NUCLEAR SCIENCE AND ENGINEERING: **157**, 117–118 (2007)

Letter to the Editor

Comments on "Evaluation and Propagation of the ^{239}Pu Fission Cross-Section Uncertainties Using a Monte Carlo Technique"

Adjustment, the term universally adopted to mean the use of integral response data for improving (i.e., adjusting) differential parameter data in reactor physics,[1,2] has already been known for over 40 yr. This methodology has since been applied in diverse areas[3–5] and most recently in criticality safety.[6,7] The crux of adjustment is that the combination of additional information, i.e., integral responses and the available parameter data, always reduces the uncertainties in the integral responses and in the differential data. These uncertainties are expressed in terms of variance-covariance matrices, and since such matrices, by definition, are positive definite and the posterior uncertainties are given as the original uncertainties minus another positive definite matrix, the uncertainties indeed always decrease.[8] Using the adjusted parameters in a new response calculation, for which there is no measured value, will thus result in a response uncertainty that is smaller than the uncertainty reflecting the propagation of the uncertainties in the original parameters (as long as there is at least a partial overlap of the sensitivities of the respectively corresponding responses to the parameters!). This indeed was the idea that motivated the development of the TSURFER module[9] of the SCALE 5.1 system[10] for criticality safety applications.

In a recent paper[11] Kawano et al. (using a Monte Carlo technique) have numerically demonstrated that the above methodology, proven in the various papers cited and in many others, indeed reduces uncertainties. This numerical demonstration necessitated the diagonalization of the parameter covariance matrix, since the a priori covariance matrix of the parameters (cross sections) in general, due to possible correlations, is not diagonal. The covariance matrix is definitely not diagonal if it already involves information from integral responses, i.e., adjusted cross sections. The covariance matrix had to be diagonalized in order to facilitate its straightforward use for sampling. Kawano et al. diagonalized the a priori uncertainty matrix **X** of the ^{239}Pu fission cross sections (also known as prior), sampled each of its eigenvalues from the corresponding Gaussian distribution, and used the inverse transformation to generate sampled sets of the ^{239}Pu fission cross sections. For each sampled parameter set, they now calculated the corresponding k_{eff} of Jezebel, the well-known bare plutonium sphere, and thus obtained the distribution of these k_{eff} values. Using a standard transport code to calculate the k_{eff} values, they indeed demonstrated their claim that, given the covariance matrix associated with the ^{239}Pu fission cross sections, one does not need the sensitivities of Jezebel's k_{eff} to each of the ^{239}Pu fission cross sections in order to estimate the uncertainty in this integral response. This seems to be the main, in fact the only, achievement in Ref. 11. However, these transport calculations were repeated with only 30 sets of sampled ^{239}Pu fission cross-section sets, and it was difficult to obtain a credible estimate of the uncertainty in k_{eff} from the demonstrated distribution. On the other hand, the distribution was also obtained using the sensitivities, **C**, and the linear approximation of k_{eff}'s dependence on the ^{239}Pu fission cross section with 1000 sets of sampled cross sections. Then, Kawano et al. used the conventional cross-section adjustment methodology, with only one integral response, the k_{eff} of Jezebel, to obtain the covariance matrix of the adjusted ^{239}Pu fission cross-section **P** (also known as posterior). Kawano et al. repeated the diagonalization and sampling procedure, this time with **P**, and to no surprise the new k_{eff} distribution is narrower and the k_{eff} uncertainty is only 0.2%, the same as in the Jezebel input used for the adjustment of the ^{239}Pu fission cross sections.

Kawano et al. state that the procedure they used to calculate **P** is the same as the cross-section adjustment technique and continue to state: "On the contrary our procedure does not change the cross section because we know that k_{eff} calculated with the prior set is 1.0 and the change only appears in the covariance." Let us rewrite Eqs. (3) and (4) of Ref. 11, although Kawano et al. use a not-transparent notation:

$$x_1 = x_0 + \mathbf{X}\mathbf{C}^t(\mathbf{C}\mathbf{X}\mathbf{C}^t + \mathbf{V})^{-1}(y - f(x_0)) \qquad (3)$$

and

$$\mathbf{P} = \mathbf{X} - \mathbf{X}\mathbf{C}^t(\mathbf{C}\mathbf{X}\mathbf{C}^t + \mathbf{V})^{-1}\mathbf{C}\mathbf{X} \ , \qquad (4)$$

where y denotes the measured value of the response, $f(x_0)$ its calculated value with the parameter set x_0, **V** the measured response covariance matrix, in the Kawano et al. example the single response variance, and the superscript t denotes a transposed matrix. Equation (3) manifests that if, usually by chance or if somebody "tuned" the parameters, y is equal to $f(x_0)$, then the parameters stay unperturbed. However, Eq. (4) makes it very clear that the additional information incorporated in the uncertainty matrices reduces the uncertainties of the parameters even in this case. As long as the uncertainty in the integral response, **V**, is not infinite, then the uncertainty of the adjusted parameters is reduced. Let us note in passing that there is no need and it is not elegant to obtain the sensitivities by brute force, i.e., "by calculating derivatives numerically" perturbing the group cross sections by 1% and recalculating k_{eff}.

Kawano et al. state in the introduction to their recent publication[11]: "The adjusted cross-section library with their covariance makes it possible to predict the uncertainty in the transport calculations if the computation of the sensitivity is feasible. In general, however, calculation of the error propagation is difficult to perform since many application codes, such

as neutron-transport Monte Carlo simulation codes require tremendous computing capabilities." It seems that this was the rationale for their recent publication. The main point in their paper is to demonstrate that it is possible to propagate, in practice, the parameter uncertainties to the predicted response uncertainty without calculating the sensitivity of the response to the parameters. But even in their simple example of a single response, Jezebel, and only the 30 group ^{239}Pu fission cross section, rather than all ^{239}Pu partial cross sections and the cross sections of gallium and the other plutonium isotopes, they relied on the linearity and performed only a very limited number of full transport calculations with the sampled ^{239}Pu cross sections. Needless to say once they repeated the calculation taking into account the results of the integral response, i.e., using **P** rather than **X**, the use of sensitivities was unavoidable.

If one really wants to reduce the parameter uncertainties, and in turn the predicted uncertainty of any future application, it is advisable to use many integral responses, rather than a single one, in order to obtain the new reduced uncertainty parameter covariance matrix **P**. This in turn necessitates calculating the sensitivities of all participating responses. We recently compared the reduced uncertainty in k_{eff} of Jezebel using various adjustments performed utilizing 15 bare and reflected metallic plutonium spheres. The original uncertainty in the calculated value of Jezebel's k_{eff}, due to all cross sections involved in the calculation, was 2.54%. Using all 15 assemblies for the adjustment, the uncertainty in k_{eff} of Jezebel dropped to a mere 0.1% and using only Jezebel itself as a sole integral response, it dropped only to the experimental 0.2%. On the other hand, using 14 integral responses for the adjustment and leaving Jezebel only as an application resulted in a reduction of the uncertainty in k_{eff} of Jezebel to 0.12%.

The TSURFER module of the SCALE system uses the information of an ever-growing number of integral responses in order to predict the lowest possible uncertainty in k_{eff} of a proposed application. The sensitivities of the application can be calculated in SCALE with either one- or three-dimensional forward and adjoint fluxes, and running times are very reasonable.

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September 7, 2006

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