

Calculation of Background Threshold Values (BTVs) for the Solid Waste Landfill (SWL) for CYs 2018, 2019, 2020, and 2021

Prepared for the U.S. Department of Energy
Assistant Secretary for Environmental Management

Contractor for the U.S. Department of Energy
under Contract 89303320DEM000030



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Calculation of Background Threshold Values (BTVs) for the Solid Waste Landfill (SWL) for CYs 2018, 2019, 2020, and 2021

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Terms

BTV	background threshold value
CPCCo	Central Plateau Cleanup Company
CRAN	Comprehensive R Archive Network
ECF	environmental calculation file
HEIS	Hanford Environmental Information System
MDL	method detection limit
SWL	solid waste landfill

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1 Purpose

This environmental calculation file (ECF) presents summary statistics and background threshold values (BTVs) for the Solid Waste Landfill (SWL) constituents for calendar year 2021.

2 Background

The SWL is a non-operating landfill located adjacent to the Nonradioactive Dangerous Waste Landfill (Figure 1).

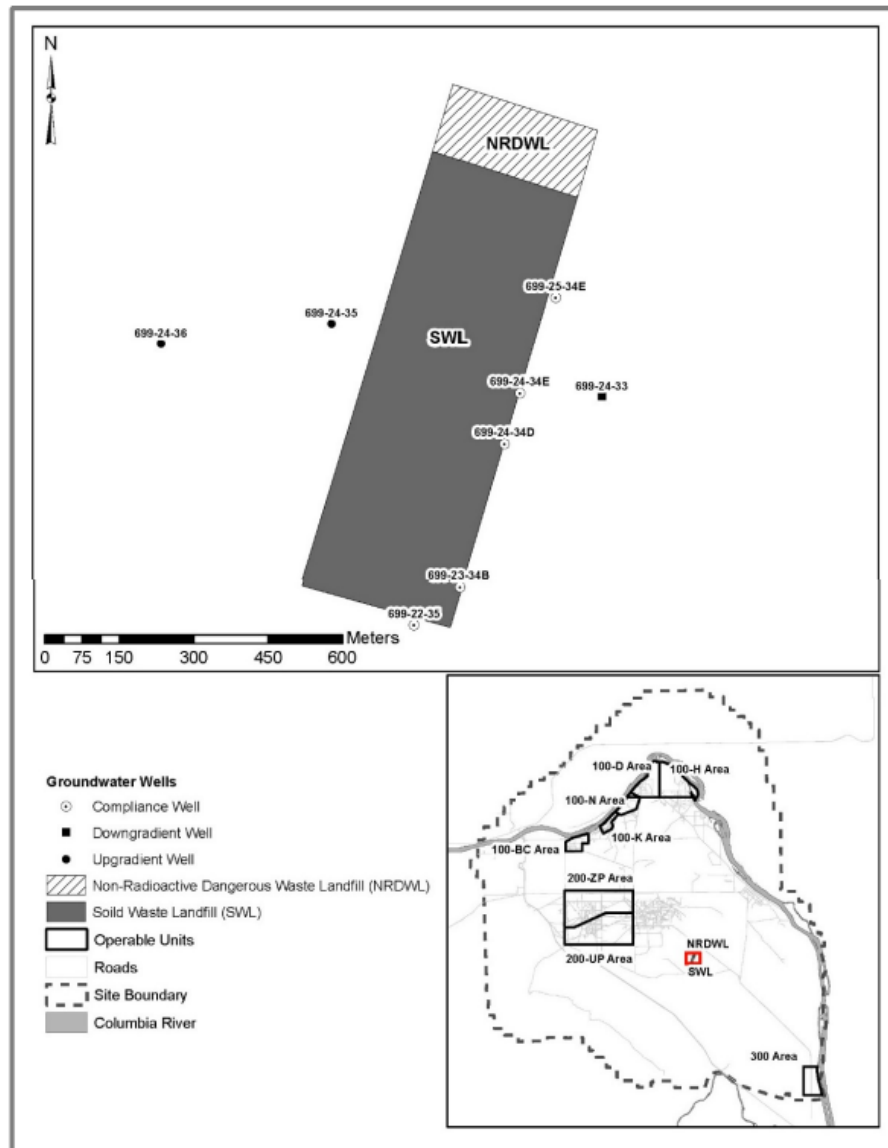


Figure 1. Solid Waste Landfill and Groundwater Wells

The SWL operated from 1973 to March 1996 and received nondangerous and nonradioactive solid waste, sewage, and garage wash water (DOE/EA-1707D, *Environmental Assessment: Closure of Nonradioactive Dangerous Waste Landfill (NRDWL) and Solid Waste Landfill (SWL), Hanford Site, Richland Washington*). Groundwater monitoring for SWL is regulated by the Washington State Department of

Ecology (WAC 173-350-500, “Solid Waste Handling Standards,” “Groundwater Monitoring”). Monitoring is conducted under DOE/RL-2015-33, *Groundwater Monitoring Plan for Solid Waste Landfill*. The set of constituents being monitored and evaluated against BTVs are listed in WAC 173-350-500(4)(h)(i), (ii), and (iii) and presented in Table 1.

Table 1. List of Constituents for Statistical Evaluation at Solid Waste Landfill

Requirement	Constituent	Type
WAC 173-350-500 (4)(h)(i), (ii), and (iii) field parameters, geochemical indicator parameters, and leachate indicators	pH	Field Parameter ^a
	Specific Conductance	
	Temperature	
	Alkalinity	
	Bicarbonate	
	Total ^b and dissolved ^c Calcium	
	Chloride	Geochemical Indicator Parameters
	Total ^b and dissolved ^c iron	
	Total ^b and dissolved ^c magnesium	
	Total ^b and dissolved ^c manganese	
	Nitrate	
	Dissolved ^{c,d} potassium	
	Dissolved ^{c,d} sodium	
	Sulfate	
	Ammonia	Leachate Indicators ^e
	Total organic carbon	
	Total dissolved solids	
WAC 173-350-500 (4)(i) site-specific constituents	Total ^b and dissolved ^c Arsenic	

Reference: WAC 173-350-500, “Solid Waste Handling Standards,” “Groundwater Monitoring.”

- Although included as a field parameter in WAC 173-350-500 (4)(h)(i). Water-level measurements will not be statistically evaluated.
- Total analyte is represented in the Hanford Environmental Information System (HEIS) database under column FILTERED_FLAG with value of “N.”
- Dissolved analyte is denoted in the HEIS database under column FILTERED_FLAG with value of “Y.”
- WAC 173-350-500 (4)(h)(ii) does not identify total potassium or total sodium as indicator parameters but were included in the analysis.
- Leachate indicators are added for sampling under this revised plan and will be statistically evaluated after the first 2 years of quarterly monitoring results (eight samples) are available to calculate background threshold values.

This document presents summary statistics and calculated BTVs for the constituents listed in Table 1 apart from static water level and the leachate indicators which have not yet completed the first 2 years of quarterly monitoring under DOE/RL-2015-33. The BTVs for each analyte were calculated based on the upgradient well 699-24-36 in the monitoring network. The statistics are based on groundwater concentrations available through the end of December 2021.

3 Methodology

This chapter discusses the data and methods used to perform summary statistics and to calculate BTVs presented in this ECF.

3.1 Data Acquisition and Processing

This section discusses the acquisition and processing of the groundwater data prior to calculation of the BTVs.

3.1.1 Chemistry Data

Groundwater chemistry data were downloaded from the Hanford Environmental Information System (HEIS) database which is maintained by the Central Plateau Cleanup Company (CPCCo) and exported into a Microsoft® Access® database (HEIS2_ADM_PNLGW_STD_RESULTS_MV_14FEB2022_COMBINED.accdb). The data were downloaded from HEIS on February 14, 2022. Table 2 presents the fields extracted from HEIS used in the calculation of summary statistics and BTVs.

Table 2. HEIS Database Fields for Constituent Data

Field Extracted	Definition
WELL_NAME	Location identification
SAMP_DATE_TIME	Sampling date
STD_CON_LONG_NAME	Analyte name
STD_VALUE_RPTD	Reported Concentration
STD_ANAL_UNITS_RPTD	Units for concentration measurement
LAB_QUALIFIER	Laboratory data qualifier
REVIEW_QUALIFIER*	Review data qualifier
COLLECTION_PURPOSE	Primary reason for sample collection
VALIDATION_QUALIFIER	Validation qualifier

*Additional information may be found in the RESULT_COMMENT field for this record (HNF-38155, *HEIS Sample, Result, and Sampling Site Data Dictionary*)

HEIS = Hanford Environmental Information System

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3.1.2 Identifying Nondetects

Nondetect data were identified by using the laboratory qualifier (LAB_QUALIFIER=U or any qualifier combination that contains U).

3.1.3 Time Period of Analysis

Consistent with previous years' BTV calculations under Revision 0 of the monitoring plan (DOE/RL-2015-33), BTVs were calculated using a 5-year data window. The time period of analysis for calendar year 2021 was January 1, 2017 to December 31, 2021.

3.1.4 Review Qualifiers

Chemistry data were removed from the dataset prior to calculation based on review qualifiers (Table 3).

Table 3. Review Qualifiers for Data Removal

Review Qualifier	Definition
R	Do not use. Further review indicates the result is not valid.
Y	Result suspect. Review - insufficient evidence to show result valid or invalid.

Table 4 presents the removed data based on review qualifiers.

Table 4. Data Removed Based on Review Qualifiers

Well Name	Sample Date	Analyte	Reported Value (µg/L)	Qualifier	
				Laboratory	Review
699-24-36	7/12/2021	Dissolved iron	637	--	Y

Laboratory qualifier:

-- = data not available or not applicable

Review qualifier:

Y = result suspect; review - insufficient evidence to show result valid or invalid

3.1.5 Daily Averaging

Daily averages were calculated for data with multiple measurements on the same day. When all measurements on the same day were nondetect data, the highest detection limit was used for the daily value. For daily duplicates where only one of the samples were nondetect data, the detected value was used for the daily value. Appendix A of this ECF presents the duplicate daily measurements and the calculated daily average.

Table 5 lists the wells for the SWL monitoring network from DOE/RL-2015-33. The BTVs for each analyte were calculated based on the upgradient well 699-24-36 in the monitoring network.

Table 5. Network Monitoring Wells

Well Name	Location (with respect to SWL)
699-24-36	Upgradient
699-25-34E	Downgradient
699-24-34E	Downgradient
699-24-34D	Downgradient
699-23-34B	Downgradient
699-22-35	Downgradient
SWL = Solid Waste Landfill	

3.1.6 Summary Statistics

Summary statistics were calculated for each analyte. The mean, median, standard deviation, coefficient of variation, minimum, and maximum were determined using detected data only, nondetected data was not included. However, nondetect data were included in determination of percent nondetects and during the comparison to the analytes' method detection limit (MDL). Each summary statistic was calculated as shown in Eq. 1 through Eq. 9.

Percent nondetects:
$$PNDs_c = \left(\frac{n_{c,0}}{n_c} \right) \times 100\% \quad (\text{Eq. 1})$$

Mean:
$$m_c = \frac{1}{n_c} \sum_{i=1}^{n_c} x_i \quad (\text{Eq. 2})$$

Median:
$$med_c = x_c \left(\frac{n_c + 1}{2} \right) \quad (\text{Eq. 3})$$

Standard deviation:
$$s_c = \sqrt{\frac{1}{n_c - 1} \sum_{i=1}^{n_c} (x_i - m_c)^2} \quad (\text{Eq. 4})$$

Coefficient of variation:
$$CV_c = \frac{s_c}{m_c} \quad (\text{Eq. 5})$$

Number of detects above MDL:
$$n_{c,a} = \sum_{i=1}^{n_c} \begin{cases} 1 & \text{if } x_i > MDL \\ 0 & \text{if } x_i < MDL \end{cases} \quad (\text{Eq. 6})$$

$$\text{Number of detects below MDL:} \quad n_{c,b} = \sum_{i=1}^{n_c} \begin{cases} 0 & \text{if } x_i > MDL \\ 1 & \text{if } x_i < MDL \end{cases} \quad (\text{Eq. 7})$$

$$\text{Minimum:} \quad \min(x_c) \quad (\text{Eq. 8})$$

$$\text{Maximum:} \quad \max(x_c) \quad (\text{Eq. 9})$$

where:

$PNDs_c$	=	percent nondetects for analyte c
$n_{c,0}$	=	number of nondetects for analyte c
n_c	=	number of measurements for analyte c
m_c	=	mean for analyte c
x_i	=	individual measurement
med_c	=	median for analyte c
x_c	=	ordered measurements for analyte c
s_c	=	composite sample standard deviation for analyte c
CV_c	=	coefficient of variation for analyte c
MDL	=	method detection limit
$n_{c,a}$	=	number of measurements above the MDL for analyte c
$n_{c,b}$	=	number of measurements below the MDL for analyte c .

3.1.7 Upper Background Threshold Values

The statistical software package ProUCL version 5.1 calculated upper BTVs (i.e., the 95% upper tolerance limit with 95% coverage) in accordance with the groundwater monitoring plan. ProUCL works with datasets that include nondetect data as well as samples with concentrations less than the MDL. There are several methods available in ProUCL for calculating upper BTVs. The methods account for the underlying distribution of the data and the presence of nondetect data. For datasets with nondetect data that follow a normal, lognormal, or nonparametric distribution, ProUCL uses the Kaplan-Meier method, a nonparametric method for calculating summary statistics and upper BTVs. For datasets with nondetect data that follow a gamma distribution, ProUCL uses a regression on order statistics method for calculating summary statistics and upper BTVs. ProUCL highlights in blue the appropriate data distributions for each dataset in its output file; however, it is important to assess all the methods available and independently verify the most appropriate method through visual inspection of the data, evaluation of the number of available data points, and the data distribution. The upper BTVs were calculated for datasets with at least four detected values. Constituents with fewer than four detections in the background dataset will use the practical quantitation limit for the BTV (not represented in this ECF).

3.1.8 Lower Background Threshold Values

The ProUCL software provides upper BTVs and not lower BTVs (i.e., the 95% lower tolerance limit with 95% coverage). For pH measurement, the lower BTV is calculated using the statistical software program

R using the data packages `data.table` and `EnvStats`. The data distribution for each pH dataset was determined using `ProUCL` (based on the method used to determine the upper BTVs as discussed in Section 3.1.7 of this ECF) and lower BTVs were calculated using the `EnvStats` package based on the appropriate data distribution (Appendix B).

4 Assumptions and Inputs

This chapter outlines the assumptions and inputs for the BTV calculations presented in this ECF.

4.1 Assumptions

The following is a summary of assumptions:

- The MDL is independent of concentration
- It is assumed that seasonal fluctuations in the data are not present
- Concentrations observed at a well are not significantly affected by active remediation activities at the site for the period over which calculations are made
- All estimated data (LAB_QUALIFIER=B or J) were treated as detected values

5 Software Applications

Software used to generate the summary statistics and BTV calculations were in accordance with CPCCo's software control management plan, CPCC-PRO-IRM-309, *Controlled Software Management*.

