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R. E. Maerker

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CONCEPTS INVOLVED IN A PROPOSED APPLICATION OF UNCERTAINTY ANALYSIS TO THE PERFORMANCE ASSESSMENT OF HIGH-LEVEL NUCLEAR WASTE ISOLATION SYSTEMS

R. E. Maerker

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ABSTRACT

This report introduces the concepts of a previously developed methodology which could readily be extended to the field of performance assessment for high-level nuclear waste isolation systems. The methodology incorporates sensitivities previously obtained with the GRESS code into an uncertainty analysis, from which propagated uncertainties in calculated responses may be derived from basic data uncertainties. Following a definition of terms, examples are provided illustrating commonly used conventions for describing the concepts of covariance and sensitivity. Examples of solutions to problems previously encountered in related fields involving uncertainty analysis and use of a generalized linear least-squares adjustment procedure are also presented.

1. NEED FOR UNCERTAINTY ESTIMATES

In the numerical solution to a complex problem such as the performance assessment of a nuclear waste isolation system, large amounts of data are usually input into the calculational scheme. It should be recognized that each datum has an uncertainty associated with it, either because the precision of measurements is limited, or because specific values for many physical properties of the system must be assumed which may only represent average conditions. Further uncertainties arise because the methods used in the calculations themselves have deficiencies or involve approximations. Consequently, the calculated result has an uncertainty that is compounded from the individual estimated uncertainties that have been propagated through the calculation from each uncertainty source.

Since there are essentially no measurements available at the present time to validate the results of complex calculated solutions to high-level nuclear waste isolation problems because of the long time intervals involved, it is of paramount importance to be able to estimate with reasonable accuracy the resulting uncertainty in the calculated values. The following sections describe a methodology that leads to the realization of this goal. Moreover, it is equally important to be able to take into account in the analysis of the system uncertainties any additional knowledge or measurements of data which may not be explicitly used in the calculational scheme but are related to some physical properties of the system. Section 6 describes how, as improved knowledge of the data becomes available, the uncertainties in the calculated values can be reduced by means of a generalized linear least-squares adjustment procedure which combines the improved knowledge of the data with the measured or assumed values used in the calculation.

2. CONCEPT AND REPRESENTATIONS OF A SIMPLE COVARIANCE

The term "covariance" is a more general definition of uncertainty than the terms "variance" or "standard deviation" because it considers not only a measure of the precision to which a quantity is perceived to be known but also how this precision is correlated with that of another quantity. One speaks of the covariance between two quantities, and there are in general as many different covariances between a given quantity (whether it be a parameter or a response) and other quantities (be they parameters or responses) as there are numbers of quantities involved. Covariances are normally expressed in terms of fractional (FSD) or percent (PSD) standard deviations and correlation coefficients. For example, if we denote two different quantities by the symbols q_1 and q_2, then

$$C_{q_1q_2} \equiv \sigma_1\sigma_2\alpha_{1,2} \quad , \tag{1}$$

where $C_{q_1q_2}$ represents the covariance between the quantities q_1 and q_2, σ_1 and σ_2 are their corresponding standard deviations, and $\alpha_{1,2}$ is the correlation coefficient.

If the quantities q_1, q_2, ...q_i, ... are represented as elements of a column vector $\bar{q} \equiv (q_i)$, then the matrix that represents their covariances and which consists of elements defined by Eq. (1) may be described by the following notation:

$$C_{qq} = \left\langle \left(\frac{\delta\bar{q}}{\bar{q}}\right)\left(\frac{\delta\bar{q}}{\bar{q}}\right)^T \right\rangle, \tag{2}$$

where the first deviation in the brackets represents a column vector and the second one its transpose - i.e., a row vector. The brackets in Eq. (2)

are used to designate an expectation value, i.e., an average over a probability distribution of possible deviations δ from the mean.

Following the usual rules of matrix multiplication, the elements of C_{qq} can be readily shown to be

$$C_{q_i q_j} = \left\langle \left(\frac{\delta q_i}{q_i}\right) \left(\frac{\delta q_j}{q_j}\right) \right\rangle = \sigma_i \sigma_j \alpha_{ij} \quad . \tag{3}$$

The covariance matrix expressed by Eq. (2) is symmetric and consists of "autocovariances" since the same quantities $\bar{q}$ appear in both factors in Eq. (2). The corresponding autocorrelation matrix is represented as a triangular matrix of correlation coefficients with ones along the diagonal, together with standard deviations for each row. For example, if there are four quantities that make up the vector $\bar{q}$, the autocorrelation matrix is shown in Table 1, where the covariances can be constructed from Eq. (3).

