4.3.4 Calculation of Upper Tolerance Limits and Summary Statistics

Upper Tolerance Limits - Calculations

Summary statistics were calculated for background analyte concentrations at Fort Polk for surface and subsurface soils for each granularity and across granularities as described above. The following statistics were also calculated: sample size, minimum, maximum, mean, one-sided 95% upper confidence limit (UCL) for the mean, median, and the 95%/95% upper tolerance limit (UTL). A UTL is an estimate of an upper bound on individual measurements from a population. It is described with two numbers. The first number is the *confidence*, the second is the *coverage*. The *coverage* of a UTL specifies the minimum percentage of the population that should lie below the UTL value. The *confidence* of a UTL indicates the certainty that the calculated UTL value provides at least the specified coverage. This certainty is a function of both the sample size and the variability among the data values used to calculate the UTL. For a 95%/95% UTL, investigators are 95% certain that 95% of the population values lie below the calculated UTL.

The results of the Shapiro-Wilk W-tests were used to determine whether parametric or non-parametric statistical methods were most appropriate for calculating the 95% UTLs. Parametric methods were used when the data distribution was normal or lognormal. Non-parametric methods (sometimes referred to as "distribution-free" methods) were used for those analytes whose data were neither normally nor lognormally distributed. Both the parametric UTLs (U.S. EPA, 1992) and the non-parametric UTLs (Conover, 1980) were calculated at the 95% confidence level.

Normal and Lognormal UTL Calculation

The normal UTL was calculated using the following equation:

$$UTL = \bar{x} + Ks$$

The Lognormal UTL was calculated as

$$UTL = e^{\bar{x} + Ks}$$

where:

$\bar{x}$ = the mean of the observations

$$= \sum_{i=1}^{n} x_i / n$$

s = the standard deviation of the observations

$$s = \sqrt{\sum_{i=1}^{n} (x_i - \bar{x}) / n - 1}$$

and

K = the one-sided normal tolerance factor selected to provide 95% coverage at the 95% confidence level for the given sample size. (Appendix B, Table 5, U.S. EPA, 1989)

The non-parametric UTL is the maximum reported value (if the samples size is less than 60) and is the second, third, forth, etc. largest result for larger sample sizes. Coverage for non-parametric UTLs is a function of the sample size and may be less than the coverage of 95% used for the normal UTLs.

Upper Tolerance Limits - Discussion

The background 95% upper tolerance limit (UTL) may be used to determine the presence or absence, and nature and extent of environmental contamination for metals, organic herbicides, and organochlorine pesticides. The UTL is the 95% upper confidence limit for the 95th percentile of the true background concentration of a constituent of interest. Results for individual samples from the site may be compared directly to the UTLs for the corresponding constituents in the same background sample medium. If a site sample concentration exceeds the UTL, it may be interpreted as indicating the presence of potential contamination.

The UTLs for 95% coverage level (i.e., the 95% upper confidence limit of the *95th percentile*) are conservative, in that only measurements that are *very* different from background will be discerned. Thus, when only the 95% UTLs are used for comparisons, there is a chance of concluding that an individual measurement is not different from background, when in fact it is from a population with results larger than background. Other factors, such as contaminant toxicity, the potential existence of "hot spots", etc., would need to be considered in the use of the UTLs to make decisions regarding site risk and clean-up levels.

All calculated statistics are presented in this report to allow the flexibility to choose statistics that are most appropriate for comparisons planned for future applications. The UTLs are presented for those instances in which decisions must be made on the basis of a comparison of individual site sample results to background (e.g., determining the presence or absence of contamination). Means, medians, and the upper confidence limits for the mean are presented for those instances in which means comparisons will be used to determine whether a site is contaminated on the average. Background UTLs and summary statistics for each depth and granularity are presented in Appendix C, Table 3. Background UTLs and summary statistics across granularities are presented (by depth) in Appendix C, Table 4.