5.1 Approved Software

The following software were used to perform calculations in addition to being approved and compliant with CPCC-PRO-IRM-309 and consistent with CHPRC-01270, *ProUCL Software Management Plan*. Following are brief descriptions of the software.

5.1.1 ProUCL (Controlled Calculation Software)

- **Software Title:** ProUCL (EPA/600/R-07/041, *ProUCL Version 5.1 Technical Guide: Statistical Software for Environmental Applications for Data Sets with and without Nondetect Observations*) uses statistical methods to estimate exposure point concentrations (EPCs), not-to-exceed values, and BTVs for datasets with detected and nondetected observations.
- **Software Version:** Version 5.1
- **Hanford Information System Inventory Identification Number:** 2831
- **Workstation type and property number (from which software is run):** INTERA Inc. workstation 00905

5.1.2 Software Installation and Checkout

Verification that the software specified in Section 5.1.1 is qualified for use is documented in the Software Installation and Checkout Form. Appendix D of this ECF provides a copy of the form.

5.2 Support Software

R is a public domain computing platform that provides data manipulation, calculation, and graphical display capabilities to support data analysis (Venables et al., 2017, *An Introduction to R, Notes on R: A Programming Environment for Data Analysis and Graphics*). It is freely available to the public and can be compiled and run on a variety of platforms. The base installation of R contains statistical and plotting functions and many more are available for download through the Comprehensive R Archive Network (CRAN). The R routines described previously were independently checked and verified by detailed review as part of this preparation of this calculation file.

The following R packages, as listed in Table 6, were downloaded from CRAN and used for data preparation and lower BTV calculations.

Table 6. R Packages Used for Data Preparation and Lower BTV Calculations

R Package	Package Description	Version
data.table	Extension of data.frame	1.14.2
EnvStats	Package for environmental statistics, including EPA guidance	2.5.0
reshape2	Restructure and aggregate data	1.4.4
XLConnect	Excel® connector for R	1.0.5

Note: Excel is a registered trademark of the Microsoft Corporation in the United States and other countries.

EPA = U.S. Environmental Protection Agency

BTV = background threshold value

6 Calculation

The following input files were used in the implementation of this analysis:

- *qryChemHeis1.txt*: concentration data from HEIS database
- *ProUCL_Datasets_2021.xlsx*: dataset for use in ProUCL 2021

Datasets were imported into ProUCL software and upper BTVs were calculated using all available methods accounting for the presence of nondetect data. The reported upper BTV was selected based on ProUCL results, including evaluation of the data distribution and sample size. Lower BTVs for pH were calculated using the R script 02_BTVs_pH.R. All R scripts (ImportData_ChemistryData, BTVs_pH, SummaryStatistics, and ExportDatasets) and R functions (bicarbonate, readCHEMHEIS) that were used in the calculation of upper and lower BTVs in addition to summary statistics. Appendix B of this ECF provides the R Code BTV calculations.

7 Results

Table 7 provides the BTVs for the analytes listed in Table 1 of this ECF. In addition to the BTVs and their associated data distributions, summary statistics such as n-value, mean, median, minimum, maximum, standard deviation, coefficient of variation, and percent nondetect data are reported in Table 7. Appendix A of this ECF lists the duplicate data and their daily averages. Appendix B of this ECF presents the various R scripts and functions that were used to determine BTVs and summary statistics. Appendix C presents the final dataset (the culmination of the abovementioned filtering steps) that were used to calculate BTVs and the output files from ProUCL.

Table 7. Summary Statistics and Background Threshold Values - 2021

Analyte	Date Range	n	Nondetects (%)	Mean	Median	Std Dev	CV	n > MDL	n < MDL	Min	Max	BTV	Units	Distribution
Alkalinity	1/27/2017 - 10/13/2021	15	0	168,433	169,000	5,577	0.033	15	0	155,000	177,000	182,744	µg/L	Normal
Dissolved Arsenic	1/27/2017 - 10/13/2021	14	43	5.7	5.6	1.8	0.308	8	6	3.7	8.6	9.1	µg/L	Normal
Total Arsenic	1/27/2017 - 10/13/2021	14	43	5.9	4.6	2.4	0.413	8	6	3.7	9.9	11.9	µg/L	Lognormal
Bicarbonate	1/27/2017 - 10/13/2021	15	0	168,433	169,000	5,577	0.033	15	0	155,000	177,000	182,744	µg/L	Normal
Dissolved Calcium	1/27/2017 - 10/13/2021	15	0	50,153	50,000	1,850	0.037	15	0	47,000	52,800	54,901	µg/L	Normal
Total Calcium	1/27/2017 - 10/13/2021	15	0	50,687	50,200	2,362	0.047	15	0	46,700	55,500	56,748	µg/L	Normal
Chloride	1/27/2017 - 10/13/2021	15	0	5,682	5,640	187	0.033	15	0	5,340	6,100	6,161	µg/L	Normal
Dissolved Iron	1/27/2017 - 10/13/2021	14	93	NA	NA	NA	NA	1	13	NA	NA	NA	µg/L	NA
Total Iron	1/27/2017 - 10/13/2021	15	93	NA	NA	NA	NA	1	14	NA	NA	NA	µg/L	NA
Dissolved Magnesium	1/27/2017 - 10/13/2021	15	0	12,713	12,700	417	0.033	15	0	12,000	13,600	13,784	µg/L	Normal
Total Magnesium	1/27/2017 - 10/13/2021	15	0	12,743	12,750	651	0.051	15	0	12,000	14,300	14,414	µg/L	Normal
Dissolved Manganese	1/27/2017 - 10/13/2021	15	60	1.3	1.0	1.1	0.880	6	9	0.4	3.4	3.0	µg/L	Normal
Total Manganese	1/27/2017 - 10/13/2021	15	60	1.0	0.5	1.0	1.01	6	9	0.3	3.0	2.8	µg/L	Gamma
Nitrate	1/27/2017 - 10/13/2021	15	0	13,517	13,500	513	0.038	15	0	12,400	14,200	14,832	µg/L	Normal
pH Measurement	1/27/2017 - 10/13/2021	15	0	7.67	7.65	0.09	0.012	15	0	7.53	7.85	7.90 (U)	unitless	Normal
												7.40 (L)		
Dissolved Potassium	1/27/2017 – 10/13/2021	15	0	6,787	6,700	483	0.071	15	0	6,110	7,800	8,026	µg/L	Normal
Total Potassium	1/27/2017 – 10/13/2021	15	0	6,765	6,630	498	0.074	15	0	6,030	7,900	8,044	µg/L	Normal
Dissolved Sodium	1/27/2017 – 10/13/2021	15	0	20,910	21,100	904	0.043	15	0	18,500	22,100	23,231	µg/L	Normal
Total Sodium	1/27/2017 – 10/13/2021	15	0	20,860	21,000	1,350	0.065	15	0	18,400	23,800	24,324	µg/L	Normal
Specific Conductance	1/27/2017 – 10/13/2021	15	0	425	438	51	0.119	15	0	245	450	450	µS/cm	Nonparametric
Sulfate	1/27/2017 – 10/13/2021	15	0	43,363	44,000	1,991	0.046	15	0	40,200	47,000	48,472	µg/L	Normal
Temperature	1/27/2017 – 10/13/2021	15	0	18.6	18.5	0.4	0.024	15	0	17.8	19.6	19.7	Deg C	Normal

NA = Constituent has fewer than four detections in the background dataset and the practical quantitation limit will be used for the BTV. Determination of the practical quantitation limit is not included in this calculation.

BTV = background threshold value

CV = coefficient of variation

L = lower BTV value (pH)

Max = maximum value

MDL = method detection limit

Min = minimum value

Std Dev = standard deviation

U = upper BTV value (pH)

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8 References

- CHPRC-01270, *ProUCL Software Management Plan*, Rev. 3, CH2M HILL. Plateau Remediation Company, Richland, Washington.
- CPCC-PRO-IRM-309, *Controlled Software Management*, Central Plateau Cleanup Company, Richland, Washington.
- DOE/EA-1707D, 2011, *Environmental Assessment: Closure of Nonradioactive Dangerous Waste Landfill (NRDWL) and Solid Waste Landfill (SWL), Hanford Site, Richland Washington*, U.S. Department of Energy, Richland Operations Office, Richland, Washington. Available at: <https://pdw.hanford.gov/document/1005170534>.
- DOE/RL-2015-33, 2021, *Groundwater Monitoring Plan for Solid Waste Landfill*, Rev 1, U.S. Department of Energy, Richland Operations Office, Richland, Washington. Available at: <https://pdw.hanford.gov/document/AR-13626>.
- EPA/600/R-07/041, 2015, *ProUCL Version 5.1 Technical Guide: Statistical Software for Environmental Applications for Data Sets with and without Nondetect Observations*, Office of Research and Development, U.S. Environmental Protection Agency, Washington, D.C. Available at: https://www.epa.gov/sites/default/files/2016-05/documents/proucl_5.1_tech-guide.pdf.
- HNF-38155, 2013, *HEIS Sample, Result, and Sampling Site Data Dictionary*, Rev. 1, CH2M HILL Plateau Remediation Company, Richland, Washington. Available at: <https://pdw.hanford.gov/document/0082589H>.
- Venables, W.N., D.M. Smith, and the R Core Team, 2017, *An Introduction to R, Notes on R: A Programming Environment for Data Analysis and Graphics*, Version 3.4.3, 105 pp. Available at: <https://cran.r-project.org/doc/manuals/r-release/R-intro.pdf>.
- WAC 173-350-500, “Solid Waste Handling Standards,” “Groundwater Monitoring,” *Washington Administrative Code*, Olympia, Washington. Available at: <http://app.leg.wa.gov/WAC/default.aspx?cite=173-350-500>.

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Appendix A

Daily Averaging Results

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Table A-1. Daily Averaged Samples

Well Name	Sample Date	Analyte	Reported Value and Laboratory Qualifier (µg/L)	Final Value (µg/L)
699-24-36	9/22/2021	Alkalinity	179,000	174,500
			170,000 X	
699-24-36	9/22/2021	Bicarbonate	179,000	174,500
			170,000 X	
699-24-36	9/22/2021	Chloride	5,550	5,625
			5,700 D	
699-24-36	9/22/2021	Dissolved Calcium	50,300	50,500
			50,700	
699-24-36	9/22/2021	Dissolved Iron	30 U	31 B
			31 B	
699-24-36	9/22/2021	Dissolved Magnesium	13,000	12,900
			12,800	
699-24-36	9/22/2021	Dissolved Manganese	1 U	1 U
			0.31 U	
699-24-36	9/22/2021	Dissolved Potassium	6,520	6,550
			6,580	
699-24-36	9/22/2021	Dissolved Sodium	20,400	20,550
			20,700	
699-24-36	9/22/2021	Nitrate	12,800	13,150
			13,500 D	
699-24-36	9/22/2021	Sulfate	41,500 D	41,150 D
			40,800 D	
699-24-36	9/22/2021	Total Calcium	51,400	50,200
			49,000	
699-24-36	9/22/2021	Total Iron	22 U	30 U
			30 U	
699-24-36	9/22/2021	Total Magnesium	13,000	12,750
			12,500	
699-24-36	9/22/2021	Total Manganese	1 U	0.5 B
			0.48 B	

Table A-1. Daily Averaged Samples

Well Name	Sample Date	Analyte	Reported Value and Laboratory Qualifier (µg/L)	Final Value (µg/L)
699-24-36	9/22/2021	Total Potassium	6,680	6,515
			6,350	
699-24-36	9/22/2021	Total Sodium	20,900	20,400
			19,900	

Laboratory Qualifiers:

- B = The analyte was detected at a value less than the contract required detection limit but greater than or equal to the instrument detection limit/method detection limit, as appropriate
- D = Analyte was reported at a secondary dilution factor, typically >1 (i.e., the primary preparation required dilution either to bring the analyte to within the calibration range or minimize interference). Required for organics/wetchem if the sample was diluted
- U = Analyzed for but not detected above limiting criteria
- X = The result-specific translation of this qualifier code is provided in the hardcopy data report and/or case narrative. Additional result-specific translation information may also be found in the RESULT_COMMENT field for this record

Appendix B

R Code Background Threshold Value Calculations

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B.1 ImportData_ChemistryData R script

```

#-----#
#--Import and Select Chemistry Data for Trend Analysis
#--by: C. Brumbaugh (INTERA)
#--Modified from: ECF-200PO1-21-0002, REV.0
#-----#
#-----#
#--Load Packages--#
library(data.table)
library(reshape2)
library(XLConnect)
#-----#
#-----#
#--Set Working Directory--#
DIR <- 'C:/Users/CBrumbaugh/OneDrive - INTERA Inc/Desktop/Projects/Critical Means and BTV
Calcs/BTV/V3_3-3-2022'
setwd(DIR)
#-----#
#-----#
#--Load Project-Specific Functions--#
source('R Functions/readCHEMHEIS.R')
source('R Functions/bicarbonate.R')
#-----#
#-----#
#--Import Chemistry Dataset--#
CHEM <- readCHEMHEIS('Data/Data Pull 2-14-2022/qryChemHeis1.txt')
CHEM2 <- CHEM
CHEM <- CHEM2
#-----#
#-----#
#--List of Wells and Analytes for Analysis--#
WELLS <- c('699-24-36')

```

```

ANALYTES <- c('pH Measurement','Specific Conductance','Temperature',
              'Alkalinity','Bicarbonate','Calcium','Chloride','Iron',
              'Magnesium','Manganese','Nitrate','Potassium','Sodium','Sulfate',
              'Arsenic', 'Ammonia', 'Total organic carbon', 'Total dissolved solids')

#-----#
#-----#
#--Limit Wells and Analytes to those found in the project well list--#
CHEM <- CHEM[ANALYTE%in% ANALYTES]
CHEM <- CHEM[NAME%in% WELLS]
CHEM <- CHEM[year(EVENT) >= 2017]

#-----#
#-----#

#--Remove Qualified Data--#
FLAG <- CHEM[REVIEWQ%like% 'Y' | REVIEWQ%like% 'R' | REVIEWQ%like% 'F']
ROWS <- which(CHEM$REVIEWQ%like% 'Y' | CHEM$REVIEWQ%like% 'R' |
CHEM$REVIEWQ%like% 'F')
CHEM <- CHEM[-ROWS,]

write.table(FLAG,file='Output/Runs 3-29-2022/Data Removed by Review
Qualifier.csv',sep=',',row.names=FALSE)

#-----#
#-----#

#---Correct Bicarbonate Values---#
bicarb <- CHEM[ANALYTE == 'Alkalinity' & EVENT %like% '2017-10-12'|
              ANALYTE == 'Alkalinity' & EVENT %like% '2018-01-08'|
              ANALYTE == 'Alkalinity' & EVENT %like% '2018-07-19'|
              ANALYTE == 'Alkalinity' & EVENT %like% '2018-10-16'|
              ANALYTE == 'Alkalinity' & EVENT %like% '2021-09-22']

bicarb[bicarb=="Alkalinity"] <- "Bicarbonate"
bicarb[, "ANALYTE"] <- "Bicarbonate"
setkey(bicarb,'Analyte')
CHEM <- rbind(CHEM,bicarb)
CHEM <- CHEM[-323,]#--Calculate Bicarbonate--#

