least in future editions of these books and in other books in nuclear science and engineering that may be published in the future, such erronous conceptual statements will not be made. It should be clearly pointed out to students in nuclear science and engineering that the area under the curve of a cross section is conserved only under the so called psi-chi approximation. The detailed equations and discussions relating to exact Doppler broadening are not reproduced here in order to save space and are readily available in Ref. 3.

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Responses to "Propagation of Knowledge Regarding Conservation During Doppler Broadening"

I hope that Ganesan[1] is overestimating the dangers of students being misled by statements such as "the total area under the resonance curve is constant when the temperature changes" and that they will ask the questions:

1. What is the variable of integration (energy, velocity, lethargy, etc.)?
2. What is the range of integration?
3. How does this relate to the quantity of relevance in reactor calculations (the integral of flux times cross section)?

The integral that remains constant when temperature changes is

$$\int_0^{\infty} E\sigma(E,T)\,dE \ .$$

I would agree that a student is unlikely to guess that it is the area under the curve of σ plotted against E^2 that remains constant. However, in most cases of practical interest the resonances are sufficiently narrow for the area to remain approximately constant when the variable of integration is energy (or even lethargy).

When the self-shielding and mutual shielding effects are small, the ratio of integrals

$$\int_{E_1}^{E_2} \phi(E)\sigma(E,T)\,dE \Big/ \int_{E_1}^{E_2} \phi(E)\,dE$$

can often be approximated as independent of temperature, but the student should carefully consider whether this is true for the particular range of integration and flux shape, $\phi(E)$, in relation to the widths and positions of the resonances in the energy interval (E_1 to E_2), and also whether $\phi(E)$ is itself a function of T.

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[1]S. GANESAN, *Nucl. Sci. Eng.*, **86**, 118 (1984).

In his Letter to the Editor, Ganesan[1] has supplied a number of references in which the details of Doppler broadening are presented. Therefore, I will only present a few comments here on conservation of "the area under the curve" of resonances and the related assumption that "Doppler broadening smooths cross sections."

First of all let me state that one should not be too hard on authors who state that "the area under the curve" of resonances is conserved. In textbooks and other references that introduce the psi-chi approximation for use in fission reactor core calculations, a natural result of introducing the psi-chi approximation is the observation that, when the psi-chi approximation is used, the "area under the curve" of a resonance is conserved, and under Doppler broadening, cross sections become smoother. If restricted to the energy and temperature ranges where the psi-chi approximation is valid, it is an excellent tool that is both economical and accurate for use in predicting the behavior of resonances under Doppler broadening. Therefore the introduction of psi-chi approximating and its consequences in textbooks is certainly worth doing, since it introduces the reader to a very practical method that is widely used in fission reactor calculations.

However, what is not stressed in textbooks is identification of the range of validity of the psi-chi method and recognition that conservation and smoothing of the cross section are a consequence of the psi-chi approximation and are not properties of the basic Doppler broadening equation. In particular, the failure to explicitly point out that conservation and smoothing of cross section are a result of using the psi-chi approximation has led readers to assume that these are general properties of Doppler broadening, and they have applied these concepts to applications where they are not valid.

The basic Doppler broadening equation conserves and smooths the reaction rate $[N\sigma(N)]$, not cross sections. In the higher energy resonance region at fission reactor temperatures, where the reaction shape is dominated by resonance profiles, distinguishing between reaction and cross-section smoothing is of little practical concern. It is in this energy range that the psi-chi approximation is valid and accurate and where, for all practical purposes, cross-section conservation and smoothing occur. However, even here care must be exercised to define the cross section accurately over the entire energy range, particularly for heavy even-even isotopes such as ^{232}Th, ^{238}U, and ^{240}Pu where the resonances are widely spaced; e.g., for ^{238}U, on average, the resonances are some 500 half-widths apart.

