using the GRESS code and was used to calculate the sensitivities of the neutron-induced reaction cross sections of ^{56}Fe and ^{55}Mn. Furthermore, as for ^{55}Mn, covariances of the model parameters were estimated by using Zhao's method[3] and a covariance file was made in the framework of File-30 of the ENDF-6 format[4].

2. Sensitivity Calculation

2.1 Methods and procedures

The GRESS code modified TNG by adding the routines of the calculation of derivatives with respect to input data. Calculated are the normalized sensitivities which are obtained by multiplying a derivative by its associate input parameter value and dividing by the associated output value. A normalized sensitivity of 0.1 means that a 1% change in that input parameter would induce a 0.1% change in the output.

The modified TNG code was used to calculate the cross sections of ^{56}Fe and ^{55}Mn together with their sensitivities. The calculated reactions are given as follows:

Reaction		1st step		2nd step
n + ^{56}Fe	→	n + ^{56}Fe	→	n + γ + ^{56}Fe
			→	2n + ^{55}Fe
			→	n + p + ^{55}Mn
			→	n + α + ^{52}Cr
	→	p + ^{56}Mn	→	p + γ + ^{56}Mn
			→	p + n + ^{55}Mn
	→	α + ^{53}Cr	→	α + γ + ^{53}Cr
			→	α + n + ^{52}Cr
n + ^{55}Mn	→	n + ^{55}Mn	→	n + γ + ^{55}Mn
			→	2n + ^{54}Mn
			→	n + p + ^{54}Cr
			→	n + α + ^{51}V
	→	p + ^{55}Cr	→	p + γ + ^{55}Cr
			→	p + n + ^{54}Cr
	→	α + ^{52}V	→	α + γ + ^{52}V
			→	α + n + ^{51}V

The input data to TNG were taken from the evaluation work[5,6] at ORNL. Cascade gamma-ray emission was calculated for each residual nucleus. The parameter for the residual interaction in the preequilibrium process, which is referred to as preequilibrium parameter hereafter, was set to be 400 MeV^3 for ^{56}Fe and 600 MeV^3 for ^{55}Mn.

Sensitivities were calculated with respect to optical-model, level density, giant-dipole resonance and preequilibrium parameters. Concerning the optical-model parameters, the sensitivities were also calculated with the SCAT-2 code[7], and it was found[8] that the SCAT-

2 results were in good agreement with the TNG ones. This means that there is no code dependence on calculated sensitivities if the same physical model is applied.

2.2 Calculated results

The sensitivities of the total, shape elastic scattering and compound nucleus formation cross sections were calculated with respect to neutron optical-model parameters, i.e., depths, radii and diffuseness for real and imaginary potentials. The calculated results of the ^{56}Fe case are shown in Figs. 1-6. It is found from the figures that the sensitivities to the diffuseness parameters are smaller than those to other parameters. The same tendency is seen in Fig. 7 for the total cross section of ^{55}Mn. Figures 8 and 9 show the first step Hauser-Feshbach calculations of ^{56}Fe. Real radius parameters affect the calculated cross sections considerably.

The effect of the level density parameters were calculated on the neutron-, proton- and α-emission cross sections. Considered were a parameters, spin cut-off factors and pairing-energy corrections for residual nuclei. As for the neutron emission from ^{56}Fe, its cross section is sensitive to the a parameters for ^{56}Fe and ^{56}Mn, as seen in Fig. 10. Figure 11 indicates that the proton-emission cross section is sensitive not only to the a parameter for its residual nuclei ^{56}Mn but also to that for the target nucleus ^{56}Fe. This is also seen in Fig. 12 where the sensitivity of the ^{55}Mn(n,p) cross section is shown.

Figure 13 shows the sensitivities of the ^{56}Fe(n,n'γ) cross section to giant dipole-resonance parameters. The calculated cross sections is not sensitive to the parameters.

Figure 14 shows that the cross sections are not very sensitive to the preequilibrium parameter. However, it is found from Fig. 15 that the higher energy part of neutron spectrum is much influenced by the parameter. This phenomenon is understandable by the preequilibrium reaction theory.

3. Estimate of Parameter Covariances

3.1 Model parameters

It is important to select the parameters which affect calculated cross sections considerably. As a result of sensitivity calculation, eight parameters were chosen to make a parameter covariance file, i.e., real well depth, real and imaginary radii for neutron optical potentials, real radii for proton and α-particle potentials and level density parameters a for ^{55}Mn, ^{55}Cr and ^{52}V. The values of the parameters mentioned above are given as follows:

real depth for n	49.747 MeV
real radius for n	1.287 fm

imag. radius for n	1.345 fm
real radius for p	1.250 fm
real radius for α	1.644 fm
a for ^{55}Mn	7.410 MeV^{-1}
a for ^{55}Cr	8.550 MeV^{-1}
a for ^{52}V	7.955 MeV^{-1}

3.2 Covariances of model parameters

Covariances of the model parameters were determined from the difference between model calculations and experimental data, as described by Zhao et al.[3] The following experimental data were taken into account to deduce parameter covariances:

Total cross section

Foster, Jr. and Glasgow[9]

(n,2n) reaction

Menlove et al.[10]

Ikeda et al.[11]

Lu-Hanlin et al.[12]

(n,α) reaction

Gabbard and Kern[13]

Bormann et al.[14]

Bahal and Pepelnik[15]

Fischer et al.[16]

Zupranska et al.[17]

Vänskä and Rieppo[18]

(n,p) reaction

Smith[19]

Ikeda et al.[11]

Bormann et al.[20]

The (n,p) cross section of ^{51}V was substituted for that of ^{55}Mn, since there were not enough data points on this reaction to deduce covariances.

The correlation matrix thus obtained is listed in Table 1. Cross-section covariances were calculated from these parameter covariances. The variances of the (n,2n) and (n,p) cross sections are shown in Figs. 16 and 17, respectively. The parameter covariances as well as sensitivities were stored in File-30 of the ENDF-6 format[4].

4. Concluding Remarks

Sensitivities of nuclear model calculations were obtained for the neutron-induced reactions on ^{56}Fe and ^{55}Mn. The multi-step Hauser-Feshbach code TNG was used to calculate cross sections together with their sensitivities to input parameters. As for ^{55}Mn, covariances of eight parameters were estimated, and a covariance file was created in the framework of File-30 of the ENDF-6 format.

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Table 1 Correlation Matrix

	σ(%)	V_n	RV_n	RW_n	RV_p	RV_α	a_n	a_p	a_α
V_n	6.1	1.000							
RV_n	3.7	−0.991	1.000						
RW_n	8.2	−0.833	0.762	1.000					
RV_p	6.6	−0.384	0.368	0.386	1.000				
RV_α	10.2	−0.325	0.300	0.379	−0.240	1.000			
a_n	3.9	−0.290	0.250	0.419	−0.286	0.214	1.000		
a_p	8.1	−0.461	0.422	0.558	0.764	−0.187	0.281	1.000	
a_α	8.1	−0.311	0.285	0.374	−0.196	0.780	0.148	−0.175	1.000

σ(%)= Standard deviation

V_n = Real well depth for neutron potential

RV_n = Real radius for neutron potential

RW_n = Imaginary radius for neutron potential

RV_p = Real radius for proton potential

RV_α = Real radius for α-particle potential

a_n = *a* parameter for ^{55}Mn

a_p = *a* parameter for ^{55}Cr

a_α = *a* parameter for ^{53}V

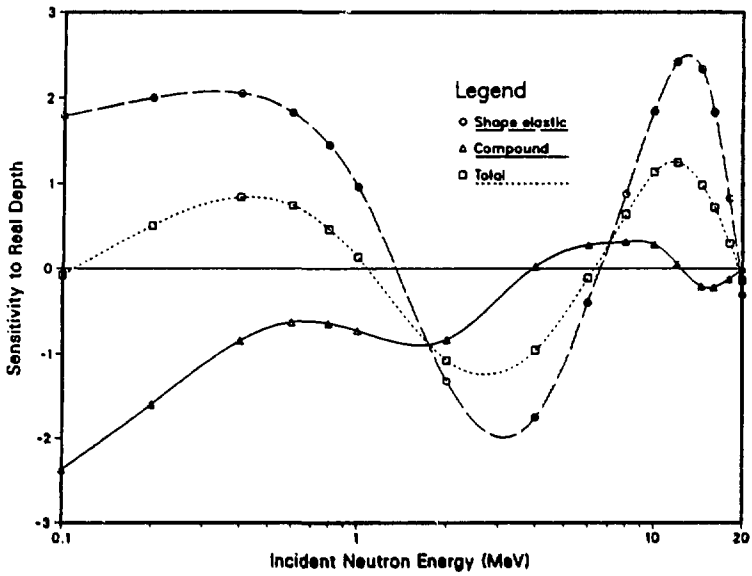

Fig. 1 Sensitivity of optical-model calculations of ^{56}Fe to real well depth

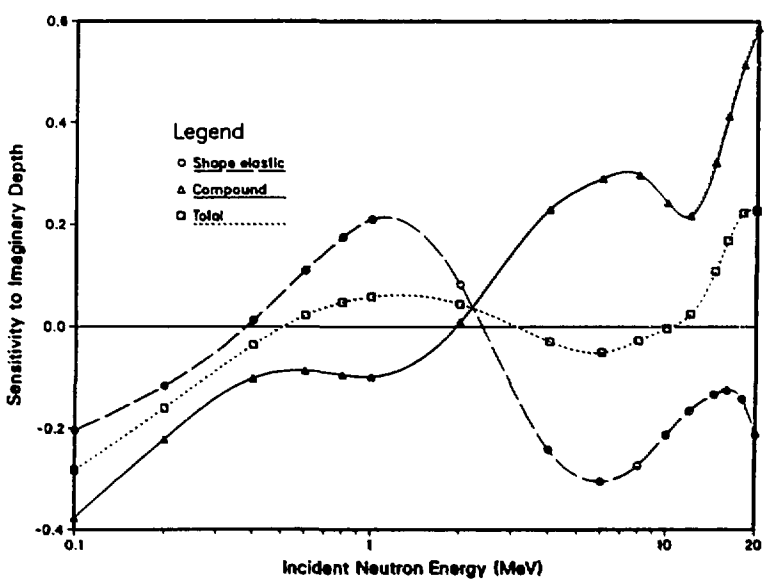

Fig. 2 Sensitivity of optical-model calculations of ^{56}Fe to imaginary well depth