```

```

#--list <- split(CHEM,CHEM$NAME)
#--bicarb <- lapply(list,bicarbonate)
#--bicarb <- do.call('rbind',bicarb)
#-----#
#-----#
#--Combine Bicarbonate into Dataset--#
#--CHEM$NDS <- ifelse(CHEM$LABQ%like% 'U',TRUE,FALSE)
#--CHEM <-
subset(CHEM,select=c("NAME","EVENT","ANALYTE","FILTERED","VAL","LABQ","UNIT","MD
L","NDS"))
#--setnames(bicarb,names(bicarb),names(CHEM))
#--CHEM <- rbind(CHEM,bicarb)
#-----#
#-----#
#--Set-up Table for Duplicate Tracking--#
duplicates <- NULL
#-----#
#-----#
#--Loop Through Each Well--#
for(i in 1:length(WELLS)){
#-----#
#--Loop Through Each Analyte--#
for(j in 1:length(ANALYTES)){
#-----#
#--Subset Data by Well and Analyte--#
sub <- CHEM[NAME == WELLS[i] & ANALYTE == ANALYTES[j]]
#-----#
#-----#
#--Find Duplicates--#
if(ANALYTES[j]%in% c('Calcium','Iron','Magnesium','Manganese','Potassium','Sodium','Arsenic')){
  sub$match <- paste0(sub$EVENT,'-',sub$FILTERED)
} else {

```

```

sub$match <- paste0(sub$EVENT)
}
dups <- sub[duplicated(sub$match),]
#-----#
#-----#
#--Duplicate Handling--#
if(nrow(dups) > 0){
  #-----#
  #--Loop Through Duplicates--#
  for(k in 1:nrow(dups)){
    #-----#
    #--Extract Duplicates--#
    subdup <- subset(sub,sub$match == dups$match[k])
    #-----#
    #-----#
    #--Remove Duplicates from Chemistry Dataset--#
    rows <- which(CHEM$NAME == WELLS[i] & CHEM$FILTERED == dups$FILTERED[k] &
CHEM$ANALYTE == ANALYTES[j] & CHEM$EVENT == dups$EVENT[k])
    CHEM <- CHEM[!rows,]
    #-----#
    #-----#
    #--Calculate Mean if All Data are Detected--#
    if(sum(subdup$NDS) == 0){

      dup <- subdup[1,]
      dup$VAL <- mean(subdup$VAL)
      #-----#
      #-----#
      #--Use Maximum Detection Limit if All Data Are Non-Detect--#
    } else if(sum(subdup$NDS) == 2){

      dup <- subdup[1,]

```



```

dup$VAL <- max(subdup$VAL)
#-----#
#-----#
#--Use the Detected Value if One is Detected and One is Non-Detect--#
} else if(sum(subdup$NDS) == 1){

dup <- subdup[1,]
dup$VAL <- subdup[NDS == FALSE]$VAL
dup$LABQ <- subdup[NDS==FALSE]$LABQ
#-----#
#-----#
#--Report Error if Scenario not supported--#
} else {
  stop('Undefined Duplicated Handling')
}
#-----#
#-----#
#--Remove Match Field--#
dup$match <- NULL
subdup$match <- NULL
#-----#
#-----#
#--Combine Processed Duplicate with Original Dataset--#
CHEM <- rbind(CHEM,dup)
#-----#
#-----#
#--Add Calculated Value for Duplicates to List of Duplicate Samples--#
subdup$NewVAL <- dup$VAL
subdup$NewQUAL <- dup$LABQ
#-----#
#-----#

```

```

#--Combine All Duplicates--#
duplicates <- rbind(duplicates,subdup)
#-----#
}
#-----#
}
#-----#
}
#-----#
}
#-----#
#-----#
#-----#

#--Set Analyte Names for Total and Dissolved--#
CHEM$ANALYTE2 <- ifelse(CHEM$ANALYTE%in%
c('Calcium','Iron','Magnesium','Manganese','Potassium','Sodium','Arsenic') & CHEM$FILTERED == 'N',
      paste0('Total ',CHEM$ANALYTE),
      ifelse(CHEM$ANALYTE%in%
c('Calcium','Iron','Magnesium','Manganese','Potassium','Sodium','Arsenic') & CHEM$FILTERED == 'Y',
      paste0('Dissolved ',CHEM$ANALYTE),CHEM$ANALYTE))
#-----#
#-----#

#--Set-up ProUCL Dataset--#
Pro <- subset(CHEM,select=c('NAME','EVENT','ANALYTE2','VAL','UNIT','LABQ'))
Pro$D_VAL <- ifelse(Pro$LABQ%like% 'U',0,1)
#-----#
#-----#

#--Subset by Year--#
Pro_2021 <- Pro[year(EVENT) <= 2021]
Well_24_36 <- Pro_2021[NAME == '699-24-36']
ProUCL <- list(`2021` = Pro_2021, Well_24_36 = Well_24_36)
#-----#
#-----#

```

```
#--Export ProUCL Datasets--#
```

```
writeWorksheetToFile('ProUCL/Runs 3-29-2022/ProUCL_Datasets_2021.xlsx',Pro_2021,sheet='ProUCL_Datasets_2021')
```

```
writeWorksheetToFile('ProUCL/Runs 3-29-2022/ProUCL_Datasets_2022_24_36.xlsx',Well_24_36,sheet='Well_24_36')
```

```
#-----#
```

```
#-----#
```

```
#--Save Datasets--#
```

```
write.table(duplicates,file='Output/Runs 3-29-2022/Duplicates_03292022.csv',sep=',',row.names=FALSE)
```

```
write.table(CHEM,file='Output/Runs 3-29-2022/ChemistryData_030292022.csv',sep=',',row.names=FALSE)
```

```
save(CHEM,file='Data/Runs 3-29-2022/ChemistryData_03292022.RData')
```

```
save(ProUCL,file='Data/Runs 3-29-2022/ProUCLDatasests.RData')
```

```
#-----#
```

B.2 BTV_pH R script

```
#-----#
```

```
#--Calculate BTVs for pH
```

```
#--by: C. Brumbaugh (INTERA)
```

```
#--Modified from: ECF-200PO1-21-0002, REV.0
```

```
#-----#
```

```
#-----#
```

```
#--Load Packages--#
```

```
library(data.table)
```

```
library(EnvStats)
```

```
#-----#
```

```
#-----#
```

```
#--Set Working Directory--#
```

```
DIR <- 'C:/Users/CBrumbaugh/OneDrive - INTERA Inc/Desktop/Projects/Critical Means and BTV Calcs/BTV/V3_3-3-2022'
```

```

setwd(DIR)
#-----#

#-----#
#--Import Chemistry Dataset--#
load('Data/Runs 3-29-2022/ChemistryData_03212022.RData')
#-----#

#-----#
#--Extract Only pH Data--#
CHEM <- CHEM[ANALYTE == 'pH Measurement']
#-----#

#-----#
#--Years and Wells for Analysis--#
yrs <- c(2021)
wells <- sort(unique(CHEM$NAME))
#-----#

#-----#
#--BTV Summary Table--#
btvs <- NULL
#-----#

#-----#
#--Loop through Each Year--#
for(i in 1:length(yrs)){

#-----#
#--Loop through Each Well--#

```

```

for(j in 1:length(wells)){

#-----#
#--Determine Start and End Years for Dataset - Rolling 5 Year--#
start <- yrs[i] - 4
end <- yrs[i]
#-----#

#-----#
#--Subset Data by Year--#
sub <- CHEM[year(EVENT) >= start & year(EVENT) <= end & NAME == wells[j]]
#-----#

#-----#
#--Determine Distribution--#
dist <- suppressWarnings(distChooseCensored(sub$VAL,sub$NDS))$decision
if(wells[j] == '699-24-36'){
  dist <- 'Normal'
}
#-----#

#-----#
#--Calculate BTVs Based on Distribution--#
if(dist == 'Normal'){

  btv <- tolIntNorm(sub$VAL,coverage = 0.95,ti.type = "two-sided")

} else if(dist == 'Lognormal'){

  btv <- tolIntLnorm(sub$VAL,coverage = 0.95,ti.type = "two-sided")

```

```

    } else if(dist == 'Gamma'){

      btv <- tolIntGamma(sub$VAL,coverage = 0.95, ti.type = 'two-
sided',conf.level=0.95,normal.approx.transform="cube.root")

    } else {

      btv <- tolIntNpar(sub$VAL,ti.type = 'two-sided',conf.level=0.95)

    }
#-----#

#-----#

#--Summarize BTV--#
btvsub <- data.table(Year = yrs[i],
                    WellName = wells[j],
                    LowerBTV = as.numeric(btv$interval$limits[1]),
                    UpperBTV = as.numeric(btv$interval$limits[2]),
                    Distribution = dist)
btvs <- rbind(btvsub,btvsub)
#-----#

}
#-----#

}
#-----#

#-----#

#--Save Table--#

```

```
write.table(btv, file='Output/Runs 3-29-2022/BTV_pH.csv', sep=',', row.names=FALSE)
```

```
#-----#
```

B.3 Summary Statistics R Script

```
#-----#
```

```
#--Summary Statistics
```

```
#--by: C. Brumbaugh (INTERA)
```

```
#--Modified from: ECF-200PO1-21-0002, REV.0
```

```
#-----#
```

```
#-----#
```

```
#--Load Packages--#
```

```
library(data.table)
```

```
library(EnvStats)
```

```
#-----#
```

```
#-----#
```

```
#--Set Working Directory--#
```

```
DIR <- 'C:/Users/CBrumbaugh/OneDrive - INTERA Inc/Desktop/Projects/Critical Means and BTV  
Calcs/BTV/V3_3-3-2022'
```

```
setwd(DIR)
```

```
#-----#
```

```
#-----#
```

```
#--Import Datasets--#
```

```
load('Data/Runs 3-29-2022/ProUCLDasetests.RData')
```

```
#-----#
```

```
ProUCL <- subset(ProUCL, names(ProUCL) %in% c('Well_24_36'))
```

```
#-----#
```

```
#--Data Summary Table--#
```

```

summary <- NULL
#-----#

#-----#
#--Loop Through Each Dataset--#
for(i in 1:length(ProUCL)){

#-----#
#--Extract Dataset--#
sub <- ProUCL[[i]]
nm <- names(ProUCL)[i]
#-----#

#-----#
#--Extract Analytes--#
an <- sort(unique(sub$ANALYTE2))
#-----#

#-----#
#--Loop Through each Analyte--#
for(j in 1:length(an)){

#-----#
#--Subset by Analyte--#
ansub <- sub[ANALYTE2 == an[j]]
#-----#

#-----#
#--Calculate Summary Statistics--#
if(all(ansub$D_VAL == 1)){

```



```

dt <- data.table(Dataset=nm,
  Analyte=an[j],
  MinDate=min(ansub$EVENT),
  MaxDate=max(ansub$EVENT),
  PNDs=0,
  Mean=mean(ansub$VAL),
  Median=median(ansub$VAL),
  Stdev=sd(ansub$VAL),
  CV=sd(ansub$VAL)/mean(ansub$VAL),
  N=nrow(ansub),
  `N > MDL` = nrow(ansub),
  `N < MDL` = 0,
  MinValue=min(ansub$VAL),
  MaxValue=max(ansub$VAL))

summary <- rbind(summary,dt)

} else if(all(ansub$D_VAL == 0) | nrow(ansub[D_VAL == 1]) < 4){

dt <- data.table(Dataset=nm,
  Analyte=an[j],
  MinDate=min(ansub$EVENT),
  MaxDate=max(ansub$EVENT),
  PNDs=nrow(ansub[D_VAL == 0])/nrow(ansub),
  Mean=NA,
  Median=NA,
  Stdev=NA,
  CV=NA,
  N=nrow(ansub),

```

```

`N > MDL` = nrow(ansub[D_VAL == 1]),
`N < MDL` = nrow(ansub[D_VAL == 0]),
MinValue=NA,
MaxValue=NA)

summary <- rbind(summary,dt)

} else {

stats <- subset(ansub, ansub$D_VAL == 1)

dt <- data.table(Dataset=nm,
  Analyte=an[j],
  MinDate=min(ansub$EVENT),
  MaxDate=max(ansub$EVENT),
  PNDs=nrow(ansub[D_VAL == 0])/nrow(ansub),
  Mean=mean(stats$VAL),
  Median=median(stats$VAL),
  Stdev=sd(stats$VAL),
  CV=sd(stats$VAL)/mean(stats$VAL),
  N=nrow(ansub),
  `N > MDL` = nrow(ansub[D_VAL == 1]),
  `N < MDL` = nrow(ansub[D_VAL == 0]),
  MinValue=min(stats$VAL),
  MaxValue=max(stats$VAL))

summary <- rbind(summary,dt)

}

#-----#

```

```

}
#-----#

}
#-----#

#-----#
#--Export Dataset--#
write.table(summary,file='ProUCL/Runs 3-29-2022/DataSummary.csv',sep=',',row.names=FALSE)
#-----#

B.4 Export Dataset R Script
#-----#
#--Export Dataset
#--by: C. Brumbaugh (INTERA)
#--Modified from: ECF-200PO1-21-0002, REV.0
#-----#
#-----#
#--Load Packages--#
library(data.table)
library(EnvStats)
library(XLConnect)
#-----#
#-----#
#--Set Working Directory--#
DIR <- 'C:/Users/CBrumbaugh/OneDrive - INTERA Inc/Desktop/Projects/Critical Means and BTV
Calcs/BTV/V3_3-3-2022'
setwd(DIR)
#-----#
#-----#
#--Import Chemistry Dataset--#

```

```

load('Data/Runs 3-29-2022/ChemistryData_03292022.RData')
#-----#
#-----#
#--Years of Analysis--#
yrs <- c(2021)
#-----#
#-----#
#--Loop through Each Year--#
for(i in 1:length(yrs)){
  #-----#
  #--Determine Start and End Years for Dataset - Rolling 5 Year--#
  start <- yrs[i] - 4
  end <- yrs[i]
  #-----#
  #-----#
  #--Subset Data by Year--#
  sub <- CHEM[year(EVENT) >= start & year(EVENT) <= end]
  #-----#
  #-----#
  #--Export Entire Dataset--#
  sh <- yrs[i]
  writeWorksheetToFile('Output/Runs 3-29-2022/BTV Datasets.xlsx',sub,sheet=paste0(sh))
  #-----#
}
#-----#

B.5 Bicarbonate R function
=====
=====

#' Calculate Bicarbonate Alkalinity from Total Alkalinity
#'
#' @param X data.table or data.frame of chemistry data