Other Summary Statistics

In addition to comparisons of individual site sample results to background UTLs, means comparisons are also appropriate for other environmental applications (e.g., estimating the volume of contaminated media requiring corrective action, demonstrating attainment of required clean-up levels, performing statistical comparisons for risk assessments, etc.). Means comparisons, or central tendency tests, are used to indicate whether or not differences exist between two sample populations (e.g., "background" and "site").

A one-sided 95% upper confidence limit (UCL) for the mean is calculated as $\bar{x} + t_{\alpha,n-1} s / \sqrt{n}$ where $\bar{x}$ and s are the mean and standard deviation of the data, n is the sample size and t is value from the Students t distribution with α level of significance and n-1 degrees of freedom. For all cases, normal theory UCLs were considered appropriate by the Central Limit Theorem.

The one-sided 95% upper confidence limit (UCL) for the mean can be used when comparing average site concentrations to background. A one-sided 95% lower confidence limit (LCL) for the site average can be calculated and compared to the UCL for the background average. If the LCL for the site average is less than the UCL for the background average, then one may conclude that there is no difference between the background and site concentrations, on the average. For a conservative check, one may also calculate the site average and compare the site average to the background UCL. If the site average is less than the background UCL, then one may conclude that there is no difference between the background and site concentrations, on the average. For a more thorough analysis between site and background averages, a statistician should be consulted.

4.4 Conclusions

Plots illustrating the data for each of the individual analytes are presented in Appendix D. For each analyte, box plots are shown to compare the coarse and fine granularity data along with their combined blank UTLs. Raw data used for the statistical evaluations are given in Appendix B. All tests of normality, UTLs and summary statistics are presented in Appendix C.

Surface and subsurface soils were segregated for the background study and should be segregated for future investigations. Coarse and fine-grained soils were segregated for this background study and it is recommended that they be segregated for future investigations. Summary statistics for coarse and fine granularities for each depth are presented in Appendix C, Table 3. Because information will not always be available about the granularity of future samples, UTLs and other summary statistics are also provided for the combined granularities. Combining data across granularities reduces the ability of the study to determine true differences between potential releases and background, but may be necessary in some cases. The process of deriving the combined UTLs and summary statistics was the same as that for the segregated data. Summary statistics for combined coarse and fine granularities are presented in Appendix C, Table 4. Measurement imprecision indicated by the analysis of the field duplicate data may contribute to the overall uncertainty of our analyses.

Metals concentrations in fine-grained soils tended to be higher than metals concentrations in coarse-grained soils. These differences in concentrations were statistically significant, except for antimony, calcium, cobalt, manganese, mercury, molybdenum, and silver in subsurface soils and antimony, barium, beryllium, cobalt, manganese, mercury, molybdenum, selenium, silver, sodium, and thallium in surface soils. No significant differences in granularity were observed for herbicides or pesticides, however there were in general few detected results for these analytes.

For comparison purposes of individual sample results to background concentrations, the background 95% UTL may be used to determine the presence or absence of environmental contamination for metals, organic herbicides, and organochlorine pesticides. For those samples in which the soil type is known, refer to Table 4.4-1. If the soil type is unknown, refer to Table 4.4-2.