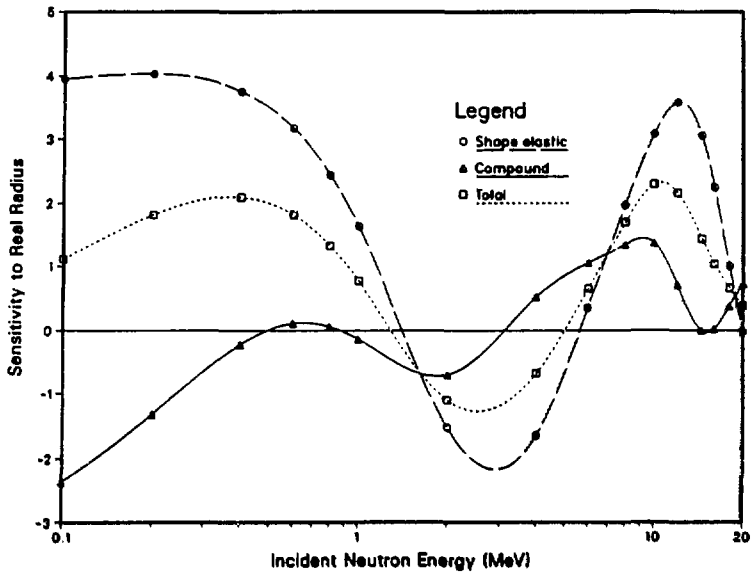

Fig. 3 Sensitivity of optical-model calculations of ^{56}Fe to real radius

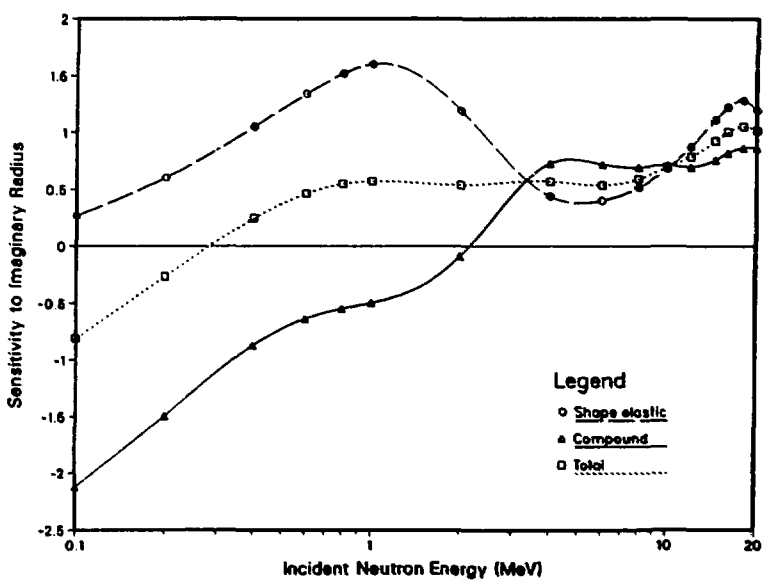

Fig. 4 Sensitivity of optical-model calculations of ^{56}Fe to imaginary radius

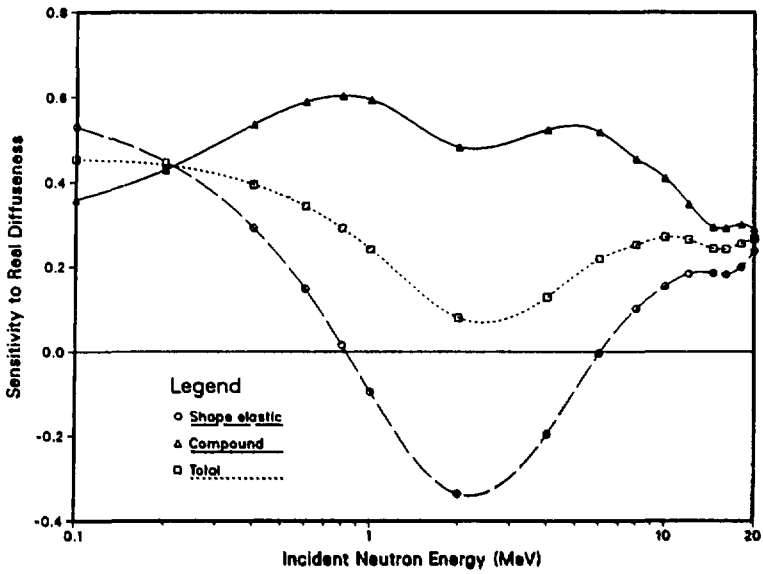

Fig. 5 Sensitivity of optical-model calculations of ^{56}Fe to real diffuseness

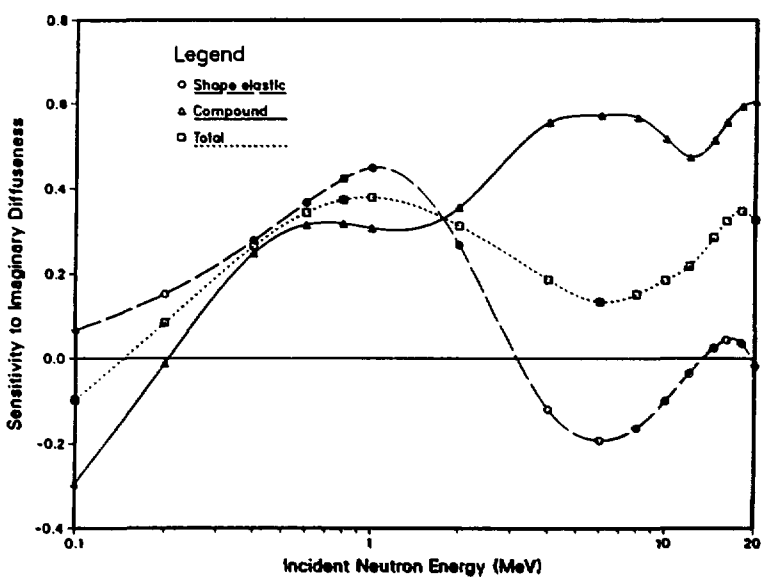

Fig. 6 Sensitivity of optical-model calculations of ^{56}Fe to imaginary diffuseness

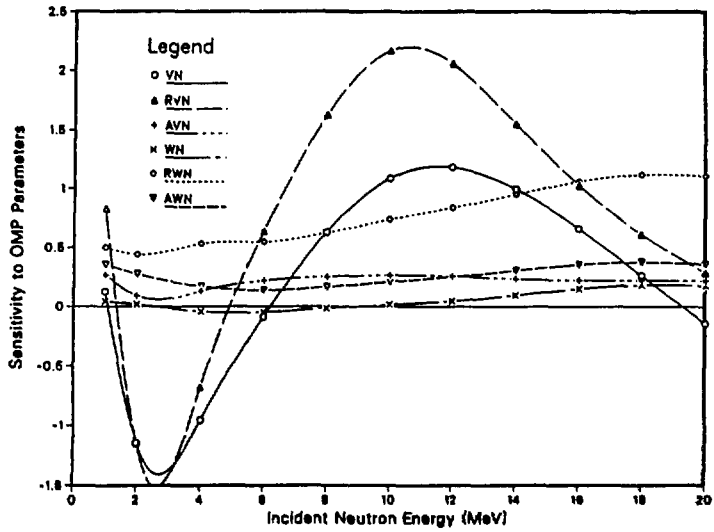

Fig. 7 Sensitivity of total cross section of ^{55}Mn to neutron optical potentials
VN=real depth, RVN=real radius, AVN=real diffuseness, WN=imaginary depth, RWN=imaginary radius, AWN=imaginary diffuseness

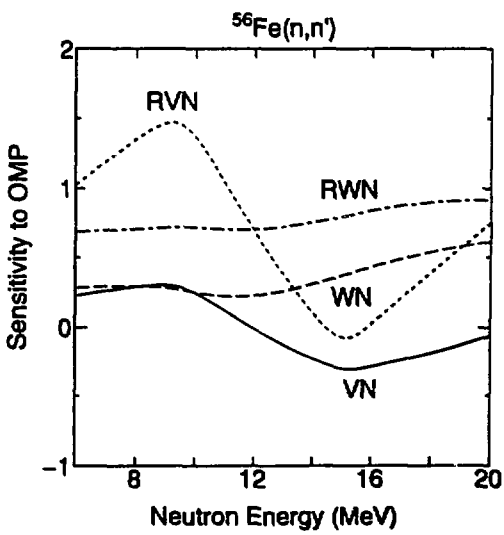

Fig. 8 Sensitivity of ^{56}Fe(n,n') cross sections to neutron optical potentials

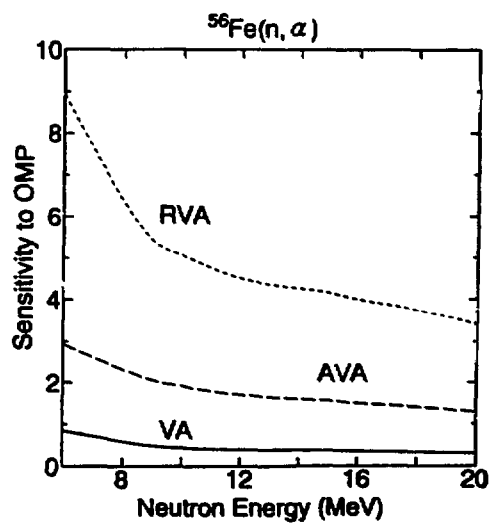

Fig. 9 Sensitivity of ^{56}Fe(n,α) cross sections to α-particle optical potentials
VA=real depth, RVA=real radius, AVA=real diffuseness

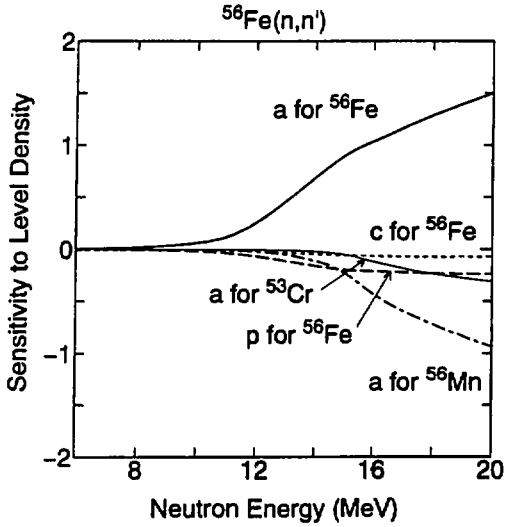

Fig. 10 Sensitivity of $^{56}Fe(n,n')$ cross sections to level density parameters
a=*a* parameter, p=pairing-energy correction, c=spin cut-off factor

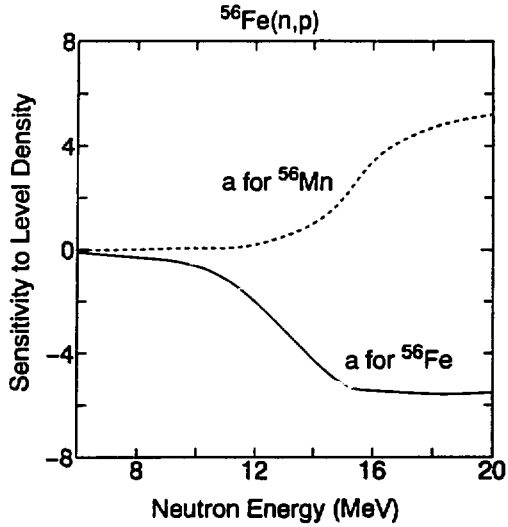

Fig. 11 Sensitivity of $^{56}Fe(n,p)$ cross sections to level density parameters

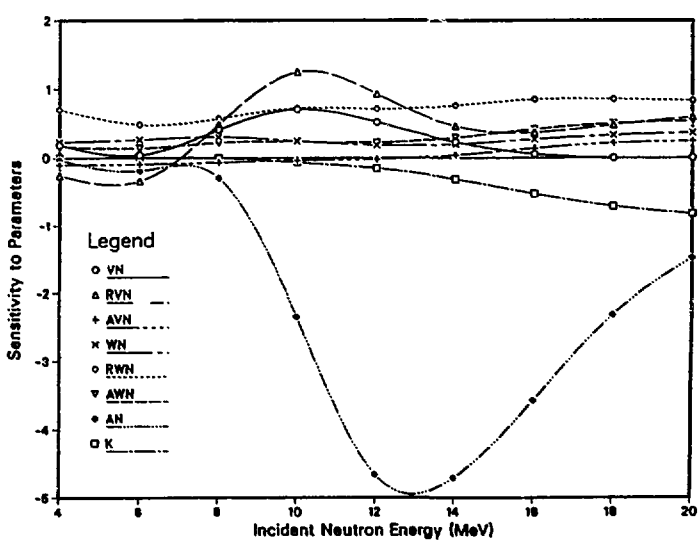

Fig. 12 Sensitivity of $^{55}Mn(n,p)$ cross sections
AN=*a* parameter for ^{55}Mn, K=preequilibrium parameter
For other symbols, see the caption of Fig. 7.

