

## Webinar 3: ProUCL A to Z

74: could not find superfund download. found TCE NDs...

\* Polona(privately): Look for SuperFund.xls

**X 84:** When you were discussing the background threshold value options at the start, you mentioned that when you get more than 10 samples you should be using hypothesis testing. Are you referring to more than 10 background samples? Or are you saying if your background is based on <10 samples and your data set for comparison has more than 10 samples?

Hypothesis testing is used when many (at least 10) observations for site and for background are available. For smaller sample sizes results of hypothesis testing are not reliable.

85. The Download Files button is greyed out

\* Moderator Jean Balent(privately): You have to click the file name in the list in that window and then click "download" files.

**X 89. :** I was instructed to not remove outliers when computing BTVs, do you agree

Outliers are extremely large or small values relative to the rest of the data. Although they are a suspect to misrepresent the data, they shouldn't be removed from the calculation unless there is a clear underlying reason to do so such as:

- Transcription errors
- Data-coding errors
- Laboratory measurement errors

Therefore, they need to be investigated as they can provide quite some useful information regarding the site such as:

- Indicate hot spots that are consequence of previous use of the site
- Multiple soil types in background areas
- Naturally occurring spots with high concentrations of analytes

Good practice is to perform analysis with and without outliers and document well all the reasoning behind analysis and results of investigations of outliers.

**X 92.:** What is difference between WH and HW Gamma estimates?

For mildly skewed to moderately skewed gamma distributed data sets, HW and WH approximations yield fairly comparable UTLs. However, for highly skewed data sets ( $k < 0.5-1.0$ ) with higher variability, the HW method tends to yield higher limits than the WH method.

**X 93.:** Do you recommend outlier removal from background?

Outliers are extremely large or small values relative to the rest of the data. Although they are a suspect to misrepresent the data, they shouldn't be removed from the calculation unless there is a clear underlying reason to do so such as:

- Transcription errors
- Data-coding errors
- Laboratory measurement errors

Therefore, they need to be investigated as they can provide quite some useful information regarding the site such as:

- Indicate hot spots that are consequence of previous use of the site
- Multiple soil types in background areas
- Naturally occurring spots with high concentrations of analytes

Good practice is to perform analysis with and without outliers and document well all the reasoning behind analysis and results of investigations of outliers.

94: Some regulators require outlier removal from background, but not site data.

\* Moderator Jean Balent(privately): Thanks for the comment!

**X 96.**: Question - what should you do if ProUCL recommends the 99% UCL as the best option when running for a 95% UCL??

This ProUCL output indicates that mean value is not well characterized. Most likely reasons are:

- Distribution of data is very skewed or multimodal
- Sample size is too small
- Sampling is biased

Statistician should be consulted for further steps with data analysis.

**X 97.**: What reason is there for removing an outlier besides showing lab error; is just mathematical reasoning good enough?

Removing outliers based on outcome of statistical test is not a good practice. Not removing true outliers or removing false outliers both lead to distorted estimates of population parameters" (QA/G-9S). Recommended approach is to investigate all confirmed outliers for possible underlying cause like area with high naturally occurring concentration, multiple soil types in background area, higher variability than expected, historical not well documented use of the area. Then perform analysis with and without outliers and document all reasoning and results of outlier investigation.

**X 98.**: Why not run an outlier test available in ProUCL to confirm the presence of outliers?

Outlier test to confirm a suspect outlier should be performed, however outliers shouldn't be removed only based on test outcome. They need to be investigated and decision to remove should only be made based on finding underlying cause for outlier. Rather than removing outliers, performing analysis with and without outliers and documenting well the reasoning and outcome of outlier investigation is recommended.

**X 99.**: Do you recommend doing outlier testing in addition to visualizing data on plot before removing outliers?

Graphical display and statistical tests for outliers are both very useful methods. However, outliers shouldn't be removed only based on statistical testing or visualization. All outliers need to be investigated for presence of underlying cause before they are removed from further analysis. Rather than removing outliers, performing analysis with and without outliers and documenting well the reasoning and outcome of outlier investigation is recommended.

