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Foundations for Sensitivity-Based Criticality Validation Techniques

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Foundations for Sensitivity-Based Criticality Validation Techniques

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1. Introduction

The current validation techniques for criticality safety computer codes and data require a considerable amount of judgement in order to establish the area of applicability. Key to the establishment of bias values is the use of benchmark systems that are deemed to be similar to the application area. The current procedures for relating similar system parameters (ratio of hydrogen-to-fissile concentration (H/X), poison concentration, enrichment, etc.) are based largely on the practitioner's judgement. A more rigorous and less judgement-based approach is needed for the wide variety of application areas that are seen today.

This work describes the development of sensitivity coefficients as a gauge of system similarity. Sensitivity coefficients are defined physically such that they represent the percentage effect on some response due to a fractional (e.g., typically a 1%) change in an input parameter. For fissionable material systems, one of the appropriate responses is the system k_{eff} value, relative to input parameters of interest (i.e., the nuclear reaction probabilities or cross sections). These sensitivity coefficients are typically presented as "profiles," where the change in k_{eff} due to cross sections is given as a function of the energy of the cross section. These sensitivity profiles can be generated for each material in the system and may include various reaction rates

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(e.g., scatter, absorption, fission) as well as χ and $\bar{\mathbf{n}}$. These profiles give a great deal of information about the particular system, because they provide the effect on k_{eff} for differential changes in all the system cross-section information. However, the amount of information is too large to be of general use. Some type of integral-parameter method for representing these sensitivities would be useful to reduce the amount of information to a few parameters. The sensitivity theory utilized in this work will be given in Section 2. The results of various integral methods for sensitivities will be discussed in Section 3.

2. Sensitivity Theory

The techniques used in this work to generate sensitivity information for the various critical benchmarks are based on the widely used perturbation theory approach.¹⁻⁴ The full derivation of the general procedure will not be given here; however, the specific theory for the generation of k_{eff} sensitivities is given below. For the full derivation of the general sensitivity equations the reader is referred to Ref. 5.

Considering the Boltzmann transport equation written in the form:

$$[A - I B] \mathbf{f} = 0, \quad (1)$$

where A and B are loss and production operators, \mathbf{f} is the neutron flux, and I is $1/k_{eff}$, and a perturbed system

$$[A' - I' B'] \mathbf{f}' = 0, \quad (2)$$

the equation adjoint to Eq. (1) is

$$[A^* - I B^*] \mathbf{f}^* = 0. \quad (3)$$

Eq. (2) is multiplied by \mathbf{f}^* , and integrated over all phase space,

$$\langle \mathbf{f}^* (A' - I' B') \mathbf{f}' \rangle = 0. \quad (4)$$

Defining:

$$\begin{aligned} \mathbf{A}' &= \mathbf{A} + d\mathbf{A} \\ \mathbf{B}' &= \mathbf{B} + d\mathbf{B} \\ \mathbf{I}' &= \mathbf{I} + d\mathbf{I} \end{aligned} \quad (5)$$

and using the property of adjointness for the operators \mathbf{A} , \mathbf{A}^* and \mathbf{B} , \mathbf{B}^* , we find

$$\langle \mathbf{f}^* (d\mathbf{A} - \mathbf{I} d\mathbf{B} - \mathbf{B} d\mathbf{I} - d\mathbf{I} d\mathbf{B}) \mathbf{f} \rangle = 0. \quad (6)$$

Ignoring second-order terms (d^2dB), substituting \mathbf{f}' with \mathbf{f} , and solving for the inverse k_{eff} perturbation;

$$d\mathbf{I} / \mathbf{I} = \langle \mathbf{f}^* (d\mathbf{A} - \mathbf{I} d\mathbf{B}) \mathbf{f} \rangle / \langle \mathbf{f}^* (\mathbf{I} \mathbf{B}) \mathbf{f} \rangle. \quad (7)$$