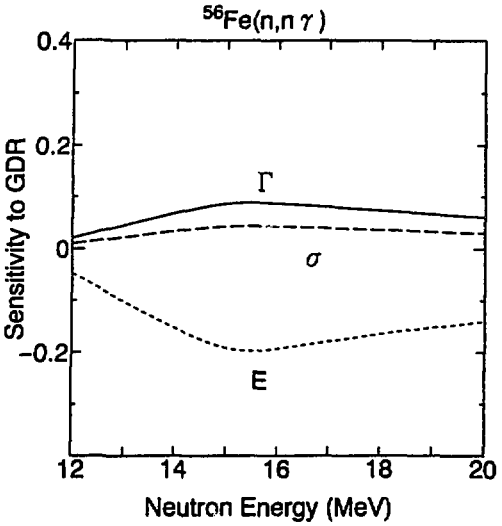

Fig. 13 Sensitivity of ^{56}Fe(n,n'γ) cross section to giant dipole-resonance parameters E=resonance energy, Γ=half width, σ=peak cross section

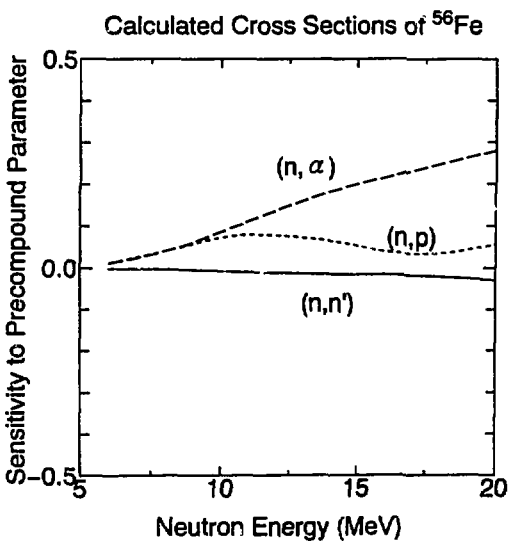

Fig. 14 Sensitivity of calculated cross sections of ^{56}Fe to preequilibrium parameter

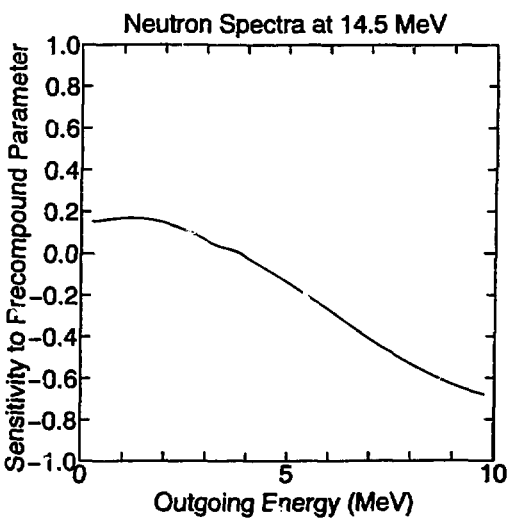

Fig. 15 Sensitivity of neutron emission spectra at 14.5 MeV to preequilibrium parameter

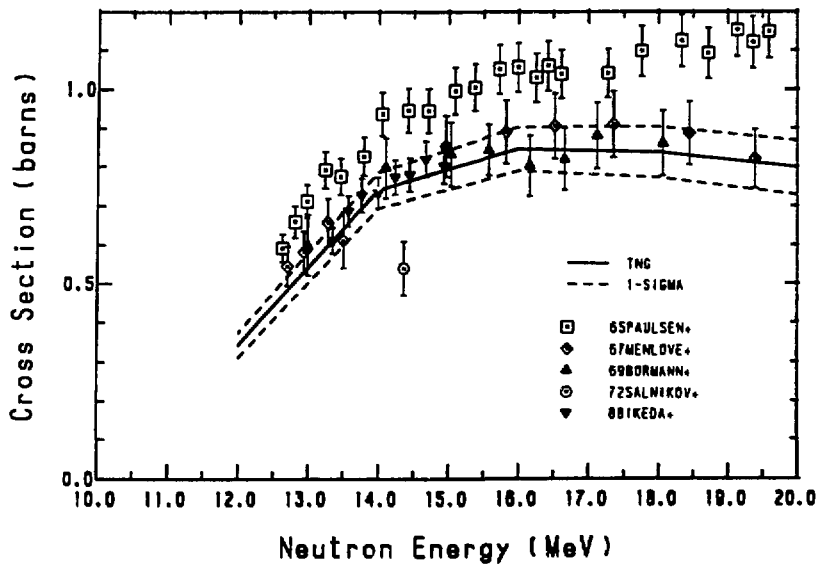

Fig. 16 ^{55}Mn(n,2n) cross sections and calculated variances

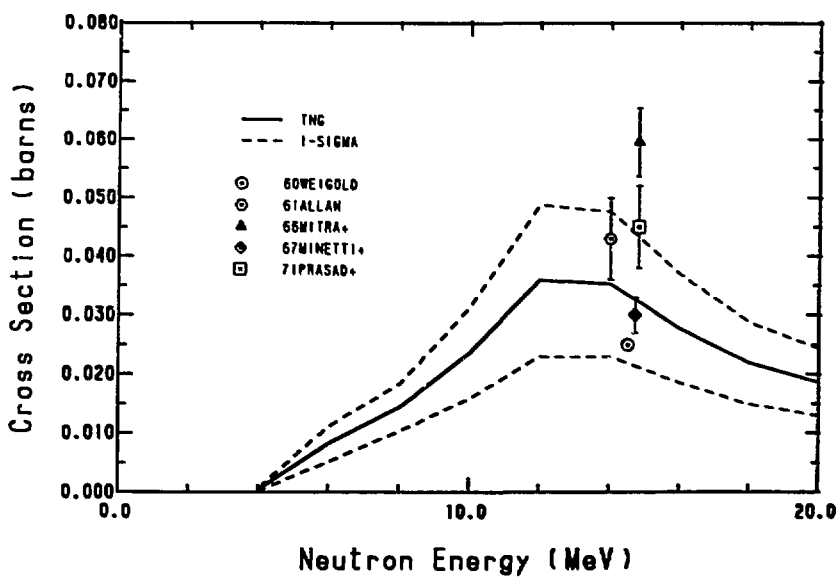

Fig. 17 ^{55}Mn(n,p) cross sections and calculated variances

4. Utilization of Covariance Data

4.1 Utilization of Cross-section Covariance Data in FBR Core Nuclear Design and Cross-section Adjustment

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Abstract

In the core design of large fast breeder reactors (FBRs), it is essentially important to improve the prediction accuracy of nuclear characteristics from the viewpoint of both reducing cost and insuring reliability of the plant. The cross-section errors, that is, covariance data are one of the most dominant sources for the prediction uncertainty of the core parameters, therefore, quantitative evaluation of covariance data is indispensable for FBR core design. The first objective of the present paper is to introduce how the cross-section covariance data are utilized in the FBR core nuclear design works. The second is to delineate the cross-section adjustment study and its application to an FBR design, because this improved design method markedly enhances the needs and importance of the cross-section covariance data.

1. FBR Core Nuclear Design

1.1 Outline

In the FBR field, a number of core critical experiments have been performed and analyzed as reactor physics benchmarks or engineering mock-ups for reactor design. Our basic policy of current design work is to make maximum use of those integral experimental information in the evaluation of both design nominal values and their prediction errors. Figure 1 shows a conventional calculational flow which has been used in FBR design works. Points to be noted in the procedure are: (a) the nuclear data used in the design calculation should be sufficiently verified and reliable, and identical to those used in the critical experimental analysis, (b) the analytical method of the design calculation ought to be as accurate as possible and almost equivalent to those of the critical experimental analysis, and (c) the calculational values are corrected by the ratio of the corresponding experimental value and the analytical value of the critical experiments, i.e., C/E values.

Uncertainty evaluation of the design nominal values are one of most crucial aspects in the design work. The sources of the design prediction errors can be classified by following components: (a) errors of the cross-section set used in the reactor core calculation, (b) approximations of analytical modeling like pin heterogeneity treatment or neutron transport effect, and (c) uncertainties of design specifications caused by fabrication tolerance, fuel compositions, reactor core temperature and so forth. Furthermore, when critical experimental information is applied, additional error sources must be considered: (d) experimental and analytical errors of the critical experiments, and (e) differences between the critical experimental cores and the design core such as plate/pin cell structure, fuel composition, reactor core size and shape, etc. All of these error components should be evaluated by analyzing those contents in detail and by quantifying the values with a consistent manner.

1.2 Design Nominal Values and Their Errors

We here consider three methods about how to reflect the integral experimental information to a design core: (a) no use of integral data, (b) the E/C bias method, and (c) the cross-section adjustment method. The evaluation of the prediction accuracy by each method is based on the matrix formulas derived by Takeda et al[1]. The cross-section covariance data play an important role in either design method as seen below.

(a) No-Information Method

If no integral information from critical experiments is used, we call it "no-information method" here for convenience, the design nominal values, $Rc^{*(2)}$, i.e. best-estimated values of core characteristics are merely calculational values, $Rc^{(2)}$, using a basic cross-section set, To, where the superscript "(2)" designates the design target core:

$$Rc^{*(2)} = Rc^{(2)}(To) \tag{1.1}$$

The error, V, of design nominal values is a simple summation of cross-section errors and analytical errors. The cross-section covariance is connected with prediction errors of nuclear characteristics by multiplying sensitivity coefficients:

$$V[Rc^{*(2)}] = G^{(2)}MG^{(2)t} + Vm^{(2)} \tag{1.2}$$

where M: covariance of a basic cross-section set To,

G: sensitivity coefficients defined by $(dR/R)/(d\sigma/\sigma)$,

Vm: analytical errors of integral parameters Rc.

The analytical errors of the design core, $Vm^{(2)}$, should include uncertainties of design specifications as mentioned above. Naturally, any errors concerned with critical experiments do not appear in Eq.1.2.

(b) E/C Bias Method

When the E/C bias method is adopted, the design nominal values are expressed as follows, where $Re^{(m)}$ designates experimental values of core characteristics and the superscript "(m)" means a mock-up experimental core.

$$Rc^{*(2)} = Rc^{(2)}(To) \times [Re^{(m)}/Rc^{(m)}] \quad (1.3)$$

Equation 1.3 assumes implicitly that the experimental values are close to true. On the other hand, the error of design nominal values by the E/C bias method is:

$$V[Rc^{*(2)}] = \Delta G M \Delta G^t + Ve^{(m)} + \Delta Vm \quad (1.4)$$

where $\Delta G \equiv G^{(2)} - G^{(m)}$: difference of sensitivity coefficients,

$Ve^{(m)}$: experimental errors of a mock-up core,

$\Delta Vm \equiv Vm^{(m)} + Vm^{(2)} - Vm^{(m2)} - Vm^{(m2)t}$: contribution of analytical errors remaining after the bias operation, where the superscript "(m2)" designates the correlation between the mock-up and design cores.

The first term in the right side of Eq.1.4 shows the contribution of the cross-section covariance, which is expected to be small when the mock-up core is a good copy of the design core. The second term, i.e. the experimental errors, appear as an additional contribution compared with Eq.1.2. The third term is related to analytical errors and can be reduced if their correlations are positive between both cores.

(c) Cross-Section Adjustment Method

Figure 2 shows the flow diagram of adjustment method compared with the E/C bias method. Similar to the no-information method, the design nominal values of the cross-section adjustment method are simply calculational values got by the adjusted cross sections, T':

$$Rc^{*(2)} = Rc^{(2)}(T') = Rc^{(2)}(To) + G^{(2)}(T' - To) \quad (1.5)$$

The right side of Eq.1.5 indicates the nominal values of the adjustment method can take into account the difference of sensitivity between experimental cores and a design core. Using the superscript "(12)" as the correlation between a group of experimental cores and a design core, the error of design nominal values by the adjustment method is expressed by:

$$V[Rc^{*(2)}] = G^{(2)}M'G^{(2)t} + Vm^{(2)} - NVm^{(12)} - Vm^{(12)t}N^t \quad (1.6)$$

where M': covariance of the adjusted cross-section set T'

$$N \equiv G^{(2)}MG^{(1)t}[G^{(1)}MG^{(1)t} + Ve^{(1)} + Vm^{(1)}]^{-1}$$

The definition of T' and M' is shown in the next section. Significant difference in the adjustment method from the E/C bias method appears for the first term in the right side of Eq.1.6, that is, the contribution of cross-section errors. The improvement of prediction accuracy by the adjustment method arises from the reduction of cross-section covariance (M→M') compared with the no-information

method. On the other hand, similarity of sensitivity (G→ΔG) is the improvement mechanism in the case of the E/C bias method. The second to fourth terms of Eq.1.6 are related to analytical errors and can be small like those of the E/C bias method if their correlations are strongly positive.

2. Cross-Section Adjustment

2.1 Theory

The idea of cross-section adjustment is based on the Bayesian parameter-estimation method, that is, the probability that a cross-section set, T, is true should be maximized under the condition that integral information, Re, is obtained. The theory of cross-section adjustment had been developed by a number of investigators[2,3], and the equations for adjustment were finally compiled in comprehensive matrix forms by Dragt et al[4]. The fundamental assumptions for the formulation are: (a) all kinds of errors have statistical Gaussian distributions, and (b) integral parameters are linear with respect to cross-section changes. The cross-section set after adjustment, T', is derived using the least-square technique and expressed by:

$$T' = To + MG^{(1)t}[G^{(1)}MG^{(1)t} + Ve^{(1)} + Vm^{(1)}]^{-1}[Re - Rc(To)] \qquad (2.1)$$

The covariance of the adjusted cross-section set, M', is rewritten as:

$$M' = M - MG^{(1)t}[G^{(1)}MG^{(1)t} + Ve^{(1)} + Vm^{(1)}]^{-1}G^{(1)}M \qquad (2.2)$$

In these equations, the evaluation of the covariance matrix, M, is possible to greatly affect the adjusted results. Figure 3 demonstrates the importance of correlation factors using a very simple model. This system consists of only two nuclear characteristics and three cross-sections. If a strong correlation is assumed between cross-section 1 and 2, the adjusted result is found quite different from that of reference case where no correlation exists in the covariance.