```

```

#' @param alk character vector representing alkalinity units
#' @param ALK character vector of Alkalinity (Total) Analyte Name
#' @param pH character vector of pH Name
#' @param NM character vector of Location Name field title
#' @param EVENT character vector of Date field title
#' @param ANALYTE character vector of Analyte Name field title
#' @param VAL character vector of Result field title
#'
#' @return data.table of calculated bicarbonate alkalinity
#'
#' @eXport
#' @import reshape2

#=====
=====

bicarbonate <- function (X,
                        alk = 'CaCO3',
                        ALK = 'Alkalinity',
                        pH = 'pH Measurement',
                        NM = 'NAME',
                        EVENT = 'EVENT',
                        ANALYTE = 'ANALYTE',
                        VAL = 'VAL'){

#-----#
#--Rename Columns--#
setnames(X,NM,'NAME')
setnames(X,EVENT,'EVENT')
setnames(X,ANALYTE,'ANALYTE')
setnames(X,VAL,'VAL')
#-----#

```

```

#-----#

#--Reshape Dataset to Crosstab--#

X <- melt(data=X,id.vars=
c("NAME","EVENT","ANALYTE"),measure.vars="VAL",variable_name="VAL",na.rm=TRUE)

X <- dcast(X,formula = NAME + EVENT ~ ANALYTE, fun.aggregate=mean)

X <- subset(X,!is.na(X[[ALK]]))

#-----#

#-----#

#--Molecular weight of CaCO3-----#

MW_CaCO3 <- (40.08 + 12.01115 + (3*15.9994))*10^6

#--Molecular weight of HCO3-----#

#-----#

MW_HCO3 <- (1.00797 + 12.01115 + (3*15.9994))*10^6

#-----#

X$Alk2 <- X[[ALK]]/MW_CaCO3

X$HCO3 <- (((2*X$Alk2) - (10^(-14+X[[pH]])))/(1 + 2*(10^-10.33)*10^X[[pH]]))

X$CO3 <- ((10^-10.33)*(X$HCO3)*(10^X[[pH]]))

X$HCO3 <- X$HCO3 * MW_HCO3

X$CO3 <- X$CO3 * (MW_HCO3-1.00797)

#-----#

#-----#

#--Remove Measured Bicarbonate Results--#

X <- subset(X,is.na(X$Bicarbonate))

X <- subset(X,!is.na(X$`pH Measurement`))

#-----#

#-----#

#--Add Additional Columns to Dataset--#

X$ANALYTE <- 'Bicarbonate'

```

```

X$QUAL <- "
X$UNITS <- 'ug/L as CaCO3'
X$NDS <- FALSE
X$FILTERED <- 'N'
X$MDL <- NA
#-----#

#-----#

#--Reorder and Rename Data fields--#
X <- subset(X,select =
c('NAME','EVENT','ANALYTE','FILTERED','HCO3','QUAL','UNITS','MDL','NDS'))
setnames(X,'HCO3','VAL')
#-----#

return(X)
}

```

B.6 ReadCHEMHEIS R function

```

#=====
=====

#' Read in chemistry data from the HEIS database.
#'
#' @param FILE the file name to read (text file with | separator)
#' @param EFORM the format for the dates (EVENT)
#'
#' @return the chemistry data from HEIS database
#'
#' @export
#' @import data.table

#=====
=====

readCHEMHEIS <- function(FILE, EFORM='%m/%d/%Y%H:%M:%S'){

```

```

#-----#
#--Define Column Classes and Read in Data--#
CLASS <- c('character','character','character','character','numeric',
           'character','character','character','character','numeric',
           'character','character','character','character','character','numeric')
CHEM <- fread(FILE, colClasses=CLASS, sep='|', header=TRUE, stringsAsFactors=FALSE)
#-----#

#-----#
#--Remove Discrete Depth Samples--#
#CHEM <- CHEM[DEPTH != 'm']
#-----#

#-----#
#--Remove Blank Data--#
CHEM <- CHEM[!is.na(VAL)]
#-----#

#-----#
#--Convert Dates--#
CHEM[, EVENT:=sub('EDT ', '', EVENT)]
CHEM[, EVENT:=sub('EST ', '', EVENT)]
CHEM[, LOAD_DATE_TIME:=sub('EDT ', '', LOAD_DATE_TIME)]
CHEM[, LOAD_DATE_TIME:=sub('EST ', '', LOAD_DATE_TIME)]
CHEM[, EVENT:= as.POSIXct(CHEM$EVENT, format=EFORM, tz="US/Pacific")]
CHEM[, LOAD_DATE_TIME:= as.POSIXct(CHEM$LOAD_DATE_TIME, format=EFORM,
tz="US/Pacific")]
#-----#

#-----#

```



```
#--Set key--#  
setkey(CHEM, NULL)  
CHEM <- unique(CHEM)  
#-----#  
  
return(CHEM)  
}
```

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Appendix C

Background Threshold Value Datasets and ProUCL Output

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Table C-1. BTV Dataset for 2021

Well Name	Sample Date	Analyte	Result	Laboratory Qualifier	Unit
699-24-36	1/27/2017	Alkalinity	170,000	--	µg/L
699-24-36	4/10/2017	Alkalinity	172,000	--	µg/L
699-24-36	8/7/2017	Alkalinity	177,000	--	µg/L
699-24-36	10/12/2017	Alkalinity	163,000	--	µg/L
699-24-36	1/8/2018	Alkalinity	155,000	--	µg/L
699-24-36	4/26/2018	Alkalinity	170,000	--	µg/L
699-24-36	7/19/2018	Alkalinity	168,000	--	µg/L
699-24-36	10/16/2018	Alkalinity	163,000	--	µg/L
699-24-36	4/4/2019	Alkalinity	168,000	--	µg/L
699-24-36	10/4/2019	Alkalinity	165,000	--	µg/L
699-24-36	9/30/2020	Alkalinity	169,000	--	µg/L
699-24-36	1/5/2021	Alkalinity	166,000	--	µg/L
699-24-36	7/12/2021	Alkalinity	175,000	--	µg/L
699-24-36	9/22/2021	Alkalinity ^a	174,500	--	µg/L
699-24-36	10/13/2021	Alkalinity	171,000	--	µg/L
699-24-36	7/12/2021	Ammonia	88.6	C	µg/L
699-24-36	10/13/2021	Ammonia	20.7	U	µg/L
699-24-36	1/27/2017	Bicarbonate	170,000	--	µg/L
699-24-36	4/10/2017	Bicarbonate	172,000	--	µg/L
699-24-36	8/7/2017	Bicarbonate	177,000	--	µg/L
699-24-36	10/12/2017	Bicarbonate	163,000	--	µg/L
699-24-36	1/8/2018	Bicarbonate	155,000	--	µg/L
699-24-36	4/26/2018	Bicarbonate	170,000	--	µg/L
699-24-36	7/19/2018	Bicarbonate	168,000	--	µg/L
699-24-36	10/16/2018	Bicarbonate	163,000	--	µg/L
699-24-36	4/4/2019	Bicarbonate	168,000	--	µg/L
699-24-36	10/4/2019	Bicarbonate	165,000	--	µg/L
699-24-36	9/30/2020	Bicarbonate	169,000	--	µg/L
699-24-36	1/5/2021	Bicarbonate	166,000	--	µg/L
699-24-36	7/12/2021	Bicarbonate	175,000	--	µg/L
699-24-36	9/22/2021	Bicarbonate ^a	174,500	X	µg/L

Table C-1. BTV Dataset for 2021

Well Name	Sample Date	Analyte	Result	Laboratory Qualifier	Unit
699-24-36	10/13/2021	Bicarbonate	171,000	--	µg/L
699-24-36	1/27/2017	Chloride	5,500	D	µg/L
699-24-36	4/10/2017	Chloride	5,590	--	µg/L
699-24-36	8/7/2017	Chloride	5,340	--	µg/L
699-24-36	10/12/2017	Chloride	5,600	D	µg/L
699-24-36	1/8/2018	Chloride	5,700	D	µg/L
699-24-36	4/26/2018	Chloride	5,500	D	µg/L
699-24-36	7/19/2018	Chloride	5,900	D	µg/L
699-24-36	10/16/2018	Chloride	5,800	D	µg/L
699-24-36	4/4/2019	Chloride	5,870	--	µg/L
699-24-36	10/4/2019	Chloride	6,100	D	µg/L
699-24-36	9/30/2020	Chloride	5,600	D	µg/L
699-24-36	1/5/2021	Chloride	5,730	D	µg/L
699-24-36	7/12/2021	Chloride	5,640	D	µg/L
699-24-36	9/22/2021	Chloride ^a	5,625	--	µg/L
699-24-36	10/13/2021	Chloride	5,740	D	µg/L
699-24-36	1/27/2017	Dissolved Arsenic	5.0	U	µg/L
699-24-36	4/10/2017	Dissolved Arsenic	5.3	B	µg/L
699-24-36	8/7/2017	Dissolved Arsenic	5.0	U	µg/L
699-24-36	10/12/2017	Dissolved Arsenic	8.6	B	µg/L
699-24-36	1/8/2018	Dissolved Arsenic	4.4	U	µg/L
699-24-36	4/26/2018	Dissolved Arsenic	6.1	B	µg/L
699-24-36	7/19/2018	Dissolved Arsenic	4.0	U	µg/L
699-24-36	10/16/2018	Dissolved Arsenic	7.7	B	µg/L
699-24-36	4/4/2019	Dissolved Arsenic	4.4	U	µg/L
699-24-36	10/4/2019	Dissolved Arsenic	5.8	B	µg/L
699-24-36	9/30/2020	Dissolved Arsenic	14	U	µg/L
699-24-36	1/5/2021	Dissolved Arsenic	3.7	--	µg/L
699-24-36	7/12/2021	Dissolved Arsenic	3.8	B	µg/L
699-24-36	10/13/2021	Dissolved Arsenic	4.6	BD	µg/L
699-24-36	1/27/2017	Dissolved Calcium	49,600	--	µg/L

Table C-1. BTV Dataset for 2021

Well Name	Sample Date	Analyte	Result	Laboratory Qualifier	Unit
699-24-36	4/10/2017	Dissolved Calcium	47,000	--	µg/L
699-24-36	8/7/2017	Dissolved Calcium	49,900	--	µg/L
699-24-36	10/12/2017	Dissolved Calcium	47,800	--	µg/L
699-24-36	1/8/2018	Dissolved Calcium	48,800	--	µg/L
699-24-36	4/26/2018	Dissolved Calcium	52,300	--	µg/L
699-24-36	7/19/2018	Dissolved Calcium	50,600	--	µg/L
699-24-36	10/16/2018	Dissolved Calcium	52,300	--	µg/L
699-24-36	4/4/2019	Dissolved Calcium	52,700	--	µg/L
699-24-36	10/4/2019	Dissolved Calcium	47,500	--	µg/L
699-24-36	9/30/2020	Dissolved Calcium	50,000	--	µg/L
699-24-36	1/5/2021	Dissolved Calcium	50,000	--	µg/L
699-24-36	7/12/2021	Dissolved Calcium	50,500	--	µg/L
699-24-36	9/22/2021	Dissolved Calcium ^a	50,500	--	µg/L
699-24-36	10/13/2021	Dissolved Calcium	52,800	--	µg/L
699-24-36	1/27/2017	Dissolved Iron	30	U	µg/L
699-24-36	4/10/2017	Dissolved Iron	22	U	µg/L
699-24-36	8/7/2017	Dissolved Iron	30	U	µg/L
699-24-36	10/12/2017	Dissolved Iron	22	U	µg/L
699-24-36	1/8/2018	Dissolved Iron	22	U	µg/L
699-24-36	4/26/2018	Dissolved Iron	30	U	µg/L
699-24-36	7/19/2018	Dissolved Iron	30	U	µg/L
699-24-36	10/16/2018	Dissolved Iron	22	U	µg/L
699-24-36	4/4/2019	Dissolved Iron	22	U	µg/L
699-24-36	10/4/2019	Dissolved Iron	30	U	µg/L
699-24-36	9/30/2020	Dissolved Iron	44	U	µg/L
699-24-36	1/5/2021	Dissolved Iron	44	U	µg/L
699-24-36	9/22/2021	Dissolved Iron ^a	31	B	µg/L
699-24-36	10/13/2021	Dissolved Iron	53	U	µg/L
699-24-36	1/27/2017	Dissolved Magnesium	12,900	--	µg/L
699-24-36	4/10/2017	Dissolved Magnesium	13,000	--	µg/L
699-24-36	8/7/2017	Dissolved Magnesium	12,600	--	µg/L

Table C-1. BTV Dataset for 2021

Well Name	Sample Date	Analyte	Result	Laboratory Qualifier	Unit
699-24-36	10/12/2017	Dissolved Magnesium	12,500	--	µg/L
699-24-36	1/8/2018	Dissolved Magnesium	12,500	--	µg/L
699-24-36	4/26/2018	Dissolved Magnesium	12,100	--	µg/L
699-24-36	7/19/2018	Dissolved Magnesium	12,700	--	µg/L
699-24-36	10/16/2018	Dissolved Magnesium	13,000	--	µg/L
699-24-36	4/4/2019	Dissolved Magnesium	13,000	--	µg/L
699-24-36	10/4/2019	Dissolved Magnesium	12,200	--	µg/L
699-24-36	9/30/2020	Dissolved Magnesium	13,000	--	µg/L
699-24-36	1/5/2021	Dissolved Magnesium	12,000	--	µg/L
699-24-36	7/12/2021	Dissolved Magnesium	12,700	--	µg/L
699-24-36	9/22/2021	Dissolved Magnesium ^a	12,900	--	µg/L
699-24-36	10/13/2021	Dissolved Magnesium	13,600	--	µg/L
699-24-36	1/27/2017	Dissolved Manganese	3.4	B	µg/L
699-24-36	4/10/2017	Dissolved Manganese	1.1	B	µg/L
699-24-36	8/7/2017	Dissolved Manganese	2.0	U	µg/L
699-24-36	10/12/2017	Dissolved Manganese	0.46	B	µg/L
699-24-36	1/8/2018	Dissolved Manganese	0.39	BC	µg/L
699-24-36	4/26/2018	Dissolved Manganese	4.0	U	µg/L
699-24-36	7/19/2018	Dissolved Manganese	4.0	U	µg/L
699-24-36	10/16/2018	Dissolved Manganese	0.83	BC	µg/L
699-24-36	4/4/2019	Dissolved Manganese	1.9	U	µg/L
699-24-36	10/4/2019	Dissolved Manganese	2.0	U	µg/L
699-24-36	9/30/2020	Dissolved Manganese	1.4	B	µg/L
699-24-36	1/5/2021	Dissolved Manganese	2.4	U	µg/L
699-24-36	7/12/2021	Dissolved Manganese	0.31	U	µg/L
699-24-36	9/22/2021	Dissolved Manganese ^a	1.0	U	µg/L
699-24-36	10/13/2021	Dissolved Manganese	1.5	UD	µg/L
699-24-36	1/27/2017	Dissolved Potassium	6,120	--	µg/L
699-24-36	4/10/2017	Dissolved Potassium	7,340	--	µg/L
699-24-36	8/7/2017	Dissolved Potassium	6,280	--	µg/L
699-24-36	10/12/2017	Dissolved Potassium	6,980	--	µg/L