Table 1. Representation of an Autocorrelation Matrix

	Percent Standard Deviation	q_1	q_2	q_3	q_4
q_1	σ_1	1.0			
q_2	σ_2	$\alpha_{2,1}$	1.0		
q_3	σ_3	$\alpha_{3,1}$	$\alpha_{3,2}$	1.0	
q_4	σ_4	$\alpha_{4,1}$	$\alpha_{4,2}$	$\alpha_{4,3}$	1.0

If the covariances of the quantities $\bar{q}$ with other quantities $\bar{v}$ are desired, then

$$C_{qv} = \left\langle \left(\frac{\delta\bar{q}}{\bar{q}}\right) \left(\frac{\delta\bar{v}}{\bar{v}}\right)^T \right\rangle \quad , \tag{4}$$

and the corresponding rectangular correlation matrix is now in general asymmetrical with no diagonal since the quantities $\bar{q}$ and $\bar{v}$ may be dimensioned differently. The resulting matrix now involves cross-covariances or cross-correlations between the quantities $\bar{q}$ and $\bar{v}$. If $\bar{q}$ once again represents four quantities and $\bar{v}$ three other quantities, then the resulting cross-correlation matrix may be represented as shown in Table 2.

Table 2. Representation of a Cross-Correlation Matrix

	v_1	v_2	v_3
q_1	$\alpha_{1,1}$	$\alpha_{1,2}$	$\alpha_{1,3}$
q_2	$\alpha_{2,1}$	$\alpha_{2,2}$	$\alpha_{2,3}$
q_3	$\alpha_{3,1}$	$\alpha_{3,2}$	$\alpha_{3,3}$
q_4	$\alpha_{4,1}$	$\alpha_{4,2}$	$\alpha_{4,3}$

Notice that the standard deviations are suppressed. Thus, if Table 2 represented the sum total of our knowledge of the uncertainties between $\bar{q}$ and $\bar{v}$, then the cross-covariances could not be determined. We should recognize, however, that the matrix in Table 2 represents an off-diagonal submatrix of a larger symmetric complete correlation matrix involving the quantities $\bar{q}$ and $\bar{v}$ which also contains as diagonal submatrix components the autocorrelations between the components of $\bar{q}$ shown in Table 1 and similar autocorrelations among the components of $\bar{v}$. This is illustrated in Table 3, where only the lower triangle is given. Notice that the three components of $\bar{v}$ have correlation coefficients designated with subscripts 5, 6, and 7 to distinguish them from those of $\bar{q}$.

Table 3. Complete Correlation Matrix Between the Quantities $\bar{q}$ and $\bar{v}$

		q_1	q_2	q_3	q_4	v_1	v_2	v_3
q_1	σ_{q1}	1.0						
q_2	σ_{q2}	$\alpha_{2,1}$	1.0	AUTO				
q_3	σ_{q3}	$\alpha_{3,1}$	$\alpha_{3,2}$	1.0				
q_4	σ_{q4}	$\alpha_{4,1}$	$\alpha_{4,2}$	$\alpha_{4,3}$	1.0			
v_1	σ_{v1}	$\alpha_{5,1}$	$\alpha_{5,2}$	$\alpha_{5,3}$	$\alpha_{5,4}$	1.0		
v_2	σ_{v2}	$\alpha_{6,1}$	$\alpha_{6,2}$ CROSS	$\alpha_{6,3}$	$\alpha_{6,4}$	$\alpha_{6,5}$	1.0	AUTO
v_3	σ_{v3}	$\alpha_{7,1}$	$\alpha_{7,2}$	$\alpha_{7,3}$	$\alpha_{7,4}$	$\alpha_{7,5}$	$\alpha_{7,6}$	1.0

The cross-covariance between q_3 and v_2 is

$$(C_{qv})_{3,2} = \sigma_{q3}\,\sigma_{v2}\,\alpha_{6,3} \quad , \tag{5}$$

while that between q_2 and v_3 is

$$(C_{qv})_{2,3} = \sigma_{q2}\,\sigma_{v3}\,\alpha_{7,2} \quad , \tag{6}$$

and they are not necessarily the same.

3. PRINCIPLES IN ESTIMATING PARAMETER COVARIANCES

By "parameters" are meant basic data, often differential in some sense, that are used in a calculation of an integral response. For application to nuclear waste isolation problems, these parameters can be broadly divided into three categories - measured data, assumed data, and bias factors arising from use of approximations in the methods employed in the calculations. The first two, in fact, represent data to which GRESS sensitivities may be readily calculated.[1] Examples of the first category include half-lives of radioactive isotopes and the energy distribution of the particles from decay of various nuclides; examples of the second include assumed hydraulic and heat transfer properties of soils and concrete, pressure differentials giving rise to slurry transport, and physical dimensions. The third category is more difficult to analyze. A bias factor may be defined to be a multiplicative correction factor that is to be applied to a calculated result that takes into account known deficiencies in the calculational method. An example of this category is the point-depletion assumption used in the ORIGEN2 code[2] to simulate nuclear fuel cycles and/or spent fuel characteristics. Although values of bias factors are often assumed to be unity, their covariances reflect uncertainties in these values and are generally non-negligible.