2.2 Data for Adjustment

Table 1 summarizes data used in the present adjustment study. The detail of each data was described elsewhere[5], therefore, we focus on only the cross-section and covariance matters here. The basic cross-sections to be adjusted is a 70-group constant set JFS-3-J2[6] generated from JENDL-2[7], which has been a standard cross-section set for FBR design and reactor physics study in Japan so far. The number of energy groups for the adjustment is 18, which is considered as most effective for FBR analysis in the capacity of current computers. For practical use in reactor analytical systems, the adjusted results were extended to the standard 70-group structure by spline-fitting technique. The nuclear data for the adjustment were selected from the viewpoint of significance in large FBR core analysis. As shown in Table 2, they include infinite cross-sections of 32 reactions

from eleven nuclides such as plutonium, uranium and structure materials, fission spectra of two nuclides, and delayed neutron fractions of six nuclides. On the contrary, matrix components of inelastic cross-sections or self-shielding factors were not adjusted in the present study.

The adjustment procedure needs a full matrix of nuclear-data covariance. JENDL does not provide any covariance files yet, therefore, 18-group covariance data of the above-mentioned reactions were newly evaluated in the present study in cooperation with JAERI nuclear data center. The variances(diagonal terms) of the cross-section errors were basically estimated from the statistical scattering of nuclear experimental values around JENDL-2 as follows:

$$\text{variance} = [\Sigma w(\sigma_{exp}-\sigma_{J2})^2/\sigma_{J2}^2]/\Sigma w \qquad (2.3)$$

where w : weight (square of experimental error)

σ_{exp} : experimental values

σ_{J2} : JENDL-2 value

The correlation factors(non-diagonal terms) were basically determined by the following policy: (a) classification of energy ranges corresponding to each evaluation method of nuclear data, (b) weak correlations in the region apart from the diagonal, and (c) smoothness between adjacent energy regions. Furthermore, the covariance data were somewhat modified iteratively according to feedback from preliminary adjustment results, so as to make the cross-section changes reasonable from the viewpoint of nuclear-data evaluators. Evaluated covariance data of Pu239 fission reaction are shown in Table 3 as a typical example.

2.3 Adjustment Results

The adjustment results for ZPPR-9 core are summarized in Table 4: (a) C/E values of criticality after the adjustment reached 1.0 very closely and dependence on core concepts almost disappeared, (b) C/E values of reaction rate ratio such as C28/F49 were quite improved, (c) radial dependence of C/E values were almost vanished, and (d) the prediction uncertainties caused by cross-section errors, GMG[4], were markedly improved through all kinds of the integral characteristics after adjustment.

The main changes of JFS-3-J2 cross-sections by the adjustment are shown in Table 5. As reported elsewhere[5], most parts of the cross-section changes were found to be reasonable from the viewpoint of nuclear data evaluation except several points such as U238 inelastic reaction.

The correlation matrix of Pu239 fission reaction after adjustment is shown in Table 6. As expected from the equations of adjustment, the correlation factors generally change to negative directions compared with Table 3. The improvement of prediction accuracy after adjustment seems to arise from these

negative correlations as well as the reduction of diagonal variances.

3. Application to a 600MWe-Class FBR Core Design

The adjusted cross-section set was applied to an FBR core design of 600MW electric power[8]. Figure 4 shows the cross-sectional view of the design core, which is a conventional two-region homogeneous one with mixed-oxide fuel. The nominal values of the design core by the adjustment method are compared with those by the no-information method and the E/C bias method in Table 7. Selection of design methods affects those nominal values in a certain range.

The prediction accuracy of each design method was evaluated using the above-mentioned formulas and summarized in Table 8. Some noticeable results are: (a) both the E/C bias and the cross-section adjustment methods generally increased the prediction accuracy compared with the no-information method, but one exception was that of control rod worths in the E/C bias method, one reason for which was considered as the influence of delayed-neuron data error, (b) the prediction accuracy of overall core parameters showed the superiority of the adjustment method to the E/C bias method, and (c) in particular, burnup-related parameters, like burnup reactivity loss and breeding ratio, are impossible to be corrected by the E/C bias method, while the adjustment method can be applied and improved the prediction accuracy by a factor of 2 from the no-information method.

4. Concluding Remarks

In the current FBR design works, the cross-section covariance data are needed to evaluate prediction accuracy of the design parameters. Especially, the cross-section adjustment method, which is most promising design method and being developed now, requires the covariance data to obtain the design nominal values as well as their accuracy. FBR core designers are strongly expecting the covariance data file to be incorporated in the JENDL library as soon as possible.

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Table 1 Basic Data and Methods Used in the Present Adjustment Study

(Target cores)
- 500~1500MWe-class large FBR cores
- Mixed oxide fuel
- Homogeneous, axially-, radially-heterogeneous cores

↓ (Data and methods must agree with targets.)

Parameter	Basic Data and Methods
Basic cross-sections	70-gorup constant set JFS-3-J2(89) → based on JENDL-2. So far, standard for FBR design and reactor physics in Japan
Number of energy group	18 group → Extended to 70-group after adjustment by spline fitting.
Nuclide and reaction for adjustment	σ_∞ of 11 nuclides(32 reactions), χ of 2 nuclides, β of 6 nuclides (totally 618) → Important nuclides and reactions for large FBR cores. Not include inelastic matrix data or f-tables.
Basic covariance	81 sub-matrices → Newly evaluated in cooperation with JAERI nuclear data center.
Integral critical experimental data	82 C/E data from JUPITER → Broad range of core size, concept and control rod arrangements. Analytical errors and their correlations were newly evaluated.
Analytical tools	SAGEP code for sensitibity, ABLE code for adjustment → Developed by Osaka Univ. Modified in the present study.

Table 2 Adjusted Nuclides and Reactions and Prepared Covariance Data

Nuclide \ Reaction	cap.	fis.	ν	ela.	inela.	μ	χ	β
U235	◎	◎	◎	–	△	–	◎	△
U238	○	◎	◎	◎	◎	○	–	△
Pu239	◎	◎	◎	–	△	○	◎	△
Pu240	○	–	◎	–	–	–	–	△
Pu241	△	○	◎	–	–	–	–	△
Pu242	–	–	–	–	–	–	–	△
C12	△			–	–	–		
O16	–			○	○	○		
Na23	○			○	–	○		
Cr	–			–	–	○		
Fe	○			○	–	○		
Ni	–			–	–	○		

△ : only diagonals ○ : diagonals and correlations between energy groups
◎ : diagonals and correlations with other nuclides or reactions – : not adjusted

Table 3 18-Group Covariance Data (Pu239 Fission Reaction)

Energy group	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1.0	0.7	0.65	0.6	0.1	0	0	0	0	0	0	0	0	0	0	0	0	0
2	0.7	1.0	0.75	0.7	0.2	0.1	0	0	0	0	0	0	0	0	0	0	0	0
3	0.65	0.75	1.0	0.75	0.3	0.2	0.1	0.1	0	0	0	0	0	0	0	0	0	0
4	0.6	0.7	0.75	1.0	0.7	0.3	0.2	0.2	0.1	0	0	0	0	0	0	0	0	0
5	0.1	0.2	0.3	0.7	1.0	0.8	0.7	0.6	0.5	0	0	0	0	0	0	0	0	0
6	0	0.1	0.2	0.3	0.8	1.0	0.8	0.7	0.6	0	0	0	0	0	0	0	0	0
7	0	0	0.1	0.2	0.7	0.8	1.0	0.8	0.7	0	0	0	0	0	0	0	0	0
8	0	0	0.1	0.2	0.6	0.7	0.8	1.0	0.8	0.1	0.1	0	0	0	0	0	0	0
9	0	0	0	0.1	0.5	0.6	0.7	0.8	1.0	0.5	0.3	0.1	0	0	0	0	0	0
10	0	0	0	0	0	0	0	0.1	0.5	1.0	0.5	0.3	0.1	0	0	0	0	0
11	0	0	0	0	0	0	0	0.1	0.3	0.5	1.0	0.5	0.3	0.1	0	0	0	0
12	0	0	0	0	0	0	0	0	0.1	0.3	0.5	1.0	0.5	0.3	0.1	0	0	0
13	0	0	0	0	0	0	0	0	0	0.1	0.3	0.5	1.0	0.5	0.3	0.1	0.1	0
14	0	0	0	0	0	0	0	0	0	0	0.1	0.3	0.5	1.0	0.5	0.3	0.2	0.1
15	0	0	0	0	0	0	0	0	0	0	0	0.1	0.3	0.5	1.0	0.5	0.3	0.2
16	0	0	0	0	0	0	0	0	0	0	0	0	0.1	0.3	0.5	1.0	0.5	0.3
17	0	0	0	0	0	0	0	0	0	0	0	0	0.1	0.2	0.3	0.5	1.0	0.5
18	0	0	0	0	0	0	0	0	0	0	0	0	0	0.1	0.2	0.3	0.5	1.0
Standard deviation(%)	5.0	2.0	2.0	2.0	3.2	6.3	6.5	7.7	7.7	3.0	3.0	3.0	2.0	6.0	6.0	4.0	4.0	4.0

(Smoothed cross-section region) (Un-resolved region) (Resolved region)

Table 4 Changes of C/Es and Uncertainties before and after Cross-Section Adjustment

Integral parameters (ZPPR-9 core)	C/E value		Uncertainty due to cross-section error (1σ, %)	
	Before adjustment	After adjustment	Before (GMG^t)	After ($GM'G^t$)
Criticality (keff)	0.994	1.001	2.5	0.3
Reaction rate ratio				
• F25/F49	1.015	0.992	4.9	1.4
• C28/F49	1.055	1.016	5.8	1.4
• F28/F49	0.972	0.981	7.7	2.2
Reaction rate distribution				
• F49、Outer Core Region	1.037	0.987	2.3	0.5
Control rod worth				
• Core center position	0.918	0.991	5.3	1.7
• Core edge position	0.990	1.010	2.5	0.6
Na void reactivity				
• Small region void	1.21	1.13	7.1	3.6
• Large region void	1.36	1.23	8.8	4.3

Table 5 JFS-3-J2 Cross-section Changes by Adjustment (Unit : %)

Energy Group	Pu239 χ	Pu239 fission	U238 fission	U238 capture	U238 inelastic	U235 fission	Na elastic
1 (10.0 MeV~)	2.5	-0.1	-0.2	0.8	-4.4	-0.6	-0.0
2 (6.07 MeV~)	1.2	-0.1	-0.2	2.0	-7.8	-0.6	-0.1
3 (3.68 MeV~)	0.5	-0.3	-0.2	2.1	-6.1	-0.6	-0.2
4 (2.23 MeV~)	-0.2	-0.4	-3.2	2.5	-7.9	-1.0	-0.5
5 (1.35 MeV~)	-0.5	-1.3	-4.2	1.4	-4.6	-1.6	-0.8
6 (821 keV~)	-0.7	-2.7	-1.2	-0.5	-3.1	-3.5	-1.2
7 (388 keV~)	-0.9	-2.5	-2.4	-1.3	-2.3	-3.0	-1.5
8 (183 keV~)	-0.9	-1.8	-3.6	-3.5	-1.5	-3.1	-1.7
9 (86.5 keV~)	-0.9	-0.6	-3.4	-5.8	-1.0	-3.1	-2.9
10 (40.9 keV~)	-0.9	1.1	-3.2	-2.1	0.0	-1.7	-1.7
11 (19.3 keV~)	-	1.6	-2.1	-2.6	0.0	-1.5	-0.4
12 (9.12 keV~)	-	1.8	-1.6	-3.4	0.0	-2.2	0.6
13 (4.31 keV~)	-	1.4	-0.2	-3.3	0.0	-1.2	1.2
14 (2.04 keV~)	-	6.8	-3.3	-4.5	0.0	0.6	1.2
15 (961 eV~)	-	6.3	-9.9	-4.1	0.0	1.4	0.6
16 (454 eV~)	-	3.8	-0.0	-2.9	0.0	0.6	0.3
17 (214 eV~)	-	2.8	-0.1	-2.0	0.0	0.2	0.2
18 (101 eV~)	-	2.2	-0.4	-0.4	0.0	-0.1	0.1
βeff (Tuttle, Saphier)	-	-0.5	-1.2	-	-	-1.0	-

