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Statistical Approach to Meeting Soil Cleanup Goals

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The establishment of health-protective soil remediation levels often relies on the results of a risk assessment, which provides a way to equate a permissible risk to a target soil contaminant concentration. Inherent in such risk assessments is the assumption that the target concentrations are representative averages. Unfortunately, soil cleanup levels thus calculated are typically misapplied on a point by point basis rather than on an average. This is not cost-effective because it results in post-remedy conditions that overshoot the target risk goals. Because environmental contamination is characterized by a distribution of concentrations, some exceedances of target averages, average risk, or average concentration can be allowed in the post-remediation distribution. This work presents a mathematical model for calculating this allowable higher than average concentration, termed the confidence response goal (CRG), which places a limit on concentrations requiring remediation while ensuring that target average concentrations are satisfied overall. The CRG is site-specific becauses it depends on the contaminant concentration distribution. The strength of the approach lies in its ability to handle typical data uncertainties quantitatively because it relies on the upper confidence limit as a measure of the mean concentration (in a manner similar to its use in risk assessment), hence the term "confidence" in the CRG. The advantages of the approach are significant. An example is given of a Superfund site where excavation volumes were reduced by 66% and $40 million was saved, about half of which could be attributed to the CRG approach.

Introduction

Soil cleanup levels at Superfund sites are determined more often by risk assessment than by any other criterion. There are two steps to this decision-making process. First, a baseline risk assessment is used to evaluate current and future "no-action" conditions. If this leads to a conclusion that cleanup is required, then the second step is to perform a risk assessment in reverse to determine contaminant concentrations that correspond to a permissible level of risk. The contaminant concentrations thus calculated may be referred to as the "cleanup level" or the "cleanup goal".

Once cleanup goals are established, it is usually assumed that any sample location with contaminant concentrations that exceed these levels requires remediation, particularly for soils. Excavation of all soils in the vicinity of such locations exceeding cleanup goals is one common remedy. In such cases, these Superfund remedies involve an excavation-sampling iteration where excavation of the sides and bottom of a pit continues until side and bottom sampling reveals no contaminant concentrations above the cleanup goal.

For risk-based cleanup goals, this approach is not cost-effective because it results in more remediation than actually required to meet the target risk goal. The logic for the most cost-effective approach is simple; so simple, in fact, that the reader may mistakenly believe that the premise proposed herein is already the *status quo* at Superfund sites. It is not. The cost-effective approach considers the cleanup goal as the post-remediation *average* concentration. The approach proposed here is not only applicable to Superfund sites, but can be used for any sites where remediation in support of a target cleanup goal is required.

Background

Relationship of Cleanup Goals to Risk. Quantitative risk assessment is used to assess the concentration of a contaminant that may remain on a site without posing an undue threat to human health or ecosystems. Risk is determined from two components, exposure and toxicity, and it is exposure that is a function of the contaminant concentration:

$$\text{risk} = \text{concentration} \times \text{other exposure factors} \times \text{toxicity} \quad (1)$$

where other exposure factors include contact rate, days exposed, etc., and toxicity is a parameter reflecting an undesirable human health response to a dose of the contaminant.

The measure of exposure appropriate for a risk assessment is the average concentration of a contaminant throughout an "exposure unit", a geographic area to which humans are exposed (*1*). This premise is based on the assumption that over a long enough time, the exposed individual has contacted (by ingestion or dermal exposure) all parts of the exposure unit. Inhalation of out-gassed soil contaminants mixed into the breathing zone also offers an averaged soil exposure. Agency guidance covering the definition of exposure units suggests that they should be homogeneous with respect to prior pollution and that differences in land use, terrain, accessibility, or media type that can affect exposure may require establishment of a number of separate exposure units (*2*). Independent cleanup decisions should be made for each exposure unit.

Assuming that an exposure unit has been adequately defined so that exposure, and therefore risk, is a function of the average contaminant concentration in the exposure unit, it is recognized that there is some uncertainty associated with environmental sampling. Agency risk

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assessment guidance (*1*) specifies that this uncertainty be addressed in the risk equation by use of an upper confidence limit (UCL) on the mean contaminant concentration of the samples, instead of simply the mean of the samples. The UCL is a function of sample size; the value of the UCL increases with decreasing sample size. Since the UCL on the mean contaminant concentration is used to assess exposure in an EPA-guided risk assessment, a higher calculated risk ensues than if simply the sample mean were used in the equation. This is a conservative (*i.e.*, health-protective) approach because it increases the likelihood that a contaminated site will be characterized as having unacceptable risk.