Table C-1. BTV Dataset for 2021

Well Name	Sample Date	Analyte	Result	Laboratory Qualifier	Unit
699-24-36	1/8/2018	Dissolved Potassium	6,740	--	µg/L
699-24-36	4/26/2018	Dissolved Potassium	6,490	--	µg/L
699-24-36	7/19/2018	Dissolved Potassium	6,630	--	µg/L
699-24-36	10/16/2018	Dissolved Potassium	6,700	--	µg/L
699-24-36	4/4/2019	Dissolved Potassium	7,120	--	µg/L
699-24-36	10/4/2019	Dissolved Potassium	6,110	--	µg/L
699-24-36	9/30/2020	Dissolved Potassium	7,800	--	µg/L
699-24-36	1/5/2021	Dissolved Potassium	7,400	--	µg/L
699-24-36	7/12/2021	Dissolved Potassium	6,580	--	µg/L
699-24-36	9/22/2021	Dissolved Potassium ^a	6,550	--	µg/L
699-24-36	10/13/2021	Dissolved Potassium	6,960	--	µg/L
699-24-36	1/27/2017	Dissolved Sodium	21,400	--	µg/L
699-24-36	4/10/2017	Dissolved Sodium	21,600	--	µg/L
699-24-36	8/7/2017	Dissolved Sodium	20,200	--	µg/L
699-24-36	10/12/2017	Dissolved Sodium	21,200	--	µg/L
699-24-36	1/8/2018	Dissolved Sodium	20,300	--	µg/L
699-24-36	4/26/2018	Dissolved Sodium	20,000	--	µg/L
699-24-36	7/19/2018	Dissolved Sodium	21,200	--	µg/L
699-24-36	10/16/2018	Dissolved Sodium	21,900	--	µg/L
699-24-36	4/4/2019	Dissolved Sodium	22,100	--	µg/L
699-24-36	10/4/2019	Dissolved Sodium	18,500	--	µg/L
699-24-36	9/30/2020	Dissolved Sodium	21,000	--	µg/L
699-24-36	1/5/2021	Dissolved Sodium	21,000	--	µg/L
699-24-36	7/12/2021	Dissolved Sodium	21,600	--	µg/L
699-24-36	9/22/2021	Dissolved Sodium ^a	20,550	--	µg/L
699-24-36	10/13/2021	Dissolved Sodium	21,100	--	µg/L
699-24-36	1/27/2017	Nitrate	14,200	D	µg/L
699-24-36	4/10/2017	Nitrate	13,900	D	µg/L
699-24-36	8/7/2017	Nitrate	12,900	--	µg/L
699-24-36	10/12/2017	Nitrate	13,700	D	µg/L
699-24-36	1/8/2018	Nitrate	14,200	D	µg/L

Table C-1. BTV Dataset for 2021

Well Name	Sample Date	Analyte	Result	Laboratory Qualifier	Unit
699-24-36	4/26/2018	Nitrate	13,300	D	µg/L
699-24-36	7/19/2018	Nitrate	14,200	D	µg/L
699-24-36	10/16/2018	Nitrate	13,700	D	µg/L
699-24-36	4/4/2019	Nitrate	13,100	--	µg/L
699-24-36	10/4/2019	Nitrate	13,300	ZD	µg/L
699-24-36	9/30/2020	Nitrate	12,400	DZN	µg/L
699-24-36	1/5/2021	Nitrate	13,500	D	µg/L
699-24-36	7/12/2021	Nitrate	13,700	D	µg/L
699-24-36	9/22/2021	Nitrate ^a	13,150	--	µg/L
699-24-36	10/13/2021	Nitrate	13,500	D	µg/L
699-24-36	1/27/2017	pH Measurement	7.57	--	unitless
699-24-36	4/10/2017	pH Measurement	7.65	--	unitless
699-24-36	8/7/2017	pH Measurement	7.60	--	unitless
699-24-36	10/12/2017	pH Measurement	7.57	--	unitless
699-24-36	1/8/2018	pH Measurement	7.76	--	unitless
699-24-36	4/26/2018	pH Measurement	7.62	--	unitless
699-24-36	7/19/2018	pH Measurement	7.53	--	unitless
699-24-36	10/16/2018	pH Measurement	7.85	--	unitless
699-24-36	4/4/2019	pH Measurement	7.67	--	unitless
699-24-36	10/4/2019	pH Measurement	7.65	--	unitless
699-24-36	9/30/2020	pH Measurement	7.67	--	unitless
699-24-36	1/5/2021	pH Measurement	7.77	--	unitless
699-24-36	7/12/2021	pH Measurement	7.76	--	unitless
699-24-36	9/22/2021	pH Measurement	7.62	--	unitless
699-24-36	10/13/2021	pH Measurement	7.75	--	unitless
699-24-36	1/27/2017	Specific Conductance	441	--	µS/cm
699-24-36	4/10/2017	Specific Conductance	450	--	µS/cm
699-24-36	8/7/2017	Specific Conductance	444	--	µS/cm
699-24-36	10/12/2017	Specific Conductance	443	--	µS/cm
699-24-36	1/8/2018	Specific Conductance	450	--	µS/cm
699-24-36	4/26/2018	Specific Conductance	245	--	µS/cm

Table C-1. BTV Dataset for 2021

Well Name	Sample Date	Analyte	Result	Laboratory Qualifier	Unit
699-24-36	7/19/2018	Specific Conductance	441	--	μS/cm
699-24-36	10/16/2018	Specific Conductance	435	--	μS/cm
699-24-36	4/4/2019	Specific Conductance	431	--	μS/cm
699-24-36	10/4/2019	Specific Conductance	422	--	μS/cm
699-24-36	9/30/2020	Specific Conductance	437	--	μS/cm
699-24-36	1/5/2021	Specific Conductance	438	--	μS/cm
699-24-36	7/12/2021	Specific Conductance	447	--	μS/cm
699-24-36	9/22/2021	Specific Conductance	427	--	μS/cm
699-24-36	10/13/2021	Specific Conductance	425	--	μS/cm
699-24-36	1/27/2017	Sulfate	44,000	D	μg/L
699-24-36	4/10/2017	Sulfate	42,900	D	μg/L
699-24-36	8/7/2017	Sulfate	41,600	D	μg/L
699-24-36	10/12/2017	Sulfate	44,000	D	μg/L
699-24-36	1/8/2018	Sulfate	47,000	D	μg/L
699-24-36	4/26/2018	Sulfate	42,000	D	μg/L
699-24-36	7/19/2018	Sulfate	46,000	D	μg/L
699-24-36	10/16/2018	Sulfate	45,000	D	μg/L
699-24-36	4/4/2019	Sulfate	44,200	D	μg/L
699-24-36	10/4/2019	Sulfate	42,000	D	μg/L
699-24-36	9/30/2020	Sulfate	41,000	D	μg/L
699-24-36	1/5/2021	Sulfate	44,600	D	μg/L
699-24-36	7/12/2021	Sulfate	44,800	D	μg/L
699-24-36	9/22/2021	Sulfate ^a	41,150	D	μg/L
699-24-36	10/13/2021	Sulfate	40,200	D	μg/L
699-24-36	1/27/2017	Temperature	18.3	--	Deg C
699-24-36	4/10/2017	Temperature	18.6	--	Deg C
699-24-36	8/7/2017	Temperature	19.2	--	Deg C
699-24-36	10/12/2017	Temperature	18.4	--	Deg C
699-24-36	1/8/2018	Temperature	18.2	--	Deg C
699-24-36	4/26/2018	Temperature	18.7	--	Deg C
699-24-36	7/19/2018	Temperature	18.4	--	Deg C

Table C-1. BTV Dataset for 2021

Well Name	Sample Date	Analyte	Result	Laboratory Qualifier	Unit
699-24-36	10/16/2018	Temperature	18.2	--	Deg C
699-24-36	4/4/2019	Temperature	18.5	--	Deg C
699-24-36	10/4/2019	Temperature	18.7	--	Deg C
699-24-36	9/30/2020	Temperature	19.1	--	Deg C
699-24-36	1/5/2021	Temperature	17.8	--	Deg C
699-24-36	7/12/2021	Temperature	19.6	--	Deg C
699-24-36	9/22/2021	Temperature	18.5	--	Deg C
699-24-36	10/13/2021	Temperature	18.4	--	Deg C
699-24-36	1/27/2017	Total Arsenic	5.0	U	µg/L
699-24-36	4/10/2017	Total Arsenic	9.9	BC	µg/L
699-24-36	8/7/2017	Total Arsenic	5.0	U	µg/L
699-24-36	10/12/2017	Total Arsenic	4.4	U	µg/L
699-24-36	1/8/2018	Total Arsenic	8.1	B	µg/L
699-24-36	4/26/2018	Total Arsenic	4.6	B	µg/L
699-24-36	7/19/2018	Total Arsenic	4.2	B	µg/L
699-24-36	10/16/2018	Total Arsenic	8.3	B	µg/L
699-24-36	4/4/2019	Total Arsenic	4.4	U	µg/L
699-24-36	10/4/2019	Total Arsenic	5.0	U	µg/L
699-24-36	9/30/2020	Total Arsenic	14	U	µg/L
699-24-36	1/5/2021	Total Arsenic	3.9	--	µg/L
699-24-36	7/12/2021	Total Arsenic	3.7	B	µg/L
699-24-36	10/13/2021	Total Arsenic	4.6	BD	µg/L
699-24-36	1/27/2017	Total Calcium	49,500	--	µg/L
699-24-36	4/10/2017	Total Calcium	49,200	--	µg/L
699-24-36	8/7/2017	Total Calcium	49,600	--	µg/L
699-24-36	10/12/2017	Total Calcium	48,500	--	µg/L
699-24-36	1/8/2018	Total Calcium	55,500	--	µg/L
699-24-36	4/26/2018	Total Calcium	52,600	--	µg/L
699-24-36	7/19/2018	Total Calcium	49,800	--	µg/L
699-24-36	10/16/2018	Total Calcium	50,500	--	µg/L
699-24-36	4/4/2019	Total Calcium	52,200	--	µg/L

Table C-1. BTV Dataset for 2021

Well Name	Sample Date	Analyte	Result	Laboratory Qualifier	Unit
699-24-36	10/4/2019	Total Calcium	46,700	--	µg/L
699-24-36	9/30/2020	Total Calcium	51,000	--	µg/L
699-24-36	1/5/2021	Total Calcium	49,000	--	µg/L
699-24-36	7/12/2021	Total Calcium	50,900	--	µg/L
699-24-36	9/22/2021	Total Calcium ^a	50,200	--	µg/L
699-24-36	10/13/2021	Total Calcium	55,100	--	µg/L
699-24-36	7/12/2021	Total dissolved solids	303,000	--	µg/L
699-24-36	10/13/2021	Total dissolved solids	271,000	--	µg/L
699-24-36	1/27/2017	Total Iron	30	U	µg/L
699-24-36	4/10/2017	Total Iron	37	B	µg/L
699-24-36	8/7/2017	Total Iron	30	U	µg/L
699-24-36	10/12/2017	Total Iron	22	U	µg/L
699-24-36	1/8/2018	Total Iron	22	U	µg/L
699-24-36	4/26/2018	Total Iron	30	U	µg/L
699-24-36	7/19/2018	Total Iron	30	U	µg/L
699-24-36	10/16/2018	Total Iron	22	U	µg/L
699-24-36	4/4/2019	Total Iron	22	U	µg/L
699-24-36	10/4/2019	Total Iron	30	U	µg/L
699-24-36	9/30/2020	Total Iron	44	U	µg/L
699-24-36	1/5/2021	Total Iron	44	U	µg/L
699-24-36	7/12/2021	Total Iron	22	U	µg/L
699-24-36	9/22/2021	Total Iron ^a	30	U	µg/L
699-24-36	10/13/2021	Total Iron	53	U	µg/L
699-24-36	1/27/2017	Total Magnesium	12,900	--	µg/L
699-24-36	4/10/2017	Total Magnesium	12,100	--	µg/L
699-24-36	8/7/2017	Total Magnesium	12,800	--	µg/L
699-24-36	10/12/2017	Total Magnesium	12,400	--	µg/L
699-24-36	1/8/2018	Total Magnesium	14,300	--	µg/L
699-24-36	4/26/2018	Total Magnesium	12,100	--	µg/L
699-24-36	7/19/2018	Total Magnesium	12,700	--	µg/L
699-24-36	10/16/2018	Total Magnesium	12,600	--	µg/L

Table C-1. BTV Dataset for 2021

Well Name	Sample Date	Analyte	Result	Laboratory Qualifier	Unit
699-24-36	4/4/2019	Total Magnesium	12,800	--	µg/L
699-24-36	10/4/2019	Total Magnesium	12,000	--	µg/L
699-24-36	9/30/2020	Total Magnesium	13,000	--	µg/L
699-24-36	1/5/2021	Total Magnesium	12,000	--	µg/L
699-24-36	7/12/2021	Total Magnesium	12,800	--	µg/L
699-24-36	9/22/2021	Total Magnesium ^a	12,750	--	µg/L
699-24-36	10/13/2021	Total Magnesium	13,900	--	µg/L
699-24-36	1/27/2017	Total Manganese	3.0	B	µg/L
699-24-36	4/10/2017	Total Manganese	1.4	BC	µg/L
699-24-36	8/7/2017	Total Manganese	2.0	U	µg/L
699-24-36	10/12/2017	Total Manganese	0.51	B	µg/L
699-24-36	1/8/2018	Total Manganese	0.26	U	µg/L
699-24-36	4/26/2018	Total Manganese	4.0	U	µg/L
699-24-36	7/19/2018	Total Manganese	4.0	U	µg/L
699-24-36	10/16/2018	Total Manganese	0.31	BC	µg/L
699-24-36	4/4/2019	Total Manganese	1.9	U	µg/L
699-24-36	10/4/2019	Total Manganese	2.0	U	µg/L
699-24-36	9/30/2020	Total Manganese	0.74	U	µg/L
699-24-36	1/5/2021	Total Manganese	2.4	U	µg/L
699-24-36	7/12/2021	Total Manganese	0.45	B	µg/L
699-24-36	9/22/2021	Total Manganese ^a	0.48	B	µg/L
699-24-36	10/13/2021	Total Manganese	1.5	UD	µg/L
699-24-36	7/12/2021	Total organic carbon	330	U	µg/L
699-24-36	10/13/2021	Total organic carbon	330	U	µg/L
699-24-36	1/27/2017	Total Potassium	6,090	--	µg/L
699-24-36	4/10/2017	Total Potassium	7,170	--	µg/L
699-24-36	8/7/2017	Total Potassium	6,410	--	µg/L
699-24-36	10/12/2017	Total Potassium	6,880	--	µg/L
699-24-36	1/8/2018	Total Potassium	7,000	--	µg/L
699-24-36	4/26/2018	Total Potassium	6,470	--	µg/L
699-24-36	7/19/2018	Total Potassium	6,510	--	µg/L