Table 6 Covariance Data after Adjustment (Pu239 Fission Reaction)

Energy group	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1.0	0.69	0.65	0.61	0.06	-0.10	-0.10	-0.09	0.06	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.00	-0.00
2	0.69	1.0	0.74	0.70	0.17	0.01	-0.17	-0.15	-0.10	0.01	0.01	0.01	0.02	0.02	0.02	0.02	0.01	-0.00
3	0.65	0.74	1.0	0.73	0.21	0.05	-0.13	-0.10	-0.23	0.01	0.01	0.02	0.02	0.03	0.03	0.02	0.01	-0.00
4	0.61	0.70	0.73	1.0	0.74	0.04	-0.16	-0.12	-0.23	-0.01	0.00	0.02	0.03	0.04	0.04	0.03	0.01	-0.01
5	0.06	0.17	0.21	0.74	1.0	0.47	0.16	-0.08	-0.19	-0.14	-0.09	-0.01	0.04	0.05	0.07	0.05	0.03	0.01
6	-0.10	0.01	0.05	0.04	0.47	1.0	0.35	0.06	-0.09	-0.21	-0.15	-0.05	0.01	0.04	0.06	0.06	0.04	0.03
7	-0.10	-0.17	-0.13	-0.16	0.16	0.35	1.0	0.29	0.09	-0.28	-0.20	-0.08	-0.01	0.01	0.04	0.04	0.04	0.04
8	-0.09	-0.15	-0.10	-0.12	-0.08	0.06	0.29	1.0	0.37	-0.13	-0.06	-0.13	-0.06	-0.05	-0.01	0.02	0.03	0.07
9	-0.06	-0.10	-0.23	-0.23	-0.19	-0.09	0.08	0.37	1.0	0.57	0.27	0.02	-0.10	-0.11	-0.06	-0.01	0.02	0.08
10	0.01	0.01	0.01	-0.01	-0.14	-0.21	-0.28	-0.13	0.57	1.0	0.44	0.24	0.03	-0.10	-0.08	-0.05	-0.01	0.04
11	0.01	0.01	0.01	0.01	-0.09	-0.15	-0.20	-0.06	0.27	0.44	1.0	0.46	0.24	0.00	-0.09	-0.05	-0.01	0.05
12	0.01	0.01	0.02	0.02	-0.01	-0.05	-0.08	-0.13	0.02	0.24	0.46	1.0	0.46	0.22	0.01	-0.07	-0.02	0.03
13	0.01	0.02	0.02	0.03	0.04	0.01	-0.01	-0.06	-0.10	0.03	0.24	0.46	1.0	0.44	0.22	0.03	0.07	0.02
14	0.01	0.02	0.03	0.04	0.05	0.04	0.01	-0.05	-0.11	-0.10	0.00	0.22	0.44	1.0	0.39	0.19	0.13	0.08
15	0.01	0.02	0.03	0.04	0.07	0.06	0.04	-0.01	-0.06	-0.08	-0.09	0.01	0.22	0.39	1.0	0.41	0.21	0.14
16	0.01	0.02	0.02	0.03	0.05	0.06	0.04	0.02	-0.01	-0.05	-0.05	-0.07	0.03	0.19	0.41	1.0	0.42	0.21
17	0.00	0.01	0.01	0.01	0.03	0.04	0.04	0.03	0.02	-0.01	-0.01	-0.02	0.07	0.13	0.21	0.42	1.0	0.37
18	-0.00	-0.00	-0.00	-0.01	0.01	0.03	0.04	0.07	0.08	0.04	0.05	0.03	0.02	0.08	0.14	0.21	0.37	1.0
Standard deviation(%)	4.96	1.97	1.93	1.85	2.02	3.61	3.37	4.04	4.41	2.82	2.83	2.88	1.90	5.41	5.40	3.64	3.63	3.01

(Smoothed cross-section region) (Un-resolved region) (Resolved region)

Table 7 Design Nominal Values of a 600MWe-class FBR Core Parameters

Nuclear characteristics	No-Infomation Method	E/C Bias Method	Cross-Section Adjustment Method (difference from E/C Bias Method)
Pu enrichment (w/o)	same as right	17.01/21.05	same as left
Criticality (keff) • BOEC / EOEC	1.0290 / 0.9997	1.0360 / 1.0067	1.0304 / 0.9986
Burnup reactivity (%Δk/kk')	2.82	same as left	3.06 (+ 9%)
Breeding ratio	1.052	same as left	1.030 (-2%)
Maxmum linear power (W/cm) • Inner / Outer core	476 / 480	476 / 480	482 (+ 6W/cm) / 477
Control rod worth (%Δk/kk') • MCR /BCR	6.49 / 2.60	6.61 / 2.65	6.59 / 2.78 (+ 5%)
Sodium void reactivity ($)	6.5	5.0	5.9 (+ 18%)
Doppler reactivity (10^{-3}Tdk/dT)	-8.9	-10.2	-9.0 (-11%)

Table 8 Design Accuracy of a 600MWe-class FBR Core Parameters

Relative values (1σ, %)

Nuclear characteristics	No-Infomation Method	E/C Bias Method	Cross-Section Adjustment Method
Criticality (keff)	2.06	0.70	0.43
Breeding ratio (C28/F49)	5.9	2.3	1.5
Power distribution (F49) • Inner core edge / Outer core center	1.7 / 2.8	1.9 / 2.5	1.3 / 2.2
Control rod worth • Center / Ring1 / Ring2	4.9 / 4.6 / 4.1	4.6 / 4.0 / 4.0	3.0 / 3.1 / 2.8
Sodium void reactivity	9.7	10.3	7.1

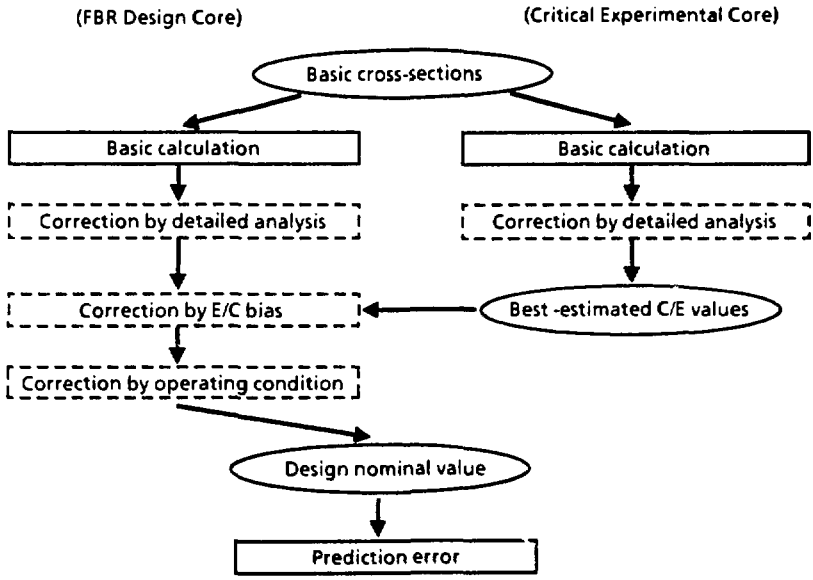


Fig.1 Conventional Flow Diagram of FBR Core Design by E/C Bias Method

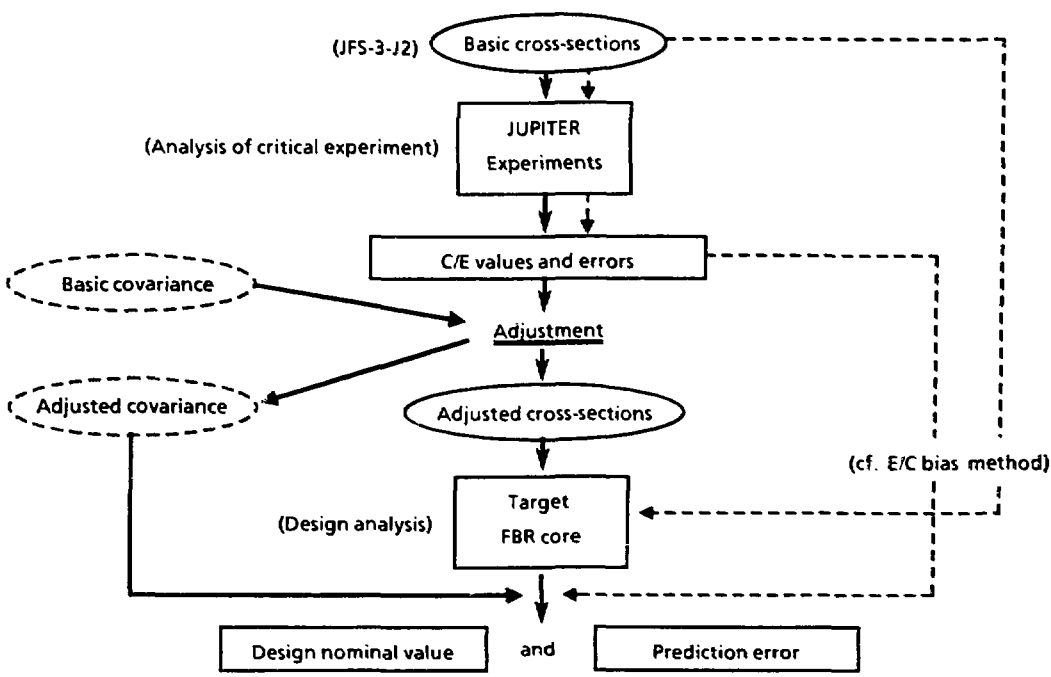


Fig.2 Advanced Flow Diagram of FBR Core Design by Cross-Section Adjustment Method

(Two nuclear characteristics and three cross-sections system)

M			G			GMGt		Vem		Re-Rc	T'-T	M'			GM'Gt	
1	0.9	0	1	1	1	4.80	4.81	0.01	0	1	0.395	0.244	0.145	-0.390	5.03E-03	4.95E-03
0.9	1	0	1.01	1	0.99	4.81	4.82	0	0.01	1	0.395	0.145	0.243	-0.390	4.95E-03	5.05E-03
0	0	1									0.208	-0.390	-0.390	0.787		
(Reference Case)																
1	0	0	1	1	1	3.00	3.00	0.01	0	1	0.334	0.659	-0.334	-0.328	5.04E-03	4.94E-03
0	1	0	1.01	1	0.99	3.00	3.00	0	0.01	1	0.333	-0.334	0.667	-0.331	4.94E-03	5.04E-03
0	0	1									0.331	-0.328	-0.331	0.666		

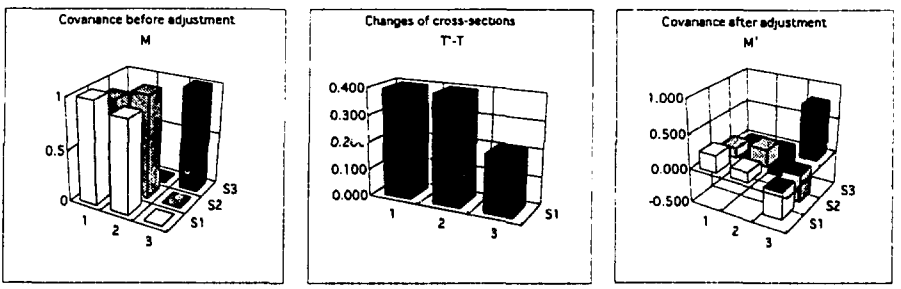
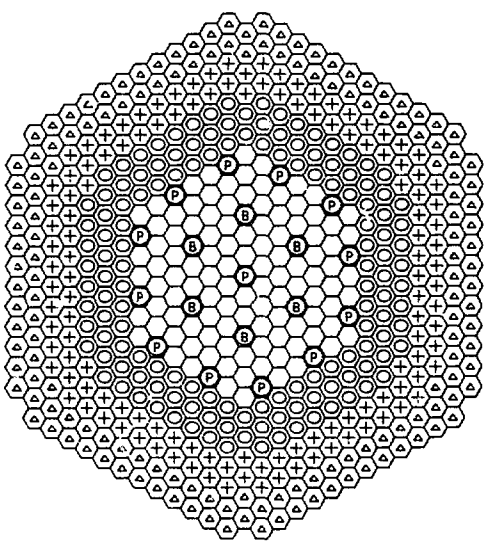
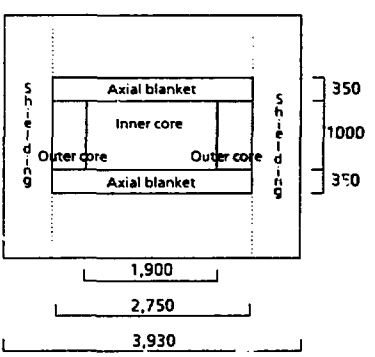