There are no recipes for obtaining parameter covariances. The standard deviations are simply educated guesses of how well the value of the quantity is perceived to be known in the case of measured data or how much the value is allowed to vary in the case of assumed data. For methods bias factors, a study sometimes has to be made using more rigorous methods of calculation that can quantify the approximations made in employing a given assumption.

Parameter correlations depend on the manner in which they were measured in the case of measured data or on relationships that may need to be satisfied between assumed values in the case of assumed data. In the first case, if a quantity is measured indirectly as a ratio to another better known quantity, then, even though in nature these two quantities are completely independent, from the method used in their measurement there is a strong correlation between them which must be reflected in their covariances. Similarly, in the case of assumed data, it may be necessary to satisfy a boundary or some other condition on two parameters simultaneously, thus correlating them.

Correlation coefficients vary between the limits -1 (complete anti-correlation) through 0 (no correlation) to +1 (complete correlation). If there is reason to suspect a positive correlation between two parameters but the magnitude of the correlation is relatively unknown, then coefficients of 0.5 may be assumed. Similarly appropriate negative coefficients of -0.5 may be assumed for suspected but difficult to assess negative correlations.

4. COVARIANCE PROPAGATION WITH SENSITIVITIES

It is, of course, fundamental to the entire development of the uncertainty concept that one be able to determine the uncertainty in a calculated response that arises as the result of an uncertainty in some parameter that is used in its calculation. This idea of covariance propagation requires knowledge of how the response changes as a result of a change in the parameter - i.e., of a sensitivity.

If sensitivity is defined as the fractional change of a response per fractional change in a parameter (often expressed as a dimensionless ratio of such units as percent per percent, etc.), then the perturbed value of the response $\bar{r}$ is related to the perturbed value of the parameter $\bar{p}$ as

$$\bar{r}(\bar{p}+\delta\bar{p}) = \bar{r}(\bar{p}) + \delta\bar{r} \simeq \bar{r}(\bar{p}) + S_r\frac{\bar{r}}{\bar{p}}\delta\bar{p} \quad , \tag{7}$$

where

$$S_r = \partial\bar{r}/\bar{r}/\partial\bar{p}/\bar{p} = \frac{\bar{p}}{\bar{r}}\,[\partial\bar{r}/\partial\bar{p}] \quad . \tag{8}$$

In Eq. (7) the right-hand side represents a linear expansion about the unperturbed value.

If the response column vector has dimensions I x 1 and the parameter column vector N x 1, where I and N are the number of responses and parameters respectively, then the sensitivity matrix S_r as defined by Eq. (8) has dimensions I x N.

The covariance matrix for $\bar{r}$ becomes, using Eqs. (7) and (8),

$$C_{\bar{r}\bar{r}} \equiv \left\langle \left(\frac{\delta\bar{r}}{\bar{r}}\right) \left(\frac{\delta\bar{r}}{\bar{r}}\right)^T \right\rangle = \left\langle \left[S_r\left(\frac{\delta\bar{p}}{\bar{p}}\right)\right]\left[S_r\left(\frac{\delta\bar{p}}{\bar{p}}\right)\right]^T \right\rangle$$

$$= S_r \left\langle \left(\frac{\delta\bar{p}}{\bar{p}}\right) \left(\frac{\delta\bar{p}}{\bar{p}}\right)^T \right\rangle S_r^T = S_r C_{pp} S_r^T \quad , \tag{9}^*$$

*Recall that $(AB)^T \equiv B^T A^T$, where A and B are matrices.

where S_r^T is the transpose of the sensitivity matrix and is of dimensions N x I. As in all cases involving matrix multiplication, the dimensions of each side of Eq. (9) must agree. The dimensions of $C_{\bar{r}\bar{r}}$ are I x I, and they must be the same as those of $S_r C_{pp} S_r^T$, which are (I x N) x (N x N) x (N x I). Recognizing that a matrix of dimensions I x N may be written as the product of two other matrices of dimensions I x 1 and 1 x N, then the dimensions of the matrix obtained by forming $S_r C_{pp} S_r^T$ become [(I x 1) x (1 x N)] x [(N x 1) x (1 x N)] x [(N x 1) x (1 x I)]. Regrouping and further recognizing that the result of multiplying 1 x N and N x 1 matrices together has dimensions of 1 x 1, i.e., is a scalar, one obtains dimensions of (I x 1) x (1 x 1) x (1 x 1) x (1 x I) = (I x 1) x (1 x I), which reduces to I x I, in agreement with those of the left-hand side of Eq. (9).