In many modern evaluations, the "resonance region" extends to very low energies, well below the energy range in which resonance peaks occur; e.g., in many ENDF/B evaluations, the resonance region extends down to 10^{-5} eV. At low energies, distinguishing between reaction and cross-section conservation can be very important. The low energy limit of Breit-Wigner resonances is not a zero cross section; the capture and fission cross sections become $1/v$ and the elastic constant. Since the capture and fission reaction rate at low energies is constant, the reaction rate is already "smooth," and as such these cross sections are essentially independent of temperature. In contrast, the constant elastic cross section is temperature dependent; this is true of all cross sections, which at zero Kelvin are constant at low energies whether they are defined by a series of resonances or simply in the tabulated form used in many modern evaluations. An initially constant cross section under Doppler broadening will develop a $1/v$ tail

[1]S. GANESAN, *Nucl. Sci. Eng.*, **86**, 118 (1984).

at low energies that smoothly joins the constant cross section at higher energies. The rate of growth of this $1/v$ tail depends on the ratio of target to projectile mass. In the worst case for hydrogen, whose zero Kelvin elastic cross section is constant at 20 b, even at room temperature (293 K), i.e., at thermal energy (0.0253 eV), the Doppler broadening equation predicts a cross section of 30 b (an increase of 50%). This result is in contrast to the prediction of the psi-chi method of cross-section smoothing. The assumption of cross-section smoothing has led many evaluated data users to examine cross sections and, if they are smooth, to assume that they need not be broadened. As pointed out above, this assumption can lead to large errors at low energies.

So far I have only been discussing fission reaction systems. As I pointed out, in these systems the psi-chi method is a practical tool for predicting the behavior of cross sections under Doppler broadening in the higher energy resonance region. There are differences at lower energies that users should be aware of. However, even more important is what happens in fusion systems. It should be pointed out that what applies to fission reactors does not necessarily apply to fusion systems. When we consider fusion ignition temperatures of 2 to 4 keV (for comparison, if 1/40 eV corresponds to 300 K, then 1 keV corresponds to 12 000 000 K), the behavior of cross sections under Doppler broadening is completely different from what one would calculate with the approximations that normally apply to fission systems. Since fusion systems contain predominantly light nuclei, differentiating between reaction and cross-section conservation and smoothing is very important, and the "low energy" effects discussed above extend well up into the kiloelectron-volt region. In fusion systems, Doppler broadening can even change the effective threshold of low-energy threshold reactions.[2] However, many of the people who are currently becoming or are involved in fusion systems were educated in fission systems, and they are propagating fission systems "folklore" into fusion systems, where it just does not apply.

Let me summarize the preceding comments by suggesting to authors who introduce the psi-chi approximation that they add a description of where the approximation applies, i.e., in what I will call the "classical" resonance region for fission systems temperatures. It is also worth pointing out that in many modern evaluations the resonance region can extend well beyond the energy range where there are actual resonance peaks. In addition, if they discuss cross-section smoothing and conservation, they should *explicitly* state that these properties are a consequence of the psi-chi approximation and as such should only be considered to apply where the psi-chi approximation is valid. In order to illustrate deviation from the predictions of the psi-chi approximation, it may be worthwhile to present an illustration from a modern evaluated data library, such as ENDF/B-V (see Ref. 3, which contains plots of all ENDF/B-V evaluations).

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[2]D. E. CULLEN, R. J. HOWERTON, and E. F. PLECHATY, *Nucl. Sci. Eng.*, **74**, 140 (1980).

[3]"Guidebook for the ENDF/B-V Nuclear Data Files," ENDF-328, Brookhaven National Laboratory (1982).

Reference 1 states that "it has been shown that, above a few eV, the Doppler broadening may be approximated by a Gaussian convolution." For a single-level Breit-Wigner resonance, this approximation leads to the usual expression:

$$\sigma_\Delta(E) = \sigma_0 \psi \left(\frac{\Gamma}{\Delta}\ ,\ \frac{E - E_0}{\Gamma/2}\right) , \tag{1}$$

where σ_0 is evaluated at the resonance energy E_0 and where ψ is the "Voigt profile." The invariance of the line area follows:

$$\int \sigma_\Delta(E)\, dE = \sigma_0 \int \psi \left(\frac{\Gamma}{\Delta}\ ,\ \frac{E - E_0}{\Gamma/2}\right) dE = 2\,\frac{\pi}{\Gamma}\,\sigma_0\ . \tag{2}$$

Of course Eq. (2) is not exact: It assumes that Eq. (1) accurately represents the Doppler-broadened line shape and neglects the resonance contribution to the integral from $-\infty$ to $-2E_0/\Gamma$ and the energy dependence of σ_0. (Although for a displacement kernel such as a Gaussian convolution, the energy independence of σ_0 is not required to validate the line area invariance.)

