APPENDIX A

STATISTICAL METHODS

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1.0 INTRODUCTION

Two estimates of exposure are used in the risk assessment process: (i) the mean, or central tendency (CT), exposure, and (ii) the reasonable maximum exposure (RME). The CT exposure scenario uses the mean value to represent probable exposure conditions. The RME scenario generally uses a conservative 95 percent upper confidence limit of the mean to estimate a reasonable maximum exposure. The determinations of the CT and RME estimates are statistically based and driven by characteristics of the data. Key factors determining the statistical methodologies employed include: (i) the probability distribution of the observed data (e.g., normal vs. lognormal, etc.), and (ii) the degree of censored data (non-detected results) present.

The following sections present the procedures used to determine the CT and RME values of the chemicals of potential concern (COPCs) in this risk assessment. A number of guidance documents will be consulted in developing the statistical methodologies including MOE (1997), USEPA (1989), USEPA (1992) updated by USEPA (2002), USEPA (1997), USEPA (2000), and USEPA (2003).

2.0 STATISTICAL PROCEDURES

The development of COPC exposure estimates for each parameter and area of concern is a three-step process consisting of (i) determining the percentage of non-detects present, (ii) data distribution testing, and (iii) selecting the appropriate statistical method for exposure estimate calculations.

The first step of the statistical evaluation is to determine the percentage of the non-detects present in each data set. Suggested approaches to account for the presence of non-detect analytical results are outlined in USEPA (2000), and USEPA (2002), and these guidelines are summarized in Table A.1.

The second step of the statistical analysis to establish COPC exposure estimates is to determine the data distribution. Each data set is tested for normality and lognormality using either the Shapiro-Wilk W-test (1965) (for sample sizes up to 50) or the Shapiro-Francia W'-test (1972) (for sample sizes of 50 to 100). Additional tests of normality for larger data sets, if needed, are presented in USEPA (2000).

Methods for determining the CT and RME values are discussed in USEPA 2002 (which updates USEPA 1992), USEPA 1997 and USEPA 2003. The alternative procedures suggested are listed in Table A.2. A summary of the selected statistical methods used to determine the CT and RME values, based on the observed distribution of the data and the proportion of non-detect values is given in Tables A.3 and A.4.

The following sections discuss the calculation procedures used to develop the CT and RME estimates. Section 2.1 deals with the statistical methods used for normally distributed data sets, Section 2.2 discusses the statistical methods used for the lognormally distributed data sets, and Section 2.3 discusses statistical methods used for non-normal data sets. Each section is organized into separate divisions to deal with the cases of a low degree of censored (non-detect) data (0 to 15 percent), moderately censored (16 to 50 percent), highly censored (51 to 75 percent), very highly censored (76 to 99 percent), and 100 percent non-detected data.

2.1 NORMAL DISTRIBUTION

2.1.1 UP TO 15 PERCENT NON-DETECTS

In order to calculate the CT and RME values, the non-detect values will be replaced with one-half the reported detection limit. The arithmetic mean and standard deviation of this substituted data set will be then calculated. The calculated mean is taken as the CT value. The RME value is established by calculating the 95 percent upper confidence limit (UCL) of the arithmetic mean for the normal distribution using the following equation.

$$95\%UCL = \bar{x} + t_{(0.05,n-1,1)} \bullet s / \sqrt{n}$$

Where:

$\bar{x}$	=	mean of the substituted data set;
$t_{(0.05,\,n\text{-}1,\,1)}$	=	student *t*-statistic for a one-tailed 95 percent confidence (α=0.05) and n-1 degrees of freedom;
s	=	standard deviation of the substituted data set; and
n	=	number of samples.

2.1.2 NON-DETECTS GREATER THAN 15 PERCENT UP TO 50 PERCENT

In this case, the mean and standard deviation of the censored data set are adjusted using Cohen's method, as recommended in USEPA 2002. This method is presented in McBean & Rovers (1998) and USEPA (2000). Cohen's method adjusts the sample mean and sample standard deviation to account for the censored data below the detection limit as follows.

Step 1) Compute the sample mean $\bar{x}_d$ using detected data only.

Step 2) Compute the sample variance s_d^2 using detected data only.

Step 3) Compute the two parameters *h* (proportion of non-detects) and γ as:

$$h = \frac{n - m}{n} \qquad \gamma = \frac{s_d^2}{(\bar{x} - DL)^2}$$

Where *m* is the number of detected data points, *n* is the total number of samples and DL is the detection limit.

Step 4) Determine the value of the parameter $\hat{\lambda}$ from the Table A.5 based on h and γ.

Step 5) Estimate the corrected sample mean ($\bar{x}$) and standard deviation (s) as:

$$\bar{x} = \bar{x}_d - \hat{\lambda}(\bar{x}_d - DL) \quad \text{and} \quad s = \sqrt{s_d^2 + \hat{\lambda}(\bar{x}_d - DL)^2}\ .$$

The Cohen-adjusted mean is taken as the CT value. The RME value is established using the Cohen-adjusted mean and standard deviation to calculate the 95 percent UCL of the arithmetic mean using the equation presented in Section 2.1.1.

2.1.3 NON-DETECTS GREATER THAN 50 PERCENT UP TO 74 PERCENT

When more than half of a data set consists of non-detect results, estimates of the mean value and standard deviation become uncertain. If the data set contains greater than 50 percent non-detects (up to 75 percent), the CT and RME values will be calculated using a bounding method estimating maximum values for the mean and 95 percent UCL, as described in Section 3.2 and Appendix A of USEPA (2002).

The CT value is calculated as the mean of the data set, substituting non-detect values with the full reported detection limit. This provides a conservative maximum value for the CT estimate.

For the RME value, an optimization process [USEPA's (2002) bounding method] is applied to find a conservative maximum bound for the 95 percent UCL of the arithmetic mean. This involved re-calculating the normal UCL (see Section 2.1.1) iteratively, allowing the non-detect values to vary between zero and the reported detection limit until a maximum value for the 95 percent UCL is obtained.

2.1.4 NON-DETECTS GREATER THAN 75 PERCENT UP TO 99 PERCENT

According to USEPA (2002), for highly censored data sets (greater than 75 percent non-detects), the recommended approach to calculate exposure estimates is to substitute non-detect results with their full detection limits and report the resulting exposure terms as values likely to be overestimated.