Following a risk management decision to remediate based on the results of a risk assessment, a cleanup goal can be derived by solving the risk equation (eq 1) backwards with risk set equal to a specified target value (or "permissible" risk). At Superfund sites, as specified by the National Contingency Plan, the EPA uses a range of permissible incremental cancer risks from 10^{-6} to 10^{-4}, with a preference for the target risk for remediation to be set at 10^{-6} once remediation is required (*3*). Rearranging eq 1, the cleanup goal (CUG) is thus obtained from

$$\text{CUG} = \frac{\text{permissible risk}}{\text{toxicity} \times \text{other exposure factors}} \tag{2}$$

The value of the CUG derived in this manner is analogous to however contamination was represented in the risk assessment, *e.g.*, average, UCL, or worst known single measurement. Because EPA risk assessment guidance dictates the use of the UCL, the CUG should be met after remediation in an analogous way. Recent articles concerning applications of risk calculations to cleanup decisions have recognized this concept (*4, 5*). Thus, an exposure unit will require remediation if its average contaminant concentration, as represented by the UCL, exceeds the CUG, **not** if individual samples exceed the CUG. There may be individual samples or observations where the contaminant concentration does exceed the CUG within this exposure unit, but as long as the UCL does not exceed the CUG, no remediation is required.

This same logic can be applied to those exposure units where some remediation is required. The attainment of acceptable risk does not necessitate remediating every location in an exposure unit where the contaminant concentration exceeds the CUG. Rather, enough remediation must be done such that the CUG and the target risk are met **on average** after remediation across the exposure unit (*4, 5*). This can be done by specifying a "response goal", a contaminant concentration higher than the CUG, such that if remediation of all areas with contaminant concentrations exceeding the response goal are carried out (or a "confidence" response goal if the target is the upper *confidence* limit rather than the mean), then the CUG would be met on average across the exposure unit. This approach in no way compromises the original risk-based goal; in fact, anything more aggressive would not be cost-effective because it would exceed the goal.

Given the premise that risk-based CUGs can tolerate individual point exceedances in the field as long as the CUG is satisfied on average, the challenge is to predict how many or how high an exceedance is allowable while still meeting the average condition and taking into consideration the uncertainty imposed by limited sampling schemes. As

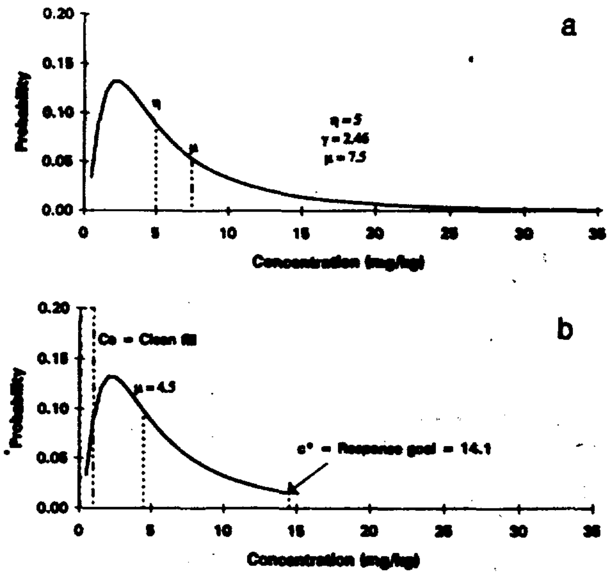

FIGURE 1. (a) Log-normal distribution of contaminant concentrations, pre-remediation. The mean concentration is 7.5 mg/kg. (b) Truncated log-normal distribution of contaminant concentrations, post-remediation. The distribution is truncated at the response goal of 14.1 mg/kg. All remediated sample locations are replaced with fill of concentration c_o = 0.1 mg/kg. This results in a post-remediation mean contaminant concentration of 4.5 mg/kg. Note that the spike representing fill is drawn arbitrarily wide for clarity in the figure.

shown below, statistical tools are available to make such predictions using site-specific data. The results will differ for each distribution, thus each analysis is site specific. For example, two distributions may have the same average, but different standard deviations. In such a case the maximum CUG exceedance allowed will differ for the two distributions.

Methodology

Pre-remediation concentrations can typically be described by a log-normal distribution (*6*). The response goal (c^*) can be expressed as a function of the geometric mean (η) and geometric standard deviation (γ) of a log-normal distribution of contaminant concentrations and the desired reduction in exposure (α), which is defined as the ratio of the average post-remediation concentration to the average pre-remediation concentration (μ'/μ). Exposure is always a function of the arithmetic mean concentration over a pre-defined exposure area regardless of the type of distribution that best describes contaminant concentrations. Post-remediation concentrations form a log-normal distribution that is truncated at the response goal, with a second distribution superimposed that represents the concentration of the contaminant in back fill (c_0) or a cover depending on the response. The second distribution is described by a δ function. The average concentration of the post-remediation distribution is a weighted average of the portion of the pre-remediation distribution with concentrations below the response goal and the concentration of the back fill/cover, which replaces all pre-remediation concentrations that exceed the response goal. See Figure 1 for an example of a pre- and post-remediation distribution of contaminant concentrations. Derivation of an analytical expression, which can be solved for the response goal, is given in the supplementary material. The resulting expression is

$$\alpha = \frac{1}{2}\left[1 + 2F\left(\frac{1}{\ln\gamma}\ln\frac{c^*}{\eta} - \ln\gamma\right) + \frac{c_o}{\eta}e^{-(\ln\gamma)^2/2}\left[1 - 2F\left(\frac{1}{\ln\gamma}\ln\frac{c^*}{\eta}\right)\right]\right] \quad (3)$$

where $F(z)$ is the area under the standard normal curve from 0 to z or the negative of the area under the standard normal curve from $-z$ to 0. When the average contaminant concentration exceeds the desired average, eq 3 can be solved for the response goal, c^*, as a function of α, η, and γ. Note that where the average contaminant concentration is below the desired average, no response goal can be calculated.