Fig.3 Effect of Correlation Factors to Adjusted Results





Inner core	108
Outer core	138
S.S. shielding	126
B_4C shielding	150
Main contol rod	13
Buckup control rod	6
Total	541

Fig.4 Cross-Sectional View of a 600MWe-Class FBR Core

4.2 Applications of Error Covariance to Fast Reactor Material Dosimetry in JOYO

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Abstract

In the JOYO dosimetry neutron specurum is analyzed by using unfolding code NEUPAC (NEutron Unfolding code PACkage) based on J1-Unfolding method. Cross section, measured reaction rate, initial guess spectrum and their error covariance are required as input data of NEUPAC. Cross section and its error covariance, which are dominant data, are processed from ENDF/B-V file with error covariance. Neutron spectrum with an uncertainty can be analyzed by using NEUPAC. This error analysis using the error covariance contributes the improvement of reliability for evaluation result such as neutron fluence. Also the present evaluation accuracy on neutron fluence reaches within about 5% for the irradiation test in core region.

1. Introduction

In JOYO various irradiation tests have been carried out to develop the fuels and materials for commercialization of FBR and to support JOYO surveillance test. In the irradiation test analysis and evaluation, irradiation information such as neutron spectrum, neutron flux or neutron fluence is a key parameter and must be estimated accurately. Therefore, neutron dosimetry method with activation technique [1] has been developed in cooperation with University of Tokyo, Hanford Engineering Development Laboratory and PNC. Analysis of neutron spectrum is performed by using unfolding code NEUPAC (NEutron Unfolding code PACkage) [2] based on J1-Unfolding method. Uncertainties of neutron spectrum, flux and fluence can be estimated by using NEUPAC according to the error covariance as input data of cross section, reaction rate and initial guess spectrum. So far a lot of evaluation on neutron fluence with uncertainty have been conducted and reflected on various irradiation tests.

This paper presents evaluation method, the analysis condition including errors and a typical example of evaluated results.

2. Outline of Reactor Dosimetry Experiment

2.1 Objectives and Evaluation Items

The objectives and evaluation items of fast reactor material dosimetry in JOYO are summarized as follows:

Objectives	Evaluation Items
(1) Fuel Development:	○Neutron flux (Total, Fast, Thermal)
High performance MOX fuel	○Neutron spectrum
(High burnup, High linear heat rate)	○Linear heat rate
Mixed nitride, Mixed carbide and TRU fuel	
(2) Material Development:	○Neutron flux (Total, Fast, Thermal)
Modified and advanced cladding materials	○Neutron spectrum
Fusion materials	○Displacement per atom
Absorber materials, etc.	
(3)Surveillance Test:	○Neutron flux (Total, Fast, Thermal)
Safety vessel	○Neutron spectrum
Reactor vessel, etc.	○Displacement per atom

2.2 Standard Dosimeter Set

In the activation method the dosimeter set is selected as the sensitivity to reaction rate covers the energy range widely. The standard dosimeter set used in JOYO, which covers energy range from 100 eV to 20MeV, is listed in Table 1. One-tenth to one milligram of fissionable materials and Sc are encapsulated separately in the tiny vanadium capsules and the others are fabricated in wire form with one to ten milligrams in weight. The purity of dosimeter materials is 99.9 to 99.999%. Almost all dosimeter materials have no impurities which obstruct the measurements of reaction rates. These dosimeters are encapsulated into the dosimeter capsule, and are loaded in the irradiation subassembly or test rig shown in Figure 1.

2.3 Analysis Method of Neutron Spectrum

Neutron spectrum is analyzed by using NEUPAC in a process shown in Figure 2. As the input data measured reaction rate, initial guess spectrum, cross section and their errors are required. The initial guess spectrum is calculated by two-dimensional discrete ordinate radiation transport code DOT3.5 [3] with the 103 neutron energy group. The 103 group cross section set based on ENDF/B-V dosimetry file with error covariance is processed by using NJOY [4] code.

Main features of NEUPAC are

1) neutron fluence as integral value based on the neutron flux and spectrum can be evaluated directly,

2) uncertainties of estimated values of neutron spectrum, flux and fluence can be assigned accurately according to the errors (variance or covariance) of input data of reaction rate, cross section and guess spectrum.

The method for unfolding the neutron spectrum $\phi(u)$ from measured reaction rate Ri is based on following equation :

$$Ri = \int \phi(u)\, \sigma i(u)\, du \quad (i=1 \sim n) \tag{1}$$

where $\sigma i(u)$ is cross section.

In this condition, the value of

$$I = \int W(u)\, \phi(u)\, du \tag{2}$$

is going to be evaluated on the assumption that the guess spectrum $\phi_o(u)$ of the unknown spectrum $\phi(u)$ is given.

In this case, the errors of the known quantities must be given as follows:

$\overline{\Delta Ri\ \Delta Rj}$: Covariance matrix of reaction rate

$\overline{\Delta \sigma i(u1)\ \Delta \sigma j(u2)}$: Covariance matrix of cross section

$\overline{\Delta \phi_o(u1)\ \Delta \phi_o(u2)}$: Covariance matrix giving the error range of the guess spectrum

$W(u)$: Given window function

The procedure for solving the J_1-Unfolding method is applied to NEUPAC. The functional J_1 with I value of equation (2) so as to be stationary for the true solution $\phi(u)$ is constructed as follows:

$$J_1 = \int W(u)\, f(u)\, du + \Sigma Ci \{ Ri - \int \phi(u)\, \sigma i(u)\, du \} \tag{3}$$

Here, operation is made so that the value J_1 with the guess spectrum $\phi_o(u)$ substituted for the unknown spectrum $\phi(u)$ may become the most likelihood estimate. The basic principle is to use

$$\Delta J_1 = \int \{W(u) - \Sigma Ci\, \sigma i(u)\} \Delta\phi_o(u) + \Sigma Ci \{\Delta Ri - \int \Delta\phi(u) \Delta \sigma i(u)\, du\} \tag{4}$$

in order to obtain the coefficient Ci in the way to attain the variance of the estimate, $(\Delta J_1)^2 = \text{Min.}$ In the present analysis error values are given as follows

Cross section (σ) :Covariance matrix from ENDF/B-V dosimetry file

Initial guess spectrum (ϕ_o):Variance of 30% for each energy group(based on experience)

Reaction rate (R) : Variance from measurement error for reaction rate and reactor power
: Covariance matrix from measurement error for reactor power

3. Example of Neutron Spectrum Analysis

Example of analysis condition and results by NEUPAC are described here. Measured dosimeters were irradiated in the core material irradiation rig in the MK-II core shown in Figure 3. 8 types of reaction rates from 8 types of dosimeters are used for analysis. Figure 4 shows the input data of errors. In the upper part of Figure 4 measured reaction rates and their errors (variance) are inputted. The variance ΔV_R is expressed by :

$$\Delta V_R = \sqrt{(\Delta R^2 + \Delta P^2)}$$

where ΔR and ΔP are measurement errors of reaction rate and reactor power respectively.

The middle part is covariance of reaction rate expressed by ΔP^2. In the lower part 30% is given as variance of initial guess spectrum. The unfolding results are shown in Figure 5, Figure 6, Figure 7, Figure8 and Table 2. Figure 5 is output list of the unfolded spectrum, its uncertainty of 1 σ % level and improvement ratio indicating the error reduction of neutron spectrum. Figure 6 indicates the relative covariance of unfolding spectrum for each energy group. The relative error is improved at the energy range of about 10^{-2} MeV and 10^{+1} MeV as shown in Figure 7. Figure 8 shows the unfolded spectrum, its uncertainty of 1 σ % level and a 90% confidence level for each reaction rate which is described in detail in Table 2. Table 3 shows neutron flux and its uncertainties including breakdown. The comparison of the measured reaction rate (E) and the calculated ones (C) by initial guess spectrum and unfolded spectrum are shown in Table 4. It is confirmed that this neutron spectrum analysis is satisfied because the reaction rate calculated by unfolded spectrum agrees well the measured one.

4. Summary

Dosimetry method with activation technique has been established in JOYO. In this method neutron fluence with an uncertainty can be obtained by using NEUPAC according to error covariance as input data. This error analysis contributes the improvement of reliability for evaluation result. Also the present evaluation accuracy on neutron fluence with an uncertainty reaches within 5% for the irradiation test in the core position. More effort will be required to improve the evaluation accuracy for the irradiation test around the core such as reflector position.

5. Future R&D Plan

Recently it is required to improved the evaluation accuracy of neutron fluence. From this point of view new cross section set processed from JENDL-3 [5),6)] with error covariance is considered to be applied to fast reactor material dosimetry.

References

1) Chatani K. and Suzuki S.: ISSN 0385-4876 81(1993) (In Japanese)
2) Odo T. and Suzuki S. : PNC TN9420 92-005 22(1992)
3) Rhoades W.A. and Mynatt F.R. : ORNL/TM-4280(1973)
4) MacFarlane R.E. and Boicourt R.M. : LA-9303, Vol. 1(ENDF-324)(1982)
5) Shibata K., et al, : JAERI 1319(1990)
6) Nakazawa M., et al, : JAERI 1325(1991)

Table 1 Standard Dosimeter Set of JOYO

Monitoring Material	Form	Dimension (mm)	Reaction	
			Non-Threshold	Threshold
Co	Wire (Co-V or Co-Al)	φ1.0	$^{59}Co(n,\gamma)$	
Sc	Vanadium Capsuled (Sc_2O_3)	φ1.5×L8.0	$^{46}Sc(n,\gamma)$	
Ti	Wire	φ0.5		$^{46}Ti(n,p)$
Fe	Wire	φ0.75	$^{58}Fe(n,\gamma)$	$^{54}Fe(n,p)$
Ni	Wire	φ0.75		$^{58}Ni(n,p)$
Cu	Wire	φ0.75		$^{63}Cu(n,\alpha)$
Ta	Wire (Ta-V or Ta-Al)	φ0.5	$^{181}Ta(n,\gamma)$	
Nb	Thin Foil	0.51μm		$^{93}Nb(n,n')$
Np-237	Vanadium Capsuled (NpO_2)	φ1.5×L8.0		$^{237}Np(n,f)$
U-235	Vanadium Capsuled (UO_2)	φ1.5×L8.0	$^{235}U(n,f)$	
U-238	Vanadium Capsuled (UO_2)	φ1.5×L8.0		$^{238}U(n,f)$
Th-232	Vanadium Capsuled (Th)	φ1.5×L8.0	$^{232}Th(n,\gamma)$	$^{232}Th(n,f)$

Table 2 90% Confidence Level for Each Reaction Type

	90% Confidence Level (MeV)			
	No.	Reaction Type	Lower Energy	Upper Energy
Core Center Row [0] D12 (+4mm above Core Midplane)	1	^{59}Co (n,γ)	1.51598E-04	8.66237E-01
	2	^{237}Np (n,f)	3.64609E-01	4.05144E+00
	3	^{235}U (n,f)	2.14692E-03	2.06537E+00
	4	^{238}U (n,f)	1.37008E+00	5.95840E+00
	5	^{46}Ti (n,p)	3.70422E+00	9.44874E+00
	6	^{54}Fe (n,p)	2.18244E+00	7.33705E+00
	7	^{58}Ni (n,p)	1.84101E+00	7.26162E+00
	8	^{63}Cu (n,α)	4.63784E+00	1.11970E+01

Table 3 Example of Output Data (Neutron Flux and Its Uncertainties)