To summarize, the covariances of each parameter used in a calculation are propagated to those of a calculated result by the use of sensitivities:

$$C_{\bar{r}\bar{r}} = S_r C_{pp} S_r^T \quad . \tag{9}$$

If sensitivities to the parameters are large, then the first-order expansion indicated by Eq. (7) becomes inaccurate and higher order terms should be considered. For the present application, it will be assumed that first-order theory is sufficiently accurate and that these sensitivities, whether they be obtained from GRESS or by adjoint methods, will provide adequate estimates of the response covariances.

5. EXAMPLES OF PARAMETER AND RESPONSE COVARIANCES

Several examples of parameter and response covariances, although completely unrelated to quantities of interest in nuclear waste disposal, will be given in order to illustrate the concepts introduced in the earlier sections.

The first example of a parameter covariance is that of the total inelastic iron cross section derived from data appearing in a recent nuclear data evaluation.[3] A portion of the correlation matrix is shown in Table 4.

Table 4. Correlation Matrix of the Total Inelastic Iron Cross Section in the 3- to 11-MeV Range*

Energy Range (MeV)	PSD (%)	Group	Group 1	Group 2	Group 3	Group 4
8.19 to 11.05	5.83	1	1.00			
6.07 to 8.19	5.37	2	0.18	1.00		
4.07 to 6.07	5.47	3	0.13	1.00	1.00	
3.01 to 4.07	5.58	4	0.16	1.00	1.00	1.00

*Matrix is symmetric; only the lower half is shown.

Several interesting features about this matrix are that there is an assumed perfect correlation in this cross section in the energy range 3 to 8 MeV, that the cross sections above 8 MeV are poorly correlated with those below 8 MeV, and that all the correlations are positive. The value of the relative covariance of this cross section between the energy limits associated with groups 1 and 4 is

$$(C_{qq})_{1,4} = (5.83\%)(5.58\%)(0.16) = 5.21\%^2 = 5.21 \times 10^{-4} \quad . \tag{10}$$

The sensitivities of the group fluxes in the same group structure as defined in Table 4 to the total inelastic iron cross section calculated by the adjoint method for a detector located behind about 28 cm of stainless steel and 11 cm of water is shown in Table 5. It is to be observed that the sensitivities are negative (i.e., an increase in the cross section results in a decrease in the flux) and that there are zeros in the upper half of the matrix (i.e., the group fluxes are not influenced by the cross-section behavior at energies lying below them).

Table 5. Group Flux Sensitivities to the Total Inelastic Iron Cross Section in the 3- to 11-MeV Range

Energy Range (MeV)	Flux Group, g	Cross Section Group, g´			
		1	2	3	4
8.19 to 11.05	1	-2.70	0	0	0
6.07 to 8.19	2	-0.16	-2.79	0	0
4.07 to 6.07	3	-0.07	-0.28	-2.68	0
3.01 to 4.07	4	-0.05	-0.20	-0.53	-1.90

By applying Eq. (9) and performing the matrix multiplication to the matrices appearing in Tables 4 and 5, the resulting correlation matrix for the fluxes in the first four groups may easily be obtained and is shown in Table 6. Notice that the perfect correlation present in the cross section in the range 3 to 8 MeV is propagated directly to the response. Notice also that the standard deviations of the fluxes have been increased by factors of about three over the corresponding values of the

Table 6. Correlation Matrix of the Group Fluxes in the 3- to 11-MeV Range Due to Uncertainties in the Total Inelastic Iron Cross Section*

Energy Range (MeV)	PSD (%)	Group	Group 1	2	3	4
8.19 to 11.05	15.8	1	1.00			
6.07 to 8.19	15.2	2	0.24	1.00		
4.07 to 6.07	16.2	3	0.16	1.00	1.00	
3.01 to 4.07	14.6	4	0.18	1.00	1.00	1.00

*Matrix is symmetric; only the lower half is shown.

cross sections. This is primarily due to the high sensitivities appearing along the diagonal in Table 5.

It is of interest to observe the changes in Table 6 which would occur if the correlation matrix in Table 4 were diagonal (i.e., if all correlations between group cross sections were zero). The results of this calculation are shown in Table 7.

Table 7. Correlation Matrix of the Group Fluxes in the 3- to 11-MeV Range Due to Uncorrelated Uncertainties in the Total Inelastic Iron Cross Section*

Energy Range (MeV)	PSD (%)	Group	Group 1	2	3	4
8.19 to 11.05	15.8	1	1.00			
6.07 to 8.19	15.0	2	0.06	1.00		
4.07 to 6.07	14.7	3	0.03	0.10	1.00	
3.01 to 4.07	11.0	4	0.03	0.10	0.27	1.00

*Matrix is symmetric; only the lower half is shown.