Table C-1. BTV Dataset for 2021

Well Name	Sample Date	Analyte	Result	Laboratory Qualifier	Unit
699-24-36	10/16/2018	Total Potassium	6,470	--	µg/L
699-24-36	4/4/2019	Total Potassium	7,010	--	µg/L
699-24-36	10/4/2019	Total Potassium	6,030	--	µg/L
699-24-36	9/30/2020	Total Potassium	7,900	--	µg/L
699-24-36	1/5/2021	Total Potassium	7,400	--	µg/L
699-24-36	7/12/2021	Total Potassium	6,630	--	µg/L
699-24-36	9/22/2021	Total Potassium ^a	6,515	--	µg/L
699-24-36	10/13/2021	Total Potassium	6,990	--	µg/L
699-24-36	1/27/2017	Total Sodium	20,200	--	µg/L
699-24-36	4/10/2017	Total Sodium	23,800	--	µg/L
699-24-36	8/7/2017	Total Sodium	20,100	--	µg/L
699-24-36	10/12/2017	Total Sodium	18,600	--	µg/L
699-24-36	1/8/2018	Total Sodium	22,200	--	µg/L
699-24-36	4/26/2018	Total Sodium	20,100	--	µg/L
699-24-36	7/19/2018	Total Sodium	21,000	--	µg/L
699-24-36	10/16/2018	Total Sodium	21,100	--	µg/L
699-24-36	4/4/2019	Total Sodium	21,800	--	µg/L
699-24-36	10/4/2019	Total Sodium	18,400	--	µg/L
699-24-36	9/30/2020	Total Sodium	21,000	--	µg/L
699-24-36	1/5/2021	Total Sodium	21,000	--	µg/L
699-24-36	7/12/2021	Total Sodium	21,700	--	µg/L
699-24-36	9/22/2021	Total Sodium ^a	20,400	--	µg/L
699-24-36	10/13/2021	Total Sodium	21,500	--	µg/L

a. Analyte result is based on the daily average since multiple sampling events occurred on the same day

BTV = background threshold value

2021 ProUCL Output**Background Statistics for Data Sets with Non-Detects****User Selected Options**

Date/Time of Computation ProUCL 5.15/24/2022 4:20:44 PM

From File ProUCL_Datasets_2021 5_24_22 updates bicarbonate.xls

Full Precision OFF

Confidence Coefficient 95%

Coverage 95%

Different or Future K Observations 1

Number of Bootstrap Operations 2000

VAL (alkalinity)

General Statistics

Total Number of Observations	15	Number of Distinct Observations	12
Minimum	155000	First Quartile	165500
Second Largest	175000	Median	169000
Maximum	177000	Third Quartile	171500
Mean	168433	SD	5577
Coefficient of Variation	0.0331	Skewness	-0.758
Mean of logged Data	12.03	SD of logged Data	0.0335

Critical Values for Background Threshold Values (BTVs)

Tolerance Factor K (For UTL)	2.566	d2max (for USL)	2.409
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Normal GOF Test

Shapiro Wilk Test Statistic	0.958	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Normal at 5% Significance Level
Lilliefors Test Statistic	0.136	Lilliefors GOF Test
5% Lilliefors Critical Value	0.22	Data appear Normal at 5% Significance Level

Data appear Normal at 5% Significance Level**Background Statistics Assuming Normal Distribution**

95% UTL with 95% Coverage	182744	90% Percentile (z)	175580
95% UPL (t)	178578	95% Percentile (z)	177607
95% USL	181868	99% Percentile (z)	181407

Gamma GOF Test

A-D Test Statistic	0.258	Anderson-Darling Gamma GOF Test
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5% A-D Critical Value 0.734 Detected data appear Gamma Distributed at 5% Significance Level

K-S Test Statistic 0.139 **Kolmogorov-Smirnov Gamma GOF Test**

5% K-S Critical Value 0.221 Detected data appear Gamma Distributed at 5% Significance Level

Detected data appear Gamma Distributed at 5% Significance Level

Gamma Statistics

k hat (MLE)	961.8	k star (bias corrected MLE)	769.5
Theta hat (MLE)	175.1	Theta star (bias corrected MLE)	218.9
nu hat (MLE)	28853	nu star (bias corrected)	23084
MLE Mean (bias corrected)	168433	MLE Sd (bias corrected)	6072

Background Statistics Assuming Gamma Distribution

95% Wilson Hilferty (WH) Approx. Gamma UPL	178808	90% Percentile	176260
95% Hawkins Wixley (HW) Approx. Gamma UPL	178838	95% Percentile	178544
95% WH Approx. Gamma UTL with Coverage	95% 183213	99% Percentile	182880
95% HW Approx. Gamma UTL with Coverage	95% 183275		
95% WH USL	182281	95% HW USL	182336

Lognormal GOF Test

Shapiro Wilk Test Statistic	0.95	Shapiro Wilk Lognormal GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.142	Lilliefors Lognormal GOF Test
5% Lilliefors Critical Value	0.22	Data appear Lognormal at 5% Significance Level

Data appear Lognormal at 5% Significance Level

Background Statistics assuming Lognormal Distribution

95% UTL with Coverage	95% 183466	90% Percentile (z)	175735
95% UPL (t)	178930	95% Percentile (z)	177888
95% USL	182504	99% Percentile (z)	181999

Nonparametric Distribution Free Background Statistics

Data appear Normal at 5% Significance Level

Nonparametric Upper Limits for Background Threshold Values

Order of Statistic, r	15	95% UTL with Coverage	95% 177000
Approx, f used to compute achieved CC	0.789	Approximate Actual Confidence Coefficient achieved by UTL	0.537
		Approximate Sample Size needed to achieve specified CC	59
95% Percentile Bootstrap UTL with Coverage	95% 177000	95% BCA Bootstrap UTL with Coverage	95% 177000
95% UPL	177000	90% Percentile	174800
90% Chebyshev UPL	185713	95% Percentile	175600

95% Chebyshev UPL 193540

99% Percentile 176720

95% USL 177000

Note: The use of USL tends to yield a conservative estimate of BTV, especially when the sample size starts exceeding 20.

Therefore, one may use USL to estimate a BTV only when the data set represents a background data set free of outliers and consists of observations collected from clean unimpacted locations.

The use of USL tends to provide a balance between false positives and false negatives provided the data represents a background data set and when many onsite observations need to be compared with the BTV.

VAL (ammonia)**General Statistics**

Total Number of Observations	2	Number of Missing Observations	0
Number of Distinct Observations	2		
Number of Detects	1	Number of Non-Detects	1
Number of Distinct Detects	1	Number of Distinct Non-Detects	1
Minimum Detect	88.6	Minimum Non-Detect	20.7
Maximum Detect	88.6	Maximum Non-Detect	20.7
Variance Detected	N/A	Percent Non-Detects	50%
Mean Detected	88.6	SD Detected	N/A
Mean of Detected Logged Data	4.484	SD of Detected Logged Data	N/A

Warning: This data set only has 2 observations!

Data set is too small to compute reliable and meaningful statistics and estimates!

The data set for variable VAL (ammonia) was not processed!

It is suggested to collect at least 8 to 10 observations before using these statistical methods!

If possible, compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

VAL (bicarbonate)**General Statistics**

Total Number of Observations	15	Number of Distinct Observations	12
Minimum	155000	First Quartile	165500
Second Largest	175000	Median	169000
Maximum	177000	Third Quartile	171500
Mean	168433	SD	5577
Coefficient of Variation	0.0331	Skewness	-0.758
Mean of logged Data	12.03	SD of logged Data	0.0335

Critical Values for Background Threshold Values (BTVs)

Tolerance Factor K (For UTL)	2.566	d2max (for USL)	2.409
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Normal GOF Test

Shapiro Wilk Test Statistic	0.958	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Normal at 5% Significance Level
Lilliefors Test Statistic	0.136	Lilliefors GOF Test
5% Lilliefors Critical Value	0.22	Data appear Normal at 5% Significance Level

Data appear Normal at 5% Significance Level**Background Statistics Assuming Normal Distribution**

95% UTL with 95% Coverage	182744	90% Percentile (z)	175580
95% UPL (t)	178578	95% Percentile (z)	177607
95% USL	181868	99% Percentile (z)	181407

Gamma GOF Test

A-D Test Statistic	0.258	Anderson-Darling Gamma GOF Test
5% A-D Critical Value	0.734	Detected data appear Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.139	Kolmogorov-Smirnov Gamma GOF Test
5% K-S Critical Value	0.221	Detected data appear Gamma Distributed at 5% Significance Level

Detected data appear Gamma Distributed at 5% Significance Level**Gamma Statistics**

k hat (MLE)	961.8	k star (bias corrected MLE)	769.5
Theta hat (MLE)	175.1	Theta star (bias corrected MLE)	218.9
nu hat (MLE)	28853	nu star (bias corrected)	23084
MLE Mean (bias corrected)	168433	MLE Sd (bias corrected)	6072

Background Statistics Assuming Gamma Distribution

95% Wilson Hilferty (WH) Approx. Gamma UPL	178808	90% Percentile	176260
95% Hawkins Wixley (HW) Approx. Gamma UPL	178838	95% Percentile	178544
95% WH Approx. Gamma UTL with Coverage	95% 183213	99% Percentile	182880
95% HW Approx. Gamma UTL with Coverage	95% 183275		
95% WH USL	182281	95% HW USL	182336

Lognormal GOF Test

Shapiro Wilk Test Statistic	0.95	Shapiro Wilk Lognormal GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.142	Lilliefors Lognormal GOF Test

5% Lilliefors Critical Value 0.22 Data appear Lognormal at 5% Significance Level

Data appear Lognormal at 5% Significance Level

Background Statistics assuming Lognormal Distribution

95% UTL with 95% Coverage	183466	90% Percentile (z)	175735
95% UPL (t)	178930	95% Percentile (z)	177888
95% USL	182504	99% Percentile (z)	181999

Nonparametric Distribution Free Background Statistics

Data appear Normal at 5% Significance Level

Nonparametric Upper Limits for Background Threshold Values

Order of Statistic, r	15	95% UTL with 95% Coverage	177000
Approx, f used to compute achieved CC	0.789	Approximate Actual Confidence Coefficient achieved by UTL	0.537
		Approximate Sample Size needed to achieve specified CC	59
95% Percentile Bootstrap UTL with 95% Coverage	177000	95% BCA Bootstrap UTL with 95% Coverage	177000
95% UPL	177000	90% Percentile	174800
90% Chebyshev UPL	185713	95% Percentile	175600
95% Chebyshev UPL	193540	99% Percentile	176720
95% USL	177000		

Note: The use of USL tends to yield a conservative estimate of BTV, especially when the sample size starts exceeding 20.

Therefore, one may use USL to estimate a BTV only when the data set represents a background data set free of outliers and consists of observations collected from clean unimpacted locations.

The use of USL tends to provide a balance between false positives and false negatives provided the data represents a background data set and when many onsite observations need to be compared with the BTV.

VAL (chloride)

General Statistics

Total Number of Observations	15	Number of Distinct Observations	13
Minimum	5340	First Quartile	5595
Second Largest	5900	Median	5640
Maximum	6100	Third Quartile	5770
Mean	5682	SD	186.6
Coefficient of Variation	0.0328	Skewness	0.473
Mean of logged Data	8.645	SD of logged Data	0.0327

Critical Values for Background Threshold Values (BTVs)

Tolerance Factor K (For UTL)	2.566	d2max (for USL)	2.409
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Normal GOF Test

Shapiro Wilk Test Statistic	0.974	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Normal at 5% Significance Level
Lilliefors Test Statistic	0.123	Lilliefors GOF Test
5% Lilliefors Critical Value	0.22	Data appear Normal at 5% Significance Level

Data appear Normal at 5% Significance Level**Background Statistics Assuming Normal Distribution**

95% UTL with 95% Coverage	6161	90% Percentile (z)	5922
95% UPL (t)	6022	95% Percentile (z)	5989
95% USL	6132	99% Percentile (z)	6117

Gamma GOF Test

A-D Test Statistic	0.229	Anderson-Darling Gamma GOF Test
5% A-D Critical Value	0.734	Detected data appear Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.123	Kolmogorov-Smirnov Gamma GOF Test
5% K-S Critical Value	0.221	Detected data appear Gamma Distributed at 5% Significance Level

Detected data appear Gamma Distributed at 5% Significance Level**Gamma Statistics**

k hat (MLE)	1001	k star (bias corrected MLE)	800.7
Theta hat (MLE)	5.678	Theta star (bias corrected MLE)	7.097
nu hat (MLE)	30024	nu star (bias corrected)	24020
MLE Mean (bias corrected)	5682	MLE Sd (bias corrected)	200.8

Background Statistics Assuming Gamma Distribution

95% Wilson Hilferty (WH) Approx. Gamma UPL	6025	90% Percentile	5941
95% Hawkins Wixley (HW) Approx. Gamma UPL	6026	95% Percentile	6017
95% WH Approx. Gamma UTL with 95% Coverage	6171	99% Percentile	6160
95% HW Approx. Gamma UTL with 95% Coverage	6172		
95% WH USL	6140	95% HW USL	6141

Lognormal GOF Test

Shapiro Wilk Test Statistic	0.978	Shapiro Wilk Lognormal GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.118	Lilliefors Lognormal GOF Test
5% Lilliefors Critical Value	0.22	Data appear Lognormal at 5% Significance Level

Data appear Lognormal at 5% Significance Level

Background Statistics assuming Lognormal Distribution

95% UTL with 95% Coverage	6176	90% Percentile (z)	5922
95% UPL (t)	6027	95% Percentile (z)	5993
95% USL	6144	99% Percentile (z)	6128

Nonparametric Distribution Free Background Statistics**Data appear Normal at 5% Significance Level****Nonparametric Upper Limits for Background Threshold Values**

Order of Statistic, r	15	95% UTL with 95% Coverage	6100
Approx, f used to compute achieved CC	0.789	Approximate Actual Confidence Coefficient achieved by UTL	0.537
		Approximate Sample Size needed to achieve specified CC	59
95% Percentile Bootstrap UTL with 95% Coverage	6100	95% BCA Bootstrap UTL with 95% Coverage	6100
95% UPL	6100	90% Percentile	5888
90% Chebyshev UPL	6261	95% Percentile	5960
95% Chebyshev UPL	6523	99% Percentile	6072
95% USL	6100		

Note: The use of USL tends to yield a conservative estimate of BTV, especially when the sample size starts exceeding 20.

