PHYSOR 2004 -The Physics of Fuel Cycles and Advanced Nuclear Systems: Global Developments
Chicago, Illinois, April 25-29, 2004, on CD-ROM, American Nuclear Society, La Grange Park, IL (2004)

The Fission Spectrum Uncertainty

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The fission spectrum uncertainty (variance covariance) matrix is needed in many nuclear data applications. Unfortunately, most modern evaluated data files, with the exception of JENDL3.3, do not include information on the fission spectrum uncertainty. In this paper, the fission spectrum relative uncertainty matrix derivation for the Watt fission spectrum is followed by a more general derivation utilizing some characteristics of any fission spectrum. In the second derivation, the Watt spectrum is used only for the calculation of sensitivity coefficients.

KEYWORDS: fission spectrum uncertainty, Watt fission spectrum, fission spectrum mean energy, fission spectrum width

1. Introduction

The fission spectrum can be analytically represented in several different forms, such as a simple Maxwellian, the Watt fission spectrum, or the more modern and physically sound Madland-Nix representation. A quantitative estimate of the uncertainty matrix associated with the fission spectrum is needed in many nuclear data applications. Criticality safety, neutron cross-section adjustment, and reactor pressure-vessel surveillance dosimetry are just a few examples. A simple way to estimate the relative uncertainty in the fission spectrum, in any representation, is to represent it in terms of the relative uncertainties in certain characteristics of the fission spectrum, such as the mean energy of the secondary fission neutrons, $\overline{E}$, and w, the relative root-mean-square width about the mean energy, which is $w = \left(1/\overline{E}\right)\sqrt{\overline{E^2} - \overline{E}^2}$, or “width” for short. [1] These two characteristics are correlated, and their correlation has to be estimated. [2] Figure 1 depicts the correlation between the mean fission energy $\overline{E}$ and the fission width w, C_{ew}, as a function of the correlation between the Watt fission spectrum parameters, C_{ab}. Even if the parameters of the Watt spectrum are not correlated (i.e. even if $C_{ab} = 0$), the mean fission energy $\overline{E}$ and the fission width w are strongly anticorrelated.

As already mentioned, our purpose is to derive the relative uncertainty (or covariance) matrix associated with a fission spectrum, utilizing the relative uncertainties in the mean fission energy $\overline{E}$ and in the fission width w. These relative uncertainties can, for instance, be derived from the raw experimental data or from the uncertainties in the parameters of a Watt fission spectrum representation of the measured fission spectrum. [3]

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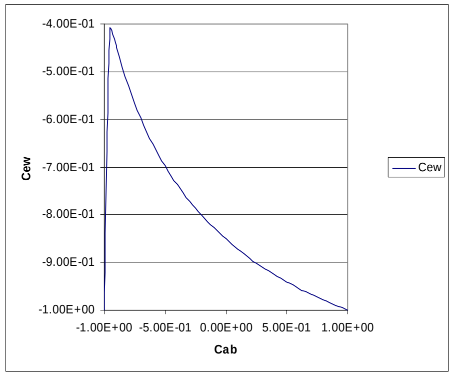

Fig. 1 The correlation between the mean fission energy $\overline{E}$ and the fission width w, C_{ew}, as a function of the correlation between the Watt fission spectrum parameters, C_{ab}.

2. The Watt Fission Spectrum

Although the Watt formula has no real physical foundation, it represents the experimental data fairly well over most of the energy range of the secondary fission neutrons. Although it depends on more than a single parameter, it is still rather simple to handle. The Watt fission spectrum is given in ENDF-102 Data Formats and Procedures [4] as

$$f(E \to E') = \sqrt{4/(\pi a^3 b)}\, e^{-ab/4} e^{-E'/a} \sinh\left(\sqrt{bE'}\right),$$

where the parameters a and b are dependent on E, the energy of the neutron-inducing fission, and E' is the energy of the secondary neutrons. The parameters a and b are usually determined by fitting the Watt formula to the measured fission spectrum data.