It can be seen that the group 1 flux is unaffected, but that the remaining flux groups have somewhat reduced uncertainties and greatly reduced correlations. Thus, the effect of introducing positive correlations among the cross sections is to increase both the variances and the correlations of the resulting calculated responses. Negative correlations would have a decreasing effect on the variances and algebraically decrease the correlations.

A second example involves two dosimeter cross sections, the $^{63}Cu(n,\alpha)^{60}Co$ reaction and the $^{46}Ti(n,p)^{46}Sc$ reaction. These cross-section covariances were taken from a modification of the ENDF/B-V nuclear data file.[4] The estimated auto-correlation matrix for the ^{63}Cu reaction is shown in Table 8 and that for the ^{46}Ti reaction is shown in Table 9. These two cross sections represent an example of cross-correlated parameters. Their cross-correlation matrix is shown in Table 10.

Table 8. Correlation Matrix of the $^{63}Cu(n,\alpha)^{60}Co$ Cross Section*

Energy Range (MeV)	PSD (%)	Group	Group 1	2	3	4	5	6	7
11.05 to 19.64	5.9	1	1.00						
8.19 to 11.05	3.1	2	0.29	1.00					
6.07 to 8.19	3.1	3	0.21	0.79	1.00				
4.07 to 6.07	3.4	4	0.17	0.60	0.56	1.00			
3.01 to 4.07	8.6	5	0.06	0.23	0.25	0.28	1.00		
2.59 to 3.01	16.1	6	0.03	0.12	0.13	0.14	0.43	1.00	
2.12 to 2.59	8.4	7	0.03	0.11	0.11	0.13	0.40	1.00	1.00

*Matrix is symmetric; only the lower half is shown.

Table 9. Correlation Matrix of the $^{46}Ti(n,p)^{46}Sc$ Cross Section*

Energy Range (MeV)	PSD (%)	Group	Group 1	2	3	4	5	6	7
11.05 to 19.64	8.7	1	1.00						
8.19 to 11.05	4.1	2	0.31	1.00					
6.07 to 8.19	3.8	3	0.24	0.55	1.00				
4.07 to 6.07	3.2	4	0.25	0.55	0.55	1.00			
3.01 to 4.07	6.5	5	0.18	0.32	0.37	0.38	1.00		
2.59 to 3.01	7.4	6	0.17	0.30	0.34	0.33	0.28	1.00	
2.12 to 2.59	8.3	7	0.15	0.26	0.29	0.29	0.23	0.26	1.00

*Matrix is symmetric; only the lower half is shown.

Table 10. Cross-Correlation Matrix Between the $^{63}Cu(n,\alpha)^{60}Co$ Cross Section and the $^{46}Ti(n,p)^{46}Sc$ Cross Section

Energy Range (MeV)	$^{46}Ti(n,p)$ Group	$^{63}Cu(n,\alpha)$ Group 1	2	3	4	5	6	7
11.05 to 19.64	1	0.02	0.05	0.05	0.04	0.01	0.01	0.01
8.19 to 11.05	2	0.03	0.13	0.12	0.08	0.03	0.02	0.01
6.07 to 8.19	3	0.03	0.10	0.21	0.15	0.04	0.02	0.02
4.07 to 6.07	4	0.03	0.10	0.15	0.18	0.06	0.03	0.03
3.01 to 4.07	5	0.01	0.05	0.07	0.07	0.03	0.02	0.01
2.59 to 3.01	6	0.01	0.05	0.06	0.06	0.02	0.01	0.01
2.12 to 2.59	7	0.01	0.04	0.06	0.05	0.02	0.01	0.01

It may be seen that neither the auto-correlations nor the cross-correlations are large, although all the values are positive. The covariance between the group 3 cross section of the $^{63}Cu(n,\alpha)$ reaction and the group 2 cross section of the $^{46}Ti(n,p)$ reaction is seen from these tables to be

$$(C_{qv})_{3,2} = (3.1\%)(4.1\%)(0.12) \approx 1.53\%^2 = 1.53 \times 10^{-4} \quad . \tag{11}$$

The response of each dosimeter d may be written as

$$r_d = \int_0^\infty \phi(E)\sigma_d(E)dE \simeq \sum_g \phi_g\sigma_{d,g} \quad , \tag{12)*$$

where ϕ_g and $\sigma_{d,g}$ are the flux and dosimeter cross section respectively in group g.