Although not rigorously exact, expression (1) and the line area invariance, Eq. (2), have become part of the folklore of nuclear engineering, as noted by Ganesan.[2] The exact Doppler broadening kernel in a crystalline solid is often not known precisely or is mathematically very unwieldy. Expressions (1) and (2) are good approximations for the temperatures likely to be found in nuclear reactors and are very useful: Line area invariance implies, for example, that the total activation induced in an optically thin target by a beam of neutrons having a constant velocity spectrum is independent of the temperature of the absorber.

Beynon[3] has shown that in general the line area invariance is not exact. This has also been illustrated by Canfield,[4] Cullen,[5] Cullen and Weisbin,[6] and others. These authors discuss in greater detail the approximations required for Eqs. (1) and (2) to hold and show the validity of these approximations for temperatures such as those existing in nuclear reactors.

Extensive reviews of the Doppler effect and of the invariance of the line area may be found in several books (for instance, Ref. 7). It is not clear that such a discussion belongs in a book on nuclear fission.

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[1]A. MICHAUDON, Ed., *Nuclear Fission and Neutron-Induced Fission Cross Sections*, p. 132, Pergamon Press (1981).

[2]S. GANESAN, *Nucl. Sci. Eng*, **86**, 118 (1984).

[3]T. D. BEYNON, *J. Nucl. Energy*, **21**, 681 (1967).

[4]E. CANFIELD, "On the Models for Calculating Effects of Thermal Moderator Motion," UCRL-50323, Lawrence Livermore National Laboratory (1967).

[5]D. E. CULLEN, *Nucl. Sci. Eng.*, **52**, 498 (1973).

[6]D. E. CULLEN and C. R. WEISBIN, *Nucl. Sci. Eng.*, **60**, 199 (1976).

[7]A. FODERARO, *The Elements of Neutron Interaction Theory*, p. 508, MIT Press, Cambridge (1971).

Whereas Ganesan[1] may have a valid point for low-energy Doppler broadening in thermal reactors, his remarks are misleading when applied to Doppler broadening in fast reactors. He implies that his remarks apply to fast as well as thermal reactors by quoting from Ref. 2.

Ganesan's quote comes from a paragraph on Doppler-broadened resonance absorption in fast reactors. The treatment of Doppler broadening presented in the book is the "psi-chi" method, which is the approximate method based on the Breit-Wigner single-level formula for resonance cross sections. The infinitely dilute group absorption cross section for absorber m is a value proportional to the reaction rate per atom of m, $\int_g \sigma_{am}(E)\, dE/E$, divided by $\int_g dE/E$. The contribution to this reaction rate integral from each resonance in the group, when calculated by the psi-chi method, is indeed independent of temperature, as stated in our text. The Cullen-Weisbin[3] paper referenced by Ganesan shows that the psi-chi method represents an excellent approximation for the calculation of Doppler-broadened cross sections for heavy elements like ^{238}U in the energy range of importance in fast reactors and for fuel temperatures involved in fast reactor safety. For resonances in fast reactors, the concept that the integral $\int \sigma_{am}(E)\, dE/E$ is unaffected by Doppler broadening is accurate, rather than erroneous as suggested by Ganesan.

It is emphasized in Ref. 2 that Doppler broadening of absorption resonances in a fast reactor must be combined with self-shielding of the neutron flux in order for there to be any variation of the effective group absorption cross section with temperature. Without self-shielding there would be no Doppler reactivity effect from changes in fuel temperature in a fast reactor.