2.1 Sensitivities

Let us first calculate the relative sensitivities of the Watt fission spectrum to its parameters a and b. We define $x = ab/6$ and take the partial derivative of f with respect to a:

$$\partial f / \partial a = \left[-3/(2a) - b/4 + E'/a^2\right] f \ .$$

The sensitivity of f with respect to a is then

$$(a/f)\partial f / \partial a = a\left[-3/(2a) - b/4 + E'/a^2\right] = E'/a - 3/2(1+x) \ .$$

Similarly,

$$\partial f / \partial b = \left[-1/(2b) - a/4 + \coth\left(\sqrt{bE'}\right)(1/2)\sqrt{E'/b}\right] f \ ,$$

and the sensitivity

$$(b/f)\partial f / \partial b = (1/2)\left[\sqrt{bE'} / \mathrm{tgh}\left(\sqrt{bE'}\right) - (1+3x)\right].$$

2.2 Relative Covariance Matrix of the Fission Spectrum Expressed by the Variation of the Parameters *a* and *b*

The relative variation in the fission spectrum $f(E \to E')$ due to the variation in the parameters a and b is given by

$$\delta f / f = \left[(a/f)\partial f / \partial a\right](\delta a / a) + \left[(b/f)\partial f / \partial b\right](\delta b / b).$$

inserting the explicit expressions of the sensitivities of the fission spectrum with respect to *a* and *b*, we obtain

$$\delta f / f = \left[E'/a - (3/2)(1+x)\right](\delta a / a) + (1/2)\left[\sqrt{bE'} / \mathrm{tgh}\left(\sqrt{bE'}\right) - (1+3x)\right](\delta b / b).$$

The relative covariance of the fission spectrum in energy group *i* and in energy group *j* is as follows:

$$\begin{aligned}
&\left\langle (\delta f / f)_i (\delta f / f)_j \right\rangle = \\
&\left[\overline{E'}^{i} / a - (3/2)(1+x)\right]\left[\overline{E'}^{j} / a - (3/2)(1+x)\right]\left\langle (\delta a / a)(\delta a / a)\right\rangle \\
&+ (1/2)\left[\overline{\sqrt{bE'} / \mathrm{tgh}\left(\sqrt{bE'}\right)}^{i} - (1+3x)\right](1/2)\left[\overline{\sqrt{bE'} / \mathrm{tgh}\left(\sqrt{bE'}\right)}^{j} - (1+3x)\right]\left\langle (\delta b / b)(\delta b / b)\right\rangle \\
&+ \left\{ \begin{aligned} &\left[\overline{E'}^{i} / a - (3/2)(1+x)\right](1/2)\left[\overline{\sqrt{bE'} / \mathrm{tgh}\left(\sqrt{bE'}\right)}^{j} - (1+3x)\right] + \\ &\left[\overline{E'}^{j} / a - (3/2)(1+x)\right](1/2)\left[\overline{\sqrt{bE'} / \mathrm{tgh}\left(\sqrt{bE'}\right)}^{i} - (1+3x)\right] \end{aligned} \right\} \left\langle (\delta a / a)(\delta b / b)\right\rangle
\end{aligned}$$

where $\overline{E'}^{i}$ is the average energy in group *i* and $\overline{\sqrt{bE'} / \mathrm{tgh}\left(\sqrt{bE'}\right)}^{i}$ is the average of $\sqrt{bE'} / \mathrm{tgh}\left(\sqrt{bE'}\right)$ in group *i*, with $f(E \rightarrow E')$ as the weighting function. The relative variances of the parameter *a* and of the parameter *b* are $\langle (\delta a / a)(\delta a / a)\rangle$ and $\langle (\delta b / b)(\delta b / b)\rangle$, respectively, and $\langle (\delta a / a)(\delta b / b)\rangle$ is their relative covariance, if they are correlated. This expression of the relative covariance of the fission spectrum in different energy groups is given in terms of the variances of the Watt fission spectrum parameters *a* and *b* and their possible covariance.