2.1.5 100 PERCENT NON-DETECTS

In any cases where all analytical data for a COPC are non-detect results, then the maximum detection limit is taken for both CT and RME scenarios.

2.2 LOGNORMAL DISTRIBUTION

USEPA (2003) presents three recommended methods for establishing CT and RME estimate from lognormally distributed data depending on the standard deviation of the log-transformed data. These methods are (i) the Student's *t* method, (ii) the Land (H-statistic) method, and (iii) the Chebyshev Inequality method.

The Student's *t* method is presented in Section 2.1.1. If the standard deviation of the lognormal data is small (less than 0.5), then USEPA recommends using the Student's *t* method.

The Land method is appropriate for calculating UCLs of lognormally distributed data. However, as USEPA (2002) notes, the method is very sensitive to deviations from lognormality, large variance or skewness of the dataset, and small datasets (fewer than thirty data points). The Land method can be used in conjunction with a modified Cohen's procedure (USEPA, 2002; Gilbert, 1987) to account for non-detect data.

The Chebyshev Inequality method may provide a more useful estimate (i.e., lower) of the UCL than obtained using the Land Method (USEPA, 2002). It is a distribution-free method that is applicable to a wide variety of data sets (not only lognormal data), as long as the skewness of the dataset is not large. The Chebyshev Inequality method using minimum variance unbiased estimators (MVUEs) of the mean and standard deviation of lognormal data sets is recommended for use by USEPA (2002). For small, moderately skewed datasets, a 99 percent UCL calculation using the Chebyshev Inequality is recommended (as opposed to the 95 percent value typically used).

A list of specific methods recommended for calculating RME estimates for lognormally distributed data sets are given in Table A.4 (USEPA, 2002).

2.2.1 UP TO 15 PERCENT NON-DETECTS

In order to calculate the CT and RME values, the non-detect values will be replaced with one-half the reported detection limit.

For the CT exposure estimate, the arithmetic mean of lognormally-distributed data ($\bar{x}$) is calculated as follows:

$$\bar{x} = e^{(\bar{y} + \frac{s_y^2}{2})}$$

Where:

$\bar{y}$	=	mean of the natural log-transformed, substituted data set; and
s_y^2	=	standard deviation of the natural log-transformed substituted data set.

If a calculated CT exposure estimate exceeded the corresponding RME estimate (see following), the CT exposure will be set equal to the RME estimate.

For the RME exposure estimate, the standard deviation of the log-transformed data will be calculated, and Table A.4 used to select the UCL method to use. The selected method will be either (i) the Student's t UCL (see Section 2.1.1 above), (ii) Land's H-UCL, or (iii) Chebyshev Inequality UCL.

Land's H-UCL is calculated as follows:

Step 1) Compute the arithmetic mean $\bar{x}_{\log}$ of the log-transformed data.

Step 2) Compute the standard deviation $s_{\log}$ of the log-transformed data.

Step 3) Look up the $H_{1-\alpha}$ statistic from Table A.6.

Step 4) Compute the one-sided $(1-\alpha)$ upper confidence limit on the mean as:

$$UCL_{1-\alpha} = e^{\left(\bar{x}_{\log} + \frac{s_{\log}^2}{2} + \frac{H_{1-\alpha} s_{\log}}{\sqrt{n-1}}\right)}$$

Where n is the number of samples.

The Chebyshev Inequality UCL is calculated as follows:

Step 1) Compute the arithmetic mean $\bar{x}_{\log}$ of the log-transformed data.

Step 2) Compute the variance $s_{\log}^2$ of the log-transformed data.

Step 3) Look up the g_n statistic from Table A.7.

Step 4) Compute the minimum-variance unbiased estimator (MVUE) of the population mean for a lognormal distribution as:

$$\hat{\mu}_{\log} = e^{\bar{x}_{\log} g_n \frac{s_{\log}^2}{2}}$$

Where n is the number of samples.

Step 5) Calculate the MVUE of the variance of this mean as:

$$\sigma_{\mu}^{2} = e^{2\bar{x}_{\log}} \left[\left(g_n \frac{s_{\log}^{2}}{2} \right)^{2} - g_n \left(\frac{n-2}{n-1} s_{\log}^{2} \right) \right].$$

Step 6) Compute the one-sided $(1-\alpha)$ upper confidence limit on the mean as:

$$UCL_{1-\alpha} = \hat{\mu}_{\log} + \sqrt{\left(\frac{1}{\alpha} - 1 \right) \sigma_{\mu}^{2}}.$$

2.2.2 NON-DETECTS GREATER THAN 15 PERCENT UP TO 50 PERCENT

When a moderate proportion of non-detect results is present in a data set, in order to calculate the CT estimate, a correction for non-detects will be made using Gilbert's modified Cohen's method (USEPA, 2002). Gilbert (1987, page 182) suggests extending Cohen's method to account for non-detect values in lognormally distributed concentrations. Cohen's method (USEPA, 2000, page 4-43) assumes the data are normally distributed, so it must be applied to the log-transformed concentration values. If $\hat{\mu}_y$ and $\hat{\sigma}_y$ are the Cohen-corrected (see Section 2.1.2) sample mean and standard deviation, respectively, of the log-transformed concentrations, then the corrected estimates of the mean and standard deviation of the underlying lognormal distribution can be obtained from the following expressions:

$$\hat{\mu} = e^{\left(\hat{\mu}_y + \frac{\hat{\sigma}_y^2}{2} \right)}$$

$$\hat{\sigma} = \hat{\mu} \sqrt{e^{\hat{\sigma}_y^2} - 1}$$

This method assumes a single detection level for all the data values. During CT calculations, if the detection limit varied, then the highest detection limit will be used for the calculations to provide a conservative estimate.

If a calculated CT exposure estimate exceeded the corresponding RME estimate (see following), the CT exposure will be set equal to the RME estimate.

For the RME value, USEPA's bounding methodology (2002) is applied to untransformed data to find a maximum value for the mean, standard deviation, and skewness. The 95 percent UCL is then calculated using Hall's Bootstrap.