When the Mean Contaminant Concentration Is Known. When the sample size of a set of data consisting of analytically determined contaminant concentrations over an exposure unit (the "data set") is very large (greater than 200–300), the true mean and standard deviation of the distribution can be assumed to be equal to the sample mean and standard deviation of the data set and are considered to be known quantities. This is a limiting case that seldom occurs in actual field studies due to both practical and financial constraints on sampling. However, we begin by describing this case because it is the most simple, mathematically.

A contaminant- and site-specific (or exposure unit-specific) response goal is calculated by solving eq 3 for c^*. As an example calculation, consider a distribution described by a geometric mean (η) of 5 mg/kg and a geometric standard deviation (γ) of 2.46. The arithmetic mean of the distribution is 7.5 mg/kg. Assume that the CUG determined from the risk assessment is 4.5 mg/kg. Therefore, α, the reduction in exposure, is equal to 0.6 (desired post-remediation mean of 4.5 mg/kg divided by the pre-remediation mean of 7.5 mg/kg). If the level of contaminant in the clean fill (c_o) is set at 0.1 mg/kg, then the solution of eq 3 for the response goal (c^*) yields a value of 14.1 mg/kg. This means that if all soils containing contaminant concentrations greater than 14.1 mg/kg are removed and back-filled with material having contaminant concentrations of 0.1 mg/kg, the average concentration of the post-remediation distribution will be the desired value of 4.5 mg/kg. Figure 1 illustrates this example.

When the Mean Contaminant Concentration Is Imprecisely Known. The decision as to whether an exposure unit must be remediated often relies on a test of whether the upper confidence limit on the arithmetic sample mean of a data set exceeds a specified target (*1*). The situation can arise where the sample mean is less than the specified target, but the upper confidence limit exceeds the specified target. A response goal cannot be calculated from the sample mean in this instance, because the sample mean is below the target. Instead, a response goal must be derived that is consistent with the uncertainty in the sample mean.

The response goal calculation described in the section above yields a value based on the assumption that the true mean and standard deviation of the distribution are known. As sample size decreases, the sample mean and standard deviation become less reliable as estimators of the true mean and standard deviation. Correspondingly, the response goal would also be uncertain. When the true mean of a distribution is imprecisely known, the procedure described above is followed for values that the true mean could attain between the upper and lower confidence limits on the sample mean. The minimum response goal calculated for the possible values of the mean between these limits is termed the confidence response goal (CRG) because it is based on confidence limits. The overall effect of less certainty in the contaminant concentrations associated with small sample sizes is that the CRG will be lower and more remediation will be required. There is a trade-off between more sampling and potentially higher action thresholds leading to less remedial cost.

The mathematical model given by eq 3 yields a response goal that is a function of the entire distribution of contaminant concentrations (f). This requires calculation of an upper and lower confidence limit on the entire distribution, not just on the mean. The distribution representing the upper confidence limit on f (corresponding to the upper confidence limit on each percentile of f) is referred to as f', while the distribution representing the lower confidence limit on f is f'' (corresponding to the lower confidence limit on each percentile of f). The distribution f' is calculated from the 95% upper confidence limit on both the arithmetic and geometric means of f, where these two values are used to define the geometric standard deviation of f' and, hence, all percentile values of f'. Likewise, the distribution f'' is calculated from the 95% lower confidence limit on the arithmetic mean and geometric mean of f.

The upper confidence limit on the arithmetic mean ($UCL_{\bar{x}}$) of a log-normal distribution is calculated after the method described by Land (*7*) from

$$UCL_{\bar{x}} = \exp\left(M + \frac{G^2}{2} + \frac{(G)(H_{G,\nu})}{\sqrt{\nu}}\right) \quad (4)$$

where M corresponds to the logarithm of the geometric mean (gm) of the data set, G represents the logarithm of the geometric standard deviation (gsd) of the data set, ν is the degrees of freedom (equal to the sample size minus one), and $H_{G,\nu}$ is the H statistic for a confidence level of 95% that can be taken from tables (*7, 8*). (The terms gm and gsd refer to the geometric mean and geometric standard deviation of the data set, as distinct from η and γ, which are the true geometric mean and geometric standard deviation of the underlying distribution. This is analogous to the use of $\bar{x}$ as the sample arithmetic mean and μ as the true arithmetic mean.) The lower confidence limit on the arithmetic mean is calculated in the same manner, but the H statistic has a negative value. Note that the H statistic for upper and lower confidence limits is not symmetrical.

