National Aeronautics and
Space Administration

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December 17, 2014

Reply to Attn of: RE-14-138

Mr. John E. Kieling, Chief
New Mexico Environment Department
Hazardous Waste Bureau
2905 Rodeo Park Drive East, Building 1
Santa Fe, NM 87505

Subject: Response to Second NMED Disapproval - NASA White Sands Test Facility Soil Background Study Investigation Report

NASA submitted the Soil Background Study Investigation Report to NMED on March 27, 2014. NMED received the report on March 31, 2014 and issued a Notice of Disapproval (NOD) with comments on June 26, 2014. All comments pertained to the statistical evaluation of the soil background data, which was performed by a professional statistician contracted by NASA. NASA submitted responses to the NOD comments in a letter dated August 27, 2014. NMED reviewed the comments and issued a second NOD on October 15, 2014. NMED stated within the second NOD, *"If NASA would like to pursue using the proposed UTLs for background over defaulting to the maximum detected concentrations or collection of additional background samples, the most straightforward approach to resolving the statistical issues is to demonstrate that the approach taken is similar to and conservative compared to ProUCL version 5.0.00 (available since September 2013) and to provide references from the statistical literature for all modifications made to existing R library modules".*

In response to the NMED comment, NASA is still recommending to use the proposed UTLs for background soil values. However, as requested, this submittal provides the ProUCL demonstration that compares the original UTLs with the UTLs calculated using the ProUCL software package. This demonstration was performed by the contracted professional statistician that developed the original proposal. This submittal also provides the requested references from statistical literature for all modifications made to the existing R library modules. Table 5 in the enclosed report provides the requested comparison of the proposed UTLs with ProUCL-generated UTLs and demonstrates that the proposed UTLs are comparable to, and in many cases more conservative, than the ProUCL values. Enclosure 1 provides a hard copy of the statistician's report. Enclosure 2 provides the same statistical report in an Adobe PDF format.

I certify under penalty of law that this document and all attachments were prepared under my direction or supervision in accordance with a system designed to assure that qualified personnel properly gather and evaluate the information submitted. Based on my inquiry of the person or persons who manage the system, or those persons directly responsible for gathering the information, the information submitted is, to the best of my knowledge and belief, true, accurate, and complete. I am aware that there are significant penalties for submitting false information, including the possibility of fine and imprisonment for known violations.

If you have any questions or comments, please contact Tim Davis of my staff at 575–524–5024.

for Radel Bunker-Farrah
Chief, Environmental Office

2 Enclosures

cc:
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Response to NMED 2014-Oct-15 Letter Regarding:
Second Notice of Disapproval – Soil Background Study Investigation Report

December 11, 2014

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Introduction

On 2014-Mar-21, I provided a report to NASA White Sands Test Facility (NASA WSTF) titled *Statistical Development of Soil Background Concentrations*. This report was used in NASA WSTF's report to the New Mexico Environmental Department (NMED) titled Soil Background Study Investigation Report, which NMED received on 2014-Mar-31. NMED responded to the NASA WSTF with a Notice of Disapproval, and enumerated four comments related to the statistical development, to which NMED requested responses. On 2014-Aug-18, I provided response to the four comments to NASA WSTF. On 2014-Oct-15, NMED responded to NASA WSTF with a Second Notice of Disapproval, and suggested that if NASA would like to pursue using the previously proposed upper tolerance limits (UTLs) for background that it would be most straightforward to demonstrate that the approach taken is similar to and conservative compared to ProUCL version 5.0.00 and to provide references from the statistical literature for all modifications made to existing R library modules. This report attempts to do this, but also notes some shortcomings in the ProUCL software and, in some cases, the general lack of appropriate statistical methodologies to handle some data sets.

Evaluation of Software Capabilities

I believe it is worth addressing the mere ability to assess the accuracy of results from the ProUCL software. There are two primary mechanisms by which statistical software can be evaluated: (1.) making the source code available for evaluation, and (2.) providing a mechanism to conduct simulations with the software. ProUCL is developed for profit under contract with Lockheed Martin, and it provides neither of these mechanisms for evaluation. The authors make numerous references to the simulations that were conducted with their source code, but there is no way for others to verify their simulations since simulations are not built into the software and the source code is not made available. This also makes it difficult to compare other software products to ProUCL. On the other hand, packages developed for the R environment make both provisions – the code is generally available and there is built-in functionality for conducting simulations. Further, some packages for the R environment have undergone public peer review. For example, and relevant to the present work, the author of the *tolerance* package (which provides the tolerance interval calculations used in recent reports on the 2014 Soil Background Investigative Study at NASA/WSTF) wrote an article for the *Journal of Statistical Software* on the *tolerance* package (Young, 2010). The *Journal of Statistical Software* is a publication of the American Statistical Association – the foremost statistical organization in the world, and its articles are peer-reviewed. It describes its review process by: "The manuscript (article/paper/manual) will be peer reviewed in the usual way. The editor-in-chief selects an editor, the editor selects two reviewers (one of them can be the editor). The review has two parts: both the manuscript and the software are reviewed. The combination of the parts should work as indicated, be clearly documented, and serve a useful purpose. The statistical part of all submissions is reviewed for both correctness and usefulness." Further, the code for the *tolerance* package is readily available for review. When either of these two mechanisms is available, the evaluation process generally requires a statistician with at least a Master's degree to conduct a thorough evaluation. On the other hand, the only peer-reviews of ProUCL that I have been able to locate only make comments on the usefulness of the methods it provides and the convenience of its user interface, not on the ability of the software to produce accurate results.

It is important to emphasize that this is *the* accepted standard in the field of statistics for evaluation of software – simulations and/or review of available source code, and ProUCL does not make either of these a viable option. The fact that the EPA contracted to have the ProUCL software developed should not make it a *de facto* standard since the potential to evaluate the ProUCL software is extremely limited, especially compared to most of the packages available for the R environment. I will comment later in this report and provide some references in the statistical literature on some of its shortcomings, particularly with regard to its Gamma Regression on Order Statistics method for imputing values for non-detects. While ProUCL certainly has many capabilities, participation in the Statistics and the Environment community group of the American Statistical Association reveals there are clearly other criticisms of the ProUCL software package.

Gamma Tolerance Interval Calculations

Given that ProUCL does not make source code available and does not have simulation capabilities, only limited example problems can be run to illustrate similarities and differences. With regard to the calculations of gamma upper tolerance limits (UTLs), ProUCL references Krishnamoorthy, Mathew, and Mukherjee (2008) for the implementation of the WH method (Wilson-Hilferty, 1931) and the HW method (Hawkins-Wixley, 1986). In their paper, Krishnamoorthy, Mathew, and Mukherjee present an example calculation of data presented by Gibbons (1994) consisting of 27 observations for alkalinity concentrations in groundwater. The data are as follows:

58, 82, 42, 28, 118, 96, 49, 54, 42, 51, 66, 89, 40, 51,
54, 55, 59, 42, 39, 40, 60, 63, 59, 70, 32, 52, 79.

Calculations for the UTL are given in Table 1 for Krishnamoorthy et al, ProUCL, and the *gamtol.int()* method in the R *tolerance* package.

Table 1. K-factor and UTL calculations from Krishnamoorthy, Mathew, and Mukherjee (2008), ProUCL, and R's *gamtol.int()* method.

Method	K Factor	UTL
Krishnamoorthy	2.2601	110.507
ProUCL	2.26	110.5
gamtol.int()	2.260045	109.2969

Clearly there is a slight difference in the *gamtol.int()* calculation of the UTL, although its K-factor is in agreement with the other two calculations. The last two sentences of Section 2 of Krishnamoorthy, Mathew, and Mukherjee (2008) state that they are not going to use the complete and sufficient statistics for the gamma distribution in their approach in order to maintain simplicity. As presented in Equations (3-8) and (3-9) of the ProUCL Version 5.0.00 Technical Guide, this is also the procedure followed by ProUCL. However, the Lehmann-Scheffé Theorem indicates that a Uniform Minimum Variance Unbiased Estimator (UMVUE) is a function of the complete and sufficient statistics – essentially saying that you get better estimators if you do use complete and sufficient statistics. In the R gamma tolerance interval method used in our calculations, *gamtol.int()*, the procedure is based on the complete and sufficient statistics for the gamma distribution parameters (the shape and rate parameter estimates), which are then used to estimate μ and σ, as given at the

end of Section 2 of Krishnamoorthy, Mathew, and Mukherjee (2008). The gamma parameters estimates are obtained via maximum likelihood estimation, and being the complete and sufficient statistics for the gamma distribution, yield the UMVUE for estimating μ and σ. The ultimate result of this is that the calculation is able to give a tighter bound for the UTL, thus being more conservative than the simpler approach followed by Krishnamoorthy et al and ProUCL.

For calculation of UTLs based on a gamma distribution for the underlying population, ProUCL reports UTLs calculated using both the WH and HW methods. The WH method uses a data transformation of $x^{1/3}$ to obtain transformed data that approximately follows a normal distribution, while the HW method uses a transformation of $x^{1/4}$ to achieve approximate normality. Krishnamoorthy, Mathew, and Mukherjee (2008) report that, "It is evident from the tabulated values ... that the WH approximation provides satisfactory coverage probabilities [i.e., confidence level] except when *a* [i.e., the shape parameter] is small." Even when the shape parameter is small, for 95% confidence and either 95% coverage or 99% coverage, the most that the estimates of confidence were off from the stated values occurred when the simulation estimate was 92.3% and the stated value was 95% – an over estimate of 2.7%. This was for samples of size n=7. When n=12, the biggest difference was an over estimate of 1.8%.

Imputation for Non-Detects for the Gamma Distribution

ProUCL imputes values for non-detects (NDs) based on what the ProcUCL Technical Guide calls the GROS (Gamma Regression on Order Statistics) method. Their methodology has been replicated in an R method named *ros()* by Eric Bailey. This code is not in a package in the usual repository at the CRAN (Comprehensive R Archive Network) web site, but is available on the GitHub web site at: *https://github.com/ebailey78/rucl/tree/master/R/* and is in the file *ros.R*. It requires the method *gMLE()* which is in the file *gMLE.R*, also available on the same web page. One slight difference exists in the ProUCL and the R *ros()* implementations – that is, when the GROS method yields a negative result (due to the regression prediction) which is used to replace an ND, ProUCL changes the negative imputed value to 0.01, while *ros()* changes the negative imputed value to 0.0001. This value can easily be altered in the *ros()* code to match the results in ProUCL by changing this value to 0.01 on line 69 in the *ros.R* file. To illustrate the equivalence of the two implementations, six samples of size n=12 were randomly generated for each of three parameter combinations for the gamma distribution, and in each sample, the lowest three values were converted to NDs. The distribution parameters combinations of shape and scale that were used are the same as those used in the previous report of 2014-August-18:

1. Gamma(3, 3),
2. Gamma(7, 1), and
3. Gamma(1, 0.2).

Note that the second parameter here is expressed as the rate, while some of the tables below express the second parameter as the scale = 1/rate.

The R method used to generate the sample data is *gamma.data.to.xlsx()* and its code is listed in the Appendix A. ProUCL and *ros()* were each used to calculate imputed values for the samples, and the resulting data sets are tabulated in Tables 3a–3f. As can be seen from the imputed values for these

two methods, the results are identical, ignoring some calculation error in the last decimal places that is a common occurrence due to differences in precision specifications. Aside from it being useful to be able to replicate the ProUCL methodology in R, it is also informative to analyze the code in *ros()* that replicates the results in ProUCL, particularly since the source code for ProUCL is not available and the documentation in the ProUCL Technical Guide of what the code does is not completely clear. Evaluation of this code reveals that the ProUCL implementation of the GROS method is naive, as it completely ignores the NDs in its estimation of the gamma distribution parameters, which is a necessary first step in performing GROS. This will generally lead to substantially biased gamma distribution parameter estimates (i.e., the shape and scale parameters). This is one of the major reasons I have been reluctant to use the ProUCL software, since gamma distributions are often indicated as being appropriate for the analyte data. Hence, use of the ProUCL software would lead to biased gamma distribution parameter estimates and subsequently to less representative imputed data values in place of the NDs.