3. General Fission Spectrum

A more general representation of the fission spectrum will not be limited to the Watt representation, and thus an alternative representation of the fission spectrum uncertainty is sought. The relative variation of the fission spectrum will be expressed in terms of the relative variations in certain characteristics of the fission spectrum, namely, $\overline{E}$ and w as

$$\delta f / f = \left[(\overline{E} / f)\partial f / \partial \overline{E}\right](\delta \overline{E} / \overline{E}) + \left[(w / f)\partial f / \partial w\right](\delta w / w).$$

These values are general characteristics of the fission spectrum; the mean energy of the secondary fission neutrons, $\overline{E}$; and the width w. In the following sections, these quantities will be calculated for the Watt spectrum representation. The sensitivities of the fission spectrum to $\overline{E}$ and *w* will then be calculated for the Watt fission spectrum representation and will be utilized for the calculation of the relative covariance of any fission spectrum as a function of the relative variance and covariance in the mean energy and in the relative width, $\overline{E}$ and *w*, respectively.

3.1 Mean Energy

The fission spectrum is normalized so that $\int f(E \to E')dE' = 1$. For the Watt fission spectrum we get, after differentiating with respect to *a*, $\int (\partial f/\partial a)dE' = 0$. Using the explicit form of the partial derivative, we get $-3/(2a) - b/4 + \overline{E}/a^2 = 0$. The explicit form of the mean energy is thus

$$\overline{E} = a(3/2 + ab/4) = (3/2)a(1 + ab/6) = (3/2)a(1 + x),$$

with partial derivatives with respect to *a* and *b* of

$$\partial\overline{E}/\partial a = \overline{E}/a + ab/4 = (3/2)(1 + 2x)$$

and

$$\partial\overline{E}/\partial b = a^2/4.$$

The sensitivities of $\overline{E}$ to *a* and *b* are

$$(a/\overline{E})(\partial\overline{E}/\partial a) = a(3/2)(1+2x)/[(3/2)a(1+x)] = (1+2x)/(1+x)$$

and

$$(b/\overline{E})(\partial\overline{E}/\partial b) = b(a^2/4)/[(3/2)a(1+x)] = x/(1+x).$$

Since, by definition, $\overline{E} = \int E' f(E \to E')dE'$, its partial derivative with respect to *a* can alternatively be derived by $\partial\overline{E}/\partial a = \int E'(\partial f/\partial a)dE'$. Using again the explicit form of $\partial f/\partial a$, we get

$$\partial\overline{E}/\partial a = -3/(2a)\overline{E} - (b/4)\overline{E} + (1/a^2)\overline{E^2} = -(1/a)(3/2 + ab/4)\overline{E} + (1/a^2)\overline{E^2} = \left(\overline{E^2} - \overline{E}^2\right)/a^2.$$

Equating the two expressions of the partial derivative of $\overline{E}$, the mean energy of the fission spectrum secondary neutrons, with respect to *a*, we get

$$\overline{E^2} - \overline{E}^2 = a\left(\overline{E} + a^2 b/4\right).$$

3.2 The Relative Root-Mean-Square Width about the Mean Energy (Relative Width)

We define the relative root-mean-square width about the mean energy of the fission spectrum as $w = (1/\overline{E})\sqrt{\overline{E^2} - \overline{E}^2}$. This relative width is for the Watt fission spectrum representation

$$w = (1/\overline{E})\sqrt{\overline{E^2} - \overline{E}^2} = \sqrt{a\left(\overline{E} + a^2 b/4\right)/\overline{E}^2} = \sqrt{2/3}\sqrt{(1+2x)}/(1+x).$$

The sensitivities of the relative width, *w*, to the Watt fission spectrum parameters *a* and *b* are $\partial w/\partial a = (\partial w/\partial x)(\partial x/\partial a)$ and $\partial w/\partial b = (\partial w/\partial x)(\partial x/\partial b)$. Since

$$\partial w/\partial x = -\sqrt{(2/3)}x/\left[\sqrt{(1+2x)}(1+x)^2\right], \; \partial x/\partial a = b/6, \text{ and } \partial x/\partial b = a/6,$$

the sensitivities of the relative width are

$$\left(a / w\right)\partial w / \partial a = \left(b / w\right)\partial w / \partial b = -x^2 / \left[\left(1 + x\right)\left(1 + 2x\right)\right].$$

