



Covariance Propagation in Spectral Indices

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The dosimetry community has a history of using spectral indices to support neutron spectrum characterization and cross section validation efforts. An important aspect to this type of analysis is the proper consideration of the contribution of the spectrum uncertainty to the total uncertainty in calculated spectral indices (SIs). This paper identifies deficiencies in the traditional treatment of the SI uncertainty, provides simple bounds to the spectral component in the SI uncertainty estimates, verifies that these estimates are reflected in actual applications, details a methodology that rigorously captures the spectral contribution to the uncertainty in the SI, and provides quantified examples that demonstrate the importance of the proper treatment the spectral contribution to the uncertainty in the SI.

I. INTRODUCTION

In reactor neutron reference benchmark fields, spectrum-averaged cross sections for reactions of interest to the dosimetry community are often given in the form of a spectral index (SI), that is, as a ratio of the spectrum-averaged cross section for the given reaction to that for a “reference” reaction. This quantity is often used because it removes the sensitivity of the metric to the reactor power and to any dependence on an absolute fluence diagnostic. This provides an experimental metric that is sensitive to the spectral shape and has a low measurement uncertainty. The calculated-to-experimental (C/E) double SI ratio is often the quantity used to validate either a neutron spectrum or a cross section determination. In calculating the uncertainty in this double ratio, the uncertainty in the calculated spectral index typically neglects consideration of the uncertainty due to the knowledge of the neutron spectrum. Arguments can be made that this spectral uncertainty cancels out when the sensitivity of the test cross section is similar to that for the “reference” reaction. However, this condition of similar sensitivity can be very dependent upon the spectral shape. The definition of a spectral definition in Ref. [1] states that “it is applicable among detector pairs with distinguishable energy response ranges”, and this is clearly in conflict with the spectral similarity condition and supports the observation that this similarity is violated in the majority of cases where SIs are reported for reactor-based reference neutron fields.

This paper examines the importance of the spectrum uncertainty in reporting uncertainties in the C/E ratios of

SIs for reactions of interest to the dosimetry community. When proper *a priori* uncertainty information is available for the reference neutron field, this paper shows how to rigorously treat the uncertainty propagation in this SI C/E double ratio.

II. SPECTRAL INDICES

A. Definitions

The community uses an integral detector response, typically the measured activity for a reaction with a well-characterized cross section, in support of the validation of dosimetry cross sections and to adjust calculated reactor spectra. The metric used is a specific activity, i.e. the activity per unit mass of a sample. In order to extract a metric that depends primarily upon the neutron spectrum but not the irradiation time or the strength of the source, i.e. the magnitudes of the neutron fluence, experimenters often report a spectrum-averaged cross section normalized to a unit fluence.

The spectrum-averaged cross section (xsec.) is one important metric that the dosimetry community uses to examine the consistency of measured reaction activities in the energy-dependent spectrum in the benchmark neutron fields. The energy-dependence of the neutron spectrum means that there is also an energy-dependence to its uncertainty (unc.) and there may be a correlation in the uncertainty between energy regions. There is typically a larger uncertainty in the low energy portion of the spectrum than in the fast, high energy, portion. This means that it is not always easy to accurately quantify the total neutron fluence in a given sample irradiation. In addition, the strength of the neutron source, for both

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accelerator and reactor-produced neutron sources, can be hard to exactly duplicate between different irradiations or to accurately and succinctly document in a manner that promotes replication of the irradiation conditions. Thus, rather than a spectrum-averaged cross section, the reported dosimetry metric is more often the ratio between the spectrum-averaged cross section for a reaction of interest and a well-known "reference" reaction. This quantity is called a spectral index, SI, and is defined as

$$SI_{\alpha,\beta} = \langle \sigma_{\alpha} \rangle / \langle \sigma_{\beta} \rangle. \quad (1)$$

While experimental measurements are often reported as spectral indices, it is the calculated-to-experimental (C/E) ratio of the SI that is the relevant metric for the validation of either cross sections or spectral representations. These are given as

$$C_{\alpha,\beta} = [SI_{\alpha,\beta}]_{\text{calc}} / [SI_{\alpha,\beta}]_{\text{expt}}. \quad (2)$$