The Expectation-Maximization algorithm (EM algorithm or method) was formally proposed by Dempster, Laird, and Rubin (1977). Their seminal paper coins the term "EM algorithm" and has been cited over 8,000 times in the literature. This paper outlines the idea of alternating back and forth between what they call the *E-step* ("E" for Expectation) – where the expected values of the missing data are calculated conditioned on an estimate of the unknown parameters, and the *M-step* ("M" for Maximization) – where the unknown parameters are estimated using maximum likelihood and conditioned on the estimates of the missing data. The EM algorithm iterates between these two steps until convergence is obtained. Ip (1994) provides an overview of the history of the EM algorithm in Sections 2.1 and 2.2, including a note that Hartley (1958) presents one of the earliest suggestions of an estimation method along the lines of the EM algorithm; gives an outline of the EM algorithm process in Section 2.3; and in Section 2.4 discusses its wide application, including its use with censored data, and notes its limitations. Helsel (2012) discusses the use of the EM algorithm to impute values for NDs in Section 13.3.2 of his book, and notes that Maul and El-Shaarawi (1993) used the EM algorithm to impute values for censored halocarbon concentrations as a first step towards doing a cluster analysis. Gleit (1985) conducts simulations to examine several methods for imputing values for NDs due to left censoring in a normal distribution. He concludes that the "truncated MLE [was] terribly biased and had huge variances" – and this is what ProUCL does for its GROS method for the gamma distribution. He also concludes that, "fill-in with expected values did a good job throughout the simulation" – where what he calls "fill-in with expected values" is an informal version of the EM algorithm. Gleit's final conclusion is that, "fill-in with expected values is by far the best estimator." Shuway, Azari, and Kayhanian (2002) compare ROS and EM algorithm methods in their ability to obtain confidence intervals for population means when data follow a lognormal or gamma distribution. While their results are targeted towards mean confidence intervals and not tolerance intervals, they note that, "it is well-known that exact MLEs are available by simple and numerically stable iterations using the EM algorithm". Ultimately they conclude that the ROS method often performs better for lognormal-distributed data and the EM algorithm performs better for gamma-distributed data, though, again, these results are for confidence intervals for a population mean and not for tolerance intervals.

Previously, I had implemented the EM algorithm as a modification to the method *fitdistr()* in the *MASS* package. However, being a more general maximum likelihood estimation method (i.e., allowing estimation for many different distributions), it was more complicated to read, understand, and to obtain convergence. Consequently, I have moved the EM algorithm calculation to a much simpler and more robust alternative that is specifically tailored to the gamma distribution.

To implement the EM algorithm for the gamma distribution, the maximum likelihood estimation technique as described in Singh, Singh, and Iaci (2002) was implemented. This technique is available in the R method *gMLE()* which is in the file *gMLE.R*, available on GitHub as noted previously. The custom written R method *em.gmle.impute()* is then used to alternate between (1.) getting the expected values of the NDs conditional on the gamma distribution parameter estimates (referred to in the aforementioned papers as the *E-step*), and (2.) calling *gMLE()* to get the maximum likelihood gamma distribution parameter estimates (referred to in aforementioned papers as the *M-step*). These two steps are then iterated until convergence is obtained. The code for the *em.gmle.impute()* method is included in Appendix A. The *em.gmle.impute()* method was used to impute values for the NDs in the same eighteen samples discussed above for the GROS and *ros()* calculations, and the results are also shown in Table 3a–3f. Immediately obvious is that the EM algorithm does not result in negative estimates for imputed values, so there are no consistent low values in place of NDs such as the 0.01 for GROS and the 0.0001 for *ros()*. Table 4 reports estimates of the gamma distribution parameters from the data sets with imputed values for the ProUCL GROS method and the EM algorithm for both the shape and the scale parameters of the gamma distribution. All of these estimates were done in ProUCL using the menu item Statistical Tests > Goodness-of-Fit Tests > Gamma. No NDs are present in the data sets with imputed values, so there are no options for using the NDs. Table 4 shows the percent difference of the actual (true) parameter value to the estimated parameter value, for each of the two gamma parameters (shape and scale). It also shows the average absolute percent differences for each method and for each parameter combination. In each case the EM algorithm is 10–20% closer to the true parameter value than the GROS method.

Nonparametric Tolerance Intervals

As discussed in the ProUCL Technical Guide, ProUCL calculates nonparametric UTLs based on the formulas given in Hahn and Meeker (1991). Section 1.10.1 of the ProUCL User Guide notes the sample sizes required to achieve the specified levels of confidence and coverage with a nonparametric UTL. However, ProUCL will still calculate a nonparametric UTL even if the sample size is not adequate to achieve the user specified confidence and coverage levels. It does report the level of confidence given by the interval, but the user must be careful to note that it is different from what was specified. In identifying that the levels are not what was specified by the user, ProUCL indicates that coverage is maintained at the specified level and notes the impact as a decrease in confidence. With a sample of n=12, as is the case in the present study, using the maximum order statistic, $x_{(12)}$, as the UTL gives a confidence of (solving using Hahn and Meeker's Equation 5.4):

$$\text{confidence} = 1 - p^n = 1 - (0.95)^{12} = 0.460, \text{ or } 46.0\%,$$

with 95% coverage, which is the same value reported by ProUCL. Clearly this is very low confidence in a UTL calculation. It's interpretation is that, 46% of the time that a sample of size n=12 is randomly selected and the largest order statistic is used as the UTL, the UTL will actually be at or above 95% of the population. Another informative way of thinking about the largest order statistic and the impact of sample size is the fact that, the variability in the data is better represented as the sample size gets larger. Hence, the maximum value will tend to be larger for bigger sample sizes even though the distribution of the population and its spread remain the same. As an illustration, consider the three gamma distributions listed above and what their expected

maximum order statistic is for samples of size n=12 versus for samples of size n=59 (the number required to achieve 95% confidence with 95% coverage), calculated as:

$$x_{(n)} = G^{-1}(n/(n+1), \text{shape}, \text{rate}),$$

where G^{-1} is the inverse gamma cumulative distribution function. These values are given in Table 2 below.

Table 2. Expected maximum order statistics for various gamma distributions and samples of size n=12 and n=59.

(shape, rate)	$x_{(12)}$	$x_{(59)}$	$x_{(59)} / x_{(12)}$
3, 3	1.899	2.584	1.361
7, 1	11.042	13.740	1.244
1, 0.2	12.825	20.472	1.596

This implies that one would typically expect the appropriate nonparametric UTL to be between 24.4% and 59.6% larger than the maximum order statistic (i.e., the reported UTL) for a sample of size n=12. This is, of course, assuming the actual distribution of the population is a gamma distribution that simply could not be identified using a goodness of fit test.

Another nonparametric UTL can be obtained via a bootstrap of a 95th percentile. But with small data sets, the bootstrap is restricted to only a few possible values it can obtain for its 95th percentile on each bootstrap sample, so this method does not yield a useful result. Hence, there are no good nonparametric UTL methods available for small sample sizes. In the 2014-Mar-31 report, the use of bootstrapping a 95% upper prediction limit (UPL) based on Chebyshev's inequality was an attempt to get an approximate nonparametric UTL. It was motivated by the notions that: (1.) being based on Chebyshev's inequality the calculation is nonparametric, and (2.) a future observation has 95% confidence of being below the calculated UTL, so bootstrapping to get a large number of these calculations and then taking the 95th percentile of these values might exceed 95% of all future observations. Unfortunately, this results in a large UTL.

Perhaps a better option would be to calculate a UTL based on lognormal and gamma distribution assumptions and taking the larger of the two values. This would seem more appropriate than merely taking the maximum sample value, $x_{(12)}$, given the above discussion of its underestimation of the appropriate nonparametric UTL of $x_{(59)}$.

ProUCL Comparison UTLs

For comparison, calculations were performed for 95%-confidence – 95% coverage UTLs using ProUCL. These are presented in Table 5. Depending on whether there are non-detects in the sample, ProUCL produces several different UTL calculations. ProUCL's calculation based on the WH and HW methods are excluded when there are non-detects. These values (WH and HW in Table 5) are very close to the calculations in my 24-Mar-2014 report but are generally slightly larger due to their simplification of not using sufficient statistics. When non-detects occur in the sample, ProUCL calculates gamma-based UTLs using a GROS method that completely ignores the non-detects in estimating the gamma parameters. This is a poor estimation method compared to the EM algorithm

and is in great contrast to the advice continually provided by EPA guidelines, ProUCL manuals, and other sources – all strongly promoting the incorporation of non-detects into environmental calculations. Also calculated by ProUCL when non-detects occur are the Kaplan-Meier (KM) estimates which estimate means and standard deviations using the nonparametric KM formulas but then substitute them into formulas for parametric UTL calculations. Regardless of the presence or absence of non-detects, ProUCL will produce a UTL estimate based on the maximum order statistic. It does not, however, provide the specified confidence and/or coverage and, in fact, is often substantially below that which is specified (such as the 46% confidence presented above when the confidence specified in the ProUCL dialog box is 95%). Finally, Table 5 also presents ProUCl's assessment of whether the gamma distribution is an appropriate fit to the data (the Gam column in Table 5). However, like the GROS UTL estimates, it ignores the non-detects in assessing the fit of a gamma distribution.

As always, if you have any questions or comments, please let me know.

Table 3a. Comparison of the GROS method in ProUCL, R's *ros()* method, and the EM method via R for imputing values in place of NDs based on a gamma distribution. Columns are: x=randomly generated gamma data; detect=1 for detection or 0 for ND; group=sample ID; GROS Est=GROS estimate from ProUCL for NDs; ros() Est= GROS estimate from R; EM est=estimates based on the EM algorithm. Six samples of n=12 were generated for each of three combinations of the gamma distributions shape and scale parameters.

X	ND	Group	Shape	Scale	GROS Est.	ros() Est.	EM Est.
2.404990257	1	1	3	0.3333	2.404990257	2.404990257	2.40499
0.622584225	1	1	3	0.3333	0.622584225	0.622584225	0.62258
1.057339971	1	1	3	0.3333	1.057339971	1.057339971	1.05734
1.819360385	1	1	3	0.3333	1.819360385	1.819360385	1.81936
1.865545979	1	1	3	0.3333	1.865545979	1.865545979	1.86555
1.033990416	1	1	3	0.3333	1.033990416	1.033990416	1.03399
0.564098148	0	1	3	0.3333	0.01	0.0001	0.03686
0.564098148	0	1	3	0.3333	0.01	0.0001	0.11959
0.67610017	1	1	3	0.3333	0.676100170	0.676100170	0.6761
0.564098148	0	1	3	0.3333	0.155526474	0.15552709	0.2124
0.802417572	1	1	3	0.3333	0.802417572	0.802417572	0.80242
0.686817195	1	1	3	0.3333	0.686817195	0.686817195	0.68682
1.40331855	1	2	3	0.3333	1.40331855	1.40331855	1.40332
0.417586213	0	2	3	0.3333	0.027989952	0.02799057	0.04003
1.241147148	1	2	3	0.3333	1.241147148	1.241147148	1.24115
0.956159641	1	2	3	0.3333	0.956159641	0.956159641	0.95616
0.417586213	0	2	3	0.3333	0.169531316	0.16953173	0.11722
0.526294481	1	2	3	0.3333	0.526294481	0.526294481	0.52629
0.417586213	0	2	3	0.3333	0.279668805	0.27966909	0.19881
1.323599808	1	2	3	0.3333	1.323599808	1.323599808	1.3236
0.420144761	1	2	3	0.3333	0.420144761	0.420144761	0.42014
1.665242645	1	2	3	0.3333	1.665242645	1.665242645	1.66524
1.032641916	1	2	3	0.3333	1.032641916	1.032641916	1.03264
0.506124426	1	2	3	0.3333	0.506124426	0.506124426	0.50612
0.6989535	1	3	3	0.3333	0.6989535	0.6989535	0.69895
1.16828533	1	3	3	0.3333	1.16828533	1.16828533	1.16829
1.32789436	1	3	3	0.3333	1.32789436	1.32789436	1.32789
0.827895358	1	3	3	0.3333	0.827895358	0.827895358	0.8279
0.558712382	0	3	3	0.3333	0.01	0.0001	0.08309
0.558712382	0	3	3	0.3333	0.15676028	0.15676038	0.1904
2.117115633	1	3	3	0.3333	2.117115633	2.117115633	2.11712
0.691418204	1	3	3	0.3333	0.691418204	0.691418204	0.69142
0.601922319	1	3	3	0.3333	0.601922319	0.601922319	0.60192
1.23240779	1	3	3	0.3333	1.23240779	1.23240779	1.23241
1.045105452	1	3	3	0.3333	1.045105452	1.045105452	1.04511
0.558712382	0	3	3	0.3333	0.283866224	0.28386629	0.28885

Table 3b. Comparison of the GROS method in ProUCL, R's *ros()* method, and the EM method via R for imputing values in place of NDs based on a gamma distribution. Columns are: x=randomly generated gamma data; detect=1 for detection or 0 for ND; group=sample ID; GROS Est=GROS estimate from ProUCL for NDs; ros() Est= GROS estimate from R; EM est=estimates based on the EM algorithm. Six samples of n=12 were generated for each of three combinations of the gamma distributions shape and scale parameters.