The use of Gilbert's modified Cohen's method for lognormal data is evaluated for use in calculating RME estimates for moderately censored data sets. However, attempts to use the procedure in conjunction with the lognormal UCL methods (e.g., Land's method, Chebyshev Inequality) most often resulted with unusable values. This resulted from either calculating UCLs much higher than the maximum data point observed, or by data characteristics being unsuitable for the required calculation (e.g., needing to use a Cohen's parameter λ that is far outside existing tabulated values for this method). As a result of persistent issues with these methods, RME estimates for lognormal, moderately censored data will be calculated using Hall's Bootstrap procedure. This procedure takes into account sample bias and skewness (such as present in lognormal distributions), and may be used with a bounding methodology to provide upper bonds on the UCL (USEPA, 2002). Hall's Bootstrap is calculated as follows.

Step 1) Compute the arithmetic mean $\bar{x}$.

Step 2) Compute the standard deviation s.

Step 3) Compute the skewness k.

Step 4) Re-sample the data a very large number of times, and calculate the each bootstrap set's mean $\bar{x}_b$, standard deviation s_b and skewness k_b.

Step 5) For each bootstrap set, calculate the studentized mean:

$$W = \frac{(\bar{x}_b - \bar{x})}{s_b}$$

Step 6) For each bootstrap set, calculate Hall's statistic:

$$Q = W + \frac{k_b W^2}{3} + \frac{k_b^2 W^3}{27} + \frac{k_b}{6n}$$

Step 7) Sort all the Q values (lowest to highest) and select the lower α^{th} quantile of the B re-sample sets. This is the $(\alpha B)^{th}$ lowest value (e.g., for 10,000 resample sets, and an α=0.05, select the 500th lowest value).

Step 8) Compute the one-sided $(1-\alpha)$ upper confidence limit on the mean as:

$$W(Q)=\frac{3}{k}\left[\sqrt[3]{1+\left(Q_{\alpha}-\frac{k}{6n}\right)}-1\right]$$

Where n is the number of samples.

Step 9) Compute the one-sided $(1-\alpha)$ upper confidence limit on the mean as:

$$UCL_{1-\alpha}=\overline{x}-W(Q_{\alpha})s.$$

In calculating Hall's bootstrap, five replicate calculations of the ten-thousand resample sets each will be generated, and the median UCL value used. These replicates will be used to determine whether or not each given data set is sensitive to small differences with the random re-sampling algorithm used by the procedure.

2.2.3 NON-DETECTS GREATER THAN 50 PERCENT UP TO 74 PERCENT

In order to calculate exposure estimates for highly-censored data sets (i.e., greater than 50 percent non-detect up to 75 percent), conservative bounding assumptions will be made, as described below.

The CT value is determined by substituting the full detection limit for non-detect values and applying a bootstrap re-sampling procedure. The bootstrap is carried out using 2,000 re-sampled data sets of the same sample size as the original data set, and the CT estimate is then taken as the average of the bootstrap means.

In this case of a highly censored data set, Hall's Bootstrap procedure fails with increasing degrees of non-detect data due to undefined skewness values if a re-sampled data set by random chance contains only non-detects. For the RME value, USEPA's Bootstrap t methodology (2003) will therefore be applied to calculate the 95 percent UCL. A modified bounding methodology is applied by considering four non-detect substitution scenarios: i) zero, ii) one-half detection limit, iii) full detection limit, and iv) alternating zero and full detection limit. These scenarios will be considered because attempting bounding procedures on each individual re-sample set in computationally impractical. The bootstrap t calculation is applied under each of the four scenarios and the largest resulting UCL will be selected as the RME estimate.

The bootstrap t is calculated as follows (USEPA, 2003):

Step 1) Calculate the arithmetic mean $\bar{x}$ of the original data.

Step 2) Re-sample the original data a very large number of times (in this case thousands of times) and calculate each resample set's mean ($\bar{x}_b$) and standard deviation (s_b).

Step 3) For each re-sample set calculate the value.

$$t_b = \frac{(\bar{x}_b - \bar{x})}{s_b} \times \sqrt{n}$$

Where n is the number of samples.

Step 4) Sort the t_b values from the lowest to the highest, and select the pivotal quantity $t_{(\alpha*N)}$, where N is the number of bootstrap sets (e.g., if 10,000 bootstrap sets are generated and α=0.05, select the 500th lowest t_b value)

Step 5) Calculate the UCL of the population mean as:

$$UCL = \bar{x} - \frac{t_{(\alpha \bullet N)} s}{\sqrt{n}}$$

2.2.4 NON-DETECTS GREATER THAN 75 PERCENT UP TO 99 PERCENT

For very highly censored data sets (greater than 75 percent non-detects), USEPA (2002) recommends calculating exposure estimates substituting non-detects with their full detection limits, and reporting the resulting values as likely to be overestimated. The CT value is calculated as the arithmetic mean of a lognormal distribution (introduced in Section 2.2.1), setting non-detects as their detection limits. If a calculated CT exposure estimate exceeded the corresponding RME estimate (see following), the CT exposure is set equal to the RME estimate. For the RME calculation, the non-detects will be substituted with the full detection limit, the standard deviation of the log-transformed data calculated, and Table A.4 will be consulted to select an appropriate UCL method. The selected methods are presented in Section 2.1.1 (Student's t method) and Section 2.2.1 (Land's Method and Chebyshev Inequality Procedure).

2.2.5 100 PERCENT NON-DETECTS

As for the normal case, in any situations where all analytical data for a COPC with a lognormal distribution will be non-detect results, then the maximum detection limit will be taken for both CT and RME scenarios.

2.3 NON-NORMAL DATASETS

For any data sets that will be neither normally, nor lognormally distributed, the non-parametric/distribution-free methods presented in USEPA (2002) will be used to calculate CT and RME exposures. The specific methods applied are presented below.

2.3.1 UP TO 15 PERCENT NON-DETECTS

For the CT exposure estimate, the arithmetic mean is calculated substituting non-detects with one-half the detection limit and using a bootstrap method to estimate the arithmetic mean. The bootstrap is carried out using 2,000 re-sampled data sets of the same sample size as the original data set. The CT value is then taken as the average of the bootstrap means.