The community routinely reports spectral indices and their associated C/E ratios but it is important that an uncertainty also be reported. The measured uncertainty of the SI is straight forward since it is the simple ratio of the measured activities. Typically the activities in the SI ratio are not correlated and the relative uncertainty can be expressed as the root-mean-square (rms) of the relative uncertainty squared for the activities in the numerator and denominator of the SI. However, when one looks at the $C_{\alpha,\beta}$ ratios, the uncertainty contribution from the calculated spectral index must also be considered. The uncertainty in the calculated spectral index involves the uncertainty due to the underlying neutron spectrum and that due to the cross section for the two reactions. The cross sections for the reactions in the numerator and denominator can generally be considered to be independent and uncorrelated, and hence the uncertainty contributions are added in quadrature. The spectrum appears in both the numerator and denominator of the SI so the treatment of the spectrum uncertainty contribution is much more difficult. As an upper bound for the uncertainty the separate spectrum contributions to the numerator and denominator could be added, corresponding to a negatively correlated uncertainty. This worst-case relative uncertainty is given as

$$\Delta SI_{\text{worst}} = \sqrt{\Delta\sigma_{\alpha}^2 + \Delta\sigma_{\beta}^2} + \Delta\Phi_{\text{num}} + \Delta\Phi_{\text{den}}. \quad (3)$$

Note, this worst case treatment is not an addition of all terms in quadrature since the contributions are not necessarily uncorrelated, but is a sum of contributions in the same manner that a systematic anti-correlated uncertainty is treated, i.e. if the spectrum-averaged cross section in the numerator increases, the spectrum-averaged cross section in the denominator would decrease, magnifying the change in the calculated SI ratio. The best-case treatment is to consider the spectral uncertainties in the numerator and denominator to be positively correlated and largely cancel out. The rationale for neglecting the

spectrum contribution to the uncertainty in the spectral index is based on an approximation that the spectrum uncertainty contribution from the numerator and denominator are correlated and cancel out in the SI ratio. Intuition supports this assumption of a cancelation of the uncertainty in the ratio in so far as the energy-dependent spectral sensitivity for the reaction in the numerator and denominator are the same. The rigorous way to treat the uncertainty in the SI is to use the covariance for the spectrum and to do an accurate nonlinear error propagation for this spectral index. The purpose of this paper is to examine the importance of a rigorous treatment of the uncertainty propagation for SIs measured in various neutron fields and using various dosimetry reactions.

B. Uncertainty Propagation in a Non-linear Expression

The straight forward way to accurately treat the contribution of the spectrum uncertainty in the SI is to use an explicit Monte Carlo approach. Here the variation in the spectrum is sampled by using the spectrum covariance matrix to draw a correlated sample that represents the spectrum variation. The covariance of a spectrum must obey two mathematical constraints. First, the covariance matrix must be positive semi-definite, i.e. it must have no negative eigenvalues. Second, since the energy-integrated spectrum is normalized to the fluence, each row of the covariance matrix must sum to zero, i.e. a positive perturbation in one portion of the spectrum must be offset by a negative perturbation in a different portion of the spectrum. Since the covariance matrix, \mathbf{C} , is a square matrix with \mathbf{N} linearly independent columns, it can be factored as

$$\mathbf{C} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^T, \quad (4)$$

where \mathbf{Q} is the square ($\mathbf{N} \times \mathbf{N}$) matrix whose i^{th} column is the eigenvector, η_i , of the covariance matrix \mathbf{C} and $\mathbf{\Lambda}$ is the diagonal matrix whose diagonal elements are the corresponding eigenvalues, i.e., $\Lambda_{ii} = \lambda_{ii}$.

Since the covariance matrix is an $\mathbf{N} \times \mathbf{N}$ real symmetric matrix, the eigenvectors can be chosen such that they are real and orthogonal. Thus the inverse of \mathbf{Q} can be replaced with the transposed matrix. Since the covariance matrix is Hermitian, i.e. it is self-adjoint or equal to its own conjugate transpose, and it is a positive-definite matrix, it has a Cholesky decomposition, that is, it can be factorized into the product of a lower triangular matrix and its conjugate transpose,

$$\mathbf{C} = \mathbf{L}\mathbf{L}^*, \quad (5)$$

where \mathbf{L} is a lower triangular matrix with real and positive diagonal entries, and \mathbf{L}^* denotes the conjugate transpose of \mathbf{L} . These two decompositions can be related as follows:

$$\mathbf{C} = \mathbf{Q}\mathbf{\Lambda}^{1/2}\mathbf{\Lambda}^{1/2*}\mathbf{Q}^* = \mathbf{Q}\mathbf{\Lambda}^{1/2}(\mathbf{Q}\mathbf{\Lambda}^{1/2})^*. \quad (6)$$

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