X	ND	Group	Shape	Scale	GROS Est.	ros() Est.	EM Est.
0.866215952	1	4	3	0.3333	0.866215952	0.866215952	0.86622
0.516872508	1	4	3	0.3333	0.516872508	0.516872508	0.51687
1.47207588	1	4	3	0.3333	1.47207588	1.47207588	1.47208
0.513443257	0	4	3	0.3333	0.237175452	0.23717548	0.15238
0.996777845	1	4	3	0.3333	0.996777845	0.996777845	0.99678
1.072461419	1	4	3	0.3333	1.072461419	1.072461419	1.07246
0.513443257	0	4	3	0.3333	0.384053327	0.38405334	0.28727
1.256415186	1	4	3	0.3333	1.256415186	1.256415186	1.25642
1.276944259	1	4	3	0.3333	1.276944259	1.276944259	1.27694
1.831766009	1	4	3	0.3333	1.831766009	1.831766009	1.83177
0.513443257	0	4	3	0.3333	0.493522709	0.49352272	0.39803
1.040303558	1	4	3	0.3333	1.040303558	1.040303558	1.0403
0.691277402	0	5	3	0.3333	0.079543104	0.0795432	0.13347
1.484184217	1	5	3	0.3333	1.484184217	1.484184217	1.48418
0.90735507	1	5	3	0.3333	0.90735507	0.90735507	0.90736
0.891712348	1	5	3	0.3333	0.891712348	0.891712348	0.89171
1.593044204	1	5	3	0.3333	1.593044204	1.593044204	1.59304
0.691277402	0	5	3	0.3333	0.28060824	0.2806083	0.28019
0.962985259	1	5	3	0.3333	0.962985259	0.962985259	0.96299
2.295793698	1	5	3	0.3333	2.295793698	2.295793698	2.29579
0.864189093	1	5	3	0.3333	0.864189093	0.864189093	0.86419
0.691277402	0	5	3	0.3333	0.432057331	0.43205737	0.40823
1.198192536	1	5	3	0.3333	1.198192536	1.198192536	1.19819
2.047203768	1	5	3	0.3333	2.047203768	2.047203768	2.0472
0.296584637	0	6	3	0.3333	0.01	0.0001	0.03548
1.502613746	1	6	3	0.3333	1.502613746	1.502613746	1.50261
0.296584637	0	6	3	0.3333	0.109055457	0.10905598	0.1081
0.296584637	0	6	3	0.3333	0.224226767	0.22422713	0.18664
0.87191506	1	6	3	0.3333	0.87191506	0.87191506	0.87192
1.732319893	1	6	3	0.3333	1.732319893	1.732319893	1.73232
0.691217496	1	6	3	0.3333	0.691217496	0.691217496	0.69122
0.337590547	1	6	3	0.3333	0.337590547	0.337590547	0.33759
1.19361755	1	6	3	0.3333	1.19361755	1.19361755	1.19362
1.242110529	1	6	3	0.3333	1.242110529	1.242110529	1.24211
0.5533398	1	6	3	0.3333	0.5533398	0.5533398	0.55334
0.813519004	1	6	3	0.3333	0.813519004	0.813519004	0.81352

Table 3c. Comparison of the GROS method in ProUCL, R's *ros()* method, and the EM method via R for imputing values in place of NDs based on a gamma distribution. Columns are: x=randomly generated gamma data; detect=1 for detection or 0 for ND; group=sample ID; GROS Est=GROS estimate from ProUCL for NDs; ros() Est= GROS estimate from R; EM est=estimates based on the EM algorithm. Six samples of n=12 were generated for each of three combinations of the gamma distributions shape and scale parameters.

X	ND	Group	Shape	Scale	GROS Est.	ros() Est.	EM Est.
6.902956786	1	7	7	1.0000	6.902956786	6.902956786	6.90296
8.426982614	1	7	7	1.0000	8.426982614	8.426982614	8.42698
3.637820303	0	7	7	1.0000	0.01	0.0001	0.33816
5.784233141	1	7	7	1.0000	5.784233141	5.784233141	5.78423
3.637820303	0	7	7	1.0000	0.318652	0.31865498	0.96845
3.637820303	0	7	7	1.0000	1.335136666	1.33513866	1.62603
3.819746793	1	7	7	1.0000	3.819746793	3.819746793	3.81975
17.33666953	1	7	7	1.0000	17.33666953	17.33666953	17.33667
9.305072768	1	7	7	1.0000	9.305072768	9.305072768	9.30507
6.766902652	1	7	7	1.0000	6.766902652	6.766902652	6.7669
9.84971947	1	7	7	1.0000	9.84971947	9.84971947	9.84972
4.037912843	1	7	7	1.0000	4.037912843	4.037912843	4.03791
18.72093693	1	8	7	1.0000	18.72093693	18.72093693	18.72094
4.691594075	0	8	7	1.0000	0.01	0.0001	0.32677
11.31855291	1	8	7	1.0000	11.31855291	11.31855291	11.31855
4.907927823	1	8	7	1.0000	4.907927823	4.907927823	4.90793
5.296939362	1	8	7	1.0000	5.296939362	5.296939362	5.29694
12.42993303	1	8	7	1.0000	12.42993303	12.42993303	12.42993
5.101834431	1	8	7	1.0000	5.101834431	5.101834431	5.10183
5.608631265	1	8	7	1.0000	5.608631265	5.608631265	5.60863
7.293852568	1	8	7	1.0000	7.293852568	7.293852568	7.29385
8.042644745	1	8	7	1.0000	8.042644745	8.042644745	8.04264
4.691594075	0	8	7	1.0000	0.01	0.0001	0.97901
4.691594075	0	8	7	1.0000	1.083079494	1.08308231	1.67756
7.59609902	1	9	7	1.0000	7.59609902	7.59609902	7.5961
8.09183478	1	9	7	1.0000	8.09183478	8.09183478	8.09183
6.135991887	0	9	7	1.0000	2.699707376	2.69970736	2.22424
6.99827375	1	9	7	1.0000	6.99827375	6.99827375	6.99827
14.00177517	1	9	7	1.0000	14.00177517	14.00177517	14.00178
8.045358045	1	9	7	1.0000	8.045358045	8.045358045	8.04536
9.836381054	1	9	7	1.0000	9.836381054	9.836381054	9.83638
6.186134593	1	9	7	1.0000	6.186134593	6.186134593	6.18613
6.135991887	0	9	7	1.0000	3.681912145	3.68191213	3.31634
6.714410879	1	9	7	1.0000	6.714410879	6.714410879	6.71441
8.231975109	1	9	7	1.0000	8.231975109	8.231975109	8.23198
6.135991887	0	9	7	1.0000	4.39606542	4.39606541	4.10354

Table 3d. Comparison of the GROS method in ProUCL, R's *ros()* method, and the EM method via R for imputing values in place of NDs based on a gamma distribution. Columns are: x=randomly generated gamma data; detect=1 for detection or 0 for ND; group=sample ID; GROS Est=GROS estimate from ProUCL for NDs; ros() Est= GROS estimate from R; EM est=estimates based on the EM algorithm. Six samples of n=12 were generated for each of three combinations of the gamma distributions shape and scale parameters.

X	ND	Group	Shape	Scale	GROS Est.	ros() Est.	EM Est.
10.2190329	1	10	7	1.0000	10.2190329	10.2190329	10.21903
10.06282765	1	10	7	1.0000	10.06282765	10.06282765	10.06283
5.395173031	1	10	7	1.0000	5.395173031	5.395173031	5.39517
9.128545887	1	10	7	1.0000	9.128545887	9.128545887	9.12855
9.298253067	1	10	7	1.0000	9.298253067	9.298253067	9.29825
8.33056162	1	10	7	1.0000	8.33056162	8.33056162	8.33056
11.29474647	1	10	7	1.0000	11.29474647	11.29474647	11.29475
5.134259828	0	10	7	1.0000	4.06700088	4.06700085	2.7573
13.37110466	1	10	7	1.0000	13.37110466	13.37110466	13.3711
5.134259828	0	10	7	1.0000	5.017132555	5.01713253	3.99404
5.134259828	0	10	7	1.0000	5.705664514	5.70566449	4.87151
8.800215286	1	10	7	1.0000	8.800215286	8.800215286	8.80022
7.113263932	1	11	7	1.0000	7.113263932	7.113263932	7.11326
7.147899541	1	11	7	1.0000	7.147899541	7.147899541	7.1479
8.195100863	1	11	7	1.0000	8.195100863	8.195100863	8.1951
8.698108621	1	11	7	1.0000	8.698108621	8.698108621	8.69811
7.025086533	1	11	7	1.0000	7.025086533	7.025086533	7.02509
8.760042481	1	11	7	1.0000	8.760042481	8.760042481	8.76004
6.584597652	0	11	7	1.0000	3.633549691	3.6335497	3.03431
13.08992249	1	11	7	1.0000	13.08992249	13.08992249	13.08992
10.70500648	1	11	7	1.0000	10.70500648	10.70500648	10.70501
8.097491484	1	11	7	1.0000	8.097491484	8.097491484	8.09749
6.584597652	0	11	7	1.0000	4.538977011	4.53897702	4.14621
6.584597652	0	11	7	1.0000	5.190531115	5.19053112	4.91042
9.212660878	1	12	7	1.0000	9.212660878	9.212660878	9.21266
8.890128015	1	12	7	1.0000	8.890128015	8.890128015	8.89013
4.745609776	1	12	7	1.0000	4.745609776	4.745609776	4.74561
10.40179012	1	12	7	1.0000	10.40179012	10.40179012	10.40179
7.592513033	1	12	7	1.0000	7.592513033	7.592513033	7.59251
4.420583324	0	12	7	1.0000	3.56066131	3.56066131	2.38056
4.420583324	0	12	7	1.0000	4.418974838	4.41897483	3.48671
11.74890078	1	12	7	1.0000	11.74890078	11.74890078	11.7489
4.420583324	0	12	7	1.0000	5.041769126	5.04176912	4.27628
8.457657192	1	12	7	1.0000	8.457657192	8.457657192	8.45766
7.40764185	1	12	7	1.0000	7.40764185	7.40764185	7.40764
8.271443652	1	12	7	1.0000	8.271443652	8.271443652	8.27144

Table 3e. Comparison of the GROS method in ProUCL, R's *ros()* method, and the EM method via R for imputing values in place of NDs based on a gamma distribution. Columns are: x=randomly generated gamma data; detect=1 for detection or 0 for ND; group=sample ID; GROS Est=GROS estimate from ProUCL for NDs; ros() Est= GROS estimate from R; EM est=estimates based on the EM algorithm. Six samples of n=12 were generated for each of three combinations of the gamma distributions shape and scale parameters.

