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Estimation of Total Error in DWPF's Reported Radionuclide Inventories (U)

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**Estimation of Total Error in DWPF's Reported
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by

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Table of Contents

Section		Page
1.0	Introduction	1
2.0	Summary	1
3.0	Estimating Radionuclide Concentrations	1
4.0	Concluding Comments	7

1.0 INTRODUCTION

This report investigates the impact of random errors due to measurement and sampling on the reported concentrations of radionuclides in DWPF's filled canister inventory resulting from each macro-batch. The objective of this investigation is to estimate the variance of the total error in reporting these radionuclide concentrations.

2.0 SUMMARY

Estimates of the total radionuclide concentrations for each DWPF macro-batch are to be determined by one of two methods. A propagation of variance for each of these two methods is completed to estimate the variance of the total error affecting these derived values. In this analysis, the errors considered reflect only random variation.

3.0 ESTIMATING RADIONUCLIDE CONCENTRATIONS

There are two methods for deriving estimates of the radionuclide concentrations for each batch of slurry comprising a DWPF macro-batch: the direct and the indirect methods. Only one of these two methods is to be used for each of the radionuclides of interest.

3.1 Radionuclide Concentrations Determined Via the Direct Method

In the direct method, the contents of each MFT batch are measured, and the curies of radionuclide r per gram of solids for this i^{th} batch, c_i , is determined. A measurement, W_i , of the weight per unit volume is also made as well as a measurement, V_i , of the volume transferred from the MFT to the melter for batch i . The estimate of the total curies of radionuclide r for the macro-batch (consisting of b batches) is given by

$$C_r = \sum_{i=1}^b (c_i W_i V_i) \quad (1)$$

The errors associated with the c_i , W_i and V_i terms of equation (1) are assumed to be random errors. The standard deviations of these errors may be expressed in absolute units or, in the case of relative errors, as a percent of value. The analyses conducted below assumes that absolute units will be used. See Section 4.0 below for a discussion on how to handle relative standard deviations.

For each batch, the errors associated with the c_i and W_i terms are expected to be positively correlated, with $\text{cov}(c_i, W_i)$ representing the covariance between the errors for these two terms. The errors associated with V_i are assumed to be independent of the

errors of the other two terms of equation (1). In addition, the errors associated with one MFT batch, i , are expected to be independent of all the other batches which make up the DWPF macro-batch. The independence of the errors across batches implies no systematic influence from tank volume calibrations or from instrument calibrations; that is, the instruments used to measure the c_i and W_i for batch i are recalibrated before being used to measure c_j and W_j for batch j .

Using a Taylor's series expansion to estimate the variance of C_r , $\text{var}(C_r)$, yields

$$\begin{aligned} \text{var}(C_r) \approx \sum_{i=1}^b & \left[\left(\frac{\partial C_r}{\partial c_i} \right)^2 \text{var}(c_i) + \left(\frac{\partial C_r}{\partial W_i} \right)^2 \text{var}(W_i) + \left(\frac{\partial C_r}{\partial V_i} \right)^2 \text{var}(V_i) \right. \\ & \left. + 2 \left(\frac{\partial C_r}{\partial c_i} \right) \left(\frac{\partial C_r}{\partial W_i} \right) \text{cov}(c_i, W_i) \right] \end{aligned} \quad (2)$$

where $\frac{\partial C_r}{\partial c_i}$ is the partial of C_r with respect to c_i , and is equal to $W_i V_i$, and similarly,

$$\frac{\partial C_r}{\partial W_i} = c_i V_i \quad \text{and} \quad \frac{\partial C_r}{\partial V_i} = c_i W_i$$

This leads to the following estimate of the variance of C_r

$$\begin{aligned} \text{var}(C_r) \approx \sum_{i=1}^b & \left[W_i^2 V_i^2 \text{var}(c_i) + c_i^2 V_i^2 \text{var}(W_i) + c_i^2 W_i^2 \text{var}(V_i) \right. \\ & \left. + 2 c_i W_i V_i^2 \text{cov}(c_i, W_i) \right] \end{aligned} \quad (3)$$

This direct approach assumes that all of the errors effecting these measurements (the c_i 's, W_i 's and V_i 's) are random quantities (with correlations as described above). To complete the determination of the variance of C_r in equation (3), the variances of c_i , W_i , and V_i must be estimated from the uncertainties of these measurements. The uncertainties of c_i and W_i , can be computed from the uncertainty of each of the corresponding procedures (sampling, which includes the tank inhomogeneity, and analytical, which includes sample preparation).