The upper confidence limit on the geometric mean (UCL_{gm}) of a log-normal distribution is calculated with the t statistic from

$$UCL_{gm} = \exp\left(M + \frac{(t_\nu)(G)}{\sqrt{n}}\right) \quad (5)$$

where n is the sample size and t_ν is the one-tailed t statistic for a confidence level of 95% and degrees of freedom ν. The lower confidence limit on the geometric mean is calculated with the negative of the t statistic used for the upper confidence limit.

The arithmetic mean of a log-normal distribution is related to the distribution's geometric mean and geometric standard deviation by

$$\mu = \exp\left(\ln \eta + \frac{1}{2}(\ln \gamma)^2\right) \quad (6)$$

Substituting $UCL_{\bar{x}}$ for μ and UCL_{gm} for η, together with algebraic rearrangement of eq 6 yields

$$gsd_{f'} = \exp\left(\sqrt{2(\ln UCL_{\bar{x}} - \ln UCL_{gm})}\right) \quad (7)$$

where $gsd_{f'}$ is the geometric standard deviation of f', the log-normal distribution defined by arithmetic mean $UCL_{\bar{x}}$ and geometric mean UCL_{gm}. In other words, $gsd_{f'}$ is the geometric standard deviation of the distribution of upper confidence limits on all percentiles of the original distribution. Note that $gsd_{f'}$ does not correspond to the upper confidence limit on the geometric standard deviation of the original distribution (UCL_{gsd}) but rather is consistent with the distribution defined by upper confidence limits on the mean and geometric mean of the original distribution (f). This distinction is important because the UCL on a distribution's standard deviation defined by the χ^2 statistic takes into consideration that some percentiles may be lower than the observed value instead of only higher. Therefore, the textbook definition of the UCL on a standard deviation results in a larger value than the $gsd_{f'}$ as defined here. As a result, if the 95% upper confidence limit on the geometric standard deviation were used together with UCL_{gm}, an arithmetic mean that is greater than $UCL_{\bar{x}}$ would result. The gsd of f'' is calculated similarly from the lower confidence limits on the arithmetic and geometric means.

An example calculation of f' is given for a sample distribution f described by $n = 61$ observations, with gm = 5 mg/kg, and a gsd of 2.46. The arithmetic mean of this distribution is 7.5 mg/kg. The upper confidence limit on the mean ($UCL_{\bar{x}}$), calculated from eq 4, is 9.657 mg/kg. The upper confidence limit on the geometric mean (UCL_{gm}), calculated from eq 5, is 6.062 mg/kg. Equation 7 yields a $gsd_{f'}$ value of 2.625. Figure 2 shows the cumulative distribution functions of f and f'. A response goal can now be calculated for a distribution of contamination described by f', where UCL_{gm} and $gsd_{f'}$ are substituted in place of η and γ in eq 3.

Percentile values of f' calculated in the manner described above can be compared with the results of various methods of calculating UCLs on percentiles of f (*8*, *9*). Note that different formulas for calculating UCLs on percentiles give slightly different results, but methods described by Gilbert (*8*) and Stedinger (*9*) give comparable results to those obtained by the method used here. The method described here has the advantage of producing a log-normal distribution, whereas other formulations for calculating upper confidence limits on percentiles of log-normal distributions result in a distribution that deviates somewhat from log-normal. A log-normal distribution is a requirement for use of eq 3 to calculate a confidence response goal; however, mathematical equations could be derived for distributions other than the log-normal.

The confidence response goal is calculated from eq 3 by setting the pre-remediation mean value between the upper and lower confidence limits on the sample mean, calculating the reduction in exposure (α) for the desired CUG and solving eq 3 for c^*. In the simplest case, the Confidence response goal is calculated from a reduction in exposure equal to the desired post-remediation mean divided by the upper confidence limit on the pre-remediation mean ($UCL_{\bar{x}}$). However, this value should only be used when no

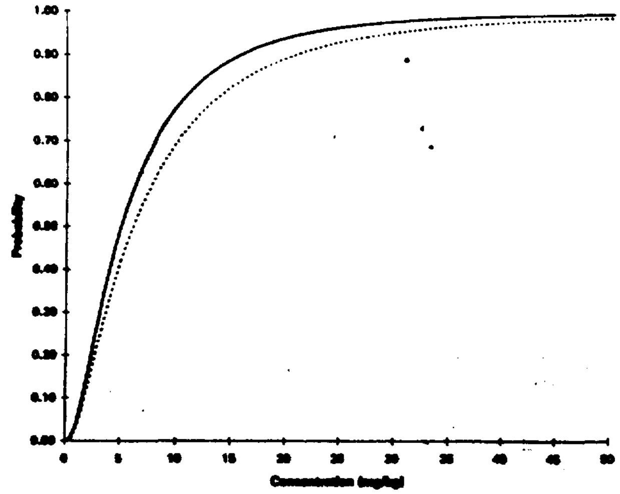

FIGURE 2. Cumulative log-normal distribution, f (solid curve), and the cumulative log-normal distribution defined by the 95% upper confidence limits on the mean and geometric mean of the data set defining f for a sample size of 61, f' (dashed curve).

lower value of the response goal is found by using any other pre-remediation mean estimate between the upper and lower confidence limits on the sample mean. The confidence response goal corresponds to the lowest value of the response goal that results for any estimate of the mean between the upper and lower confidence limits on the sample mean. This implies that although the "worst case" exposure occurs when the true mean contaminant concentration corresponds to the upper confidence limit on the sample mean, the worst case (meaning the lowest) response goal may correspond to a true mean lying at a point other than the upper confidence limit on the sample mean. This is demonstrated with example calculations below.