For the RME exposure estimate, non-detects will be substituted with one-half the detection limit, and the standard deviation calculated. If the standard deviation is below 0.75 and the number of samples is 30 or greater, then the adjusted central limit theorem (CLT) UCL is calculated. Otherwise, Hall's bootstrap 95-UCL is used.

If sample size is sufficiently large, the Central Limit Theorem (CLT) states that the mean will be normally distributed, no matter how complex the underlying distribution of concentrations might be (USEPA, 2002). An adjusted CLT UCL method is presented in USEPA (2002) and is calculated as follows.

Step 1) Compute the arithmetic mean $\bar{x}$.

Step 2) Compute the standard deviation s.

Step 3) Compute the skewness β.

Step 4) Let z_α be the $(1-\alpha)^{th}$ quantile of the standard normal distribution (for 95 percent confidence, $z_\alpha = 1.645$).

Step 5) Compute the one-sided $(1-\alpha)$ upper confidence limit on the mean as:

$$UCL_{1-\alpha} = \bar{x} + (z_\alpha + \frac{\beta}{6\sqrt{n}}(1 + 2z_\alpha^2))\frac{s}{\sqrt{n}}$$

Where n is the number of samples.

The Hall's Bootstrap procedure is calculated as described in Section 2.2.2.

2.3.2 NON-DETECTS GREATER THAN 15 PERCENT AND LESS THAN 50 PERCENT

For CT exposure estimates, a conservative approach is taken substituting non-detects with the full detection limit and calculating the bootstrap arithmetic mean (see Section 2.3.1).

For RME exposure estimates, Hall's bootstrap procedure (see Section 2.2.2) is used, applying bounding methodology to find maximum mean, standard deviation and skewness values for the original data set prior to re-sampling. These bounded estimates will be used to calculate the Hall's Bootstrap UCL for the data using 5 sets of 10,000 resamples each (as in Section 2.3.1), and the median of these five UCLs taken as the RME estimate.

2.3.3 NON-DETECTS GREATER THAN 50 PERCENT UP TO 75 PERCENT

For CT exposure estimates, the conservative method used for the moderately censored case (described in Section 2.3.2) is used. For RME exposure estimates, the Bootstrap *t* method with modified bounding procedure described in Section 2.2.3 is applied.

2.3.4 NON-DETECTS GREATER THAN 75 PERCENT UP TO 99 PERCENT

As noted for the normal (Section 2.1.4) and lognormal (Section 2.2.4) cases for very highly censored data sets (greater than 75 percent non-detects), USEPA (2002) recommends substituting non-detects with their full detection limits and reporting exposure estimates as likely to be overestimated. Both CT and RME values will be calculated accordingly, as follows.

For CT exposure estimates, a conservative approach is taken substituting non-detects with the full detection limit and calculating the bootstrap arithmetic mean (see Section 2.3.1). This is the same method used for the moderately censored 15 to 50 percent non-detect case (Section 2.3.2).

For RME estimates, the non-detects will be substituted with the full detection limit and Bootstrap *t* is used to calculate the UCL (refer to Section 2.2.3).

2.3.5 100 PERCENT NON-DETECTS

In any cases where all analytical data for a COPC will be non-detect results, then the maximum detection limit is taken for both CT and RME estimates.

3.0 MAXIMUM DETECTED VALUE

USEPA (1992 and 2002) allow an optional use of the maximum observed concentrations for the RME estimate in cases where the calculated UCL exceeds the maximum value. However, USEPA (2002) warns that this may not be appropriate for data sets with very small sample sizes, because the observed maximum may be below the population mean.

If the RME estimate calculated using any of the statistical methods presented in Section 2.0 is larger than the maximum detected value, then the maximum detected value is used for the RME.

4.0 REFERENCES

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TABLE A.1

GUIDELINES FOR ANALYZING DATA WITH NON-DETECTS [1]

Percentage of Non-detects	*Statistical Analysis Method*
<15%	Replace non-detects with detection limit/2, detection limit, or a very small number.
15% - 50%	Trimmed mean, Cohen's adjustment, Winsorized mean and standard deviation, bounding method[2], probability substitution based on specific distribution[2].
>50% - 90%	Use tests for proportions, bounding method[2][3].

Notes:

(1) adapted from USEPA, (2000), *Guidance for Data Quality Assessment Practical Methods for Data Analysis EPA QA/G-9*, EPA/600/R-96/084, July 2000.

(2) USEPA, (2002), *Calculating Upper Confidence Limits for Exposure Point Concentrations at Hazardous Waste Sites*, Office of Emergency and Remedial Response, OSWER 9285.6-10, December 2002.

(3) When greater than 75 percent non-detects present and the sample size is small (less than five samples), the bounding method should be conservatively applied setting non-detects at the detection limit (USEPA, 2002).

TABLE A.2

RECOMMENDED METHODS FOR CALCULATING UPPER CONFIDENCE LIMITS (UCLs)

Method	Applicability	Advantages	Disadvantages	Reference
(i) *For Normal or Lognormal Distributions*				
Student's *t*	means normally distributed, samples random	simple, robust if *n* is large	distribution of means must be normal	Gilbert 1987; EPA 1992
Land's *H*	lognormal data, small variance, large *n*, samples random	good coverage[(1)]	sensitive to deviations from lognormality, produces very high values for large variance or small *n*	Gilbert 1987; EPA 1992
Chebyshev Inequality (MVUE)	skewness and variance small or moderate, samples random	often smaller than Land	may need to resort to higher confidence levels for adequate coverage	Singh *et al*. 1997
Wong	gamma distribution	second order accuracy[(2)]	requires numerical solution of an improper integral	Schulz and Griffin 1999; Wong 1993
(ii) *Nonparametric/Distribution-free Methods*				
Central Limit Theorem - Adjusted	large *n*, samples random	simple, robust	sample size may not be sufficient	Gilbert 1987; Singh *et al*. 1997
Bootstrap *t* Resampling	sampling is random and representative	useful when distribution cannot be identified	inadequate coverage for some distributions; computationally intensive	Singh *et al*. 1997; Efron 1982
Hall's Bootstrap Procedure	sampling is random and representative	useful when distribution cannot be identified; takes bias and skewness into account	inadequate coverage for some distributions; computationally intensive	Hall 1988; Hall 1992; Manly 1997; Schultz and Griffin 1999
Jackknife Procedure	sampling is random and representative	useful when distribution cannot be identified	inadequate coverage for some distributions; computationally intensive	Singh *et al*. 1997
Chebyshev Inequality	skewness and variance small or moderate, samples random	useful when distribution cannot be identified	inappropriate for small sample sizes when skewness or variance is large	Singh *et al*. 1997; EPA 2000c

Notes:

This Table was taken from USEPA, 2002.