Therefore, one may use USL to estimate a BTV only when the data set represents a background data set free of outliers and consists of observations collected from clean unimpacted locations.

The use of USL tends to provide a balance between false positives and false negatives provided the data represents a background data set and when many onsite observations need to be compared with the BTV.

VAL (dissolved arsenic)**General Statistics**

Total Number of Observations	14	Number of Missing Observations	0
Number of Distinct Observations	12		
Number of Detects	8	Number of Non-Detects	6
Number of Distinct Detects	8	Number of Distinct Non-Detects	4
Minimum Detect	3.7	Minimum Non-Detect	4
Maximum Detect	8.6	Maximum Non-Detect	14
Variance Detected	3.08	Percent Non-Detects	42.86%
Mean Detected	5.701	SD Detected	1.755
Mean of Detected Logged Data	1.7	SD of Detected Logged Data	0.306

Critical Values for Background Threshold Values (BTVs)

Tolerance Factor K (For UTL)	2.614	d2max (for USL)	2.372
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Normal GOF Test on Detects Only

Shapiro Wilk Test Statistic	0.935	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.818	Detected Data appear Normal at 5% Significance Level
Lilliefors Test Statistic	0.16	Lilliefors GOF Test
5% Lilliefors Critical Value	0.283	Detected Data appear Normal at 5% Significance Level

Detected Data appear Normal at 5% Significance Level

Kaplan Meier (KM) Background Statistics Assuming Normal Distribution

KM Mean	4.973	KM SD	1.589
95% UTL95% Coverage	9.127	95% KM UPL (t)	7.886
90% KM Percentile (z)	7.01	95% KM Percentile (z)	7.587
99% KM Percentile (z)	8.67	95% KM USL	8.742

DL/2 Substitution Background Statistics Assuming Normal Distribution

Mean	4.572	SD	2.221
95% UTL95% Coverage	10.38	95% UPL (t)	8.643
90% Percentile (z)	7.418	95% Percentile (z)	8.225
99% Percentile (z)	9.738	95% USL	9.839

DL/2 is not a recommended method. DL/2 provided for comparisons and historical reasons

Gamma GOF Tests on Detected Observations Only

A-D Test Statistic	0.234	Anderson-Darling GOF Test
5% A-D Critical Value	0.715	Detected data appear Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.142	Kolmogorov-Smirnov GOF
5% K-S Critical Value	0.294	Detected data appear Gamma Distributed at 5% Significance Level

Detected data appear Gamma Distributed at 5% Significance Level

Gamma Statistics on Detected Data Only

k hat (MLE)	12.38	k star (bias corrected MLE)	7.819
Theta hat (MLE)	0.461	Theta star (bias corrected MLE)	0.729
nu hat (MLE)	198	nu star (bias corrected)	125.1
MLE Mean (bias corrected)	5.701		
MLE Sd (bias corrected)	2.039	95% Percentile of Chisquare (2kstar)	25.83

Gamma ROS Statistics using Imputed Non-Detects

GROS may not be used when data set has > 50% NDs with many tied observations at multiple DLs

GROS may not be used when kstar of detects is small such as <1.0, especially when the sample size is small (e.g., <15-20)

For such situations, GROS method may yield incorrect values of UCLs and BTVs

This is especially true when the sample size is small.

For gamma distributed detected data, BTVs and UCLs may be computed using gamma distribution on KM estimates

Minimum	3	Mean	4.873
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Maximum	8.6	Median	4.434
SD	1.676	CV	0.344
k hat (MLE)	10.33	k star (bias corrected MLE)	8.165
Theta hat (MLE)	0.472	Theta star (bias corrected MLE)	0.597
nu hat (MLE)	289.3	nu star (bias corrected)	228.6
MLE Mean (bias corrected)	4.873	MLE Sd (bias corrected)	1.705
95% Percentile of Chisquare (2kstar)	26.72	90% Percentile	7.146
95% Percentile	7.974	99% Percentile	9.688

The following statistics are computed using Gamma ROS Statistics on Imputed Data

Upper Limits using Wilson Hilferty (WH) and Hawkins Wixley (HW) Methods

	WH	HW		WH	HW
95% Approx. Gamma UTL with 95% Coverage 9.992		10.13	95% Approx. Gamma UPL	8.136	8.173
95% Gamma USL		9.488			
	9.388				

Estimates of Gamma Parameters using KM Estimates

Mean (KM)	4.973	SD (KM)	1.589
Variance (KM)	2.526	SE of Mean (KM)	0.473
k hat (KM)	9.787	k star (KM)	7.738
nu hat (KM)	274	nu star (KM)	216.7
theta hat (KM)	0.508	theta star (KM)	0.643
80% gamma percentile (KM)	6.381	90% gamma percentile (KM)	7.357
95% gamma percentile (KM)	8.231	99% gamma percentile (KM)	10.04

The following statistics are computed using gamma distribution and KM estimates

Upper Limits using Wilson Hilferty (WH) and Hawkins Wixley (HW) Methods

	WH	HW		WH	HW
95% Approx. Gamma UTL with 95% Coverage 9.661		9.755	95% Approx. Gamma UPL	7.98	7.998
95% KM Gamma Percentile		7.612	95% Gamma USL	9.116	9.181
	7.606				

Lognormal GOF Test on Detected Observations Only

Shapiro Wilk Test Statistic	0.95	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.818	Detected Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.134	Lilliefors GOF Test
5% Lilliefors Critical Value	0.283	Detected Data appear Lognormal at 5% Significance Level

Detected Data appear Lognormal at 5% Significance Level

Background Lognormal ROS Statistics Assuming Lognormal Distribution Using Imputed Non-Detects

Mean in Original Scale	4.932	Mean in Log Scale	1.552
SD in Original Scale	1.617	SD in Log Scale	0.297
95% UTL95% Coverage	10.27	95% BCA UTL95% Coverage	8.6

95% Bootstrap (%) UTL	95% Coverage	8.6	95% UPL (t)	8.143
90% Percentile (z)		6.911	95% Percentile (z)	7.7
99% Percentile (z)		9.429	95% USL	9.557

Statistics using KM estimates on Logged Data and Assuming Lognormal Distribution

KM Mean of Logged Data	1.56	95% KM UTL (Lognormal)	95% Coverage	10.09
KM SD of Logged Data	0.288	95% KM UPL (Lognormal)		8.061
95% KM Percentile Lognormal (z)	7.636	95% KM USL (Lognormal)		9.412

Background DL/2 Statistics Assuming Lognormal Distribution

Mean in Original Scale	4.572	Mean in Log Scale	1.403
SD in Original Scale	2.221	SD in Log Scale	0.51
95% UTL	95% Coverage	95% UPL (t)	10.37
90% Percentile (z)	7.825	95% Percentile (z)	9.419
99% Percentile (z)	13.34	95% USL	13.65

DL/2 is not a Recommended Method. DL/2 provided for comparisons and historical reasons.

Nonparametric Distribution Free Background Statistics

Data appear to follow a Discernible Distribution at 5% Significance Level

Nonparametric Upper Limits for BTVs(no distinction made between detects and nondetects)

Order of Statistic, r	14	95% UTL with 95% Coverage	14
Approx, f used to compute achieved CC	0.737	Approximate Actual Confidence Coefficient achieved by UTL	0.512
Approximate Sample Size needed to achieve specified CC	59	95% UPL	14
95% USL	14	95% KM Chebyshev UPL	12.14

Note: The use of USL tends to yield a conservative estimate of BTV, especially when the sample size starts exceeding 20. Therefore, one may use USL to estimate a BTV only when the data set represents a background data set free of outliers and consists of observations collected from clean unimpacted locations.

The use of USL tends to provide a balance between false positives and false negatives provided the data represents a background data set and when many onsite observations need to be compared with the BTV.

VAL (dissolved calcium)

General Statistics

Total Number of Observations	15	Number of Distinct Observations	12
Minimum	47000	First Quartile	49200
Second Largest	52700	Median	50000
Maximum	52800	Third Quartile	51450
Mean	50153	SD	1850

Coefficient of Variation	0.0369	Skewness	-0.14
Mean of logged Data	10.82	SD of logged Data	0.037

Critical Values for Background Threshold Values (BTVs)

Tolerance Factor K (For UTL)	2.566	d2max (for USL)	2.409
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Normal GOF Test

Shapiro Wilk Test Statistic	0.936	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Normal at 5% Significance Level
Lilliefors Test Statistic	0.144	Lilliefors GOF Test
5% Lilliefors Critical Value	0.22	Data appear Normal at 5% Significance Level

Data appear Normal at 5% Significance Level**Background Statistics Assuming Normal Distribution**

95% UTL with 95% Coverage	54901	90% Percentile (z)	52524
95% UPL (t)	53519	95% Percentile (z)	53196
95% USL	54610	99% Percentile (z)	54457

Gamma GOF Test

A-D Test Statistic	0.406	Anderson-Darling Gamma GOF Test
5% A-D Critical Value	0.734	Detected data appear Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.15	Kolmogorov-Smirnov Gamma GOF Test
5% K-S Critical Value	0.221	Detected data appear Gamma Distributed at 5% Significance Level

Detected data appear Gamma Distributed at 5% Significance Level**Gamma Statistics**

k hat (MLE)	784.2	k star (bias corrected MLE)	627.4
Theta hat (MLE)	63.95	Theta star (bias corrected MLE)	79.94
nu hat (MLE)	23526	nu star (bias corrected)	18822
MLE Mean (bias corrected)	50153	MLE Sd (bias corrected)	2002

Background Statistics Assuming Gamma Distribution

95% Wilson Hilferty (WH) Approx. Gamma UPL	53579	90% Percentile	52736
95% Hawkins Wixley (HW) Approx. Gamma UPL	53587	95% Percentile	53492
95% WH Approx. Gamma UTL with 95% Coverage	55040	99% Percentile	54929
95% HW Approx. Gamma UTL with 95% Coverage	55058		
95% WH USL	54731	95% HW USL	54746

Lognormal GOF Test

Shapiro Wilk Test Statistic	0.935	Shapiro Wilk Lognormal GOF Test
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5% Shapiro Wilk Critical Value	0.881	Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.142	Lilliefors Lognormal GOF Test
5% Lilliefors Critical Value	0.22	Data appear Lognormal at 5% Significance Level

Data appear Lognormal at 5% Significance Level

Background Statistics assuming Lognormal Distribution

95% UTL with 95% Coverage	55114	90% Percentile (z)	52556
95% UPL (t)	53612	95% Percentile (z)	53267
95% USL	54795	99% Percentile (z)	54628

Nonparametric Distribution Free Background Statistics

Data appear Normal at 5% Significance Level

Nonparametric Upper Limits for Background Threshold Values

Order of Statistic, r	15	95% UTL with 95% Coverage	52800
Approx, f used to compute achieved CC	0.789	Approximate Actual Confidence Coefficient achieved by UTL	0.537
		Approximate Sample Size needed to achieve specified CC	59
95% Percentile Bootstrap UTL with 95% Coverage	52800	95% BCA Bootstrap UTL with 95% Coverage	52800
95% UPL	52800	90% Percentile	52540
90% Chebyshev UPL	55885	95% Percentile	52730
95% Chebyshev UPL	58482	99% Percentile	52786
95% USL	52800		

Note: The use of USL tends to yield a conservative estimate of BTV, especially when the sample size starts exceeding 20.

Therefore, one may use USL to estimate a BTV only when the data set represents a background data set free of outliers and consists of observations collected from clean unimpacted locations.

The use of USL tends to provide a balance between false positives and false negatives provided the data represents a background data set and when many onsite observations need to be compared with the BTV.

VAL (dissolved iron)

General Statistics

Total Number of Observations	14	Number of Missing Observations	0
Number of Distinct Observations	5		
Number of Detects	1	Number of Non-Detects	13
Number of Distinct Detects	1	Number of Distinct Non-Detects	4
Minimum Detect	30.7	Minimum Non-Detect	22
Maximum Detect	30.7	Maximum Non-Detect	53
Variance Detected	N/A	Percent Non-Detects	92.86%
Mean Detected	30.7	SD Detected	N/A

Mean of Detected Logged Data 3.424

SD of Detected Logged Data N/A

Warning: Only one distinct data value was detected! ProUCL (or any other software) should not be used on such a data set!
It is suggested to use alternative site specific values determined by the Project Team to estimate environmental parameters (e.g., EPC, BTV).

The data set for variable VAL (dissolved iron) was not processed!

VAL (dissolved magnesium)

General Statistics

Total Number of Observations	15	Number of Distinct Observations	9
Minimum	12000	First Quartile	12500
Second Largest	13000	Median	12700
Maximum	13600	Third Quartile	13000
Mean	12713	SD	417.2
Coefficient of Variation	0.0328	Skewness	0.0618
Mean of logged Data	9.45	SD of logged Data	0.0328

Critical Values for Background Threshold Values (BTVs)

Tolerance Factor K (For UTL)	2.566	d2max (for USL)	2.409
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Normal GOF Test

Shapiro Wilk Test Statistic	0.945	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Normal at 5% Significance Level
Lilliefors Test Statistic	0.179	Lilliefors GOF Test
5% Lilliefors Critical Value	0.22	Data appear Normal at 5% Significance Level

Data appear Normal at 5% Significance Level

Background Statistics Assuming Normal Distribution

95% UTL with 95% Coverage	13784	90% Percentile (z)	13248
95% UPL (t)	13472	95% Percentile (z)	13400
95% USL	13718	99% Percentile (z)	13684

Gamma GOF Test

A-D Test Statistic	0.416	Anderson-Darling Gamma GOF Test
5% A-D Critical Value	0.734	Detected data appear Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.17	Kolmogorov-Smirnov Gamma GOF Test
5% K-S Critical Value	0.221	Detected data appear Gamma Distributed at 5% Significance Level

Detected data appear Gamma Distributed at 5% Significance Level

Gamma Statistics

k hat (MLE)	994.6	k star (bias corrected MLE)	795.8
Theta hat (MLE)	12.78	Theta star (bias corrected MLE)	15.98
nu hat (MLE)	29839	nu star (bias corrected)	23873
MLE Mean (bias corrected)	12713	MLE Sd (bias corrected)	450.7

Background Statistics Assuming Gamma Distribution

95% Wilson Hilferty (WH) Approx. Gamma UPL	13483	90% Percentile	13294
95% Hawkins Wixley (HW) Approx. Gamma UPL	13485	95% Percentile	13464
95% WH Approx. Gamma UTL with 95% Coverage	13810	99% Percentile	13785
95% HW Approx. Gamma UTL with 95% Coverage	13813		
95% WH USL	13741	95% HW USL	13744

Lognormal GOF Test

Shapiro Wilk Test Statistic	0.946	Shapiro Wilk Lognormal GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.177	Lilliefors Lognormal GOF Test
5% Lilliefors Critical Value	0.22	Data appear Lognormal at 5% Significance Level

Data appear Lognormal at 5% Significance Level**Background Statistics assuming Lognormal Distribution**

95% UTL with 95% Coverage	13824	90% Percentile (z)	13253
95% UPL (t)	13489	95% Percentile (z)	13412
95% USL	13753	99% Percentile (z)	13715

Nonparametric Distribution Free Background Statistics**Data appear Normal at 5% Significance Level****Nonparametric Upper Limits for Background Threshold Values**

Order of Statistic, r	15	95% UTL with 95% Coverage	13600
Approx, f used to compute achieved CC	0.789	Approximate Actual Confidence Coefficient achieved by UTL	0.537
		Approximate Sample Size needed to achieve specified CC	59
95% Percentile Bootstrap UTL with 95% Coverage	13600	95% BCA Bootstrap UTL with 95% Coverage	13600
95% UPL	13600	90% Percentile	13000
90% Chebyshev UPL	14006	95% Percentile	13180
95% Chebyshev UPL	14592	99% Percentile	13516
95% USL	13600		

Note: The use of USL tends to yield a conservative estimate of BTV, especially when the sample size starts exceeding 20.