Example Calculations of Confidence Response Goals

The example calculations presented in this section are designed to capture the range of possible results that may occur when calculating CRGs.

Assume that we have a data set with 15 observations, with gm = 5 mg/kg, gsd = 4.4817 ($G = 1.5$), consistent with $\bar{x} = 15.40$ mg/kg. The desired post-remediation average concentration (or CUG) is 12.32 mg/kg. Using eqs 4, 5, and 7, we calculate $UCL_{\bar{x}} = 65.5$ mg/kg, $UCL_{gm} = 9.9$ mg/kg, and $gsd_{f'} = 7.0$. The desired ratio of reduction in exposure for an assumed mean at its upper confidence limit is 0.19 (12.32/65.5), and solving eq 3 with $c_0 = 0.1$ mg/kg yields a response goal of 77.5 mg/kg. In this case, the calculated value of 77.5 mg/kg is the minimum response goal that will be calculated for a pre-remediation mean between the upper and lower confidence limits on the sample mean, and the confidence response goal is therefore 77.5 mg/kg.

In contrast, consider a distribution with identical properties but consisting of hundreds of observations. This is an extreme example that will rarely occur in the field, but we include it here because it represents an end point in the calculation. Reduction in exposure is calculated from the arithmetic mean on the pre-remediation data set because for a large sample size the upper confidence limit and the sample mean are essentially equal. The value of the reduction in exposure is 0.8 (12.32/15.40) and solution of eq 3 yields a response goal of 167.5 mg/kg. In this example, limiting the number of samples to 15 results in a confidence

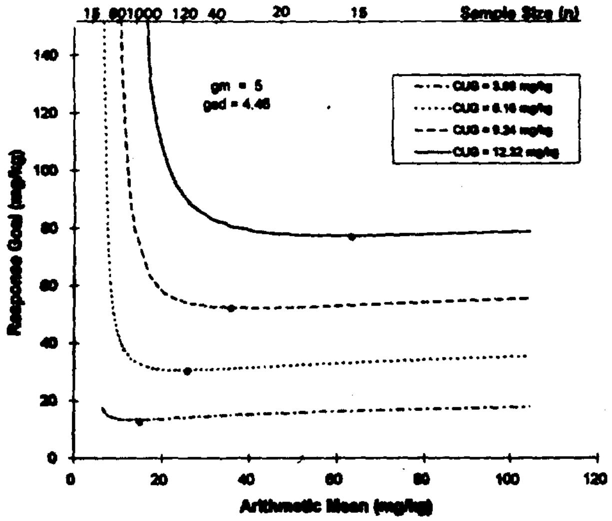

FIGURE 3. Calculated response goals for the first example given in the text as a function of the assumed mean of the data set where the assumed mean varies between the upper and lower confidence limits on the sample mean. Each assumed value of the mean also corresponds to an upper or lower confidence limit for some sample size. In this way, sample size can also be shown on the horizontal axis. Four cases are demonstrated for various cleanup goals (CUGs). The open circles correspond to the minima on the response goal curves or the confidence response goals.

response goal that is less than half that which would result with unlimited sampling (77.5 mg/kg versus 167.5 mg/kg). This ensures lower CRGs for cases characterized by fewer samples and, hence, higher uncertainty. This also demonstrates the tension that can exist between minimizing sampling costs and remediation costs.

To further illustrate this case and others, Figure 3 summarizes the response goal calculation as a function of the postulated arithmetic mean of the distribution and various CUG values for the example above. Response goals are calculated for four CUG values (12.32, 9.24, 6.16, and 3.08 mg/kg) as a function of possible pre-remediation arithmetic means for the distribution that may vary from the lower to upper confidence limits on the sample mean. Because the confidence limits on the mean are a function of sample size, postulated values of the mean that are intermediate between the sample mean and its confidence limits for a specific sample size are also equivalent to a confidence limit for a larger sample size. In this way, both the postulated mean and sample size can be shown on the horizontal axis, where the sample size is labeled at the mean value where its corresponding upper (or lower) confidence limit falls. Sample size is shown on this figure to illustrate the effect that it has on the confidence response goal.