(1) Coverage refers to whether a UCL method performs in accordance with its definition.

(2) As opposed to maximum likelihood estimation, which offers first order accuracy.

TABLE A.3

STATISTICAL METHODS USED FOR DETERMINING EXPOSURE ESTIMATES UNDER CENTRAL TENDENCY (CT) AND REASONABLE MAXIMUM EXPOSURE (RME) SCENARIOS

Percentage of Non-detect Values	*Data Distribution*		
	Normal	*Lognormal*	*Not Normal*
I) Central Tendency (CT) Exposure Scenarios			
0-15 percent	Substitute non-detect results with one-half detection limit. Calculate arithmetic mean.	Substitute non-detect results with one-half detection limit. Calculate arithmetic mean of lognormal distribution.	Substitute non-detect results with one-half detection limit. Calculate arithmetic mean of 2000 bootstrap resample set means.
>15-50 percent	Use Cohen's method to determine non-detect-adjusted estimate of arithmetic mean.	Use Gilbert's modified Cohen's method to determine non-detect-adjusted estimate of arithmetic mean for lognormal data.	Substitute non-detect results with full detection limit. Calculate arithmetic mean of 2000 bootstrap resample set means.
>50-74 percent	Substitute non-detect results with full detection limit. Calculate arithmetic mean.	Substitute non-detect results with full detection limit. Calculate arithmetic mean of 2000 bootstrap resample set means.	Substitute non-detect results with full detection limit. Calculate arithmetic mean of 2000 bootstrap resample set means.
>75-99 percent	Substitute non-detect results with full detection limit. Calculate arithmetic mean.	Substitute non-detect results with full detection limit. Calculate arithmetic mean of lognormal distribution.	Substitute non-detect results with full detection limit. Calculate arithmetic mean of 2000 bootstrap resample set means.
100 percent	Use maximum detection limit.	Use maximum detection limit.	Use maximum detection limit.

TABLE A.3

STATISTICAL METHODS USED FOR DETERMINING EXPOSURE ESTIMATES UNDER CENTRAL TENDENCY (CT) AND REASONABLE MAXIMUM EXPOSURE (RME) SCENARIOS

Percentage of Non-detect Values	*Data Distribution*		
	Normal	*Lognormal*	*Not Normal*
II) Reasonable Maximum Exposure (RME) Scenarios [(1)]			
0-15 percent[(2)]	Substitute non-detect results with one-half detection limit. Calculate Student's *t* 95-percent UCL of arithmetic mean.	Substitute non-detect results with one-half detection limit. Calculate standard deviation of log-transformed data. Use Table D.4 to select UCL method.	Substitute non-detect results with one-half detection limit. If *s* >0.75 and n>29: Use Adjusted Central Limit Theorem 95-percent UCL of mean. Otherwise, calculate Hall's bootrap 95-UCL.
>15-50 percent[(2)]	Use Cohen's method to determine non-detect-adjusted estimates of mean and standard deviation. Calculate Student's *t* 95-percent UCL of arithmetic mean.	Use Cohen's method to determine non-detect-adjusted estimates of mean and standard deviation of log-transformed data. Use Table D.4 to select UCL method.	Use bounding methodology[(3)] to find maximum mean, standard deviation and skewness. Calculate Hall's bootstrap 95-percent UCL.
>50-74 percent[(2)]	Use a bounding methodology[(3)] to find maximum Student's *t* 95-percent UCL of arithmetic mean.	Considering data set with ND=0, ND=0.5 DL, ND=DL and alternating NDs 0 and DL. Calculate bootstrap-*t* 95-percent UCL for each of the four data sets. Select the largest value as "bounded" UCL.	Considering data set with ND=0, ND=0.5 DL, ND=DL and alternating NDs 0 and DL. Calculate bootstrap-*t* 95-percent UCL for each of the four data sets. Select the largest value as "bounded" UCL.
>75-99 percent[(2)]	Substitute non-detects with their full detection limit. Calculate Student's *t* UCL of arithmetic mean (likely to be overestimated - per USEPA 2002).	Substitute non-detects with their full detection limit. Calculate standard deviation of log-transformed data. Use Table D.4 to select UCL method (likely to be overestimated - per USEPA 2002).	Substitute non-detects with their full detection limit. Calculate bootstrap-*t* 95-percent UCL (likely to be overestimated - per USEPA 2002).
100 percent	Use maximum detection limit.	Use maximum detection limit.	Use maximum detection limit.

Notes:

(1) RMEs are calculated as 95 percent upper confidence limits of the mean. Specific UCL methods were chosen based on Figure 1 and the text of USEPA (2002) and (2003).

(2) As per USEPA 2002, if the calculated UCL value exceeds the maximum detected value and a sufficient number of samples have been collected to meet data quality objectives, then the maximum detected value is used for the UCL.

(3) See Appendix A of USEPA 2002 for description of bounding methodology (note that "Step 9" of the appendix should say "less than", not "greater than").

(4) For Student's *t* UCL, use Cohen's method; for Land's H UCL, use Gilbert's modified Cohen's method; for Chebyshev UCL, use Cohen's method on log-transformed data.

TABLE A.4

95 PERCENT UPPER CONFIDENCE LIMIT (UCL) CALCULATION METHODS FOR LOGNORMAL DATA

Standard deviation of log-transformed data (s)	*Number of Samples (n)*	*Selected Upper Confidence Limit Method* [1]
$0 \leq s < 0.5$	For all n (≥ 5)	Student's *t* UCL
$0.5 \leq s < 1.0$	For all n	Land's H-UCL
$1.0 \leq s < 1.5$	$n < 25$ $n \geq 25$	Chebyshev UCL (95% MVUE) Land's H-UCL
$1.5 \leq s < 2.0$	$n < 20$ $20 \leq n \leq 50$ $n \geq 50$	Chebyshev UCL (99% MVUE) Chebyshev UCL (95% MVUE) Land's H-UCL
$2.0 \leq s < 2.5$	$n < 25$ $25 \leq n \leq 70$ $n \geq 70$	Chebyshev UCL (99% MVUE) Chebyshev UCL (95% MVUE) Land's H-UCL
$2.5 \leq s < 3.0$	$n < 30$ $30 \leq n \leq 70$ $n \geq 70$	Chebyshev UCL (max of 99% MVUE or 99% mean) Chebyshev UCL (max of 95% MVUE or 95% mean) Land's H-UCL
$s \geq 3.0$	Small n $n > 100$	Further investigation required Land's H-UCL

Note:

(1) Source: Table A1 of USEPA (2003) -- ProUCL User's Guide Version 2.1, February, 2003.