The sensitivities of each response to the parameters ϕ_g and $\sigma_{d,g}$ are the same for a given dosimeter and are readily calculated to be

$$(S^d_\phi)_g \equiv \frac{\phi_g}{r_d}\frac{\partial r_d}{\partial \phi_g} = \frac{\phi_g}{r_d}\sigma_{d,g} = \frac{\phi_g\sigma_{d,g}}{\sum_g \phi_g\sigma_{d,g}} = \frac{\sigma_{d,g}}{r_d}\frac{\partial r_d}{\partial \sigma_{d,g}} = (S^d_{\sigma_d})_g \quad . \tag{13}$$

Thus, once the fluxes are known, these sensitivities may be calculated from the propagation function $\phi_g\sigma_{d,g}/\sum_g \phi_g\sigma_{d,g}$, which is just the fractional contribution of each group to the calculated response. Let us assume the values in Table 11 for purposes of illustration and calculate the sensitivities using Eq. (13), also shown in Table 11.

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*It is unfortunate that the symbol σ has been used historically to represent both a standard deviation and a microscopic cross section. It should be clear from the text as to which quantity is meant.

Table 11. Assumed Values of Group Fluxes and Dosimetry Cross Sections and Derived Sensitivities of Each Response for Second Example

Energy Range (MeV)	Group	ϕ_g	$\sigma_{Cu,g}$	$\sigma_{Ti,g}$	$S^{Cu}_{\phi g}$	$S^{Ti}_{\phi g}$
11.05 to 19.64	1	1.1(7)*	4.0(-26)†	2.6(-25)	0.066	0.041
8.19 to 11.05	2	7.0(7)	2.5(-26)	2.3(-25)	0.262	0.230
6.07 to 8.19	3	1.7(8)	1.2(-26)	1.6(-25)	0.305	0.389
4.07 to 6.07	4	3.5(8)	7.0(-27)	6.5(-26)	0.366	0.325
3.01 to 4.07	5	1.0(8)	1.0(-28)	1.0(-26)	0.001	0.014
2.59 to 3.01	6	2.6(8)	4.0(-30)	2.5(-28)	0	0.001
2.12 to 2.59	7	5.0(8)	5.0(-31)	1.0(-30)	0	0

*Read 1.1 x 10^7 neut/cm^2-s, etc.
†Read 4.0 x 10^{-26} cm^2/target nucleus, etc.

Finally, let us assume the covariances of the flux to be the values shown in Table 12, terminating after group 5 because the sensitivities are negligible for groups 6 and 7.

Table 12. Assumed Correlation Matrix of the Flux*

Energy Range (MeV)	PSD (%)	Group	Group 1	2	3	4	5
11.05 to 19.64	20.3	1	1.0				
8.19 to 11.05	18.9	2	0.95	1.0			
6.07 to 8.19	17.5	3	0.68	0.68	1.0		
4.07 to 6.07	18.1	4	0.59	0.60	0.95	1.0	
3.01 to 4.07	17.9	5	0.61	0.62	0.95	0.96	1.0

*Matrix is symmetric; only the lower half is shown.

The covariance of each dosimeter response arises as a result of the propagation of the parameter covariances, which in this example are those of the flux and the reaction cross section. Hence, by Eq. (9), for each dosimeter d,

$$C_{r_d r_d} = S_\phi^d \, C_{\phi\phi} \, S_\phi^{d^T} + S_{\sigma_d}^d \, C_{\sigma_d \sigma_d} \, S_{\sigma_d}^{d^T} \quad , \tag{14}$$

and since the sensitivities to the flux and the cross section are the same,

$$C_{r_d r_d} = S_\phi^d (C_{\phi\phi} + C_{\sigma_d \sigma_d}) S_\phi^{d^T} \quad . \tag{15}$$

Substituting in the sensitivities for each dosimeter given in Table 10 and the covariance matrices of the flux and cross sections given in Tables 12, 8 and 9 permits one to calculate the uncertainty in each response. Thus,

$$\sigma_{Cu}^2 = (.066 \;\; .262 \;\; .305 \;\; .366 \;\; .001) \begin{pmatrix} 447 & 369 & 246 & 220 & 225 \\ 369 & 367 & 233 & 211 & 216 \\ 246 & 233 & 316 & 307 & 305 \\ 220 & 211 & 307 & 340 & 319 \\ 225 & 216 & 305 & 319 & 394 \end{pmatrix} \begin{pmatrix} .066 \\ .262 \\ .305 \\ .366 \\ .001 \end{pmatrix}$$

$$= (282 \;\; 269 \;\; 286 \;\; 288 \;\; 282) \begin{pmatrix} .066 \\ .262 \\ .305 \\ .366 \\ .001 \end{pmatrix} = (16.8\%)^2 \quad , \tag{16}$$