Hence, the sensitivity of λ , with respect to the reaction x cross section, Σ_x , becomes

$$\frac{d\mathbf{I} / \mathbf{I}}{d\Sigma_x / \Sigma_x} = \frac{\Sigma_x \langle \mathbf{f}^* (d\mathbf{A}/d\Sigma_x - \mathbf{I} d\mathbf{B}/d\Sigma_x) \mathbf{f} \rangle}{\langle \mathbf{f}^* (\mathbf{I} \mathbf{B}) \mathbf{f} \rangle}. \quad (8)$$

Note that since $\lambda = 1/k_{eff}$, then $d\lambda/\lambda = -dk_{eff}/k_{eff}$ such that the above equation is essentially the defining equation for the k_{eff} sensitivity, S_x , where

$$S_x = \frac{dk_{eff} / k_{eff}}{d\Sigma_x / \Sigma_x} = \frac{-d\mathbf{I} / \mathbf{I}}{d\Sigma_x / \Sigma_x}. \quad (9)$$

In practice, the $d\mathbf{A}$ and $d\mathbf{B}$ terms in Eq. (8) are simple functions of the scattering, capture, and fission cross sections represented symbolically as S_x . The evaluation of Eq. (8) then becomes an integration of the forward and adjoint fluxes and the cross sections over the entire phase space.

Typically, the energy dependence of the cross sections is represented by averaging the S_x quantities over an energy group i , represented as Σ_{x_i} . Insertion of these group quantities into Eq. (8) yields the

definition of a sensitivity $S_{x_i} = \frac{dk_{eff} / k_{eff}}{d\Sigma_{x_i} / \Sigma_{x_i}}$, where i is varied to obtain the sensitivity for all groups,

which span the energy range of interest.

3. SENSITIVITY-BASED INTEGRAL PARAMETERS

The development of a number of different sensitivity-based integral parameters has been studied in this work. The objective was to produce a single parameter that would quantify the similarities between two systems, such that this single parameter could be used for determination of applicability and as a trending parameter.

Initially, parameters (D values) using the absolute value of the sensitivity differences by group were developed. These AD@ values are defined as:

$$\begin{aligned}
 D_n &= \sum_{j=1}^N \sum_{i=1}^g |S_{naij} - S_{neij}| \\
 D_c &= \sum_{j=1}^N \sum_{i=1}^g |S_{caij} - S_{ceij}| \\
 D_s &= \sum_{j=1}^N \sum_{i=1}^g |S_{saij} - S_{seij}| \quad \text{and} \\
 D_{\text{sum}} &= D_n + D_c + D_s,
 \end{aligned} \tag{10}$$

where S is the sensitivity of k_{eff} for the safety application, a, or experimental configuration, e, to the capture and scattering cross sections, or to ν (c, s, or n, respectively) for group i and nuclide j.

These parameters proved to be useful in that they showed clear patterns when used in traditional trending analyses for criticality safety validation purposes. However, these parameters were unnormalized and exhibited somewhat confusing limiting values. Therefore, an alternate form of sensitivity-based integral parameters was developed. These parameters (denoted E values) correspond to the summation of the product of the sensitivity coefficients for two systems over energy groups and nuclides, normalized such that an E value of 0 indicates the systems are totally dissimilar, and an E value of 1 indicates the two systems are precisely the same. The E values are defined as:

$$\begin{aligned}
E_f &= M^{-1} \sum_{j=1}^N \sum_{i=1}^g S_{faij} S_{feij} \\
E_s &= M^{-1} \sum_{j=1}^N \sum_{i=1}^g S_{saij} S_{seij}, \text{ where} \\
E_c &= M^{-1} \sum_{j=1}^N \sum_{i=1}^g S_{caij} S_{ceij} \\
M &= \sum_x \left\{ \sum_{j=1}^N \sum_{i=1}^g (S_{xaij})^2 \sum_{j=1}^N \sum_{i=1}^g (S_{xeij})^2 \right\}^{1/2}, \text{ and } x \text{ is } f, c, \text{ or } s \text{ (note the use of fission reaction,}
\end{aligned}
\tag{11}$$

f, as opposed to \bar{n} in eq. 10).