TABLE A.5

VALUES OF LAMBDA (λ) FOR COHEN'S METHOD

λ	Percentage of Non-detects (h) 0.01	0.05	0.10	0.15	0.25	0.40	0.50
0.01	0.0102	0.0530	0.1111	0.1747	0.3205	0.5989	0.8403
0.05	0.0105	0.0547	0.1143	0.1793	0.3279	0.6101	0.8540
0.10	0.0110	0.0566	0.1180	0.1848	0.3366	0.6234	0.8703
0.15	0.0113	0.0584	0.1215	0.1898	0.3448	0.6361	0.8860
0.20	0.0116	0.0600	0.1247	0.1946	0.3525	0.6483	0.9012
0.30	0.0122	0.0630	0.1306	0.2034	0.3670	0.6713	0.9300
0.40	0.0128	0.0657	0.1360	0.2114	0.3803	0.6927	0.9570
0.50	0.0133	0.0681	0.1409	0.2188	0.3928	0.7129	0.9826
0.60	0.0137	0.0704	0.1455	0.2258	0.4045	0.7320	1.0070
0.70	0.0142	0.0726	0.1499	0.2323	0.4156	0.7502	1.0303
0.80	0.0146	0.0747	0.1540	0.2386	0.4261	0.7676	1.0527
0.90	0.0150	0.0766	0.1579	0.2445	0.4362	0.7844	1.0743
1.00	0.0153	0.0785	0.1617	0.2502	0.4459	0.8005	1.0951
1.10	0.0157	0.0803	0.1653	0.2557	0.4553	0.8161	1.1152
1.20	0.0160	0.0820	0.1688	0.2610	0.4643	0.8312	1.1347
1.30	0.0164	0.0836	0.1722	0.2661	0.4730	0.8458	1.1537
1.40	0.0167	0.0853	0.1754	0.2710	0.4815	0.8600	1.1721
1.50	0.0170	0.0868	0.1786	0.2758	0.4897	0.8738	1.1901
1.60	0.0173	0.0883	0.1817	0.2805	0.4977	0.8873	1.2076
1.70	0.0176	0.0898	0.1846	0.2851	0.5055	0.9005	1.2248
1.80	0.0179	0.0913	0.1876	0.2895	0.5132	0.9133	1.2415
1.90	0.0181	0.0927	0.1904	0.2938	0.5206	0.9259	1.2579
2.00	0.0184	0.0940	0.1932	0.2981	0.5279	0.9382	1.2739
2.10	0.0187	0.0954	0.1959	0.3022	0.5350	0.9502	1.2897
2.20	0.0189	0.0967	0.1986	0.3062	0.5420	0.9620	1.3051
2.30	0.0192	0.0980	0.2012	0.3102	0.5488	0.9736	1.3203
2.40	0.0194	0.0992	0.2037	0.3141	0.5555	0.9850	1.3352
2.50	0.0197	0.1005	0.2062	0.3179	0.5621	0.9962	1.3498
2.60	0.0199	0.1017	0.2087	0.3217	0.5686	1.0072	1.3642
2.70	0.0202	0.1029	0.2111	0.3254	0.5750	1.0180	1.3784
2.80	0.0204	0.1040	0.2135	0.3290	0.5812	1.0287	1.3924
2.90	0.0206	0.1052	0.2158	0.3326	0.5874	1.0392	1.4061

TABLE A.5

VALUES OF LAMBDA (λ) FOR COHEN'S METHOD

	Percentage of Non-detects (h)						
λ	***0.01***	***0.05***	***0.10***	***0.15***	***0.25***	***0.40***	***0.50***
3.00	0.0209	0.1063	0.2182	0.3361	0.5935	1.0495	1.4197
3.10	0.0211	0.1074	0.2204	0.3396	0.5995	1.0597	1.4330
3.20	0.0213	0.1085	0.2227	0.3430	0.6054	1.0697	1.4462
3.30	0.0215	0.1096	0.2249	0.3464	0.6112	1.0796	1.4592
3.40	0.0217	0.1107	0.2270	0.3497	0.6169	1.0894	1.4720
3.50	0.0219	0.1118	0.2292	0.3529	0.6226	1.0990	1.4847
3.60	0.0221	0.1128	0.2313	0.3562	0.6282	1.1086	1.4972
3.70	0.0223	0.1138	0.2334	0.3594	0.6337	1.1180	1.5096
3.80	0.0225	0.1148	0.2355	0.3625	0.6391	1.1273	1.5218
3.90	0.0227	0.1158	0.2375	0.3656	0.6445	1.1364	1.5339
4.00	0.0229	0.1168	0.2395	0.3687	0.6498	1.1455	1.5458
4.10	0.0231	0.1178	0.2415	0.3717	0.6551	1.1545	1.5577
4.20	0.0233	0.1188	0.2435	0.3747	0.6603	1.1634	1.5693
4.30	0.0235	0.1197	0.2454	0.3777	0.6654	1.1722	1.5809
4.40	0.0237	0.1207	0.2473	0.3806	0.6705	1.1809	1.5924
4.50	0.0239	0.1216	0.2492	0.3836	0.6755	1.1895	1.6037
4.60	0.0241	0.1225	0.2511	0.3864	0.6805	1.1980	1.6149
4.70	0.0242	0.1235	0.2530	0.3893	0.6855	1.2064	1.6260
4.80	0.0244	0.1244	0.2548	0.3921	0.6903	1.2148	1.6370
4.90	0.0246	0.1253	0.2567	0.3949	0.6952	1.2230	1.6479
5.00	0.0248	0.1262	0.2585	0.3977	0.7000	1.2312	1.6587
5.10	0.0249	0.1270	0.2603	0.4004	0.7047	1.2394	1.6694
5.20	0.0251	0.1279	0.2621	0.4031	0.7094	1.2474	1.6800
5.30	0.0253	0.1288	0.2638	0.4058	0.7141	1.2554	1.6905
5.40	0.0255	0.1296	0.2656	0.4085	0.7187	1.2633	1.7010
5.50	0.0256	0.1305	0.2673	0.4111	0.7233	1.2711	1.7113
5.60	0.0258	0.1313	0.2690	0.4137	0.7278	1.2789	1.7215
5.70	0.0260	0.1322	0.2707	0.4163	0.7323	1.2866	1.7317
5.80	0.0261	0.1330	0.2724	0.4189	0.7368	1.2943	1.7418
5.90	0.0263	0.1338	0.2741	0.4215	0.7412	1.3019	1.7518
6.00	0.0264	0.1346	0.2757	0.4240	0.7456	1.3094	1.7617