3.2 Radionuclide Concentrations Determined Via the Indirect Method

This method is deemed indirect since its estimates of the curie concentration (for the radionuclide of interest) per MFT batch depend on analytical results of SRS Tank Farm

samples as opposed to samples taken directly from the DWPF MFT. The radionuclides which are to be estimated using this method must occur only in either the sludge or the PHA.

For each radionuclide, r (determined with this indirect method), the estimate of the curie concentration for each MFT batch is given by

$$C_{i,r} = \frac{1}{x} \sum_{a=1}^x (C_{\text{stream};i,r} f_{i;a}) \quad (4)$$

where $C_{\text{stream};i,r}$ is the measured concentration of the radionuclide of interest in the stream (either sludge or PHA); that is, $C_{\text{stream};i,r}$ is the curies per gram of stream feeding into batch i ; and $f_{i;a}$ is a measure of the dilution factor for the stream (grams of solids in the MFT relative to grams of solids in the stream) relative to element a for a total of x elements.

Each $f_{i;a}$ is computed as the ratio of two measurement averages ($\bar{m}_{i;a}$ and $\bar{s}_a$). The errors associated with these two measurements are expected to be independent. The average $\bar{m}_{i;a}$ is the estimate of the content of element a in MFT batch i , and it is computed from a collection of p_i analyses. The average $\bar{s}_a$ is the estimate of the content of element a in the input stream (e.g., sludge or PHA) to the MFT, and it is computed from a collection of q analyses. These q analyses of the input stream are conducted only once for a DWPF macro-batch, and these results are used in the determination of each of the $f_{i;a}$ values. The uncertainties of $\bar{m}_{i;a}$ and $\bar{s}_a$ can be readily computed from the uncertainty of each of the corresponding procedures (sampling {includes tank uniformity} and analytical) used in their respective derivation.

Specifically,

$$\text{var}(\bar{m}_{i;a}) = \frac{\text{var}(m_{i;a})}{p_i} \quad (5)$$

and

$$\text{var}(\bar{s}_a) = \frac{\text{var}(s_a)}{q} \quad (6)$$

where $\text{var}(m_{i;a})$ represents the variance of the random errors associated with a single $m_{i;a}$ measurement and $\text{var}(s_a)$ represents the same for a single s_a measurement. The variances for these single measurements are to be estimated to allow equations (5) and (6) to be computed. Note that to ensure the reduction in variability suggested by equation (5), the p_i values of $m_{i;a}$ must share consistent sources of variation. A similar argument holds for the q values of s_a .

Using the indirect approach and the notation developed above, we get the following estimate for the total curies of radionuclide r , C_r , for a DWPF macro-batch:

$$C_r = \sum_{i=1}^b \left[\frac{C_{\text{stream};i;r}}{x} W_i V_i \sum_{a=1}^x \frac{\bar{m}_{i;a}}{\bar{s}_a} \right] \quad (7)$$

where W_i and V_i are defined as in equation (1).

The variance of C_r in equation (7) will be estimated using a Taylor's series expansion as in equation (2) above. However, some of the error terms affecting equation (7) may not be independent, and this possibility must be addressed appropriately in the estimation of the variance of C_r .

Specifically, the errors for the factors $\bar{m}_{i;a}$ derived from samples from each MFT batch i (the index a ranges over x factors: Fe, Al, Mn, and Ca, for a given MFT batch) may be correlated. The errors for these measurements are assumed to be positively correlated; for example, if the estimate of the Fe tends to be high then the estimates of the other three elements will also tend to be high. Therefore, the Taylor's series expansion must involve the covariances for these factors. In addition, the errors of the $\bar{m}_{i;a}$ may also be correlated with the errors of the measurement W_i , since all of these measurements are made on the same samples.