X	ND	Group	Shape	Scale	GROS Est.	ros() Est.	EM Est.
2.153859758	0	13	1	5.0000	0.01	0.0001	0.09114
11.7011345	1	13	1	5.0000	11.7011345	11.7011345	11.70113
4.961209759	1	13	1	5.0000	4.961209759	4.961209759	4.96121
4.970988629	1	13	1	5.0000	4.970988629	4.970988629	4.97099
2.153859758	0	13	1	5.0000	0.01	0.0001	0.40132
6.455714049	1	13	1	5.0000	6.455714049	6.455714049	6.45571
14.045522	1	13	1	5.0000	14.045522	14.045522	14.04552
2.153859758	0	13	1	5.0000	0.124946348	0.12496159	0.81743
3.445692109	1	13	1	5.0000	3.445692109	3.445692109	3.44569
9.331594746	1	13	1	5.0000	9.331594746	9.331594746	9.33159
2.537929649	1	13	1	5.0000	2.537929649	2.537929649	2.53793
3.060788741	1	13	1	5.0000	3.060788741	3.060788741	3.06079
14.59852189	1	14	1	5.0000	14.59852189	14.59852189	14.59852
3.17408711	1	14	1	5.0000	3.17408711	3.17408711	3.17409
6.445271454	1	14	1	5.0000	6.445271454	6.445271454	6.44527
7.992297191	1	14	1	5.0000	7.992297191	7.992297191	7.9923
1.354455961	0	14	1	5.0000	0.01	0.0001	0.01213
1.354455961	0	14	1	5.0000	0.01	0.0001	0.11191
13.06827726	1	14	1	5.0000	13.06827726	13.06827726	13.06828
2.35312312	1	14	1	5.0000	2.35312312	2.35312312	2.35312
1.568251322	1	14	1	5.0000	1.568251322	1.568251322	1.56825
1.46423312	1	14	1	5.0000	1.46423312	1.46423312	1.46423
1.354455961	0	14	1	5.0000	0.01	0.0001	0.31809
4.732068567	1	14	1	5.0000	4.732068567	4.732068567	4.73207
15.14768549	1	15	1	5.0000	15.14768549	15.14768549	15.14769
1.076786715	0	15	1	5.0000	0.01	0.0001	0.00215
26.47173236	1	15	1	5.0000	26.47173236	26.47173236	26.47173
1.184903241	1	15	1	5.0000	1.184903241	1.184903241	1.1849
1.114725661	1	15	1	5.0000	1.114725661	1.114725661	1.11473
4.917528406	1	15	1	5.0000	4.917528406	4.917528406	4.91753
6.630872462	1	15	1	5.0000	6.630872462	6.630872462	6.63087
2.465776086	1	15	1	5.0000	2.465776086	2.465776086	2.46578
2.616890175	1	15	1	5.0000	2.616890175	2.616890175	2.61689
5.695137397	1	15	1	5.0000	5.695137397	5.695137397	5.69514
1.076786715	0	15	1	5.0000	0.01	0.0001	0.04108
1.076786715	0	15	1	5.0000	0.01	0.0001	0.16263

Table 3f. Comparison of the GROS method in ProUCL, R's *ros()* method, and the EM method via R for imputing values in place of NDs based on a gamma distribution. Columns are: x=randomly generated gamma data; detect=1 for detection or 0 for ND; group=sample ID; GROS Est=GROS estimate from ProUCL for NDs; ros() Est= GROS estimate from R; EM est=estimates based on the EM algorithm. Six samples of n=12 were generated for each of three combinations of the gamma distributions shape and scale parameters.

X	ND	Group	Shape	Scale	GROS Est.	ros() Est.	EM Est.
0.455791679	1	16	1	5.0000	0.455791679	0.455791679	0.45579
0.817855182	1	16	1	5.0000	0.817855182	0.817855182	0.81786
0.301228981	0	16	1	5.0000	0.01	0.0001	0.00008
8.562745622	1	16	1	5.0000	8.562745622	8.562745622	8.56275
27.05689842	1	16	1	5.0000	27.05689842	27.05689842	27.0569
0.301228981	0	16	1	5.0000	0.01	0.0001	0.00455
3.815964029	1	16	1	5.0000	3.815964029	3.815964029	3.81596
2.577845714	1	16	1	5.0000	2.577845714	2.577845714	2.57785
0.367808057	1	16	1	5.0000	0.367808057	0.367808057	0.36781
0.951733159	1	16	1	5.0000	0.951733159	0.951733159	0.95173
0.301228981	0	16	1	5.0000	0.01	0.0001	0.02995
1.3933363	1	16	1	5.0000	1.3933363	1.3933363	1.39334
0.291053325	0	17	1	5.0000	0.01	0.0001	0.00141
15.3007581	1	17	1	5.0000	15.3007581	15.3007581	15.30076
0.593338496	1	17	1	5.0000	0.593338496	0.593338496	0.59334
11.20218475	1	17	1	5.0000	11.20218475	11.20218475	11.20218
0.291053325	0	17	1	5.0000	0.01	0.0001	0.02739
0.291053325	0	17	1	5.0000	0.01	0.0001	0.10931
3.791994738	1	17	1	5.0000	3.791994738	3.791994738	3.79199
3.265990866	1	17	1	5.0000	3.265990866	3.265990866	3.26599
0.333344144	1	17	1	5.0000	0.333344144	0.333344144	0.33334
4.002383342	1	17	1	5.0000	4.002383342	4.002383342	4.00238
3.251070765	1	17	1	5.0000	3.251070765	3.251070765	3.25107
3.726345719	1	17	1	5.0000	3.726345719	3.726345719	3.72635
0.623626732	1	18	1	5.0000	0.623626732	0.623626732	0.62363
0.461120965	0	18	1	5.0000	0.01	0.0001	0.00258
2.262001696	1	18	1	5.0000	2.262001696	2.262001696	2.262
1.539286765	1	18	1	5.0000	1.539286765	1.539286765	1.53929
0.643019909	1	18	1	5.0000	0.643019909	0.643019909	0.64302
0.461120965	0	18	1	5.0000	0.01	0.0001	0.02862
0.586457743	1	18	1	5.0000	0.586457743	0.586457743	0.58646
0.461120965	0	18	1	5.0000	0.01	0.0001	0.08838
3.908599787	1	18	1	5.0000	3.908599787	3.908599787	3.9086
0.886137252	1	18	1	5.0000	0.886137252	0.886137252	0.88614
6.724009395	1	18	1	5.0000	6.724009395	6.724009395	6.72401
1.852662064	1	18	1	5.0000	1.852662064	1.852662064	1.85266

Table 4. Actual parameter (shape and scale) values used to generate data in Table 3; estimates from the GROS method in ProUCL; estimates from the EM method via R; percent differences from the actual parameter values; and the average absolute percent differences across the six samples for each parameter combination.

Actual		GROS Estimates		EM Estimates		GROS % Difference		EM % Difference	
Shape	Scale	Shape	Scale	Shape	Scale	Shape	Scale	Shape	Scale
3	0.3333	0.7585	1.2244	1.2178	0.7758	-74.72	267.32	-59.41	132.74
3	0.3333	1.4081	0.5653	1.3562	0.5795	-53.06	69.59	-54.79	73.85
3	0.3333	1.1910	0.7110	1.8610	0.4600	-60.30	113.30	-37.97	38.00
3	0.3333	3.5554	0.2682	2.6343	0.3533	18.51	-19.54	-12.19	5.99
3	0.3333	1.8925	0.5740	2.1448	0.5077	-36.92	72.20	-28.51	52.31
3	0.3333	1.0929	0.7077	1.2991	0.5945	-63.57	112.31	-56.70	78.35
				Average Absolute % Differences:		51.18	109.04	41.59	63.54
7	1	0.7600	8.1024	1.3905	4.5044	-89.14	710.24	-80.14	350.44
7	1	0.5625	11.8266	1.3227	5.1475	-91.96	1082.66	-81.10	414.75
7	1	6.0809	1.1851	5.0688	1.4031	-13.13	18.51	-27.59	40.31
7	1	8.7778	0.9559	5.6773	1.4315	25.40	-4.41	-18.90	43.15
7	1	9.1318	0.8413	7.4047	1.0233	30.45	-15.87	5.78	2.33
7	1	8.4302	0.8872	5.4293	1.3334	20.43	-11.28	-22.44	33.34
				Average Absolute % Differences:		45.09	307.16	39.32	147.39
1	5	0.5058	9.9924	0.9326	5.5238	-49.42	99.85	-6.74	10.48
1	5	0.4213	10.9635	0.5896	7.8925	-57.87	119.27	-41.04	57.85
1	5	0.3799	14.5391	0.4264	12.9861	-62.01	190.78	-57.36	159.72
1	5	0.3391	11.3127	0.2922	13.1289	-66.09	126.25	-70.78	162.58
1	5	0.3975	9.5390	0.4235	8.9739	-60.25	90.78	-57.65	79.48
1	5	0.4847	3.2760	0.5389	2.9604	-51.53	-34.48	-46.11	-40.79
				Average Absolute % Differences:		57.86	110.24	46.61	85.15

Table 5 Key

Distr: The distribution determined to be the most appropriate in my original analysis, which used the EM algorithm to impute and evaluate the gamma distribution parameters, or KM for a nonparametric method.

utl.95: The 95 -95 UTL from my calculations, which is based on the WH method, and for the gamma distribution uses the EM algorithm to impute NDs and estimate gamma distribution parameters.

Gam: ProUCL's estimate of whether a gamma distribution fits the data well. When there are NDs, this is based on a GROS method that completely ignores the NDs and is a poor estimation choice.

ros.W: ProUCL's 95-95 UTL based on the WH method discussed in the ProUCL manuals based on imputing using the GROS method. Only calculated if there are NDs. This is based on a GROS method that completely ignores the NDs in estimating the gamma parameters and is a poor estimation choice.

ros.H: ProUCL's 95-95 UTL based on the HW method discussed in the ProUCL manuals based on imputing using the GROS method. Only calculated if there are NDs. This is based on a GROS method that completely ignores the NDs in estimating the gamma parameters and is a poor estimation choice.

km.W: ProUCL's 95-95 UTL based on the WH method discussed in the ProUCL manuals based on imputing using the GROS method. Only calculated if there are NDs.

km.H: The 95-95 UTL based on the HW method discussed in the ProUCL manuals based on imputing using the GROS method. Only calculated if there are NDs.

WH: ProUCL's 95-95 UTL based on the WH method discussed in the ProUCL manuals when no NDs are present.

HW: ProUCL's 95-95 UTL based on the HW method discussed in the ProUCL manuals when no NDs are present.

NonP: ProUCL's 95-95 UTL from the order statistic based nonparametric estimate. This value is wrong as it does not obtain the confidence/coverage specified and is often substantially off. To obtain this the specified confidence/coverage a sample of n=59 would be required.

Table 5a. Area 1, depth shallow – 95% coverage Upper Tolerance Limits with 95% confidence from background data for 34 analytes along with various values reported by ProUCL.