$$\text{and } \sigma^2_{Ti} = (.041\ \ .230\ \ .389\ \ .325\ \ .014) \begin{pmatrix} 488 & 375 & 250 & 224 & 232 \\ 375 & 374 & 234 & 212 & 219 \\ 250 & 234 & 320 & 308 & 307 \\ 224 & 212 & 308 & 338 & 319 \\ 232 & 219 & 307 & 319 & 362 \end{pmatrix} \begin{pmatrix} .041 \\ .230 \\ .389 \\ .325 \\ .014 \end{pmatrix}$$

$$= (280\ \ 264\ \ 293\ \ 292\ \ 288) \begin{pmatrix} .041 \\ .230 \\ .389 \\ .325 \\ .014 \end{pmatrix} = (16.9\%)^2 \ . \qquad (17)$$

The two standard deviations are thus virtually the same in this case and are dominated by the uncertainties in the flux. It is also of interest to obtain the correlation between these two responses. This correlation arises as a result of two sources. First, the flux is a common parameter to both responses [see Eq. (12)], and hence its covariance propagated with each of the response sensitivities is a common source of uncertainty in the two responses. Second, the two dosimeter cross sections are somewhat correlated (see Table 10), so that they also contribute to the response correlation. Both of these terms appear in Eq. (18), where the remaining terms involving correlations between the flux and the cross sections are assumed to be zero:

$$C_{r_d r_{d'}} = \left\langle \left(\frac{\delta \bar{r}_d}{\bar{r}_d}\right)\left(\frac{\delta \bar{r}_{d'}}{\bar{r}_{d'}}\right)^T \right\rangle = \left\langle S_\phi^d \left(\frac{\delta\bar{\phi}}{\bar{\phi}} + \frac{\delta\bar{\sigma}_d}{\bar{\sigma}_d}\right)\left(\frac{\delta\bar{\phi}}{\bar{\phi}} + \frac{\delta\bar{\sigma}_{d'}}{\bar{\sigma}_{d'}}\right)^T S_\phi^{d'^T} \right\rangle$$

$$= S_\phi^d \left\langle \left(\frac{\delta\bar{\phi}}{\bar{\phi}}\right)\left(\frac{\delta\bar{\phi}}{\bar{\phi}}\right)^T \right\rangle S_\phi^{d'^T} + S_\phi^d \left\langle \left(\frac{\delta\bar{\sigma}_d}{\bar{\sigma}_d}\right)\left(\frac{\delta\bar{\sigma}_{d'}}{\bar{\sigma}_{d'}}\right)^T \right\rangle S_\phi^{d'^T}$$

$$= S_\phi^d (C_{\phi\phi} + C_{\sigma_d \sigma_{d'}}) S_\phi^{d'^T} . \qquad (18)$$

Performing the calculations leads to contributions from each term in Eq. (18) of 275%^{2} and 1.6%^{2} respectively, thus leading to the response correlation matrix shown in Table 13.

Table 13. Correlation Matrix of the Two Dosimeter Responses

PSD (%)		$^{63}Cu(n,\alpha)$	$^{46}Ti(n,p)$
16.8	$^{63}Cu(n,\alpha)$	1.0	0.976
16.9	$^{46}Ti(n,p)$	0.976	1.0

6. ADJUSTMENTS OF RESPONSES AND PARAMETERS

Once specific estimates of parameters and their covariances have been made, sensitivities of various calculated responses to these parameters obtained, and values of the calculated responses and their propagated covariances found, improvement in the knowledge of the responses may be effected in two ways. First, attention may be devoted to obtaining more accurate values of the more important parameters [i.e., those which have appreciable contributions to the response covariances calculated using Eq. (9)]. (Notice that the relative importance of a given parameter is measured by the product of a response sensitivity to this parameter and the parameter uncertainty, so that a high sensitivity to a given parameter does not necessarily imply that the parameter is important.) In the case of high-level waste isolation analysis, more accurate values of the important parameters may be obtained by measurement in an actual waste storage facility or mock up thereof of various of the assumed parameters, or in a laboratory for some of the more basic data.

The second way in which the response covariances may be reduced is by adding the results of measurements of these or other related responses or parameters performed in a facility or mock up to the list of information accumulated above, together with an estimate of these covariances. A generalized linear least-squares adjustment procedure may then be invoked to combine all the information, resulting in the most consistent set of data containing the parameters, the calculated responses, the measurements of the related data, and all covariances and sensitivities. Because of the mathematically imposed condition of maximizing the joint probability distribution, the adjusted values all have reduced covariances.