4. Relative Covariance Matrix of the Fission Spectrum Expressed by the Relative Variation of $\overline{E}$ and w

We now express the relative variation of the fission spectrum in terms of its characteristics $\overline{E}$ and w,

$$\delta f / f = \left[\left(\overline{E} / f\right)\partial f / \partial \overline{E}\right]\left(\delta \overline{E} / \overline{E}\right) + \left[\left(w / f\right)\partial f / \partial w\right]\left(\delta w / w\right).$$

However, the sensitivities in the square brackets cannot be directly calculated since *f* is not represented explicitly as a function of $\overline{E}$ and w. In order to calculate these sensitivities, we utilize the simple Watt fission spectrum representation. The relative variations in $\overline{E}$ and in *w*, as functions of the relative variations in the Watt fission spectrum parameters *a* and *b*, are

$$\delta \overline{E} / \overline{E} = \left(a / \overline{E}\right)\left(\partial \overline{E} / \partial a\right)\left(\delta a / a\right) + \left(b / \overline{E}\right)\left(\partial \overline{E} / \partial b\right)\left(\delta b / b\right)$$

and

$$\delta w / w = \left(a / w\right)\left(\partial w / \partial a\right)\left(\delta a / a\right) + \left(b / w\right)\left(\partial w / \partial b\right)\left(\delta b / b\right).$$

Inverting the 2 × 2 matrix relating the relative variations of $\overline{E}$ and w to the relative variations of *a* and *b*, we get

$$\left(\delta a / a\right) = 1/\det\left[\left(b / w\right)\left(\partial w / \partial b\right)\delta \overline{E} / \overline{E} - \left(b / \overline{E}\right)\left(\partial \overline{E} / \partial b\right)\delta w / w\right]$$

and

$$\left(\delta b / b\right) = 1/\det\left[-\left(a / w\right)\left(\partial w / \partial a\right)\delta \overline{E} / \overline{E} + \left(a / \overline{E}\right)\left(\partial \overline{E} / \partial a\right)\delta w / w\right],$$

where det is the determinant of the transformation matrix and is equal to

$$\det = \left(a / \overline{E}\right)\left(\partial \overline{E} / \partial a\right)\left(b / w\right)\left(\partial w / \partial b\right) - \left(b / \overline{E}\right)\left(\partial \overline{E} / \partial b\right)\left(a / w\right)\left(\partial w / \partial a\right) = -x^2 / \left[\left(1 + x\right)\left(1 + 2x\right)\right].$$

These expressions of the relative variations in the Watt fission spectrum parameters *a* and *b*, in terms of the relative variations in $\overline{E}$ and in *w*, can be substituted into the equation of the relative variation in $f\left(E \rightarrow E'\right)$, expressed in terms of the variations in the parameters *a* and *b*, given by

$$\delta f / f = \left[\left(a / f\right)\partial f / \partial a\right]\left(\delta a / a\right) + \left[\left(b / f\right)\partial f / \partial b\right]\left(\delta b / b\right).$$

The sensitivities in these square brackets were analytically calculated in Section 2.1 and averaged over the respective energy groups with the fission spectrum as the weighting function in Section 2.2. Utilizing these group-averaged sensitivities ultimately leads to the multigroup fission spectrum covariance matrix as a function of the relative variances of $\overline{E}$ and *w* and their covariance.