**X 101.**: Does ProUCL have a function to mathematically determine if a value is a true outlier?

ProUCL has a module for testing outliers. Please refer to the first webinar in this series and ProUCL 5.1 User guide Chapter 7.

**X 102.**: Where is the recommended UCL shown?

Recommended UCL is displayed on the bottom of analysis output and is labeled *Suggested UCL to Use*.

**X 104.**: There is also an option for non-parametric in UTLs . How does the presence of non-detects affect the non-parametric (ROS) UTL value that is generated by ProUCL in the output ? Is this non-parametric UTL option sensitive to outliers etc?

The presence of outliers influences regression estimates for slope and intercept that are used to impute NDs with ROS method. Please refer to ProUCL 5.1 Technical Guide Chapter 4.5 for detailed discussion on impact of outliers on ROS estimated of imputed values.

**X 106.**: Is there any way to calculate lower confidence limits in proUCL?

ProUCL does not have a capability to directly to compute LCL. Please refer to Note in ProUCL 5.1 User Guide Chapter 11 and Chapters 6.4.1.4 and 10.1.2 in ProUCL 5.1 Technical Guide for some discussion on computing LCLs

**X 107.**: If a particular 95% UCL for soil shows a value above an action limit, and you excavate the hot

spot and re-run the statistics, is it appropriate to look at the SAME UCL distribution in the re-analysis (particularly if the re-analysis wants to use a different distribution).

After removing a hot spot, data for confirmation samples or backfill samples are added to the original data set, and data for excavated samples are removed. This changes the data set, which may or may not change the family of the distributions. So it is not surprising if ProUCL suggests a different distribution for the new data set.

**X 108:** If multiple UCLs are recommended what should be selected?

The answer to this question depends on the situation. We recommend consulting a statistician.

**X 110:** when calculating BTV values, would you ever change the assumed K value to something other than 1?

K larger than 1 is often used in groundwater monitoring applications.

**X 111:** I was told to not use Chebyshev output. Comment.

Chebyshev is very conservative and depends on the quality of estimate for standard deviation. It should be used with caution. If it is recommended by ProUCL then we suggest to consult a statistician as there may be some issues with the data set like extreme skewedness, multimodality or biased sampling and some more advanced statistical methods are needed for analysis.

**X 112:** Question: The gamma UTLs always give more significant digits than another distribution. Is it ok to round-up these values to less significant digits that are more in-line with what a normal distribution or other distribution would provide?

Reasonable practice would be to report UTLs to the same number of significant digits as the raw data.

114.: Sure thing - something I've been grappling with. If I have follow-up questions, we can email you/presenters afterwards?

\* Moderator Jean Balent(privately): Yes, that's correct!

**X 115:** I have learned that using UTL testing can lead to false negatives. Specifically, site data that are below the UTL will be identified as background when really it is not. Therefore, we request mean testing to support UTL testing. Is this necessary?

Testing of the mean or median is always preferable and the UTL for BTV is effective mainly in detecting high values above background.

116: thus it is very possible that many contaminants will fall below this value and thus considered to be below background when in fact, they are not.

117. \* Moderator Jean Balent: Thanks for joining us!

Seminar slides and other materials can be accessed from <https://clu-in.org/conf/tio/ProUCLAtZ3/#tabs-4>  
Please submit feedback after the event at <https://clu-in.org/conf/tio/ProUCLAtZ3/#tabs-5>

118.: Thank you for putting this on. Will we have access to the closed captioning as well?

\* Moderator Jean Balent(privately): Yes, the closed captioning will be included in the online archive

119.: The feedback link is not working.

\* Moderator Jean Balent(privately): <https://clu-in.org/conf/tio/ProUCLAtZ3/#tabs-5>

126.: ITRC & states discourage use of ProUCL for calculation of Incremental Sampling Method (ISM) UCLs. Instead they recommend substituting LODs for NDs and calculating UCLs. They do not recommend using a max concentration even when there is just 1 detection from the triplicate samples. Why? Can ProUCL be used for ISM background calcs & comparison to site ISM sample data?

OUTSIDE THE OF THE PRESENTATION TOPIC

128.: would be nice to see something illustrating all this talk rather than looking at 10-12 data points

**X 129.** : What's a K value?

The K value represents the number of future observations that you are comparing your BTV to.