Source: McBean & Rovers, 1998

TABLE A.6

VALUES OF H(0.95) FOR LAND'S METHOD

Standard deviation of log-transformed data (S_{log})	*Number of Samples*												
	3	*5*	*7*	*10*	*12*	*15*	*21*	*31*	*51*	*101*	*301*	*601*	*1001*
0.10	2.750	2.035	1.886	1.802	1.775	1.749	1.722	1.701	1.684	1.670	1.659	1.656	1.654
0.20	3.295	2.198	1.992	1.881	1.843	1.809	1.771	1.742	1.718	1.697	1.680	1.674	1.671
0.30	4.109	2.402	2.125	1.977	1.927	1.882	1.833	1.793	1.761	1.733	1.709	1.700	1.696
0.40	5.220	2.651	2.282	2.089	2.026	1.968	1.905	1.856	1.813	1.777	1.746	1.734	1.728
0.50	6.495	2.947	2.465	2.220	2.141	2.068	1.989	1.928	1.876	1.830	1.790	1.776	1.769
0.60	7.807	3.287	2.673	2.368	2.271	2.181	2.085	2.010	1.946	1.891	1.843	1.825	1.816
0.70	9.120	3.662	2.904	2.532	2.414	2.306	2.191	2.102	2.025	1.960	1.902	1.881	1.870
0.80	10.43	4.062	3.155	2.710	2.570	2.443	2.307	2.202	2.112	2.035	1.968	1.944	1.931
0.90	11.74	4.478	3.420	2.902	2.738	2.589	2.432	2.310	2.206	2.117	2.040	2.012	1.997
1.00	13.05	4.905	3.695	3.103	2.915	2.744	2.564	2.423	2.306	2.205	2.117	2.085	2.068
1.25	16.33	6.001	4.426	3.639	3.389	3.163	2.923	2.737	2.580	2.447	2.330	2.288	2.266
1.50	19.60	7.120	5.184	4.207	3.896	3.612	3.311	3.077	2.881	2.713	2.566	2.514	2.486
1.75	22.87	8.250	5.960	4.795	4.422	4.081	3.719	3.437	3.200	2.997	2.820	2.757	2.723
2.00	26.14	9.387	6.747	5.396	4.962	4.564	4.141	3.812	3.533	3.295	3.088	3.013	2.974
2.50	32.69	11.67	8.339	6.621	6.067	5.557	5.013	4.588	4.228	3.920	3.650	3.553	3.503
3.00	39.23	13.97	9.945	7.864	7.191	6.570	5.907	5.388	4.947	4.569	4.238	4.119	4.057
3.50	45.77	16.27	11.56	9.118	8.326	7.596	6.815	6.201	5.681	5.233	4.842	4.700	4.627
4.00	52.31	18.58	13.18	10.38	9.469	8.630	7.731	7.024	6.424	5.908	5.456	5.293	5.208
4.50	58.85	20.88	14.80	11.64	10.62	9.669	8.652	7.854	7.174	6.590	6.077	5.892	5.796
5.00	65.39	23.19	16.43	12.91	11.77	10.71	9.579	8.688	7.929	7.277	6.704	6.497	6.390
6.00	78.47	27.81	19.68	15.45	14.08	12.81	11.44	10.36	9.449	8.661	7.968	7.718	7.588
7.00	91.55	32.43	22.94	18.00	16.39	14.90	13.31	12.05	10.98	10.05	9.242	8.949	8.797
8.00	104.6	37.06	26.20	20.55	18.71	17.01	15.18	13.74	12.51	11.45	10.52	10.19	10.01
9.00	117.7	41.68	29.46	23.10	21.03	19.11	17.05	15.43	14.05	12.85	11.81	11.43	11.23
10.00	130.8	46.31	32.73	25.66	23.35	21.22	18.93	17.13	15.59	14.26	13.10	12.67	12.45

Sources: Land (1975) and Gilbert (1987).