$$E_{\text{sum}} = E_f + E_c + E_s.$$

These D and E parameters are considered “global” in nature, in that they are a single quantity that identifies “similarity” between two systems based only on the magnitude and shape of the sensitivity profiles for fission, capture and scatter components. It is also possible and sometimes desirable to produce similar values for each isotope/reaction pair, such that similar information can be computed on a more differential level. For this purpose, an additional parameter dE is defined from the equations above by omitting the nuclide summation in the numerator and the reaction summation in the denominator terms. The dE values then relate on a system-to-system basis the similarity of various isotopic/reaction pairs. These values sum to unity for a given reaction-type (i.e., capture, fission, scatter) and thus allow for similarity determinations for that reaction among various isotopes.

These dE values provide insight into the physics of the system, since their magnitudes show the relative importances of each nuclide with respect to capture, fission, or scattering reactions. In addition, since the sum over a given reaction will only be unity if the two systems are exactly the same, the sum over

the dE values for each reaction gives an additional indicator of the systems' similarity. A method of utilizing this information in a simple manner was to define a T value which is the ratio of the dE value relating the two systems, to the dE value of the application system to itself. This T quantity has a value less than unity if the nuclide/reaction pair is less important in the benchmark than the application. T is greater than or equal to unity if the importance of the nuclide/reaction pair in the benchmark is equal to or greater than the importance in the application. Thus, the number of benchmark systems with T values near or greater than unity is a good indicator of benchmark coverage for a given isotope/reaction pair. Interestingly, this test is appropriate even if the material is not an important material in the application.

Thus, the recommended procedure for ensuring the applicability of the benchmark dataset in criticality safety validation problems is as follows:

1. Process sensitivity coefficients for all benchmark and application systems,
2. Quantify values of E , dE , and T relating each application to the entire benchmark set,
3. Count the number of systems with E values greater than 0.8 (approximately 15-20 systems are needed for validation),
4. For important isotope/reaction pairs, count number of systems with T values greater than 0.95 (approximately 5-10 systems are needed).

The number of systems and the acceptance criterion for T and dE values are not rigorously defined. These values are based on experience with other parameters⁶ and may change over time with additional experience with these parameters.

4. References

1. E. M. OBLOW, "Sensitivity Theory from a Differential Viewpoint," *Nucl. Sci. Eng.* **59**, 187 (1976).
2. W. M. STACEY, JR., "Variational Estimates and Generalized Perturbation Theory for the Ratios of Linear and Bilinear Functionals," *J. Math. Phys.*, **13**, 1119 (1972); see also W. M. Stacey, Jr., "Variational Estimates of Reactivity Worths and Reaction Rate Ratios in Critical Nuclear Reactors," *Nucl. Sci. Eng.* **48**, 444 (1972).
3. L. N. USACHEV, "Perturbation Theory for the Breeding Ratio and for Other Number Ratios Pertaining to Various Reactor Processes," *J. Nucl. Energy Pts. A/B*, **18**, 571 (1964).
4. A. GANDINI, "A Generalized Perturbation Method for Bilinear Functionals of the Real and Adjoint Neutron Fluxes," *J. Nucl. Energy* **21**, 755 (1967).
5. C. R. WEISBIN, J. H. MARABLE, J. L. LUCIUS, E. M. OBLOW, F. R. MYNATT, R. W. PEELLE, and F. G. PEREY, *Application of FORSS Sensitivity and Uncertainty Methodology to Fast Reactor Benchmark Analysis*, ORNL/TM-5563, Union Carbide Corp., Oak Ridge National Lab., December 1976.
6. B. L. BROADHEAD, C. M. HOPPER, R. L. CHILDS, and C. V. PARKS, *Sensitivity and Uncertainty Analyses Applied to Criticality Safety Validation*, NUREG/CR-6655, Vols. 1 and 2 (ORNL/TM-13692/V1 and V2), U.S. Nuclear Regulatory Commission, Oak Ridge National Laboratory, November 1999.