Inserting these values of the relative variations in *a* and *b* into the relative variation of the fission spectrum *f*, $\delta f / f = \left[\left(a / f\right)\partial f / \partial a\right]\left(\delta a / a\right) + \left[\left(b / f\right)\partial f / \partial b\right]\left(\delta b / b\right)$, we get

$$(\bar{E}/f)\partial f/\partial\bar{E} = 1/\det\{(a/f)\partial f/\partial a(b/w)\partial w/\partial b - (b/f)\partial f/\partial b(a/w)\partial w/\partial a\}$$

and

$$(w/f)\partial f/\partial w = 1/\det\{(b/f)\partial f/\partial b(a/\bar{E})\partial\bar{E}/\partial a - (a/f)\partial f/\partial a(b/\bar{E})\partial\bar{E}/\partial b\} \quad .$$

The relative variation of the fission spectrum is thus expressed by

$$\begin{aligned}
&\delta f/f = [(\bar{E}/f)\partial f/\partial\bar{E}](\delta\bar{E}/\bar{E}) + [(w/f)\partial f/\partial w](\delta w/w) = \\
&1/\det\{(a/f)\partial f/\partial a(b/w)\partial w/\partial b - (b/f)\partial f/\partial b(a/w)\partial w/\partial a\}(\delta\bar{E}/\bar{E}) + \\
&1/\det\{(b/f)\partial f/\partial b(a/\bar{E})\partial\bar{E}/\partial a - (a/f)\partial f/\partial a(b/\bar{E})\partial\bar{E}/\partial b\}(\delta w/w)
\end{aligned}$$

Using this expression, the relative covariance matrix relating the relative variance of the mean energy of the fission spectrum, the relative variance of the spectrum's relative width, and their possible covariance will be given by

$$\begin{aligned}
&\langle(\partial f/f)_i(\partial f/f)_j\rangle = \\
&1/\det\{\overline{(a/f)\partial f/\partial a}^{\,i}(b/w)\partial w/\partial b - \overline{(b/f)\partial f/\partial b}^{\,i}(a/w)\partial w/\partial a\}\bullet \\
&1/\det\{\overline{(a/f)\partial f/\partial a}^{\,j}(b/w)\partial w/\partial b - \overline{(b/f)\partial f/\partial b}^{\,j}(a/w)\partial w/\partial a\}\bullet \\
&\langle(\delta\bar{E}/\bar{E})(\delta\bar{E}/\bar{E})\rangle + \\
&1/\det\{\overline{(b/f)\partial f/\partial b}^{\,i}(a/\bar{E})\partial\bar{E}/\partial a - \overline{(a/f)\partial f/\partial a}^{\,i}(b/\bar{E})\partial\bar{E}/\partial b\}\bullet \\
&1/\det\{\overline{(b/f)\partial f/\partial b}^{\,j}(a/\bar{E})\partial\bar{E}/\partial a - \overline{(a/f)\partial f/\partial a}^{\,j}(b/\bar{E})\partial\bar{E}/\partial b\}\bullet \\
&\langle(\delta w/w)(\delta w/w)\rangle + \\
&\left(\begin{aligned}
&1/\det\{\overline{(a/f)\partial f/\partial a}^{\,i}(b/w)\partial w/\partial b - \overline{(b/f)\partial f/\partial b}^{\,i}(a/w)\partial w/\partial a\}\bullet \\
&1/\det\{\overline{(b/f)\partial f/\partial b}^{\,j}(a/\bar{E})\partial\bar{E}/\partial a - \overline{(a/f)\partial f/\partial a}^{\,j}(b/\bar{E})\partial\bar{E}/\partial b\} + \\
&1/\det\{\overline{(a/f)\partial f/\partial a}^{\,j}(b/w)\partial w/\partial b - \overline{(b/f)\partial f/\partial b}^{\,j}(a/w)\partial w/\partial a\}\bullet \\
&1/\det\{\overline{(b/f)\partial f/\partial b}^{\,i}(a/\bar{E})\partial\bar{E}/\partial a - \overline{(a/f)\partial f/\partial a}^{\,i}(b/\bar{E})\partial\bar{E}/\partial b\}
\end{aligned}\right)\bullet \\
&\langle(\delta\bar{E}/\bar{E})(\delta w/w)\rangle
\end{aligned}$$