A sample size of infinity corresonds to the confidence limits equaling the sample mean ($\mu = \bar{x}$). The postulated mean can fall between its upper and lower confidence limits, where these confidence limits broaden for decreasing sample sizes. Reduction in exposure (α) is the ratio of the CUG to the postulated mean. When the postulated mean is less than the CUG, α exceeds 1 and no response goal calculation is made. As before, a back fill/cover concentration of 0.1 mg/kg is used in the solution of eq 3. Confidence response goals, corresponding to the minima of the curves, are shown by the open circle symbols. Note that the curves must be truncated on both ends at the sample size, and the CRG corresponds to the minimum on the curve between its points of truncation. Increasing sample size will change the CRG if the points of truncation are moved beyond the open circle symbols that are shown such that the minimum falls at a new location. The minima on the curves are determined with an interative computer algorithm that approximates interval halving.

When the CUG equals 12.32 mg/kg, there is a simple relationship between the response goal and the sample size where n is greater than or equal to 15. As the number of samples decreases, the response goal drops. This is equivalent to stating that as the upper confidence limit on the sample mean increases due to decreasing sample size, the response goal decreases. The confidence response goal for any particular n value is the response goal calculated at the upper confidence limit on the mean for that sample size.

When the CUG equals 9.24 mg/kg, the minimum response goal calculated for pre-remediation mean values between the upper and lower confidence limit on the sample mean for $n = 15$ does not correspond to UCL_α at $n = 15$. Rather, the minimum in the curve of approximately 52.4 mg/kg occurs at a postulated mean of 35.8 mg/kg. This mean value corresponds to an upper confidence limit for a sample size of 31. In this case, whether the sample size is 15, 20, or 30, the confidence response goal is the same value, at 52.4 mg/kg. For a sample size of 41, the confidence response goal increases to 52.8 mg/kg, and for unlimited samples the confidence response goal increases to 69.3 mg/kg.

When the CUG equals 6.16 mg/kg, a similar case results where the confidence response goal of 30.7 mg/kg is found at the minimum in the curve corresponding to a postulated mean of 26.6 mg/kg, which would be the upper confidence limit for a sample size of 61. In this case, the number of samples makes little difference in the confidence response goal, as it will change from 30.7 mg/kg for sample sizes less than 60 to 32.4 mg/kg at $n = \infty$. Finally, when the CUG equals 3.08 mg/kg, the confidence response goal is approximately 13.3 mg/kg regardless of sample size.

A second example is used to further illustrate the calculation of confidence response goals. This example differs from the first example illustrated in Figure 3 only in that the gsd = 2.46 ($G = 0.9$). For a gm of 5 mg/kg, this is consistent with $\bar{x} = 7.5$ mg/kg. Four cases are shown in Figure 4, for CUGs of 6, 4.5, 3, and 1.5 mg/kg. The confidence response goals are shown as the minima in the curves by the open circle symbol.

An interesting case results when the CUG equals 1.5 mg/kg. Here the minimum in the curve falls on the lower confidence limit side of the sample mean, and the confidence response goal is approximately 4.58 mg/kg at a sample size of 10. As the sample size increases, the confidence response goal also increases to 4.75 mg/kg at $n = 41$ and to 5.16 mg/kg at $n = \infty$. In this case, uncertainty about the true mean of the distribution will require more remediation if the true mean is less than the sample mean and less remediation if the true mean is greater than the sample mean. Because we do not know the true mean, we set the confidence response goal to correspond to the worst case, and in this instance the worst case is where the true mean is less than the sample mean. This is illustrated in Figure 5 where two distributions are graphed. The top diagram shows the post-remediation distribution for the case where $n = \infty$ (truncated at 5.16 mg/kg), and the bottom diagram shows the post-remediation distribution that corresponds to f'' for $n = 15$ (truncated at the lower value

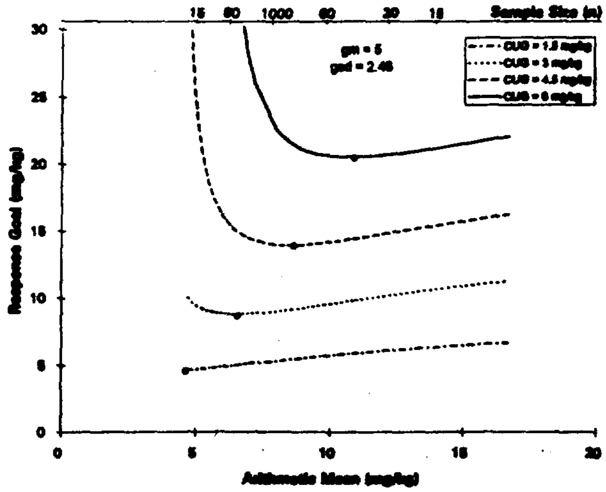

FIGURE 4. Calculated response goals for the second example given in the text as a function of the assumed mean of the data set where the assumed mean varies between the upper and lower confidence limits on the sample mean. Each assumed value of the mean also corresponds to an upper or lower confidence limit for some sample size. In this way, sample size can also be shown on the horizontal axis. Four cases are demonstrated for various cleanup goals (CUGs). The open circles correspond to the minima on the response goal curves or the confidence response goals.