TABLE A.7

VALUES OF g_n FOR CHEBYSHEV'S METHOD

Variance ÷ 2 of log-transformed data ($S_{log}^2 \div 2$)	*Number of Samples* 2	5	8	10	13	15	20	25	30	50	70	90	100	150	200	500	∞
0.05	1.025	1.041	1.045	1.046	1.047	1.048	1.049	1.049	1.049	1.050	1.050	1.051	1.051	1.051	1.051	1.051	1.051
0.10	1.050	1.082	1.091	1.093	1.096	1.097	1.099	1.100	1.101	1.103	1.103	1.104	1.104	1.104	1.105	1.105	1.105
0.15	1.076	1.125	1.138	1.143	1.147	1.149	1.152	1.154	1.155	1.158	1.159	1.160	1.160	1.161	1.161	1.161	1.162
0.20	1.102	1.169	1.187	1.194	1.200	1.203	1.207	1.210	1.212	1.216	1.217	1.218	1.218	1.219	1.220	1.221	1.221
0.25	1.128	1.214	1.238	1.247	1.255	1.259	1.265	1.268	1.271	1.276	1.278	1.280	1.280	1.281	1.282	1.283	1.284
0.30	1.154	1.260	1.291	1.302	1.312	1.317	1.325	1.330	1.333	1.340	1.342	1.344	1.345	1.346	1.347	1.349	1.350
0.35	1.180	1.307	1.345	1.359	1.372	1.378	1.387	1.393	1.398	1.406	1.410	1.412	1.412	1.415	1.416	1.418	1.419
0.40	1.207	1.356	1.401	1.418	1.433	1.441	1.453	1.460	1.465	1.476	1.480	1.483	1.484	1.486	1.488	1.490	1.492
0.45	1.234	1.406	1.459	1.479	1.498	1.506	1.521	1.530	1.536	1.548	1.554	1.557	1.558	1.562	1.563	1.566	1.568
0.50	1.261	1.457	1.519	1.542	1.564	1.574	1.592	1.602	1.610	1.625	1.631	1.635	1.637	1.641	1.643	1.646	1.649
0.55	1.288	1.509	1.581	1.608	1.633	1.645	1.666	1.678	1.687	1.705	1.713	1.717	1.719	1.724	1.726	1.730	1.733
0.60	1.315	1.563	1.645	1.675	1.705	1.719	1.743	1.757	1.768	1.789	1.798	1.803	1.805	1.811	1.813	1.819	1.822
0.65	1.343	1.618	1.711	1.746	1.780	1.796	1.823	1.840	1.852	1.876	1.887	1.893	1.895	1.902	1.905	1.911	1.916
0.70	1.371	1.675	1.779	1.818	1.857	1.876	1.907	1.926	1.940	1.968	1.981	1.988	1.990	1.998	2.002	2.009	2.014
0.75	1.399	1.733	1.849	1.894	1.938	1.959	1.994	2.016	2.032	2.064	2.079	2.087	2.090	2.099	2.103	2.111	2.117
0.80	1.427	1.792	1.922	1.971	2.021	2.045	2.085	2.110	2.128	2.165	2.182	2.191	2.194	2.205	2.210	2.219	2.226
0.85	1.456	1.853	1.996	2.052	2.108	2.134	2.179	2.208	2.228	2.270	2.289	2.300	2.304	2.316	2.322	2.332	2.340
0.90	1.485	1.915	2.074	2.135	2.197	2.227	2.278	2.310	2.333	2.381	2.402	2.415	2.419	2.432	2.439	2.451	2.460
0.95	1.514	1.979	2.153	2.221	2.291	2.323	2.380	2.417	2.442	2.496	2.521	2.535	2.539	2.555	2.562	2.576	2.586
1.00	1.543	2.044	2.235	2.310	2.387	2.424	2.487	2.528	2.557	2.617	2.645	2.660	2.666	2.683	2.692	2.707	2.718
1.05	1.573	2.111	2.320	2.403	2.487	2.528	2.598	2.644	2.676	2.744	2.774	2.792	2.798	2.818	2.827	2.845	2.858
1.10	1.602	2.180	2.407	2.498	2.591	2.636	2.714	2.765	2.800	2.876	2.911	2.930	2.938	2.959	2.970	2.990	3.004
1.15	1.632	2.250	2.497	2.596	2.699	2.748	2.834	2.891	2.930	3.014	3.053	3.075	3.083	3.108	3.120	3.143	3.158
1.20	1.662	2.321	2.589	2.698	2.810	2.864	2.960	3.022	3.066	3.159	3.203	3.227	3.236	3.263	3.277	3.303	3.320
1.25	1.693	2.395	2.685	2.803	2.926	2.985	3.090	3.159	3.207	3.311	3.359	3.387	3.397	3.427	3.442	3.471	3.490
1.30	1.724	2.470	2.783	2.911	3.045	3.111	3.226	3.301	3.354	3.470	3.523	3.554	3.565	3.599	3.616	3.648	3.669
1.35	1.754	2.547	2.884	3.023	3.169	3.241	3.367	3.450	3.508	3.636	3.695	3.729	3.741	3.779	3.798	3.833	3.857
1.40	1.786	2.626	2.988	3.139	3.298	3.376	3.513	3.604	3.669	3.809	3.875	3.912	3.926	3.968	3.989	4.028	4.055
1.45	1.817	2.706	3.096	3.259	3.431	3.515	3.666	3.766	3.836	3.991	4.063	4.105	4.120	4.166	4.190	4.233	4.263
1.50	1.849	2.788	3.206	3.382	3.569	3.661	3.825	3.933	4.011	4.181	4.260	4.307	4.323	4.374	4.400	4.448	4.482
1.55	1.880	2.873	3.320	3.510	3.711	3.811	3.990	4.108	4.193	4.379	4.467	4.518	4.536	4.592	4.621	4.675	4.711
1.60	1.913	2.959	3.437	3.642	3.859	3.967	4.161	4.291	4.383	4.587	4.683	4.739	4.759	4.821	4.853	4.912	4.953
1.65	1.945	3.047	3.558	3.777	4.012	4.129	4.339	4.480	4.581	4.804	4.910	4.971	4.993	5.062	5.097	5.162	5.207
1.70	1.977	3.137	3.682	3.918	4.171	4.297	4.525	4.678	4.788	5.031	5.147	5.215	5.239	5.314	5.353	5.424	5.474
1.75	2.010	3.229	3.810	4.062	4.334	4.471	4.717	4.883	5.003	5.269	5.395	5.469	5.496	5.578	5.621	5.700	5.755
1.80	2.043	3.323	3.942	4.212	4.504	4.651	4.917	5.097	5.227	5.517	5.655	5.736	5.766	5.856	5.903	5.990	6.050
1.85	2.077	3.420	4.077	4.366	4.680	4.838	5.125	5.320	5.461	5.776	5.927	6.016	6.048	6.147	6.198	6.294	6.360
1.90	2.110	3.518	4.216	4.525	4.861	5.031	5.341	5.552	5.705	6.048	6.212	6.309	6.344	6.453	6.509	6.613	6.686
1.95	2.144	3.619	4.359	4.688	5.049	5.232	5.566	5.794	5.959	6.331	6.511	6.617	6.655	6.773	6.834	6.949	7.029
2.00	2.178	3.721	4.506	4.858	5.243	5.439	5.799	6.045	6.224	6.628	6.823	6.938	6.980	7.109	7.176	7.302	7.389

Source: After Gilbert (1987).