To illustrate the kind of results obtained from an adjustment procedure, we present the following simple problem. Suppose the two sides of a rectangle ℓ and w were measured and found to be 5 and 2 units with standard deviations of 2 and 3 percent, respectively. Then the calculated value of the area A is 10 square units with a standard deviation that depends not only on the standard deviations of the individual side measurements but also on the correlation between these measurements. If no correlation is assumed, then the covariance matrix of the two parameters may be written as

$$C_{\ell w} = \begin{pmatrix} (2\%)^2 & 0 \\ 0 & (3\%)^2 \end{pmatrix} . \tag{19}$$

If there is a perfect correlation between the two parameters, then

$$C_{\ell w} = \begin{pmatrix} (2\%)^2 & (2\%)(3\%) \\ (2\%)(3\%) & (3\%)^2 \end{pmatrix} , \tag{20}$$

while a perfect anticorrelation may be represented as

$$C_{\ell w} = \begin{pmatrix} (2\%)^2 & -(2\%)(3\%) \\ -(2\%)(3\%) & (3\%)^2 \end{pmatrix} . \tag{21}$$

Since the sensitivities of the calculated "response" A to each of the parameters ℓ and w are

$$S_A = \frac{\ell}{A}\frac{\partial A}{\partial \ell} = \frac{w}{A}\frac{\partial A}{\partial w} = 1 , \tag{22}$$

then the propagated uncertainties in the calculated area may be readily obtained for each of the three assumed forms of $C_{\ell w}$ appearing in Eqs. (19-21) to be

$$C_{AA} = (1\ 1)C_{\ell w}\begin{pmatrix}1\\1\end{pmatrix} , \tag{23}$$

leading to standard deviations of 3.6%, 5%, and 1%, respectively.

So far the above analysis presents nothing new and is just another example illustrating covariance propagation. Let us now introduce the further information that a direct measurement of the area by means of a planimeter yields the value 10.2 square units with an uncertainty of 1%, the measurement being uncorrelated with the previous measurements of ℓ and w. In this case, a measurement of a perfectly related response (i.e., the area itself) is added to the database. Then, combining this information with the earlier information leads to the adjusted data with uncertainties shown in Table 14.[5]

Table 14. Results of Adjustment Using a Generalized Linear Least-Squares Combination Procedure

Assumed Parameter Correlation, $\alpha_{\ell w}$	Adjusted Value of A, A'	Adjusted Value of ℓ, ℓ'	Adjusted Value of w, w'	Standard Deviation of A', $\sigma_{A'}$	Standard Deviation of ℓ', $\sigma_{\ell'}$	Standard Deviation of w', $\sigma_{w'}$	Correlation Between ℓ' and w', $\alpha_{\ell'w'}$
0	10.186	5.028	2.025	0.964%	1.69%	1.79%	-0.59
+1	10.192	5.038	2.023	0.981%	0.39%	0.59%	+1
-1	10.100	4.902	2.059	0.707%	1.41%	2.12%	-1

Among the interesting conclusions that these results illustrate are the exactness of the linear approximation (i.e., $\ell'w'$ and A' are virtually identical), the significant reduction in the uncertainties of the adjusted parameters as well as that of the response (which are always less than those of the unadjusted values) effected by the inclusion of measured response information [compare with previously derived values using Eq. (23)], and the fact that, if the assumed parameter correlations are either +1 or -1, they remain so after adjustment as well. Finally, the adjusted value of A is virtually the same as the measured value of A when the uncertainty in the measured value is considerably less than that of the calculated value. For the case of perfect anticorrelation between the parameters, the calculated and measured areas have the same uncertainties (1%) and hence the adjusted value lies halfway between these two values.

The above example represents an extreme illustration of the effect of introducing additional measured information to the data to be combined, of course, and, more generally, measured information on less correlated responses and parameters will be combined, leading to somewhat less dramatic reductions in the parameter and response uncertainties than those just presented.

7. CONCLUSIONS

Covariances should be estimated for many of the parameters considered to be of importance in nuclear waste isolation in order to better assess the accuracy of calculated quantities depending on these parameters, since no confirmatory measurements of these quantities will be available. The importance of each parameter can be better judged with the help of sensitivities derived from use of GRESS or other methods, for its contribution to the uncertainty of a calculated response involves the product of the parameter uncertainty with an appropriate sensitivity. It is anticipated that a folding code can easily be written which would automate the procedure of matrix multiplication of GRESS sensitivities with parameter covariances. Thus, once covariances of the parameters become available, one could readily obtain covariances of various responses which should help to evaluate their state-of-the-art uncertainties and point out areas where improved knowledge of the more important parameters can lead to significantly better accuracies in the calculated quantities. Adjustment procedures that combine results of measurements of quantities correlated with those used in the calculations with the original database eventually can also be performed to reduce the uncertainties in the responses and some of the more important parameters.

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