Analyte	Distr	utl.95	Gam[1]	ros.W[1]	ros.H[1]	km.W[2]	km.H[2]	WH[3]	HW[3]	NonP[4]
Aluminum, Tot	gam	11475	Yes					11645	11695	9930
Antimony, Tot	KM	1.76	No	1.466	1.638	0.929	0.943			0.7
Arsenic, Tot	gam	12	No					12.39	12.6	10.1
Barium, Tot	gam	400	Yes					414.8	424.2	383
Beryllium, Tot	gam	0.762	Yes					0.754	0.758	0.7
Boron, Tot	KM	104	Yes	52.77	56.19	64.5	71.31			30
Cadmium, Tot		.	Yes							0.7
Calcium, Tot	KM	289240	Yes					245477	254971	149000
Chloride	gam	362	Yes	463.7	645.1	347.5	399.3			171
Chromium, Hex	gam	1.21	Yes	1.948	2.456	1.356	1.499			0.71
Chromium, Tot	gam	10.4	Yes					10.54	10.59	9.65
Cobalt, Tot	gam	6.96	Yes					7.098	7.146	6.28
Copper, Tot	gam	11	Yes					11.21	11.32	9.49
Cyanide, Tot		.								
Iron, Tot	KM	33200	No					31379	34490	16100
Lead, Tot	gam	12	Yes					12.13	12.21	10.3
Magnesium, Tot	KM	36610	Yes					29493	30782	19000
Manganese, Tot	gam	382	Yes					392.1	396.8	320
Mercury, Tot	KM	.0411	Yes	0.0208	0.0211	0.0209	0.0213			0.017
Molybd, Tot	gam	1.1	Yes					1.156	1.253	0.7
Nickel, Tot	gam	14.9	Yes					15	15.07	13
Nitrogen	gam	2.12	Yes					2.172	2.198	1.7
Perchlorate	KM	2.44	Yes	1.845	2.276	0.868	0.876			0.75
Potassium, Tot	gam	2644	Yes					2711	2751	2110
Selenium, Tot	KM	3.97	No	3.381	4.297	1.884	1.965			1.2
Silver, Tot	KM	3.35	Yes	2.778	3.536	2.032	2.275			0.9
Sodium, Tot	gam	597	Yes					627.9	667.4	330
Strontium, Tot	gam	778	Yes					812.5	847.9	564
Thallium, Tot		.								
Tin, Tot		.								
Titanium, Tot	gam	242	Yes					248.6	254.5	172
Uranium, Tot	gam	1.32	Yes					1.341	1.351	1.14
Vanadium, Tot	gam	49.1	Yes					50.68	51.47	45.2
Zinc, Tot	gam	45.6	Yes					46.44	46.75	37.2

[1] These methods ignore the NDs in obtaining estimates of the gamma parameters.

[2] KM methods are a mixture of nonparametric estimates placed into a parametric formula.

[3] Based on the sample mean and not on sufficient statistics, and thus usually slightly higher than necessary.

[4] Based on the maximum order statistic, which gives substantially overstated confidence and/or coverage for the specified sample size.

Table 5b. Area 1, depth middle – 95% coverage Upper Tolerance Limits with 95% confidence from background data for 34 analytes along with various values reported by ProUCL.

Analyte	Distr	utl.95	Gam[1]	ros.W[1]	ros.H[1]	km.W[2]	km.H[2]	WH[3]	HW[3]	NonP[4]
Aluminum, Tot	gam	11509	Yes					11712	11784	9970
Antimony, Tot	KM	2.17	No	2	2.52	0.894	0.905			0.7
Arsenic, Tot	gam	12.9	Yes					13.35	13.67	10.4
Barium, Tot	gam	240	Yes					248.6	254.9	183
Beryllium, Tot	gam	0.683	Yes					0.697	0.701	0.6
Boron, Tot	KM	102	Yes	47.98	50.3	64.18	71.02			29
Cadmium, Tot		.	Yes							0.7
Calcium, Tot	KM	227833	Yes					184550	190281	121000
Chloride	gam	746	Yes					789.1	891.4	337
Chromium, Hex	gam	1.2	Yes	0.717	0.786	0.647	0.695			0.35
Chromium, Tot	gam	9.83	Yes					9.971	10.01	8.44
Cobalt, Tot	gam	6.24	Yes					6.408	6.452	5.57
Copper, Tot	gam	8.58	Yes					8.666	8.686	7.58
Cyanide, Tot		.								
Iron, Tot	KM	38182	No					44549	51639	15700
Lead, Tot	gam	13.5	Yes					13.72	13.84	10.6
Magnesium, Tot	KM	40333	Yes					32542	33402	21900
Manganese, Tot	gam	322	Yes					326.8	328.3	298
Mercury, Tot	KM	0.0259	Yes	0.0142	0.0143	0.0088	0.0088			0.009
Molybd, Tot	gam	1.2	Yes					1.237	1.278	1
Nickel, Tot	gam	18.3	Yes					18.72	18.93	14.9
Nitrogen	gam	2.23	Yes					2.281	2.306	2
Perchlorate	KM	4.42	Yes	3.789	4.686	2.203	2.303			1.5
Potassium, Tot	gam	2714	Yes					2800	2864	1890
Selenium, Tot	KM	2.6	Yes	2.59	3.322	1.192	1.217			0.9
Silver, Tot	KM	2.65	Yes	2.096	2.618	1.412	1.537			0.7
Sodium, Tot	gam	1036	Yes					1082	1153	610
Strontium, Tot	gam	1543	No					1628	1723	1210
Thallium, Tot		.								
Tin, Tot		.								
Titanium, Tot	gam	280	Yes					288.5	292.5	267
Uranium, Tot	gam	1.85	Yes					1.842	1.859	1.54
Vanadium, Tot	gam	74.9	No					78.34	81.38	51.8
Zinc, Tot	gam	53.4	No					54.25	54.63	46.4

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[3] Based on the sample mean and not on sufficient statistics, and thus usually slightly higher than necessary.

[4] Based on the maximum order statistic, which gives substantially overstated confidence and/or coverage for the specified sample size.

Table 5c. Area 1, depth deep – 95% coverage Upper Tolerance Limits with 95% confidence from background data for 34 analytes along with various values reported by ProUCL.

Analyte	Distr	utl.95	Gam[1]	ros.W[1]	ros.H[1]	km.W[2]	km.H[2]	WH[3]	HW[3]	NonP[4]
Aluminum, Tot	gam	13524	No					13781	13817	13900
Antimony, Tot	KM	2.35	Yes	1.464	1.585	1.218	1.272			0.7
Arsenic, Tot	gam	12.3	No					12.67	12.81	12.4
Barium, Tot	gam	216	Yes					223.3	229.3	161
Beryllium, Tot	gam	0.777	Yes					0.777	0.781	0.74
Boron, Tot	KM	113	Yes	37.27	37.59	77.87	87.53			31
Cadmium, Tot	KM	1.17	Yes	0.791	0.947	0.499	0.525			0.37
Calcium, Tot	KM	181223	Yes					132396	133406	117000
Chloride	gam	984	Yes					1033	1109	717
Chromium, Hex	gam	0.6	Yes	0.628	0.673	0.603	0.644			0.345
Chromium, Tot	gam	10.8	Yes					10.92	10.95	10.2
Cobalt, Tot	gam	7.61	Yes					7.687	7.74	6.39
Copper, Tot	gam	10.8	Yes					10.97	11.01	10.7
Cyanide, Tot		.								
Iron, Tot	KM	45137	No					51826	59559	19800
Lead, Tot	gam	16.6	Yes					16.94	17.11	14.2
Magnesium, Tot	gam	20356	Yes					20799	21004	17600
Manganese, Tot	gam	401	No					409	410.4	402
Mercury, Tot		.	Yes							0.7
Molybd, Tot	gam	1.81	Yes					1.871	1.923	1.6
Nickel, Tot	gam	18.3	Yes					18.58	18.68	15.3
Nitrogen	gam	1.91	Yes					1.933	1.949	1.7
Perchlorate	gam	1.67	Yes	2.068	2.173	1.871	1.938			1.3
Potassium, Tot	gam	2866	Yes					2954	3005	2430
Selenium, Tot	KM	1.95	Yes	1.002	1.036	0.87	0.885			0.7
Silver, Tot	KM	2.09	Yes	1.839	2.287	1.21	1.309			0.61
Sodium, Tot	gam	1203	Yes					1248	1285	1050
Strontium, Tot	gam	1078	No					1132	1181	763
Thallium, Tot		.								
Tin, Tot		.								
Titanium, Tot	gam	224	Yes					229.4	231.2	211
Uranium, Tot	gam	2.76	Yes					2.854	2.911	2.34
Vanadium, Tot	gam	88.5	Yes					91.97	94.12	89
Zinc, Tot	gam	58.4	Yes					59.38	59.71	51.7

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[4] Based on the maximum order statistic, which gives substantially overstated confidence and/or coverage for the specified sample size.

Table 5d. Area 2, depth shallow – 95% coverage Upper Tolerance Limits with 95% confidence from background data for 34 analytes along with various values reported by ProUCL.

Analyte	Distr	utl.95	Gam[1]	ros.W[1]	ros.H[1]	km.W[2]	km.H[2]	WH[3]	HW[3]	NonP[4]
Aluminum, Tot	gam	13211	Yes					13459	13573	11200
Antimony, Tot	KM	2.22	Yes	2.013	2.578	0.929	0.952			0.8
Arsenic, Tot	gam	12.2	No					12.51	12.64	10.8
Barium, Tot	gam	624	No					648.6	665.2	600
Beryllium, Tot	gam	0.628	No					0.646	0.652	0.56
Boron, Tot	KM	106	No	61.29	65.73	75.79	84.79			31
Cadmium, Tot		.	Yes							0.7
Calcium, Tot	KM	204319	Yes					158253	158979	139000
Chloride	gam	548	No					586.1	645.2	355
Chromium, Hex	gam	0.824	No					7.898	8.36	7.84
Chromium, Tot	gam	9.38	Yes					9.486	9.519	8.81
Cobalt, Tot	gam	5.34	Yes					5.416	5.44	4.95
Copper, Tot	gam	10.3	Yes					10.53	10.63	9.08
Cyanide, Tot		.								
Iron, Tot	KM	31537	No					31527	35236	14200
Lead, Tot	gam	10.3	Yes					10.47	10.5	9.2
Magnesium, Tot	KM	56705	Yes					47667	50061	28200
Manganese, Tot	gam	292	Yes					297.8	301.3	220
Mercury, Tot	KM	0.321	No	0.116	0.116	0.111	0.111			0.138
Molybd, Tot	KM	2.29	No	1.385	1.617	1.016	1.051			1
Nickel, Tot	gam	12.9	Yes					13	13.02	12.5
Nitrogen	gam	1.94	No					1.987	2.004	1.7
Perchlorate	KM	3.42	Yes	3.217	4.078	1.603	1.65			1.2
Potassium, Tot	gam	3260	Yes					3343	3399	2660
Selenium, Tot		.								
Silver, Tot	KM	2.77	Yes	1.679	2.042	1.127	1.198			0.7
Sodium, Tot	gam	932	Yes					979.5	1030	700
Strontium, Tot	gam	1067	Yes					1110	1147	821
Thallium, Tot		.								
Tin, Tot		.								
Titanium, Tot	gam	284	Yes					290.9	294.7	224
Uranium, Tot	gam	1.9	Yes					1.965	1.999	1.51
Vanadium, Tot	gam	46.5	Yes					47.59	47.99	41.8
Zinc, Tot	gam	43.5	Yes					44.19	44.52	38

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[3] Based on the sample mean and not on sufficient statistics, and thus usually slightly higher than necessary.

[4] Based on the maximum order statistic, which gives substantially overstated confidence and/or coverage for the specified sample size.

Table 5e. Area 2, depth middle – 95% coverage Upper Tolerance Limits with 95% confidence from background data for 34 analytes along with various values reported by ProUCL.

Analyte	Distr	utl.95	Gam[1]	ros.W[1]	ros.H[1]	km.W[2]	km.H[2]	WH[3]	HW[3]	NonP[4]
Aluminum, Tot	gam	13914	No					14193	14247	13900
Antimony, Tot	gam	0.909	Yes	1.126	1.178	0.902	0.915			0.8
Arsenic, Tot	gam	12.8	Yes					13.16	13.37	9.3
Barium, Tot	gam	160	Yes					163.2	165.1	135
Beryllium, Tot	gam	0.638	Yes					0.637	0.638	0.63
Boron, Tot	gam	94.1	No	101.2	115.5	92.91	104.2			41
Cadmium, Tot	KM	1.58	Yes	1.018	1.233	0.683	0.726			0.41
Calcium, Tot	KM	195044	Yes					164352	170146	101000
Chloride	gam	894	Yes					941.6	1010	763
Chromium, Hex	KM	0.5653	Yes					2.905	3.418	1.4
Chromium, Tot	gam	9.59	Yes					9.793	9.836	8.77
Cobalt, Tot	gam	5.31	Yes					5.384	5.402	4.82
Copper, Tot	gam	10	Yes					10.21	10.28	9.18
Cyanide, Tot		.								
Iron, Tot	KM	38321	No					38765	43400	16600
Lead, Tot	gam	14.6	Yes					14.69	14.77	12.6
Magnesium, Tot	gam	26959	Yes					27417	27599	23500
Manganese, Tot	gam	371	Yes					378.2	382.1	292
Mercury, Tot		.	Yes							0.7
Molybd, Tot	gam	1.82	Yes					1.929	2.102	1.1
Nickel, Tot	gam	16.5	Yes					16.67	16.73	15
Nitrogen	gam	3.3	Yes					3.43	3.536	2.8
Perchlorate	KM	4.8	Yes	3.096	3.315	2.927	3.102			1.7
Potassium, Tot	gam	3108	Yes					3176	3193	3060
Selenium, Tot		.								
Silver, Tot	KM	1.94	Yes	1.196	1.441	0.755	0.792			0.5
Sodium, Tot	gam	974	Yes					1004	1026	820
Strontium, Tot	gam	1385	Yes					1455	1528	980
Thallium, Tot		.								
Tin, Tot		.	Yes							0.7
Titanium, Tot	gam	284	Yes					290.3	292.4	263
Uranium, Tot	gam	2.64	Yes					2.703	2.748	2.12
Vanadium, Tot	gam	79.6	Yes					81.86	83.47	64.1
Zinc, Tot	gam	63.2	Yes					64.35	64.7	57.6

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[4] Based on the maximum order statistic, which gives substantially overstated confidence and/or coverage for the specified sample size.