Table 4.4-1
Background UTLs by Depth and Granularity

Granularity	Analyte	Depth	Units	Background UTL
Coarse	Aluminum	Subsurface	mg/kg	10353.31
Coarse	Aluminum	Surface	mg/kg	20500.00
Coarse	Antimony	Subsurface	mg/kg	0.53
Coarse	Antimony	Surface	mg/kg	0.80
Coarse	Arsenic	Subsurface	mg/kg	10.10
Coarse	Arsenic	Surface	mg/kg	6.69
Coarse	Barium	Subsurface	mg/kg	58.90
Coarse	Barium	Surface	mg/kg	60.43
Coarse	Beryllium	Subsurface	mg/kg	0.69
Coarse	Beryllium	Surface	mg/kg	0.74
Coarse	Cadmium	Subsurface	mg/kg	0.43
Coarse	Cadmium	Surface	mg/kg	0.92
Coarse	Calcium	Subsurface	mg/kg	1320.00
Coarse	Calcium	Surface	mg/kg	488.91
Coarse	Chromium	Subsurface	mg/kg	12.03
Coarse	Chromium	Surface	mg/kg	26.10
Coarse	Cobalt	Subsurface	mg/kg	6.46
Coarse	Cobalt	Surface	mg/kg	3.22
Coarse	Copper	Subsurface	mg/kg	7.84
Coarse	Copper	Surface	mg/kg	9.40
Coarse	Iron	Subsurface	mg/kg	12872.56
Coarse	Iron	Surface	mg/kg	24500.00
Coarse	Lead	Subsurface	mg/kg	8.96
Coarse	Lead	Surface	mg/kg	11.10
Coarse	Magnesium	Subsurface	mg/kg	902.00
Coarse	Magnesium	Surface	mg/kg	686.00
Coarse	Manganese	Subsurface	mg/kg	215.00
Coarse	Manganese	Surface	mg/kg	270.00
Coarse	Molybdenum	Subsurface	mg/kg	0.72
Coarse	Molybdenum	Surface	mg/kg	0.82
Coarse	Nickel	Subsurface	mg/kg	6.90
Coarse	Nickel	Surface	mg/kg	7.41
Coarse	Potassium	Subsurface	mg/kg	655.00
Coarse	Potassium	Surface	mg/kg	600.00
Coarse	Selenium	Subsurface	mg/kg	0.45
Coarse	Selenium	Surface	mg/kg	0.49
Coarse	Silver	Subsurface	mg/kg	0.12
Coarse	Silver	Surface	mg/kg	0.23
Coarse	Sodium	Subsurface	mg/kg	39.40
Coarse	Sodium	Surface	mg/kg	43.28
Coarse	Thallium	Subsurface	mg/kg	0.57
Coarse	Thallium	Surface	mg/kg	0.73
Coarse	Vanadium	Subsurface	mg/kg	29.33

Table 4.4-1
Background UTLs by Depth and Granularity

Granularity	Analyte	Depth	Units	Background UTL
Coarse	Vanadium	Surface	mg/kg	58.20
Coarse	Zinc	Subsurface	mg/kg	15.30
Coarse	Zinc	Surface	mg/kg	20.80
Coarse	Mercury	Subsurface	mg/kg	0.03
Coarse	Mercury	Surface	mg/kg	0.05
Coarse	4,4'-DDD	Surface	ug/kg	3.12
Coarse	4,4'-DDE	Surface	ug/kg	0.37
Coarse	4,4'-DDT	Surface	ug/kg	0.86
Coarse	Aldrin	Surface	ug/kg	2.80
Coarse	Chlordane	Surface	ug/kg	33.80
Coarse	Dieldrin	Surface	ug/kg	3.34
Coarse	Endosulfan I	Surface	ug/kg	1.65
Coarse	Endosulfan II	Surface	ug/kg	6.04
Coarse	Endosulfan Sulfate	Surface	ug/kg	6.48
Coarse	Endrin	Surface	ug/kg	19.20
Coarse	Endrin Aldehyde	Surface	ug/kg	0.48
Coarse	Endrin Ketone	Surface	ug/kg	7.16
Coarse	Heptachlor	Surface	ug/kg	0.95
Coarse	Heptachlor epoxide	Surface	ug/kg	8.08
Coarse	Isodrin	Surface	ug/kg	1.49
Coarse	Methoxychlor	Surface	ug/kg	12.90
Coarse	Mirex	Surface	ug/kg	1.98
Coarse	Toxaphene	Surface	ug/kg	286.00
Coarse	alpha-BHC	Surface	ug/kg	1.73
Coarse	alpha-Chlordane	Surface	ug/kg	3.20
Coarse	beta-BHC	Surface	ug/kg	3.48
Coarse	delta-BHC	Surface	ug/kg	2.98
Coarse	gamma-BHC	Surface	ug/kg	1.98
Coarse	gamma-Chlordane	Surface	ug/kg	0.30
Coarse	2,4,5-T	Surface	ug/kg	4.94
Coarse	2,4,5-TP (Silvex)	Surface	ug/kg	5.68
Coarse	2,4-D	Surface	ug/kg	38.80
Coarse	2,4-DB	Surface	ug/kg	17.30
Coarse	Dalapon	Surface	ug/kg	746.00
Coarse	Dicamba	Surface	ug/kg	12.88
Coarse	Dichloroprop	Surface	ug/kg	24.80
Coarse	Dinoseb	Surface	ug/kg	47.80
Coarse	MCPA	Surface	ug/kg	7180.00
Coarse	MCPP	Surface	ug/kg	4900.00
Fine	Aluminum	Subsurface	mg/kg	24486.58
Fine	Aluminum	Surface	mg/kg	20401.37
Fine	Antimony	Subsurface	mg/kg	0.78
Fine	Antimony	Surface	mg/kg	0.78