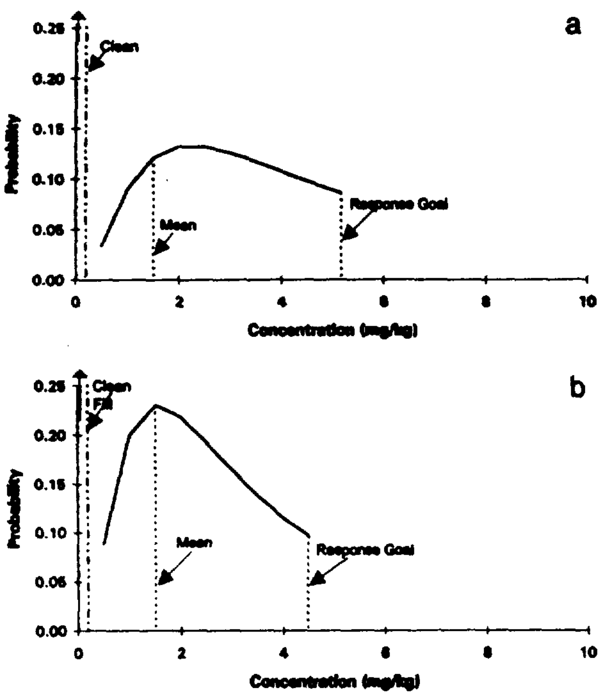

FIGURE 5. Log-normal distributions of concentrations truncated at their calculated response goals for (a) $n = \infty$ and (b) $n = 15$ corresponding to the curve labeled CUG = 1.5 mg/kg in Figure 4. These diagrams represent the situation where the confidence response goal for $n = 15$ falls on the lower confidence limit side of the sample mean. Uncertainty about the true mean of the distribution will require more remediation if the true mean is less than the sample mean. See text for discussion.

of 4.6 mg/kg). In both diagrams, the desired average post-remediation value of 1.5 mg/kg is shown as the line labeled mean. Note that the distribution corresponding to the lower confidence limit on the mean at $n = 15$ must be truncated at a lower value to obtain the same post-remediation average as the distribution corresponding to the true mean with $n = \infty$.

Discussion

When the true mean and standard deviation of a log-normal distribution are known as a result of a very large (greater than 200) sample size, the results of the response goal calculation described above can be checked by simple hand calculations. This is done by replacing the highest concentration values in the data set by values representing the level of contaminant expected in clean fill or in a cover and recalculating the average over the data set. This calculation is done successively, replacing the next highest value, until the re-calculated average meets the target or desired average. This is a "brute force" method for checking that the analytical methodology described here gives a correct answer.

Unfortunately, there is no analogous simple iterative calculation that can be used to check the value of the confidence response goal developed for considering the uncertainty inherent in smaller sample sizes and based on UCLs. This is because the confidence response goal is calculated for a hypothetical distribution that has a mean contaminant concentration different than the mean contaminant concentration of the data set, *e.g.*, it could be as high as the upper confidence limit on the mean. Since the observed data points do not describe this new distribution that has a mean at the upper confidence limit, the procedure described above of replacing high values in the data set and re-averaging does not result in the confidence response goal. That is why the mathematical approach described herein is needed.

There are at least three advantages to the analytical technique outlined here for the calculation of confidence response goals. First, the analytical technique allows a calculation that explicitly considers the uncertainties inherent in sampling, as described above.

The second advantage of the analytical approach over the simple hand calculation is that a response goal can be estimated even if it falls between two widely disparate data points. For example, suppose we had a sample with a concentration of 100 mg/kg and another with a concentration of 500 mg/kg, and the simple calculation of the response goal described above suggests that the sample at 500 mg/kg represents an area that must be remediated. However, we cannot determine which areas between 100 and 500 mg/kg should be remediated. That is, should an area with a concentration of 400 mg/kg be remediated? By using the analytical technique presented here to calculate a response goal, the samples at 100 and 500 mg/kg are assumed to form part of a continuous distribution, and a specific response goal at a concentration level between 100 and 500 mg/kg can be derived.

A third advantage of this general analytical approach is that it can be used together with various methods of assessing the concentration of contaminants in samples that have been determined analytically to be nondetectable. The assumption that the distribution of contamination is log-normal can be used as a basis to form a predictive model for nondetect values and thus incorporate additional information into the calculation of summary statistics of the data set and, thereby, the confidence response goals. For data sets that include nondetectable values, it can be assumed that those measurements above the detection limit represent a portion of a log-normal distribution from which the entire distribution can be constructed. Methods exist (*10*) to predict summary statistics for log-normal data sets that include nondetectable values at multiple detection limits. The method and computer program described in ref 10 can be used together with the analytical approach given here to further refine the calculation of the confidence response goal.