Table 5f. Area 2, depth deep – 95% coverage Upper Tolerance Limits with 95% confidence from background data for 34 analytes along with various values reported by ProUCL.

Analyte	Distr	utl.95	Gam[1]	ros.W[1]	ros.H[1]	km.W[2]	km.H[2]	WH[3]	HW[3]	NonP[4]
Aluminum, Tot	gam	12577	Yes					12809	12863	12200
Antimony, Tot	KM	1.77	No	0.599	0.602	0.821	0.846			0.5
Arsenic, Tot	gam	14.2	Yes					14.7	14.96	13.1
Barium, Tot	gam	137	Yes					139.9	141.2	127
Beryllium, Tot	gam	0.609	Yes					0.616	0.617	0.55
Boron, Tot	gam	76.4	Yes	104.5	122.8	86.42	95.54			46
Cadmium, Tot	KM	1.42	Yes	1.082	1.322	0.693	0.739			0.45
Calcium, Tot	KM	109364	Yes					90099	90611	73800
Chloride	gam	579	Yes					604.9	635.3	354
Chromium, Hex	gam	0.793	Yes					4.098	4.673	2.205
Chromium, Tot	gam	9.41	Yes					9.559	9.594	8.3
Cobalt, Tot	gam	5.49	Yes					5.569	5.591	4.82
Copper, Tot	gam	8.29	Yes					8.407	8.449	7.5
Cyanide, Tot		.								
Iron, Tot	KM	39313	No					38719	42876	17900
Lead, Tot	gam	21.6	No					22.11	22.12	23.6
Magnesium, Tot	KM	47233	Yes					31426	31881	28400
Manganese, Tot	gam	404	Yes					411.9	413.8	398
Mercury, Tot		.								
Molybd, Tot	gam	3.22	No	4.571	5.586	3.653	4.021			2.7
Nickel, Tot	gam	17.1	Yes					17.36	17.46	14.5
Nitrogen	gam	3.1	Yes					3.198	3.237	3.1
Perchlorate	gam	3.19	Yes	4.027	4.448	3.282	3.431			2.1
Potassium, Tot	gam	2942	Yes					3013	3037	2830
Selenium, Tot		.								
Silver, Tot	KM	1.63	No	0.54	0.548	0.73	0.771			0.4
Sodium, Tot	gam	796	Yes					815.2	826.6	640
Strontium, Tot	gam	896	Yes					934.5	969.4	739
Thallium, Tot		.								
Tin, Tot		.								
Titanium, Tot	gam	273	Yes					279.6	280.9	277
Uranium, Tot	gam	3.26	Yes					3.365	3.45	2.55
Vanadium, Tot	gam	50.1	Yes					51.32	52.02	38.3
Zinc, Tot	gam	96.5	Yes					99.15	99.98	95

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[3] Based on the sample mean and not on sufficient statistics, and thus usually slightly higher than necessary.

[4] Based on the maximum order statistic, which gives substantially overstated confidence and/or coverage for the specified sample size.

Table 5g. Area 3, depth shallow – 95% coverage Upper Tolerance Limits with 95% confidence from background data for 34 analytes along with various values reported by ProUCL.

Analyte	Distr	utl.95	Gam[1]	ros.W[1]	ros.H[1]	km.W[2]	km.H[2]	WH[3]	HW[3]	NonP[4]
Aluminum, Tot	gam	16701	Yes					17177	17617	11200
Antimony, Tot	KM	2.84	Yes	1.697	1.778	1.886	2.017			1
Arsenic, Tot	gam	25.3	Yes					26.33	27.16	20.6
Barium, Tot	gam	730	Yes					760.7	786.8	572
Beryllium, Tot	gam	0.708	Yes					0.729	0.739	0.56
Boron, Tot	KM	104	No	87.36	108.1	64.04	69.75			43
Cadmium, Tot		.								
Calcium, Tot	KM	435836	Yes					334335	347447	240000
Chloride	KM	2752	Yes	3232	4533	2753	3453			1100
Chromium, Hex	gam	6.66	Yes					2.052	2.238	1.205
Chromium, Tot	gam	11.1	Yes					11.36	11.63	8.48
Cobalt, Tot	gam	7.93	Yes					8.134	8.214	7.71
Copper, Tot	gam	12.9	Yes					13.31	13.6	10.1
Cyanide, Tot		.	Yes							0.7
Iron, Tot	gam	18962	Yes					19494	19849	15100
Lead, Tot	gam	13.6	Yes					14.01	14.39	9.5
Magnesium, Tot	KM	118899	Yes					108234	120539	49900
Manganese, Tot	gam	378	Yes					390.1	400.6	268
Mercury, Tot	gam	0.0269	Yes					0.0281	0.0288	0.021
Molybd, Tot	gam	9.37	No					9.879	10.54	8.2
Nickel, Tot	gam	18.8	Yes					19.38	19.67	16.7
Nitrogen	gam	4.72	Yes					4.927	5.151	3.5
Perchlorate	KM	14.4	Yes	11.62	15.81	6.811	7.32			4.3
Potassium, Tot	gam	4311	Yes					4439	4549	3510
Selenium, Tot	KM	2.88	Yes	1.831	1.982	1.431	1.481			1
Silver, Tot	gam	4.15	Yes	4.999	5.681	5.365	6.301			2.2
Sodium, Tot	gam	2444	Yes					2635	2976	1500
Strontium, Tot	gam	4499	Yes					4803	5354	3510
Thallium, Tot		.								
Tin, Tot		.								
Titanium, Tot	gam	374	Yes					389.5	407.5	234
Uranium, Tot	gam	4.59	Yes					4.826	5.093	3.42
Vanadium, Tot	gam	44.8	No					45.97	46.36	38.6
Zinc, Tot	gam	54.3	Yes					56	57.41	40.6

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[4] Based on the maximum order statistic, which gives substantially overstated confidence and/or coverage for the specified sample size.

Table 5h. Area 3, depth middle – 95% coverage Upper Tolerance Limits with 95% confidence from background data for 34 analytes along with various values reported by ProUCL.

Analyte	Distr	utl.95	Gam[1]	ros.W[1]	ros.H[1]	km.W[2]	km.H[2]	WH[3]	HW[3]	NonP[4]
Aluminum, Tot	gam	15409	Yes					15853	16440	9650
Antimony, Tot	KM	4.93	Yes	4.289	5.345	2.911	3.143			2.1
Arsenic, Tot	gam	50.2	No					52.41	54.09	44.5
Barium, Tot	gam	565	Yes					590.5	630.1	388
Beryllium, Tot	gam	0.995	Yes					1.007	1.023	0.87
Boron, Tot	KM	127	Yes	129.1	179.9	86.75	96.28			50
Cadmium, Tot		.								
Calcium, Tot	KM	530734	No					381543	391109	279000
Chloride	gam	1819	Yes					1921	2078	1230
Chromium, Hex	gam	3.92	Yes	1.079	1.13	1.594	1.821			0.71
Chromium, Tot	gam	10.8	Yes					10.99	11.11	8.48
Cobalt, Tot	exp	.	No					13.06	13.3	10.5
Copper, Tot	gam	18.6	Yes					19.22	19.61	17.9
Cyanide, Tot		.								
Iron, Tot	KM	46667	No					27654	27975	25200
Lead, Tot	gam	17.4	Yes					17.9	18.25	14.2
Magnesium, Tot	KM	92799	Yes					67641	69422	47900
Manganese, Tot	gam	445	No					458.7	463.2	457
Mercury, Tot	KM	0.0973	No	0.0398	0.04	0.0382	0.0383			0.044
Molybd, Tot	gam	18.5	No					19.76	21.39	11.3
Nickel, Tot	exp	.	No					37.16	38.03	29.8
Nitrogen	KM	5.25	Yes	5.055	6.396	3.038	3.214			2.1
Perchlorate	KM	10.4	Yes	12.54	17.71	7.073	7.774			4.1
Potassium, Tot	gam	2923	Yes					2979	2999	2640
Selenium, Tot	KM	2.98	Yes	1.796	1.878	1.733	1.805			1.1
Silver, Tot	gam	5.67	Yes	6.971	8.824	5.78	6.729			2.7
Sodium, Tot	gam	1607	Yes					1664	1703	1490
Strontium, Tot	gam	2865	Yes					3007	3169	2100
Thallium, Tot		.								
Tin, Tot		.								
Titanium, Tot	gam	355	Yes					373.3	404.3	189
Uranium, Tot	gam	4.93	Yes					5.113	5.22	4.32
Vanadium, Tot	gam	58.4	Yes					60.15	62.14	39.3
Zinc, Tot	gam	79.4	No					81.81	82.24	87

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[2] KM methods are a mixture of nonparametric estimates placed into a parametric formula.

[3] Based on the sample mean and not on sufficient statistics, and thus usually slightly higher than necessary.

[4] Based on the maximum order statistic, which gives substantially overstated confidence and/or coverage for the specified sample size.

Table 5i. Area 3, depth deep – 95% coverage Upper Tolerance Limits with 95% confidence from background data for 34 analytes along with various values reported by ProUCL.

Analyte	Distr	utl.95	Gam[1]	ros.W[1]	ros.H[1]	km.W[2]	km.H[2]	WH[3]	HW[3]	NonP[4]
Aluminum, Tot	gam	12982	Yes					13399	13878	9040
Antimony, Tot	KM	4.13	Yes	2.558	2.713	2.554	2.712			1.5
Arsenic, Tot	gam	73.6	Yes					77.62	82.14	45.7
Barium, Tot	gam	405	Yes					422.8	452.3	244
Beryllium, Tot	gam	0.718	Yes					0.741	0.748	0.61
Boron, Tot	KM	112	Yes	54.78	56.49	84.25	94.67			38
Cadmium, Tot		.								
Calcium, Tot	KM	391178	Yes					285622	289823	228000
Chloride	gam	1491	Yes					1552	1655	1120
Chromium, Hex	KM	2.37	No	1.695	1.914	1.72	1.954			0.79
Chromium, Tot	gam	11.1	Yes					11.31	11.42	9.2
Cobalt, Tot	gam	13.1	Yes					13.62	14.01	10.8
Copper, Tot	gam	19.6	Yes					20.42	21.33	13.6
Cyanide, Tot		.	Yes							0.7
Iron, Tot	gam	23714	Yes					24373	24806	19200
Lead, Tot	gam	15.3	Yes					15.69	15.97	13.4
Magnesium, Tot	KM	163967	Yes					126703	134425	82300
Manganese, Tot	gam	366	Yes					374.2	378.1	306
Mercury, Tot	KM	0.0456	Yes	0.0145	0.0145	0.0159	0.0161			0.014
Molybd, Tot	gam	24.3	Yes					26.03	28.64	13.3
Nickel, Tot	gam	26	Yes					26.76	27.25	22.9
Nitrogen	gam	2.39	Yes	2.882	3.115	2.471	2.583			1.7
Perchlorate	gam	3.62	Yes					3.778	3.931	2.8
Potassium, Tot	gam	3074	Yes					3152	3226	2450
Selenium, Tot	KM	4.11	Yes	2.117	2.227	2.179	2.302			1.3
Silver, Tot	gam	4.29	Yes	4.728	5.32	4.82	5.522			2.2
Sodium, Tot	gam	1303	Yes					1336	1361	1000
Strontium, Tot	gam	3555	Yes					3697	3838	3400
Thallium, Tot		.								
Tin, Tot		.								
Titanium, Tot	gam	225	Yes					235.8	248.7	142
Uranium, Tot	gam	7.92	Yes					8.254	8.583	5.57
Vanadium, Tot	gam	74.7	Yes					77.39	78.94	66.4
Zinc, Tot	gam	51.3	Yes					52.45	52.96	45.8

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[2] KM methods are a mixture of nonparametric estimates placed into a parametric formula.