Similarly, the errors for the factors $\bar{s}_a$ derived from samples of the input stream (sludge or PHA) of the DWPF macro-batch may be correlated. The errors for these measurements for Fe, Al, Mn, and Ca are assumed to be positively correlated; for example, if the estimate of the Fe tends to be high then the estimates of the other three elements will also tend to be high.

The errors for the other measurements of equation (7) are assumed to be independent since they are made on different samples and either by different labs or different techniques.

This leads to the following estimate of the variance of C_r :

$$\begin{aligned} \text{var}(C_r) \approx & \sum_{i=1}^b \left[\left(\frac{\partial C_r}{\partial C_{\text{stream};i;r}} \right)^2 \text{var}(C_{\text{stream};i;r}) + \left(\frac{\partial C_r}{\partial W_i} \right)^2 \text{var}(W_i) + \left(\frac{\partial C_r}{\partial V_i} \right)^2 \text{var}(V_i) \right. \\ & + \sum_{a=1}^x \left(\frac{\partial C_r}{\partial \bar{m}_{i;a}} \right)^2 \text{var}(\bar{m}_{i;a}) + \sum_{a=1}^x \sum_{\substack{c=1 \\ a \neq c}}^x \left(\frac{\partial C_r}{\partial \bar{m}_{i;a}} \right) \left(\frac{\partial C_r}{\partial \bar{m}_{i;c}} \right) \text{cov}(\bar{m}_{i;a}, \bar{m}_{i;c}) \end{aligned}$$

$$\begin{aligned}
& + 2 \sum_{a=1}^x \left(\frac{\partial C_r}{\partial \bar{m}_{i;a}} \right) \left(\frac{\partial C_r}{\partial W_i} \right) \text{cov}(\bar{m}_{i;a}, W_i) \Big] + \sum_{a=1}^x \left(\frac{\partial C_r}{\partial \bar{s}_a} \right)^2 \text{var}(\bar{s}_a) \\
& + \sum_{a=1}^x \sum_{\substack{c=1 \\ a \neq c}}^x \left(\frac{\partial C_r}{\partial \bar{s}_a} \right) \left(\frac{\partial C_r}{\partial \bar{s}_c} \right) \text{cov}(\bar{s}_a, \bar{s}_c)
\end{aligned} \tag{8}$$

where $\text{cov}(\bar{m}_{i;a}, \bar{m}_{i;c})$, $\text{cov}(\bar{m}_{i;a}, W_i)$, and $\text{cov}(\bar{s}_a, \bar{s}_c)$ represent the covariance between the errors for the two factors indicated,

and for each i

$$\frac{\partial C_r}{\partial C_{\text{stream};i;r}} = W_i V_i \frac{1}{x} \sum_{a=1}^x \frac{\bar{m}_{i;a}}{\bar{s}_a} ;$$

$$\frac{\partial C_r}{\partial W_i} = C_{\text{stream};i;r} V_i \frac{1}{x} \sum_{a=1}^x \frac{\bar{m}_{i;a}}{\bar{s}_a} ;$$

$$\frac{\partial C_r}{\partial V_i} = C_{\text{stream};i;r} W_i \frac{1}{x} \sum_{a=1}^x \frac{\bar{m}_{i;a}}{\bar{s}_a} ; \text{ and}$$

for each i and a

$$\frac{\partial C_r}{\partial \bar{m}_{i;a}} = \frac{C_{\text{stream};i;r} W_i V_i}{x \bar{s}_a} ; \text{ and}$$

for each a

$$\frac{\partial C_r}{\partial \bar{s}_a} = - \sum_{i=1}^b \frac{C_{\text{stream};i;r} \bar{m}_{i;a} W_i V_i}{x \bar{s}_a^2}$$