INTEGRAL QUANTITY OUTPUT		Initial Spectrum	Final Spectrum	Error of Final Spectrum	Break down of Error			Relative Error of Initial Spectrum / Relative Error of Final Spectrum
					Reaction Rate	Cross Section	Initial Spectrum	
ID NO.	TYPE OF W.FUNCTION	INITIAL I.Q.	FINAL I.Q.	ERROR (%)	CP1 (%)	CP2 (%)	CP3 (%)	IMPROVEMENT RATIO
1	TOTAL FLUX	4.37708E+15	4.03301E+15	4.774E+00	5.035E+01	1.369E+01	3.383E+01	2.31158E+00
2	FLUX GREATER THAN 1MEV	8.77232E+14	6.29668E+14	7.262E+00	2.490E+01	1.222E+01	6.288E+01	2.42280E+00
3	FLUX GREATER THAN 100KEV	3.27717E+15	2.89730E+15	8.117E+00	1.505E+01	1.175E+01	7.378E+01	1.51387E+00
4	DISPLACEMENT RATE(DPA/S)	1.64728E-06	1.34646E-06	5.078E+00	3.836E+01	1.709E+01	4.457E+01	2.25578E+00

Table 4 Comparison of Measured and Calculated Reaction Rates for before/after Spectrum Unfolding

Item / Position	Measured Reaction Rate ($\times 10^{24}$ reaction/sec/atom/100MWt)			Calculated/Measured	
	ID No.		Reaction Rate	before Unfolding	after Unfolding
Core Center Row [0] D12 (+4mm above Core Midplane)	1	^{59}Co (n,γ)	9.851E+13	0.840	0.832
	2	^{237}Np (n,f)	1.666E+15	1.396	1.081
	3	^{235}U (n,f)	6.168E+15	1.087	1.017
	4	^{238}U (n,f)	2.256E+14	1.484	1.025
	5	^{46}Ti (n,p)	5.464E+12	1.521	1.014
	6	^{54}Fe (n,p)	4.439E+13	1.564	1.048
	7	^{58}Ni (n,p)	6.261E+13	1.473	0.990
	8	^{63}Cu (n,α)	2.607E+11	1.525	1.044
			Averaged C/E	1.361	1.006

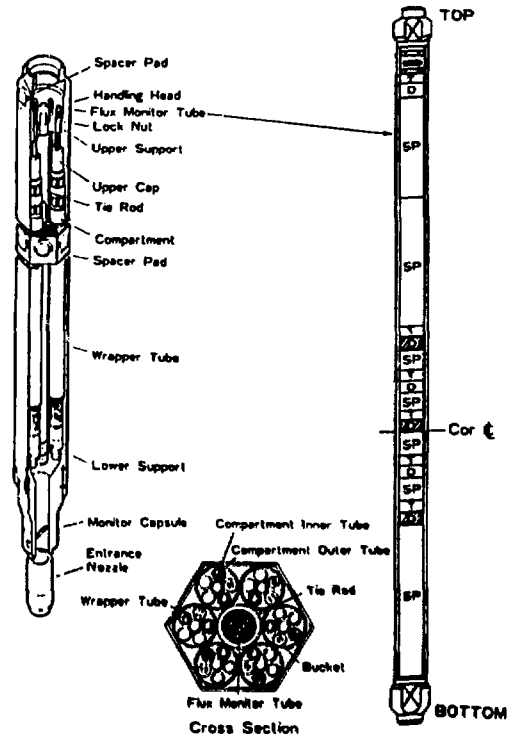

Fig. 1 Example of Loaded Dosimeters (Core Material Irradiation Rig)

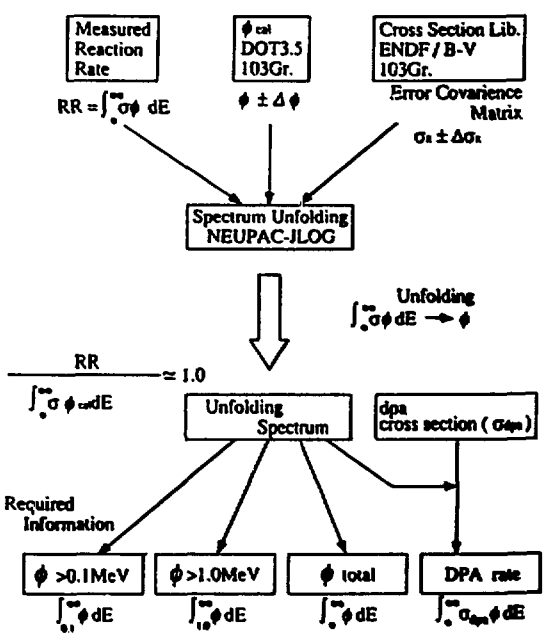

Fig. 2 Calculation Flow of NEUPAC

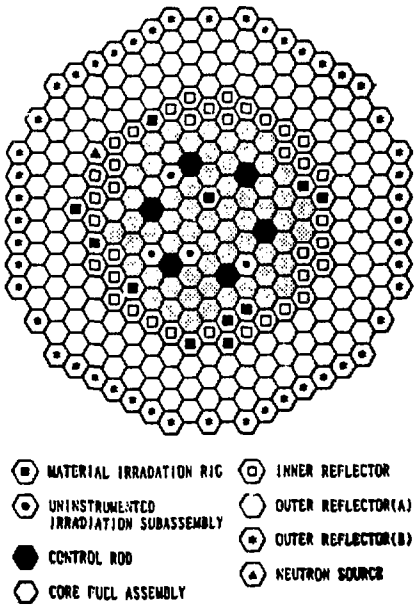

Fig. 3 Core Configuration of MK-II Core

REACTION RATE

ID NO.	REACTION TYPE	REACTION RATE *	R.R. ERROR **
1	59CO(N,G)	9.85100E+13	4.59358E-02
2	237NP(N,F)	1.66600E+15	4.44002E-02
3	235U(N,F)	6.16800E+15	3.98038E-02
4	238U(N,F)	2.25600E+14	4.14107E-02
5	46TI(N,P)	5.46400E+12	4.50309E-02
6	54FE(N,P)	4.43900E+13	5.44802E-02
7	58NI(N,P)	6.26100E+13	5.42492E-02
8	63CU(N,A)	2.60700E+11	4.59358E-02

* : $\times 10^{24}$ reaction/sec/atom/100MWt

** : $\sqrt{\Delta R^2 + \Delta P^2}$

ΔR : Measurement error of reaction rate

ΔP : Measurement error of reactor power

REACTION RATE COVARIANCE

	1	2	3	4	5	6	7	8
1	2.110E-03	1.204E-03	1.204E-03	1.204E-03	1.204E-03	1.204E-03	1.204E-03	1.204E-03
2	1.204E-03	1.971E-03	1.204E-03	1.204E-03	1.204E-03	1.204E-03	1.204E-03	1.204E-03
3	1.204E-03	1.204E-03	1.584E-03	1.204E-03	1.204E-03	1.204E-03	1.204E-03	1.204E-03
4	1.204E-03	1.204E-03	1.204E-03	1.715E-03	1.204E-03	1.204E-03	1.204E-03	1.204E-03
5	1.204E-03	1.204E-03	1.204E-03	1.204E-03	2.928E-03	1.204E-03	1.204E-03	1.204E-03
6	1.204E-03	1.204E-03	1.204E-03	1.204E-03	1.204E-03	2.968E-03	1.204E-03	1.204E-03
7	1.204E-03	1.204E-03	1.204E-03	1.204E-03	1.204E-03	1.204E-03	2.943E-03	1.204E-03
8	1.204E-03	1.204E-03	1.204E-03	1.204E-03	1.204E-03	1.204E-03	1.204E-03	2.110E-03

ΔP^2

INITIAL SPECTRUM

GROUP NO.	ENERGY RANGE	MID POINT	LETHARGY	FLUX	VARIANCE (%)
1	2.000E+01 - 1.822E+01	1.911E+01	9.321E-02	1.07282E+07	3.00000E+01
2	1.822E+01 - 1.649E+01	1.735E+01	9.976E-02	1.00236E+08	3.00000E+01
3	1.649E+01 - 1.492E+01	1.570E+01	1.002E-01	9.98144E+08	3.00000E+01
4	1.492E+01 - 1.350E+01	1.421E+01	9.995E-02	3.27017E+11	3.00000E+01
5	1.350E+01 - 1.221E+01	1.286E+01	1.000E-01	9.23797E+11	3.00000E+01

30%

Fig. 4 Example of Input Data (Corresponding to Error)

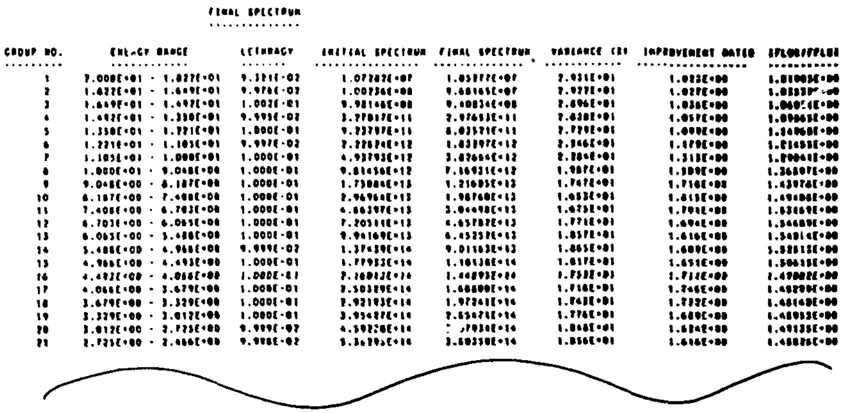

Fig. 5   Example of Output Data (Unfolded Neutron Spectrum)

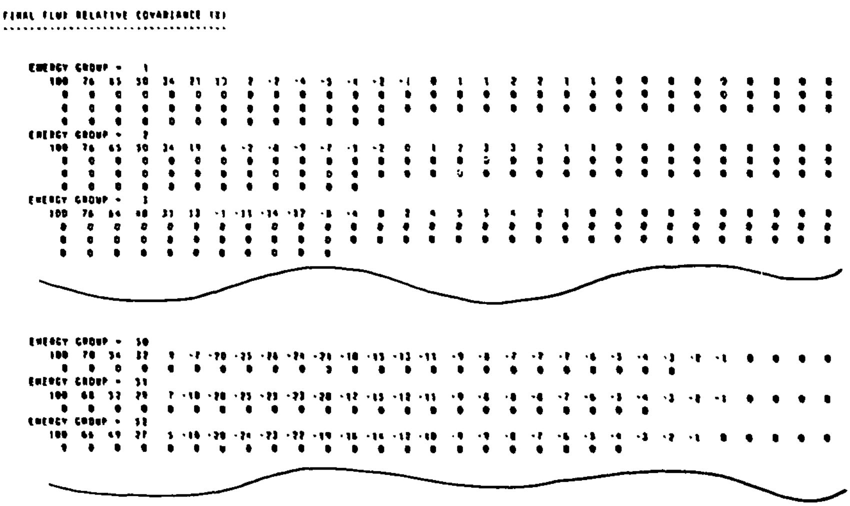

Fig. 6   Example of Output Data (Relative Covariance Matrix)