130.: Based on what the speaker said, if there are multiple detection limits what are the challenges KM method face (when there are non-detects in the data)?

That statement was made thinking specifically of hypothesis testing with the 2 sample Wilcoxon test. Where it moves multiple ND values to the highest ND in the data group.

**X 131.** : I asked this question during the first ProUCL webinar but never received a response. So, here it is again: When ProUCL provides a UCL, but  $UCL > \max$ , do you use the UCL or the max? Also, if a Chebyshev UCL  $> \max$ , do you use the Chebyshev UCL or max?

POLONA:  $UCL > \max$  indicates that there are issues with the data set. Further steps depend on a specific application and we recommend consulting a statistician. Chebyshev is very conservative and depends on the quality of estimate for standard deviation. It should be used with caution.

**X 132.** In the manganese example. the UTL and UTL values from the non-parametric calculations were set at the maximum of the dataset. What's the rationale?

The specifics of the UTL methodology are outlined in the ProUCL Tech guide, but the values returned are artifacts of creating the upper confidence limit around a given percentile of the data.

**X 133.** : The following sentence came from a document I am reviewing on calculating BTVs for metals in soil. "The USEPA (2009) generally recommends the use of the KM method when evaluating multiple censored data sets." Is this sentence correct?

134.: I could foresee regulator requiring outlier removal & then using USL.

135.: Wilson-Hilferty involves a cube root transformation to normality; and the Hawkins-Wixley uses a fourth root transform to convert gamma data to normal distribution.

**X 138.** : Are you still recommending use of Wilcoxon Rank Sum testing for comparing site data to background data

We are recommending using an appropriate hypothesis testing method when you have more than roughly 10 samples in both your background and site sample datasets. As to which hypothesis test, that is more of a site/problem specific question.

**X 139.** : How do we make a comparison of site data with a background UCL?

You generally wouldn't use a background UCL. Comparisons could be made between a site UCL and a risk level, or background UTLs and isolated sample sites though. When at least 10 data points are available for both background and the site, then using hypothesis testing is recommended.

140. : Some consider site all background unless outliers are identified as potential source areas.

**X 141.** The decision logic within ProUCL's general selection of gamma over lognormal distribution in upper bounds estimates is not really clear. In the Mn example given, goodness-of-fit testing indicates a markedly better fit to a LN distribution, especially in the more influential upper range of the data. Granted, the H-UCL sort of blows up in this circumstance as often does with low n and moderate to high variability. Travis; There are certainly situations when a UCL from the lognormal distribution could be the best fit. However, when standard deviation for lognormally distributed data is larger than 1 and data set size is less than 30 lognormal distribution tends to result in unstable and overestimated UCLs. Therefore, if users are not exceptionally well versed in distributional tendencies, relying on Gamma when both Lognormal and Gamma are available can be a general rule of thumb. If you have good reason to disagree in specific situations that is why it's a rule of thumb and not a law.

142. Luis Enrique Loaiza Guillen: and also the outlier tests with ND, makes you to ignore them or replace them with 1/2 DL

X 143.: or is it other way to use the ND in the outlier tests?

Travis; Within ProUCL those are currently the only methods, however outside of ProUCL there are certainly more.

X 144.: I was told that data with non-detects are almost never normally distributed.

Data with non-detects are censored and therefore skewed to the left.

145: Can you demonstrate how best to ID multiple populations within a data set?

Please consult with a statistician.

146: Actually ITRC ISM guidance recommends only either the t-test or Chebychev UCL or IISM UCLs.

X 147.: If given this error "It is therefore recommended to avoid the use of H-statistic based 95% UCLs." and no other UCLs are recommended, should you use the recommended H-value anyways, default to the max detect, or possibly use the BCA method as you mentioned.

As I mentioned, in the case of only the H-UCL being recommended, as long as all of the sample size requirements are met, if you need to return a UCL i would look at the non-parametric options such as BCA or another bootstrap option.

148.: Will you be compiling and sharing Q&As?

Yes!

149.: I would like to see ProUCL be able to do Multivariate Regression and Chi-square tests to help with MNA analyses.