Reference 2 describes methods applicable to fast reactors. We clearly had no intention of generalizing our remarks on Doppler broadening either to low-energy resonances where, according to Cullen and Weisbin,[3] the "psi-chi" approximation deviates from exact methods for calculating Doppler broadening or to $1/v$ absorbers, which are also treated in detail by those authors.

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[1]S. GANESAN, *Nucl. Sci. Eng.*, **86**, 118 (1984).

[2]A. E. WALTAR and A. B. REYNOLDS, *Fast Breeder Reactors*, Pergamon Press, New York (1981).

[3]D. E. CULLEN and C. R. WEISBIN, *Nucl. Sci. Eng.*, **60**, 199, (1976).

Comment on "Error Due to Nuclear Data Uncertainties in the Prediction of Large Liquid-Metal Fast Breeder Reactor Core Performance Parameters"

In a recent paper by Kamei and Yoshida[1] on the use of mock-up experiments to correct calculated performance parameters of planned power reactors and to estimate the errors in these predicted parameters, the authors state, among other things, that "There are, in principle, two different approaches to utilize the information from the mock-up experiments in the core design calculations. One is the cross-section adjustment method, and the second is the so-called bias-factor method." This, hyperbolically, corresponds to the statement that there are two approaches to treating a bacterial infection: one is to use the right antibiotics, and the other, to take a couple of aspirins. Undeniably, some people *are* allergic to antibiotics, and indeed aspirin *may* bring some (temporary) relief. Still, aspirin is certainly not the treatment of choice for infections.

As the authors of Ref. 1 state, "The (cross-section adjustment) methodology rests on a firm theoretical and mathematical foundation." They may be familiar with the paper on generalized bias operators by Ronen et al.[2] in which this statement is made and which further elaborates on the fact that the adjustment technique requires a great deal of input data, which generally necessitates expensive and time-consuming work to obtain and of which the quality and validity are sometimes still open to question. Thus, only when this information is lacking or is seriously in doubt, may the recourse to the bias-factor method be justified. And yet, in their paper, Kamei and Yoshida derive a prescription for the evaluation of the uncertainties in reactor performance parameters derived by the bias-factor method, a prescription based on the very data only the lack or deficiency of which would have justified the employment of the method in the first place.

The primary purpose of this Letter is to demonstrate how the uncertainties in power reactor performance parameters *should* be evaluated. In other words, we propose to establish the way in which the uncertainties in a given nuclear data ("cross sections") set, the results of any relevant integral experiment (mock-up, benchmark, etc.), and the necessary sensitivity profiles should be properly combined to produce the actual "error" in any performance parameter of a given reactor design and the correlations between the different parameters, i.e., the complete uncertainty matrix of the evaluated performance parameters. We shall also show that the prescription of Ref. 1 is a problematic approximation of the correct expression for the uncertainty matrix of the performance parameters, even in the special case discussed in that paper, the rather unrealistic case of absolutely precise mock-up measurements, the case of integral data of which the associated uncertainty matrix vanishes.

We should, first of all, call attention to the fact that the problem under discussion is mathematically identical to that of extrapolating surveillance dosimetry information to predict radiation damage in power reactor pressure vessels. Traditionally, the bias-factor method was being applied in the latter extrapolation. But more recently, the objective advantages of the adjustment approach have been recognized, so much so that the American Society for Testing and Materials is now considering a new draft standard on the subject.[3] Apparently we could have just quoted the relevant reference,[4] of which the formulas (with the right notation) in fact express the complete and correct solution to extrapolating the mock-up results to the reactor design. However, we feel that the very effort to evaluate the uncertainties in the values of the reactor

[1]T. KAMEI and T. YOSHIDA, *Nucl. Sci. Eng.*, **84**, 83 (1983).

[2]Y. RONEN, D. G. CACUCI, and J. J. WAGSCHAL, *Nucl. Sci. Eng.*, **77**, 426 (1981).

[3]F. B. K. KAM, Private Communication.

[4]J. J. WAGSCHAL, R. E. MAERKER, and Y. YEIVIN, *Trans. Am. Nucl. Soc.*, **34**, 631 (1980).