[3] Based on the sample mean and not on sufficient statistics, and thus usually slightly higher than necessary.

[4] Based on the maximum order statistic, which gives substantially overstated confidence and/or coverage for the specified sample size.

Table 5j. Area 4, depth shallow – 95% coverage Upper Tolerance Limits with 95% confidence from background data for 34 analytes along with various values reported by ProUCL.

Analyte	Distr	utl.95	Gam[1]	ros.W[1]	ros.H[1]	km.W[2]	km.H[2]	WH[3]	HW[3]	NonP[4]
Aluminum, Tot	gam	17681	Yes					18167	18746	12000
Antimony, Tot		.	Yes							0.7
Arsenic, Tot	gam	11.1	Yes					11.4	11.51	10.2
Barium, Tot	gam	215	Yes					221.4	224	202
Beryllium, Tot	gam	1.1	No					1.134	1.186	0.72
Boron, Tot		.								
Cadmium, Tot	KM	0.696	Yes	0.469	0.54	0.275	0.282			0.21
Calcium, Tot	KM	302460	Yes					287945	326866	136000
Chloride	KM	1317	Yes	1076	1662	736	856.7			567
Chromium, Hex	KM	1.2	Yes	0.812	0.963	0.523	0.55			0.35
Chromium, Tot	gam	11.1	Yes					11.35	11.48	9.3
Cobalt, Tot	gam	5.35	Yes					5.494	5.527	4.6
Copper, Tot	gam	11.7	Yes					11.94	12.08	9.53
Cyanide, Tot		.								
Iron, Tot	KM	39911	Yes					27969	28603	23100
Lead, Tot	gam	15.9	Yes					16.3	16.57	12.3
Magnesium, Tot	gam	14149	No					14568	14653	15100
Manganese, Tot	gam	444	Yes					457.5	475.1	296
Mercury, Tot	KM	0.0709	Yes	0.0344	0.0352	0.0366	0.0379			0.025
Molybd, Tot	gam	1.33	No					1.385	1.433	1
Nickel, Tot	gam	15.4	Yes					15.73	15.85	12.9
Nitrogen	gam	6.61	Yes	8.566	10.75	6.391	7.018			3.3
Perchlorate	KM	11.2	Yes	6.064	7.785	3.451	3.511			3.8
Potassium, Tot	gam	4151	Yes					4255	4383	2770
Selenium, Tot	KM	1.96	Yes	1.173	1.278	0.767	0.776			0.6
Silver, Tot		.								
Sodium, Tot	gam	643	Yes					680.1	732	520
Strontium, Tot	gam	476	Yes					498.2	524.6	379
Thallium, Tot		.								
Tin, Tot		.								
Titanium, Tot	gam	359	Yes					368.1	376.7	283
Uranium, Tot	gam	1.66	Yes					1.711	1.736	1.58
Vanadium, Tot	gam	33.9	No					34.41	34.5	32.7
Zinc, Tot	gam	59.7	Yes					61.3	63.14	44.8

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[3] Based on the sample mean and not on sufficient statistics, and thus usually slightly higher than necessary.

[4] Based on the maximum order statistic, which gives substantially overstated confidence and/or coverage for the specified sample size.

Table 5k. Area 4, depth middle – 95% coverage Upper Tolerance Limits with 95% confidence from background data for 34 analytes along with various values reported by ProUCL.

Analyte	Distr	utl.95	Gam[1]	ros.W[1]	ros.H[1]	km.W[2]	km.H[2]	WH[3]	HW[3]	NonP[4]
Aluminum, Tot	gam	12154	Yes					12489	12752	8610
Antimony, Tot		.	Yes							0.7
Arsenic, Tot	gam	12.6	Yes					12.97	13.34	8.66
Barium, Tot	gam	398	Yes					413.3	425	383
Beryllium, Tot	gam	0.713	Yes					0.733	0.741	0.57
Boron, Tot		.								
Cadmium, Tot		.								
Calcium, Tot	KM	214770	Yes					171417	174635	124000
Chloride	gam	1026	Yes					1099	1207	568
Chromium, Hex		.	Yes	2.522	2.889	1.954	1.993			2.34
Chromium, Tot	gam	11.7	Yes					11.98	12.15	9.8
Cobalt, Tot	gam	5.35	Yes					5.471	5.536	4.2
Copper, Tot	gam	9.2	Yes					9.4	9.45	9.1
Cyanide, Tot		.								
Iron, Tot	gam	15794	Yes					16005	16069	14000
Lead, Tot	gam	10.3	Yes					10.31	10.36	9.4
Magnesium, Tot	KM	31298	Yes					22846	23455	18000
Manganese, Tot	gam	296	No					303.5	306.3	267
Mercury, Tot	KM	0.0576	Yes	0.0201	0.0203	0.0195	0.0196			0.02
Molybd, Tot	gam	2.85	Yes					2.996	3.142	1.9
Nickel, Tot	gam	12.3	Yes					12.56	12.62	11
Nitrogen	gam	2.92	Yes	4.216	5.185	2.839	2.977			2.1
Perchlorate	KM	4.95	Yes	4.462	5.959	2.027	2.083			1.7
Potassium, Tot	gam	3038	Yes					3121	3182	2310
Selenium, Tot	KM	1.7	Yes	0.983	1.032	0.73	0.737			0.63
Silver, Tot		.								
Sodium, Tot	gam	1242	Yes					1307	1390	800
Strontium, Tot	gam	833	Yes					868.1	906.4	537
Thallium, Tot		.								
Tin, Tot		.								
Titanium, Tot	gam	352	Yes					361.7	369.7	271
Uranium, Tot	gam	3.97	Yes					4.092	4.117	4.34
Vanadium, Tot	gam	56.3	Yes					57.95	59.14	42.1
Zinc, Tot	gam	40.8	Yes					41.54	41.86	34.8

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[3] Based on the sample mean and not on sufficient statistics, and thus usually slightly higher than necessary.

[4] Based on the maximum order statistic, which gives substantially overstated confidence and/or coverage for the specified sample size.

Table 5l. Area 4, depth deep – 95% coverage Upper Tolerance Limits with 95% confidence from background data for 34 analytes along with various values reported by ProUCL.

Analyte	Distr	utl.95	Gam[1]	ros.W[1]	ros.H[1]	km.W[2]	km.H[2]	WH[3]	HW[3]	NonP[4]
Aluminum, Tot	gam	13653	Yes					14074	14418	10700
Antimony, Tot		.								
Arsenic, Tot	gam	11.9	Yes					12.24	12.57	9.9
Barium, Tot	gam	310	Yes					321.3	329	312
Beryllium, Tot	gam	0.814	Yes					0.85	0.865	0.63
Boron, Tot		.								
Cadmium, Tot		.	Yes							0.7
Calcium, Tot	KM	332558	Yes					205686	210744	182000
Chloride	gam	918	Yes					974.1	1059	585
Chromium, Hex	KM	1.23	Yes	0.611	0.662	0.602	0.643			0.33
Chromium, Tot	gam	11.3	Yes					11.62	11.83	9
Cobalt, Tot	gam	5.28	Yes					5.334	5.381	4.34
Copper, Tot	gam	13.5	No					13.97	14.13	13.3
Cyanide, Tot		.								
Iron, Tot	gam	18759	Yes					19150	19377	16400
Lead, Tot	gam	15.6	Yes					16.05	16.37	13.6
Magnesium, Tot	KM	33658	No					27804	28943	16700
Manganese, Tot	gam	393	Yes					406.7	417	338
Mercury, Tot	KM	0.0302	Yes	0.0139	0.014	0.0108	0.0108			0.011
Molybd, Tot	gam	1.98	Yes					2.068	2.191	1.3
Nickel, Tot	gam	14.1	Yes					14.49	14.76	11.2
Nitrogen	KM	4.82	Yes	4.525	5.679	2.788	2.969			1.7
Perchlorate	KM	3.37	Yes	2.165	2.552	1.255	1.281			0.96
Potassium, Tot	gam	3125	Yes					3210	3260	2500
Selenium, Tot	KM	2.45	Yes	2.081	2.644	0.892	0.901			0.8
Silver, Tot		.								
Sodium, Tot	gam	1297	Yes					1366	1493	700
Strontium, Tot	gam	841	Yes					879.7	920.2	653
Thallium, Tot		.								
Tin, Tot		.								
Titanium, Tot	gam	330	Yes					338	341.7	274
Uranium, Tot	gam	3.25	Yes					3.369	3.477	2.28
Vanadium, Tot	gam	42.4	Yes					43.48	44.18	34.7
Zinc, Tot	gam	52.9	Yes					54.46	55.63	39.5

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[4] Based on the maximum order statistic, which gives substantially overstated confidence and/or coverage for the specified sample size.

Table 5m. Area 5, depth shallow – 95% coverage Upper Tolerance Limits with 95% confidence from background data for 34 analytes along with various values reported by ProUCL.

Analyte	Distr	utl.95	Gam[1]	ros.W[1]	ros.H[1]	km.W[2]	km.H[2]	WH[3]	HW[3]	NonP[4]
Aluminum, Tot	gam	15954	No					16327	16707	12100
Antimony, Tot	KM	1.77	Yes	1.184	1.285	0.771	0.781			0.6
Arsenic, Tot	gam	11.1	Yes					11.31	11.48	9.3
Barium, Tot	gam	775	Yes					810.7	861.7	511
Beryllium, Tot	gam	0.817	Yes					0.823	0.829	0.73
Boron, Tot	KM	72.7	Yes	33.83	35.71	37.47	40.09			20
Cadmium, Tot		.	Yes							0.7
Calcium, Tot	KM	269204	Yes					210892	214352	163000
Chloride	gam	683	Yes					737.1	844.6	470
Chromium, Hex		.	Yes							0.7
Chromium, Tot	gam	14.7	Yes					15.03	15.26	11.6
Cobalt, Tot	gam	6.83	Yes					6.967	7.061	5.5
Copper, Tot	gam	13.3	Yes					13.6	13.8	11.3
Cyanide, Tot		.								
Iron, Tot	gam	14465	Yes					14674	14738	13000
Lead, Tot	gam	10.4	Yes					10.6	10.68	8.6
Magnesium, Tot	gam	8924	Yes					9079	9147	7830
Manganese, Tot	gam	265	Yes					272.3	273.7	269
Mercury, Tot	KM	0.0443	Yes	0.0204	0.0207	0.0236	0.0242			0.017
Molybd, Tot	gam	1.33	Yes	1.686	2.006	1.33	1.453			0.8
Nickel, Tot	gam	13.1	Yes					13.34	13.5	10.4
Nitrogen	exp	.	No					173.6	204.4	93.4
Perchlorate	KM	8.69	Yes	7.748	10.68	3.917	4.127			3.3
Potassium, Tot	gam	3878	Yes					3991	4124	2690
Selenium, Tot	KM	1.33	Yes	0.85	0.914	0.511	0.513			0.5
Silver, Tot	KM	2.45	Yes	2.471	3.111	1.717	1.899			1
Sodium, Tot	gam	538	Yes					559	576.9	450
Strontium, Tot	gam	486	Yes					499.6	509.1	370
Thallium, Tot		.								
Tin, Tot		.								
Titanium, Tot	gam	292	Yes					298.9	304.4	217
Uranium, Tot	gam	1.12	No					1.138	1.148	0.89
Vanadium, Tot	gam	42.2	Yes					43.17	43.68	37.2
Zinc, Tot	gam	41.1	Yes					41.87	42.19	35.2

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[4] Based on the maximum order statistic, which gives substantially overstated confidence and/or coverage for the specified sample size.