Case Study of PCBs at a Superfund Site

The confidence response goal approach has been applied at a midwestern Superfund site in a heavily industrialized area with 11 chemicals requiring cleanup, including PCBs, which resulted from the operation of several chemical and metal processing plants over a period of several decades. A portion of the site is in a residential area, and a risk-based CUG for PCBs in the residential area had been set by the U.S. EPA at 1325 μg/kg. Sample analyses for PCBs in one of the residential exposure units showed that concentrations ranged from nondetectable values to as high as 47 000 μg/kg, with over half (12/20) of the sampled locations exceeding the CUG. The sample mean of 8032 μg/kg (as well as the UCL) also exceeded the CUG.

A confidence response goal was calculated following the methodology outlined in this paper to determine the threshold concentration requiring remediation in order to comply with the CUG of 1325 μg/kg on average once remediation was complete. This calculation resulted in a CRG value of 6900 μg/kg. Eight out of 20 sample locations exceeded the CRG, indicating that a substantial portion of the exposure unit must be remediated to obtain the target risk goal.

In contrast, if the confidence response goal approach had not been used, and instead each area determined to exceed the CUG were remediated, there would have been a much different result. The area requiring remediation would have increased by approximately 50%, and the average concentration of PCBs following remediation would have been approximately 150 μg/kg rather than the 1325 μg/kg required by the risk assessment. This result would far exceed the target risk goal with substantial additional remediation costs.

The confidence response goal approach has been applied to 11 chemicals over 10 exposure units at this Superfund site, with an overall result that remediation volumes have been reduced by about 66% for a cost savings of approximately $40 million. About half of this savings was based on modified CUGs associated with a revised risk assessment, while half was based on applying those CUGs using the CRG approach. This has been accomplished with no compromise to the public health goals.

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Supporting Information Available

The mathematical derivation of equation 3 (similar to that published in a conference proceedings volume, but not easily obtainable) (8 pages) will appear following these pages in the microfilm edition of this volume of the journal. Photocopies of the supporting information from this paper or microfiche (105 × 148 mm, 24× reduction, negatives) may be obtained from Microforms Office, American Chemical Society, 1155 16th St. NW, Washington, DC 20036. Full bibliographic citation (journal, title of article, names of authors, inclusive pagination, volume number, and issue number) and prepayment, check or money order for $19.50 for photocopy ($21.50 foreign) or $12.00 for microfiche ($13.00 foreign), are required. Canadian residents should add 7% GST. Supporting information is available to subscribers electronically via the Internet at http://pubs.acs.org (WWW) and pubs.acs.org (Gopher).

Glossary of Symbols

c — contaminant concentration value corresponding to an observation

c_0 — concentration of the contaminant in the clean fill, back fill, or cover

c^* — contaminant concentration corresponding to the response goal, where all observations with concentrations greater than c^* must be remediated

f — log-normal distribution, also referred to as $f(c)$

$f(c)$ — log-normal distribution of concentrations c, also referred to as f

f' — log-normal distribution defined by the 95% upper confidence limits on the sample mean and geometric mean of the data set forming distribution f

f'' — log-normal distribution defined by the 95% lower confidence limits on the sample mean and geometric mean of the data set forming distribution f

$F(z)$ — area under the standard normal curve from 0 to z

$g(c)$ — arbitrary function of concentration

gm — sample geometric mean of a data set; derived by calculating the arithmetic mean of the natural logarithm of each observation in the data set and exponentiating the result

gsd — sample geometric standard deviation of a data set; derived by calculating the standard deviation of the natural logarithm of each observation in the data set and exponentiating the result

$\mathrm{gsd}_{f'}$ — geometric standard deviation of the distribution f'

G — natural logarithm of gsd, equivalent to the standard deviation of the natural logarithm of all observations

H — H statistic, used for calculating upper confidence limits on the arithmetic mean of data sets that form log-normal distributions; function of the confidence level (specified here to be 95%), the standard deviation of the logarithms of observations (G) and of the degrees of freedom (ν); also written as $H_{G,\nu}$; values tabulated in statistical textbooks (*7, 8*)

M — natural logarithm of gm, equivalent to the arithmetic mean of the natural logarithm of all observations

n — sample size, equal to the number of observations

t — t statistic, used for calculating upper confidence limits on the mean of data sets that form normal distributions; function of the confidence level (specified here to be 95%), and the degrees of freedom (ν); also written as t_ν; values tabulated in standard statistical textbooks

UCL_{gm} — 95% upper confidence limit on the geometric mean of the data set forming the distribution f

$UCL_{\bar{x}}$ — 95% upper confidence limit on the mean of the data set forming the distribution f

$\bar{x}$ — arithmetic sample mean of a data set

α — reduction in exposure, defined as the average of the post-remediation distribution of concentrations divided by the average of the pre-remediation distribution of concentrations (μ'/μ)

γ — geometric standard deviation of a distribution or the true geometric standard deviation of a population

δ — delta function, used to describe the distribution of contaminant concentrations in clean fill or back fill/cover that is added upon remediation

η — geometric mean of a distribution or the true geometric mean of a population

μ — arithmetic mean of a distribution, equivalent to the average value, or the true mean of a population

μ' — arithmetic mean of a post-remediation distribution

ν — degrees of freedom, equal to the sample size $(n) - 1$

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