The building blocks of this expression are the sensitivities of the mean energy and of relative width to *a* and *b*, which do not depend on the energy; the group-averaged sensitivities of the fission spectrum to *a* and *b*; det, the determinant of the transformation matrix; the variances of $\bar{E}$ and w; and their covariance. Inserting all these building blocks, the explicit form of the fission spectrum relative covariance matrix is

$$
\begin{aligned}
&\left\langle (\partial f / f)_i (\partial f / f)_j \right\rangle = \\
&\left\{ \left(\overline{E'}^{\,i} / a - (3/2)(1+x) \right) - (1/2) \left[\overline{\sqrt{bE'} / \mathrm{tgh}\left(\sqrt{bE'}\right)}^{\,\mathrm{i}} - (1+3x) \right] \right\} \bullet \\
&\left\{ \left(\overline{E'}^{\,j} / a - (3/2)(1+x) \right) - (1/2) \left[\overline{\sqrt{bE'} / \mathrm{tgh}\left(\sqrt{bE'}\right)}^{\,\mathrm{j}} - (1+3x) \right] \right\} \bullet \\
&\left\langle \left(\delta\overline{E} / \overline{E}\right)\left(\delta\overline{E} / \overline{E}\right) \right\rangle + \\
&\left[-(1+2x)/x^2 \right] \left\{ (1/2) \left[\overline{\sqrt{bE'} / \mathrm{tgh}\left(\sqrt{bE'}\right)}^{\,\mathrm{i}} - (1+3x) \right] (1+2x) - \left(\overline{E'}^{\,i} / a - (3/2)(1+x) \right) x \right\} \bullet \\
&\left[-(1+2x)/x^2 \right] \left\{ (1/2) \left[\overline{\sqrt{bE'} / \mathrm{tgh}\left(\sqrt{bE'}\right)}^{\,\mathrm{j}} - (1+3x) \right] (1+2x) - \left(\overline{E'}^{\,j} / a - (3/2)(1+x) \right) x \right\} \bullet \\
&\left\langle (\delta w / w)(\delta w / w) \right\rangle + \\
&\left(\begin{aligned}
&\left\{ \left(\overline{E'}^{\,i} / a - (3/2)(1+x) \right) - (1/2) \left[\overline{\sqrt{bE'} / \mathrm{tgh}\left(\sqrt{bE'}\right)}^{\,\mathrm{i}} - (1+3x) \right] \right\} \bullet \\
&\left[-(1+2x)/x^2 \right] \left\{ (1/2) \left[\overline{\sqrt{bE'} / \mathrm{tgh}\left(\sqrt{bE'}\right)}^{\,\mathrm{j}} - (1+3x) \right] (1+2x) - \left(\overline{E'}^{\,j} / a - (3/2)(1+x) \right) x \right\} + \\
&\left\{ \left(\overline{E'}^{\,j} / a - (3/2)(1+x) \right) - (1/2) \left[\overline{\sqrt{bE'} / \mathrm{tgh}\left(\sqrt{bE'}\right)}^{\,\mathrm{j}} - (1+3x) \right] \right\} \bullet \\
&\left[-(1+2x)/x^2 \right] \left\{ (1/2) \left[\overline{\sqrt{bE'} / \mathrm{tgh}\left(\sqrt{bE'}\right)}^{\,\mathrm{i}} - (1+3x) \right] (1+2x) - \left(\overline{E'}^{\,i} / a - (3/2)(1+x) \right) x \right\}
\end{aligned} \right) \bullet \\
&\left\langle \left(\delta\overline{E} / \overline{E}\right)(\delta w / w) \right\rangle
\end{aligned}
$$

5. Conclusion

The relative covariance matrix associated with the fission spectrum was expressed in terms of the relative uncertainties in the mean fission energy $\overline{E}$ and in the fission width w. This expression is valid even when the relative uncertainties in the Watt fission spectrum parameters are not known. The Watt fission spectrum was used only to calculate the sensitivities of the fission spectrum to the uncertainties in the mean fission energy $\overline{E}$ and in the fission width w.

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