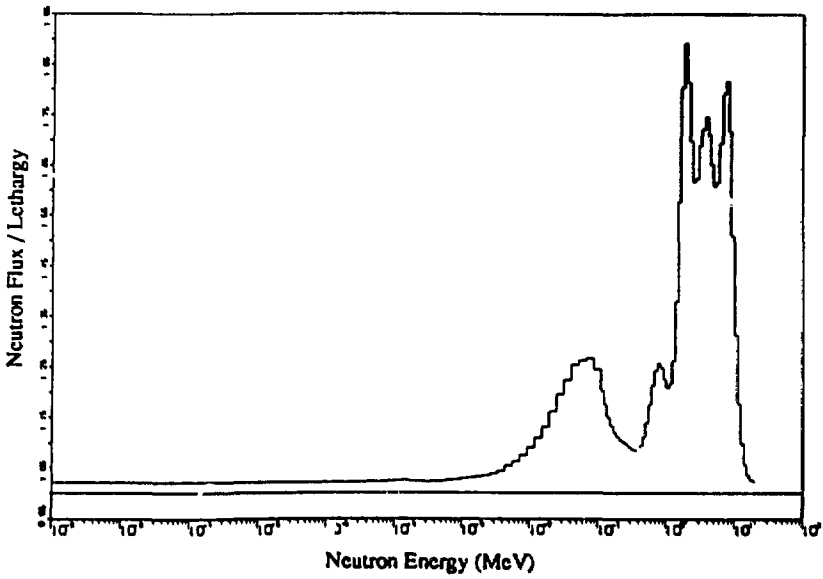

Fig. 7 Improvement Ratio of Unfolded Spectrum

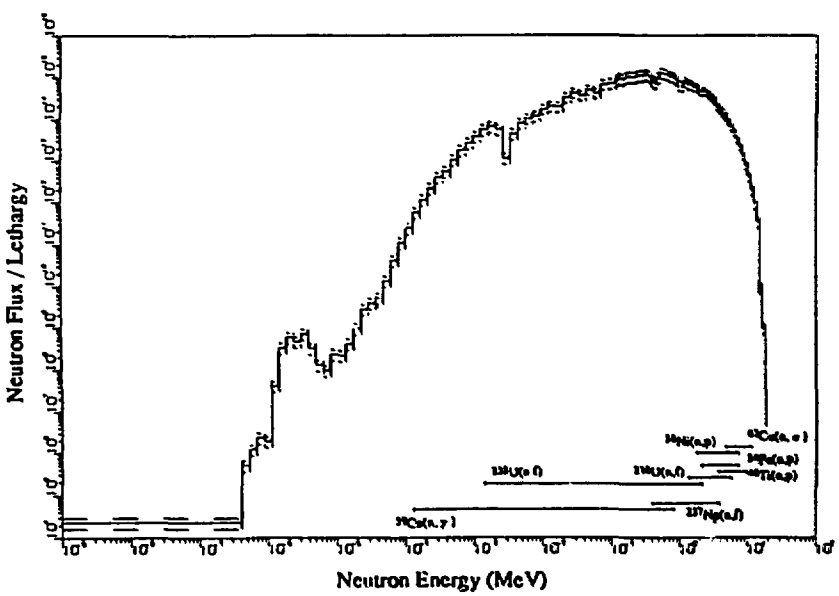

Fig. 8 Unfolded Neutron Spectrum and Its Uncertainty Range

Appendix 1 The Program of the Specialists' Meeting on Covariance Data

July 15 (Thursday)

13:30 ~ 14:50

1. Meaning of Covariance

Chairman: Y. Kikuchi (JAERI)

2.1 Covariance of Nuclear Data — Y. Kanda (Kyushu U.)

2.1 Some Comments on Peelle's Pertinent Puzzle — S. Chiba (JAERI)

15:20 ~ 17:10

2. Processing of Covariance Data and their Format

Chairman: K. Maki (Hitachi)

2.1 ENDF Format for Covariance Data — T. Nakagawa (JAERI)

2.2 Processing of Covariance File and Related Problems

A. Hasegawa (JAERI)

2.3 Experience on Preparation of a Covariance Library for the NEUPAC Code

T. Iguchi (Tokyo U.)

18:00 ~ 20:00 Reception at Akogigaura Club

July 16 (Friday)

9:20 ~ 12:00

3. Evaluation Method of Covariance Data (1)

Chairman: Y. Uenohara (Toshiba)

3.1 An Experience of Preparation of Covariance Matrices of the Simultaneous Evaluation of Heavy Nuclide Cross Sections

T. Murata (NNFDC)

3.2 Evaluation Method for FP Nuclear Cross Section Data

M. Kawai (Toshiba)

3.3 Evaluation of Covariance Data with Nuclear Model

T. Kawano (Kyushu U.)

3.2 Covariance Analysis of Experimental Data K. Kobayashi (Kyoto U.)

13:00 ~ 14:00

4. Evaluation Method of Covariance Data (2)

Chairman: Y. Nakajima (JAERI)

4.1 Sensitivities of Nuclear Model Calculation and Parameter Covariances

K. Shibata (JAERI)

4.2 Comparison of Covariances Calculated with Nuclear Model and Estimated with Least Squares Method

S. Iwasaki (Tohoku U.)

14:00 ~ 15:30

5. Utilization of Covariance Data

Chairman: S. Iwasaki (Tohoku U.)

5.1 Utilization of Cross-section Covariance Data in FBR Core Nuclear Design and Cross-section Adjustment

M. Ishikawa (PNC)

5.2 Applications of Error Covariances to Fast Reactor Material Dosimetry in JOYO

K. Chatani (PNC)

15:40 ~ 16:30

6. Discussion

Chairman: Y. Kanda (Kyushu U.)

Appendix 2 List of Participants for the Specialists' Meeting on Covariance Data

Participant		Affiliation
Keiji	CHATANI	Power Reactor and Nuclear Fuel Development Corp.
Satoshi	CHIBA	Japan Atomic Energy Research Institute
Tokio	FUKAHORI	Japan Atomic Energy Research Institute
Tetsuo	IGUCHI	Tokyo University
Makoto	ISHIKAWA	Power Reactor and Nuclear Fuel Development Corp.
Chikara	ITO	Power Reactor and Nuclear Fuel Development Corp.
Shin	IWASAKI	Tohoku University
Akira	HASEGAWA	Japan Atomic Energy Research Institute
Yukinori	KANDA	Kyushu University
Masayoshi	KAWAI	Toshiba Corp.
Toshihiko	KAWANO	Kyushu University
Yasuyuki	KIKUCHI	Japan Atomic Energy Research Institute
Kensuke	KITAO	Data Engineering Inc.
Katsuhei	KOBAYASHI	Kyoto University
Koichi	MAKI	Hitachi Ltd.
Hiroyuki	MATSUNOBU	Sumitomo Atomic Energy Industries Ltd.
Alberto	MENGONI	Japan Atomic Energy Research Institute
Toru	MURATA	Nippon Nuclear Fuel Development Co.
Tsuneo	NAKAGAWA	Japan Atomic Energy Research Institute
Yutaka	NAKAJIMA	Japan Atomic Energy Research Institute
Naoteru	ODANO	Ship Research Institute
O.	SHCHERBAKOV	Kyoto University
Keiichi	SHIBATA	Japan Atomic Energy Research Institute
Masayoshi	SUGIMOTO	Japan Atomic Energy Research Institute
Yuji	UENOHARA	Toshiba Corp.
Naoki	YAMANO	Sumitomo Atomic Energy Industries Ltd.

国際単位系 (SI) と換算表

表 1　SI 基本単位および補助単位

量	名称	記号
長さ	メートル	m
質量	キログラム	kg
時間	秒	s
電流	アンペア	A
熱力学温度	ケルビン	K
物質量	モル	mol
光度	カンデラ	cd
平面角	ラジアン	rad
立体角	ステラジアン	sr

表 2　SI と併用される単位

名称	記号
分，時，日	min，h，d
度，分，秒	°，′，″
リットル	l，L
トン	t
電子ボルト	eV
原子質量単位	u

1 eV = 1.60218 × 10^{-19} J

1 u = 1.66054 × 10^{-27} kg

表 3　固有の名称をもつ SI 組立単位

量	名称	記号	他の SI 単位による表現
周波数	ヘルツ	Hz	s^{-1}
力	ニュートン	N	m·kg/s^2
圧力，応力	パスカル	Pa	N/m^2
エネルギー，仕事，熱量	ジュール	J	N·m
工率，放射束	ワット	W	J/s
電気量，電荷	クーロン	C	A·s
電位，電圧，起電力	ボルト	V	W/A
静電容量	ファラド	F	C/V
電気抵抗	オーム	Ω	V/A
コンダクタンス	シーメンス	S	A/V
磁束	ウェーバ	Wb	V·s
磁束密度	テスラ	T	Wb/m^2
インダクタンス	ヘンリー	H	Wb/A
セルシウス温度	セルシウス度	℃	
光束	ルーメン	lm	cd sr
照度	ルクス	lx	lm/m^2
放射能	ベクレル	Bq	s^{-1}
吸収線量	グレイ	Gy	J/kg
線量当量	シーベルト	Sv	J/kg

表 4　SI と共に暫定的に維持される単位

名称	記号
オングストローム	Å
バーン	b
バール	bar
ガル	Gal
キュリー	Ci
レントゲン	R
ラド	rad
レム	rem

1 Å = 0.1 nm = 10^{-10} m

1 b = 100 fm^2 = 10^{-28} m^2

1 bar = 0.1 MPa = 10^5 Pa

1 Gal = 1 cm/s^2 = 10^{-2} m/s^2

1 Ci = 3.7 × 10^{10} Bq

1 R = 2.58 × 10^{-4} C/kg

1 rad = 1 cGy = 10^{-2} Gy

1 rem = 1 cSv = 10^{-2} Sv

表 5　SI 接頭語

倍数	接頭語	記号
10^{18}	エクサ	E
10^{15}	ペタ	P
10^{12}	テラ	T
10^{9}	ギガ	G
10^{6}	メガ	M
10^{3}	キロ	k
10^{2}	ヘクト	h
10^{1}	デカ	da
10^{-1}	デシ	d
10^{-2}	センチ	c
10^{-3}	ミリ	m
10^{-6}	マイクロ	μ
10^{-9}	ナノ	n
10^{-12}	ピコ	p
10^{-15}	フェムト	f
10^{-18}	アト	a

（注）

1. 表 1 ～ 5 は「国際単位系」第 5 版，国際度量衡局 1985 年刊行による。ただし，1 eV および 1 u の値は CODATA の 1986 年推奨値によった
2. 表 4 には海里，ノット，アール，ヘクタールも含まれているが日常の単位なのでここでは省略した
3. bar は，JIS では流体の圧力を表わす場合に限り表 2 のカテゴリーに分類されている。
4. EC 閣僚理事会指令では bar，barn および「血圧の単位」mmHg を表 2 のカテゴリーに入れている。

換算表

力	N(=10^5 dyn)	kgf	lbf
	1	0.101972	0.224809
	9.80665	1	2.20462
	4.44822	0.453592	1

粘度　1 Pa·s(N·s/m^2) = 10 P(ポアズ)(g/(cm·s))

動粘度　1 m^2/s = 10^4 St(ストークス)(cm^2/s)

圧力	MPa(=10 bar)	kgf/cm^2	atm	mmHg(Torr)	lbf/in^2(psi)
	1	10.1972	9.86923	7.50062 × 10^3	145.038
	0.0980665	1	0.967841	735.559	14.2233
	0.101325	1.03323	1	760	14.6959
	1.33322 × 10^{-4}	1.35951 × 10^{-4}	1.31579 × 10^{-3}	1	1.93368 × 10^{-2}
	6.89476 × 10^{-3}	7.03070 × 10^{-2}	6.80460 × 10^{-2}	51.7149	1

エネルギー・仕事・熱量	J(=10^7 erg)	kgf·m	kW·h	cal(計量法)	Btu	ft·lbf	eV
	1	0.101972	2.77778 × 10^{-7}	0.238889	9.47813 × 10^{-4}	0.737562	6.24150 × 10^{18}
	9.80665	1	2.72407 × 10^{-6}	2.34270	9.29487 × 10^{-3}	7.23301	6.12082 × 10^{19}
	3.6 × 10^6	3.67098 × 10^5	1	8.59999 × 10^5	3412.13	2.65522 × 10^6	2.24694 × 10^{25}
	4.18605	0.426858	1.16279 × 10^{-6}	1	3.96759 × 10^{-3}	3.08747	2.61272 × 10^{19}
	1055.06	107.586	2.93072 × 10^{-4}	252.042	1	778.172	6.58515 × 10^{21}
	1.35582	0.138255	3.76616 × 10^{-7}	0.323890	1.28506 × 10^{-3}	1	8.46233 × 10^{18}
	1.60218 × 10^{-19}	1.63377 × 10^{-20}	4.45050 × 10^{-26}	3.82743 × 10^{-20}	1.51857 × 10^{-22}	1.18171 × 10^{-19}	1

1 cal = 4.18605 J(計量法)

= 4.184 J　(熱化学)

= 4.1855 J　(15 °C)

= 4.1868 J(国際蒸気表)

仕事率　1 PS(仏馬力)

= 75 kgf·m/s

= 735.499 W

放射能	Bq	Ci
	1	2.70270 × 10^{-11}
	3.7 × 10^{10}	1

吸収線量	Gy	rad
	1	100
	0.01	1

照射線量	C/kg	R
	1	3876
	2.58 × 10^{-4}	1