Table 4.4-1
Background UTLs by Depth and Granularity

Granularity	Analyte	Depth	Units	Background UTL
Fine	Arsenic	Subsurface	mg/kg	11.30
Fine	Arsenic	Surface	mg/kg	10.83
Fine	Barium	Subsurface	mg/kg	279.25
Fine	Barium	Surface	mg/kg	118.05
Fine	Beryllium	Subsurface	mg/kg	1.90
Fine	Beryllium	Surface	mg/kg	1.68
Fine	Cadmium	Subsurface	mg/kg	2.47
Fine	Cadmium	Surface	mg/kg	1.87
Fine	Calcium	Subsurface	mg/kg	8140.00
Fine	Calcium	Surface	mg/kg	2682.01
Fine	Chromium	Subsurface	mg/kg	57.60
Fine	Chromium	Surface	mg/kg	44.84
Fine	Cobalt	Subsurface	mg/kg	17.30
Fine	Cobalt	Surface	mg/kg	4.81
Fine	Copper	Subsurface	mg/kg	14.25
Fine	Copper	Surface	mg/kg	15.50
Fine	Iron	Subsurface	mg/kg	48645.79
Fine	Iron	Surface	mg/kg	44431.40
Fine	Lead	Subsurface	mg/kg	17.87
Fine	Lead	Surface	mg/kg	162.00
Fine	Magnesium	Subsurface	mg/kg	3228.00
Fine	Magnesium	Surface	mg/kg	2159.34
Fine	Manganese	Subsurface	mg/kg	209.00
Fine	Manganese	Surface	mg/kg	525.00
Fine	Molybdenum	Subsurface	mg/kg	1.26
Fine	Molybdenum	Surface	mg/kg	1.33
Fine	Nickel	Subsurface	mg/kg	18.50
Fine	Nickel	Surface	mg/kg	9.77
Fine	Percent moisture	Subsurface	%	28.78
Fine	Percent moisture	Surface	%	23.57
Fine	Potassium	Subsurface	mg/kg	1174.52
Fine	Potassium	Surface	mg/kg	1119.94
Fine	Selenium	Subsurface	mg/kg	0.47
Fine	Selenium	Surface	mg/kg	0.43
Fine	Silver	Subsurface	mg/kg	0.12
Fine	Silver	Surface	mg/kg	0.36
Fine	Sodium	Subsurface	mg/kg	228.00
Fine	Sodium	Surface	mg/kg	68.42
Fine	Thallium	Subsurface	mg/kg	1.10
Fine	Thallium	Surface	mg/kg	1.18
Fine	Vanadium	Subsurface	mg/kg	69.70
Fine	Vanadium	Surface	mg/kg	99.27
Fine	Zinc	Subsurface	mg/kg	30.40