Thus, the variance of C_r given by equation (8) is estimated by

$$\begin{aligned}
 \text{var}(C_r) \approx & \sum_{i=1}^b \left[\left(W_i V_i \frac{1}{x} \sum_{a=1}^x \frac{\bar{m}_{i;a}}{\bar{s}_a} \right)^2 \text{var}(C_{\text{stream};i;r}) + \left(C_{\text{stream};i;r} V_i \frac{1}{x} \sum_{a=1}^x \frac{\bar{m}_{i;a}}{\bar{s}_a} \right)^2 \text{var}(W_i) \right. \\
 & + \left(C_{\text{stream};i;r} W_i \frac{1}{x} \sum_{a=1}^x \frac{\bar{m}_{i;a}}{\bar{s}_a} \right)^2 \text{var}(V_i) + \sum_{a=1}^x \sum_{\substack{c=1 \\ a \neq c}}^x \frac{\left(\frac{1}{x} C_{\text{stream};i;r} W_i V_i \right)^2}{\bar{s}_a \bar{s}_c} \text{cov}(\bar{m}_{i;a}, \bar{m}_{i;c}) \\
 & + \sum_{a=1}^x \left(\frac{C_{\text{stream};i;r} W_i V_i}{x \bar{s}_a} \right)^2 \text{var}(\bar{m}_{i;a}) \\
 & + 2 \sum_{a=1}^x \left(\frac{C_{\text{stream};i;r} V_i}{x} \right)^2 \frac{W_i}{\bar{s}_a} \left(\sum_{c=1}^x \frac{\bar{m}_{i;c}}{\bar{s}_c} \right) \text{cov}(\bar{m}_{i;a}, W_i) \Big] \\
 & + \sum_{a=1}^x \left(- \sum_{i=1}^b \frac{C_{\text{stream};i;r} \bar{m}_{i;a} W_i V_i}{x \bar{s}_a^2} \right)^2 \text{var}(\bar{s}_a) \\
 & + \sum_{\substack{a=1 \\ a \neq c}}^x \sum_{c=1}^x \left(- \sum_{i=1}^b \frac{C_{\text{stream};i;r} \bar{m}_{i;a} W_i V_i}{x \bar{s}_a^2} \right) \left(- \sum_{i=1}^b \frac{C_{\text{stream};i;r} \bar{m}_{i;c} W_i V_i}{x \bar{s}_c^2} \right) \text{cov}(\bar{s}_a, \bar{s}_c) \quad (9)
 \end{aligned}$$

This indirect approach assumes that all of the errors effecting these measurements (except for those discussed above) are independent, random quantities. To complete the determination of the variance of C_r in equation (9), the variances of the $C_{\text{stream};i;r}$, W_i , $\bar{m}_{i;a}$, $\bar{s}_a$, and V_i must be estimated from the uncertainties of these measurements. The covariances of the correlated errors must also be estimated.

A note regarding estimates of the covariances of the $\bar{m}_{i;a}$ and $\bar{s}_a$. These covariances may be difficult to estimate. If the errors affecting these factors are positively correlated,

then a bounding (conservative) estimate of the covariance between any two of these factors is the product of their standard deviations. These estimates may be used in equation (7) to provide the estimate of the variance of C_r .

4.0 CONCLUDING COMMENTS

As more definitive estimates of the errors affecting these measurements are identified, they may be used in these calculations to provide a representative estimate of the total error in the reported radionuclide inventory for each DWPF macro-batch. Specifically, if some of the errors are relative errors, then estimates of the corresponding variances should be entered appropriately into equations (3) or (9). For example, if y is a measurement with a relative standard deviation of $n\%$, then the estimate of the variance of the error associate with the measurement y is equal to $(\frac{yn}{100})^2$.

The approach presented in this memo assumes that the reported radionuclide concentrations and other measurements will be corrected for known biases associated with vessel uniformity, sampling, and analysis. If not accounted for or if steps are not taken (such as recalibrating instrumentation between MFT batches), the systematic errors from these sources could be significant contributors to the overall uncertainty. In this analysis, the errors considered reflect only random variation.