Table 5n. Area 5, depth middle – 95% coverage Upper Tolerance Limits with 95% confidence from background data for 34 analytes along with various values reported by ProUCL.

Analyte	Distr	utl.95	Gam[1]	ros.W[1]	ros.H[1]	km.W[2]	km.H[2]	WH[3]	HW[3]	NonP[4]
Aluminum, Tot	gam	14948	Yes					15376	15695	10500
Antimony, Tot	KM	2.49	Yes	2.254	2.75	1.16	1.182			0.9
Arsenic, Tot	gam	8.69	Yes					8.842	8.917	7.5
Barium, Tot	gam	237	Yes					244.7	251.6	208
Beryllium, Tot	gam	0.86	Yes					0.898	0.914	0.65
Boron, Tot	KM	79.3	Yes	28.44	28.91	44.89	48.61			21
Cadmium, Tot		.								
Calcium, Tot	KM	186172	Yes					132664	133642	120000
Chloride	gam	743	Yes					805.4	955.4	372
Chromium, Hex		.								
Chromium, Tot	gam	14.5	Yes					14.83	15.01	11.3
Cobalt, Tot	gam	6.83	Yes					6.991	7.081	5.4
Copper, Tot	gam	10.9	Yes					11.19	11.34	8.3
Cyanide, Tot		.								
Iron, Tot	gam	15258	Yes					15482	15572	13100
Lead, Tot	gam	12.8	Yes					13.05	13.14	11.7
Magnesium, Tot	gam	12962	Yes					13224	13324	11400
Manganese, Tot	gam	271	Yes					278.6	284.4	213
Mercury, Tot	KM	0.0322	Yes	0.0145	0.0147	0.0136	0.0137			0.012
Molybd, Tot	gam	1.35	Yes					1.397	1.428	1.2
Nickel, Tot	gam	12.5	Yes					12.78	12.94	10.3
Nitrogen	KM	17.3	Yes	13.35	17.78	8.842	9.525			7
Perchlorate		.	Yes							0.7
Potassium, Tot	gam	2800	Yes					2877	2930	2270
Selenium, Tot	KM	1.5	Yes	0.822	0.859	0.584	0.588			0.5
Silver, Tot	KM	1.75	Yes	0.759	0.79	0.962	1.043			0.5
Sodium, Tot	gam	730	Yes					767.2	819.7	466
Strontium, Tot	gam	456	Yes					468.2	474.9	386
Thallium, Tot		.								
Tin, Tot		.								
Titanium, Tot	gam	386	Yes					399.2	414.9	274
Uranium, Tot	gam	2.04	Yes					2.087	2.121	1.67
Vanadium, Tot	gam	40.7	Yes					41.54	41.89	35.3
Zinc, Tot	gam	45	Yes					45.89	46.34	35.1

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[4] Based on the maximum order statistic, which gives substantially overstated confidence and/or coverage for the specified sample size.

Table 5o. Area 5, depth deep – 95% coverage Upper Tolerance Limits with 95% confidence from background data for 34 analytes along with various values reported by ProUCL.

Analyte	Distr	utl.95	Gam[1]	ros.W[1]	ros.H[1]	km.W[2]	km.H[2]	WH[3]	HW[3]	NonP[4]
Aluminum, Tot	gam	16863	Yes					17338	17743	13800
Antimony, Tot	KM	1.87	Yes	1.277	1.378	1.022	1.058			0.7
Arsenic, Tot	gam	8.31	Yes					8.493	8.554	6.7
Barium, Tot	gam	167	Yes					171.6	174	146
Beryllium, Tot	gam	0.953	Yes					0.947	0.957	0.86
Boron, Tot	KM	68.3	No	66.94	90.52	40.74	43.66			24
Cadmium, Tot		.	Yes							0.7
Calcium, Tot	KM	206942	Yes					143017	144806	126000
Chloride	gam	535	Yes					575.6	671.6	257
Chromium, Hex		.	Yes							0.7
Chromium, Tot	gam	15.3	Yes					15.67	15.88	12.4
Cobalt, Tot	gam	7.28	Yes					7.446	7.546	6.1
Copper, Tot	gam	11.5	Yes					11.8	11.89	10.8
Cyanide, Tot		.								
Iron, Tot	gam	16607	Yes					16882	16980	15000
Lead, Tot	gam	12.2	Yes					12.41	12.5	10.4
Magnesium, Tot	gam	12737	Yes					13014	13131	11500
Manganese, Tot	gam	360	Yes					371.3	377.2	319
Mercury, Tot	KM	0.0242	Yes	0.0146	0.0147	0.0088	0.0088			0.009
Molybd, Tot	gam	1.51	Yes					1.565	1.616	1.1
Nickel, Tot	gam	13.8	Yes					14.16	14.31	12.2
Nitrogen	gam	5.46	Yes	8.336	10.93	5.235	5.522			4.9
Perchlorate	KM	1.32	Yes	0.449	0.449	0.484	0.485			0.43
Potassium, Tot	gam	3649	Yes					3770	3873	2750
Selenium, Tot	KM	2.18	Yes	1.689	2.083	0.758	0.764			0.7
Silver, Tot	KM	1.89	Yes	1.549	1.932	0.953	1.021			0.58
Sodium, Tot	gam	1004	Yes					1061	1134	750
Strontium, Tot	gam	374	Yes					382.7	386.2	343
Thallium, Tot		.								
Tin, Tot		.								
Titanium, Tot	gam	389	Yes					403	415.8	283
Uranium, Tot	gam	1.58	Yes					1.611	1.617	1.39
Vanadium, Tot	gam	36.5	Yes					37.22	37.59	29.8
Zinc, Tot	gam	55	Yes					56.42	57.09	48.9

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[3] Based on the sample mean and not on sufficient statistics, and thus usually slightly higher than necessary.

[4] Based on the maximum order statistic, which gives substantially overstated confidence and/or coverage for the specified sample size.

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Appendix A – R Code

```
library(xlsx)

#---------------------------------------
# Define a function to generate random gamma data from the specified gamma
# parameters, sample size, number of groups, and detection limit; and save
# to the specified .xlsx file.
gamma.data.to.xlsx <- function(shape, rate, n, num.groups, det.limit=0,
                                          num.nds=NULL, file.out=NULL) {

      #Initialize the data.frame for the specified data.
      new.data <- data.frame(x=numeric(), d_x=numeric(), group=character(),
                                    stringsAsFactors=FALSE)

      #Loop through each group to be generated.
      for(i.group in 1:num.groups) {

            #Generate the data.frame for the current group.
            x <- rgamma(n, shape=shape, rate=rate)

            #If num.nds is not NULL, use it to determine the det.limit.
            if(! is.null(num.nds)) {
                  sorted.x <- sort(x)
                  if(num.nds < n)
                        det.limit <- (sorted.x[num.nds] + sorted.x[num.nds + 1]) / 2
            }

            #Identify the NDs in a separate column - 0's denote NDs, 1's
            #denote detects.
            d_x <- rep(1, n)
            tf.nd <- x < det.limit
            d_x[tf.nd] <- 0
            x[tf.nd] <- det.limit

            #Create the group variable as a character vector.
            group <- as.character(rep(i.group, n))

            #Append the new data to the existing data.frame.
            new.data <- rbind(new.data,
                              data.frame(x=x, d_x=d_x, group=group, shape=shape,
                                    rate=rate, stringsAsFactors=FALSE))
      }

      # If the output file specification is not NULL, then write the data out as
      # a .xlsx file.
      if(! is.null(file.out) ) write.xlsx2(x=new.data, file=file.out,
                                          row.names=FALSE)

      #Return the new data frame.
      return(new.data)
}
```

```
# Example usage.
# Set the specific Excel file name.
data.path <- "/2014-Soils/"
file.base <- "test.gamma.01"
file.ext <- ".xlsx"
file.out <- paste(data.path, file.base, file.ext, sep="")


#----------------------------------------
# Get some randomly generated gamma data sets and store the data in a
# .xlsx file to be used by ProUCL to calculate UTLs.  Save the data
# sets as data.frames and get calculate UTLs using the tolerance
# package for comparison with ProUCL's results.

test.data.02 <-
      gamma.data.to.xlsx(shape=3, rate=3, n=12, num.groups=6, det.limit,
                                 num.nds=0, file.out=file.out)
test.data.02$group <- factor(test.data.02$group)
str(test.data.02)

for(i in 1:nlevels(test.data.02$group)) {
      print(gamtol.int(x=test.data.02$x[test.data.02$group == i],
                                 alpha=0.05, P=0.95, side=1)[[4]])
}
```

```
library(MASS)

#---------------------------------------
# Define a function to take a vector of x data having NDs replaced by
# detection limits and a vector indicating detects and ND with 1s and 0s,
# respectively, and return a list with a vector of x-values with 0's for
# NDs and a vector of detection limits - suitable for use with
# em.gmle.impute().
convert.dls.to.zeros <- function(x, d) {
	tf.nds <- which(d == 0)
	tf.detects <- ! tf.nds
	d <- rep(0, length(d))
	d[tf.nds] <- x[tf.nds]
	x[tf.nds] <- 0
	return( list(x=x, det.limits=d) )
}


#---------------------------------------
# Define a function to implement the EM algorithm in solving for the gamma
# distribution parameters and imputing for NDs.
em.gmle.impute <- function(x, detect.limits, precision=1e-4,
                                        bias.correct=TRUE, na.rm=FALSE,
                                neg="small", max.iters=100, ...) {
	tf.nds <- x == 0
	wh.nds <- which(tf.nds)
	wh.detects <- which(! tf.nds)

	n.total <- length(x)
	n.nds <- length(wh.nds)
	n.detects <- n.total - n.nds

	k.plus.1 <- n.total - n.detects + 1
	ord <- order(x, na.last=FALSE)
	p <- ((1:n.total - 0.5) / n.total)[order(ord)]

	dl2 <- 0.5 * detect.limits
	p.detects <- p[wh.detects]
	p.nds <- p[wh.nds]
	x[wh.nds] <- dl2[wh.nds]


	# Use the algorithm in Singh, Singh, and Iaci3 (2008) to get the
	# gamma initial MLE estimates.
	params <- gmle(x, precision=precision*0.01, bias.correct=bias.correct,
                                na.rm=na.rm, neg=neg, ...)
	# Update the estimated imputed values based on the current gamma
	# parameter estimates.
	x[wh.nds] <- qgamma(p.nds, shape=params$shape, rate=params$rate)

	#Iterate between solving for the MLE estimates and the getting updated
	#imputed values for the NDs, until convergence.
	convergence <- 1
	for(iter in 1:max.iters) {

		params.old <- params
```

```
            # Use the algorithm in Singh, Singh, and Iaci3 (2008) to get the gamma
            # MLE estimates.
            params <- gmle(x, precision=precision*0.01, bias.correct=bias.correct,
                              na.rm=na.rm, neg=neg, ...)

            # Update the estimated imputed values based on the current gamma
            # parameter estimates.
            x[wh.nds] <- qgamma(p.nds, shape=params$shape, rate=params$rate)

            #If the desired precision is reached then set the convergence level
            #to 0 and break out.
            if(abs(params$shape - params.old$shape) < precision) {
                  convergence <- 0
                  break
            }
      }
      cat("convergence = ", convergence, "\n", sep="")
      return( list(x=x, params=params, convergence=convergence, iters=iter) )
}

# Example usage.  Note DL's are inserted in the x vector where there are NDs.
x <- c(14.59852189, 3.17408711, 6.445271454, 7.992297191, 1.354455961, 1.354455961, 13.06827726,
2.35312312, 1.568251322, 1.46423312, 1.354455961, 4.732068567)
d <- c(1, 1, 1, 1, 0, 0, 1, 1, 1, 1, 0, 1)

xd <- convert.dls.to.zeros(x, d)
em.out <- em.gmle.impute(xd$x, xd$det.limits, max.iters=100)
```