Therefore, one may use USL to estimate a BTV only when the data set represents a background data set free of outliers and consists of observations collected from clean unimpacted locations.

The use of USL tends to provide a balance between false positives and false negatives provided the data represents a background data set and when many onsite observations need to be compared with the BTV.

VAL (dissolved manganese)

General Statistics

Total Number of Observations	15	Number of Missing Observations	0
Number of Distinct Observations	13		
Number of Detects	6	Number of Non-Detects	9
Number of Distinct Detects	6	Number of Distinct Non-Detects	7
Minimum Detect	0.39	Minimum Non-Detect	0.31
Maximum Detect	3.39	Maximum Non-Detect	4
Variance Detected	1.233	Percent Non-Detects	60%
Mean Detected	1.262	SD Detected	1.11
Mean of Detected Logged Data	-0.042	SD of Detected Logged Data	0.791

Critical Values for Background Threshold Values (BTVs)

Tolerance Factor K (For UTL)	2.566	d2max (for USL)	2.409
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Normal GOF Test on Detects Only

Shapiro Wilk Test Statistic	0.797	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.788	Detected Data appear Normal at 5% Significance Level
Lilliefors Test Statistic	0.284	Lilliefors GOF Test
5% Lilliefors Critical Value	0.325	Detected Data appear Normal at 5% Significance Level

Detected Data appear Normal at 5% Significance Level

Kaplan Meier (KM) Background Statistics Assuming Normal Distribution

KM Mean	0.918	KM SD	0.805
95% UTL95% Coverage	2.984	95% KM UPL (t)	2.383
90% KM Percentile (z)	1.95	95% KM Percentile (z)	2.242
99% KM Percentile (z)	2.791	95% KM USL	2.857

DL/2 Substitution Background Statistics Assuming Normal Distribution

Mean	1.142	SD	0.817
95% UTL95% Coverage	3.238	95% UPL (t)	2.628
90% Percentile (z)	2.189	95% Percentile (z)	2.485
99% Percentile (z)	3.042	95% USL	3.11

DL/2 is not a recommended method. DL/2 provided for comparisons and historical reasons

Gamma GOF Tests on Detected Observations Only

A-D Test Statistic	0.311	Anderson-Darling GOF Test
5% A-D Critical Value	0.704	Detected data appear Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.183	Kolmogorov-Smirnov GOF
5% K-S Critical Value	0.336	Detected data appear Gamma Distributed at 5% Significance Level

Detected data appear Gamma Distributed at 5% Significance Level

Gamma Statistics on Detected Data Only

k hat (MLE)	1.972	k star (bias corrected MLE)	1.097
Theta hat (MLE)	0.64	Theta star (bias corrected MLE)	1.15
nu hat (MLE)	23.67	nu star (bias corrected)	13.17
MLE Mean (bias corrected)	1.262		
MLE Sd (bias corrected)	1.204	95% Percentile of Chisquare (2kstar)	6.363

Gamma ROS Statistics using Imputed Non-Detects

GROS may not be used when data set has > 50% NDs with many tied observations at multiple DLs

GROS may not be used when kstar of detects is small such as <1.0, especially when the sample size is small (e.g., <15-20)

For such situations, GROS method may yield incorrect values of UCLs and BTVs

This is especially true when the sample size is small.

For gamma distributed detected data, BTVs and UCLs may be computed using gamma distribution on KM estimates

Minimum	0.01	Mean	0.797
Maximum	3.39	Median	0.541
SD	0.813	CV	1.02
k hat (MLE)	1.145	k star (bias corrected MLE)	0.96
Theta hat (MLE)	0.696	Theta star (bias corrected MLE)	0.83
nu hat (MLE)	34.34	nu star (bias corrected)	28.81
MLE Mean (bias corrected)	0.797	MLE Sd (bias corrected)	0.814
95% Percentile of Chisquare (2kstar)	5.836	90% Percentile	1.854
95% Percentile	2.423	99% Percentile	3.748

The following statistics are computed using Gamma ROS Statistics on Imputed Data**Upper Limits using Wilson Hilferty (WH) and Hawkins Wixley (HW) Methods**

	WH	HW		WH	HW
95% Approx. Gamma UTL with 95% Coverage		4.564	95% Approx. Gamma UPL	2.547	2.764
95% Gamma USL		4.129			
	3.618				

Estimates of Gamma Parameters using KM Estimates

Mean (KM)	0.918	SD (KM)	0.805
Variance (KM)	0.648	SE of Mean (KM)	0.265
k hat (KM)	1.302	k star (KM)	1.086
nu hat (KM)	39.07	nu star (KM)	32.59

theta hat (KM)	0.705	theta star (KM)	0.846
80% gamma percentile (KM)	1.468	90% gamma percentile (KM)	2.072
95% gamma percentile (KM)	2.673	99% gamma percentile (KM)	4.058

The following statistics are computed using gamma distribution and KM estimates

Upper Limits using Wilson Hilferty (WH) and Hawkins Wixley (HW) Methods

	WH	HW		WH	HW
95% Approx. Gamma UTL with 95% Coverage		3.501	95% Approx. Gamma UPL	2.348	2.366
95% KM Gamma Percentile	2.143	2.146	95% Gamma USL	3.137	3.234

Lognormal GOF Test on Detected Observations Only

Shapiro Wilk Test Statistic	0.955	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.788	Detected Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.157	Lilliefors GOF Test
5% Lilliefors Critical Value	0.325	Detected Data appear Lognormal at 5% Significance Level

Detected Data appear Lognormal at 5% Significance Level

Background Lognormal ROS Statistics Assuming Lognormal Distribution Using Imputed Non-Detects

Mean in Original Scale	0.834	Mean in Log Scale	-0.433
SD in Original Scale	0.775	SD in Log Scale	0.684
95% UTL95% Coverage	3.749	95% BCA UTL95% Coverage	3.39
95% Bootstrap (%) UTL95% Coverage	3.39	95% UPL (t)	2.25
90% Percentile (z)	1.558	95% Percentile (z)	1.997
99% Percentile (z)	3.182	95% USL	3.367

Statistics using KM estimates on Logged Data and Assuming Lognormal Distribution

KM Mean of Logged Data	-0.356	95% KM UTL (Lognormal)95% Coverage	4.154
KM SD of Logged Data	0.694	95% KM UPL (Lognormal)	2.474
95% KM Percentile Lognormal (z)	2.192	95% KM USL (Lognormal)	3.725

Background DL/2 Statistics Assuming Lognormal Distribution

Mean in Original Scale	1.142	Mean in Log Scale	-0.105
SD in Original Scale	0.817	SD in Log Scale	0.756
95% UTL95% Coverage	6.266	95% UPL (t)	3.562
90% Percentile (z)	2.372	95% Percentile (z)	3.122
99% Percentile (z)	5.228	95% USL	5.565

DL/2 is not a Recommended Method. DL/2 provided for comparisons and historical reasons.

Nonparametric Distribution Free Background Statistics

Data appear to follow a Discernible Distribution at 5% Significance Level

Nonparametric Upper Limits for BTVs(no distinction made between detects and nondetects)

Order of Statistic, r	15	95% UTL with 95% Coverage	4
Approx, f used to compute achieved CC	0.789	Approximate Actual Confidence Coefficient achieved by UTL	0.537
Approximate Sample Size needed to achieve specified CC	59	95% UPL	4
95% USL	4	95% KM Chebyshev UPL	4.542

Note: The use of USL tends to yield a conservative estimate of BTV, especially when the sample size starts exceeding 20.

Therefore, one may use USL to estimate a BTV only when the data set represents a background data set free of outliers and consists of observations collected from clean unimpacted locations.

The use of USL tends to provide a balance between false positives and false negatives provided the data represents a background data set and when many onsite observations need to be compared with the BTV.

VAL (dissolved potassium)**General Statistics**

Total Number of Observations	15	Number of Distinct Observations	15
Minimum	6110	First Quartile	6520
Second Largest	7400	Median	6700
Maximum	7800	Third Quartile	7050
Mean	6787	SD	483.1
Coefficient of Variation	0.0712	Skewness	0.512
Mean of logged Data	8.82	SD of logged Data	0.0704

Critical Values for Background Threshold Values (BTVs)

Tolerance Factor K (For UTL)	2.566	d2max (for USL)	2.409
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Normal GOF Test

Shapiro Wilk Test Statistic	0.962	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Normal at 5% Significance Level
Lilliefors Test Statistic	0.138	Lilliefors GOF Test
5% Lilliefors Critical Value	0.22	Data appear Normal at 5% Significance Level

Data appear Normal at 5% Significance Level

Background Statistics Assuming Normal Distribution

95% UTL with 95% Coverage	8026	90% Percentile (z)	7406
95% UPL (t)	7666	95% Percentile (z)	7581
95% USL	7951	99% Percentile (z)	7911

Gamma GOF Test

A-D Test Statistic	0.217	Anderson-Darling Gamma GOF Test
5% A-D Critical Value	0.734	Detected data appear Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.131	Kolmogorov-Smirnov Gamma GOF Test
5% K-S Critical Value	0.221	Detected data appear Gamma Distributed at 5% Significance Level
Detected data appear Gamma Distributed at 5% Significance Level		

Gamma Statistics

k hat (MLE)	214.9	k star (bias corrected MLE)	172
Theta hat (MLE)	31.58	Theta star (bias corrected MLE)	39.46
nu hat (MLE)	6447	nu star (bias corrected)	5159
MLE Mean (bias corrected)	6787	MLE Sd (bias corrected)	517.5

Background Statistics Assuming Gamma Distribution

95% Wilson Hilferty (WH) Approx. Gamma UPL	7685	90% Percentile	7458
95% Hawkins Wixley (HW) Approx. Gamma UPL	7687	95% Percentile	7660
95% WH Approx. Gamma UTL with 95% Coverage	8080	99% Percentile	8048
95% HW Approx. Gamma UTL with 95% Coverage	8088		
95% WH USL	7996	95% HW USL	8002

Lognormal GOF Test

Shapiro Wilk Test Statistic	0.968	Shapiro Wilk Lognormal GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.126	Lilliefors Lognormal GOF Test
5% Lilliefors Critical Value	0.22	Data appear Lognormal at 5% Significance Level

Data appear Lognormal at 5% Significance Level**Background Statistics assuming Lognormal Distribution**

95% UTL with 95% Coverage	8111	90% Percentile (z)	7410
95% UPL (t)	7696	95% Percentile (z)	7602
95% USL	8022	99% Percentile (z)	7975

Nonparametric Distribution Free Background Statistics**Data appear Normal at 5% Significance Level****Nonparametric Upper Limits for Background Threshold Values**

Order of Statistic, r	15	95% UTL with 95% Coverage	7800
Approx, f used to compute achieved CC	0.789	Approximate Actual Confidence Coefficient achieved by UTL	0.537
		Approximate Sample Size needed to achieve specified CC	59
95% Percentile Bootstrap UTL with 95% Coverage	7800	95% BCA Bootstrap UTL with 95% Coverage	7800
95% UPL	7800	90% Percentile	7376

90% Chebyshev UPL	8284	95% Percentile	7520
95% Chebyshev UPL	8962	99% Percentile	7744
95% USL	7800		

Note: The use of USL tends to yield a conservative estimate of BTV, especially when the sample size starts exceeding 20.

Therefore, one may use USL to estimate a BTV only when the data set represents a background data set free of outliers and consists of observations collected from clean unimpacted locations.

The use of USL tends to provide a balance between false positives and false negatives provided the data represents a background data set and when many onsite observations need to be compared with the BTV.

VAL (dissolved sodium)

General Statistics

Total Number of Observations	15	Number of Distinct Observations	12
Minimum	18500	First Quartile	20425
Second Largest	21900	Median	21100
Maximum	22100	Third Quartile	21500
Mean	20910	SD	904.4
Coefficient of Variation	0.0433	Skewness	-1.325
Mean of logged Data	9.947	SD of logged Data	0.0445

Critical Values for Background Threshold Values (BTVs)

Tolerance Factor K (For UTL)	2.566	d2max (for USL)	2.409
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Normal GOF Test

Shapiro Wilk Test Statistic	0.904	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Normal at 5% Significance Level
Lilliefors Test Statistic	0.206	Lilliefors GOF Test
5% Lilliefors Critical Value	0.22	Data appear Normal at 5% Significance Level

Data appear Normal at 5% Significance Level

Background Statistics Assuming Normal Distribution

95% UTL with 95% Coverage	23231	90% Percentile (z)	22069
95% UPL (t)	22555	95% Percentile (z)	22398
95% USL	23089	99% Percentile (z)	23014

Gamma GOF Test

A-D Test Statistic	0.531	Anderson-Darling Gamma GOF Test
5% A-D Critical Value	0.734	Detected data appear Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.213	Kolmogorov-Smirnov Gamma GOF Test

5% K-S Critical Value 0.221 Detected data appear Gamma Distributed at 5% Significance Level

Detected data appear Gamma Distributed at 5% Significance Level

Gamma Statistics

k hat (MLE)	552.3	k star (bias corrected MLE)	441.9
Theta hat (MLE)	37.86	Theta star (bias corrected MLE)	47.32
nu hat (MLE)	16570	nu star (bias corrected)	13257
MLE Mean (bias corrected)	20910	MLE Sd (bias corrected)	994.7

Background Statistics Assuming Gamma Distribution

95% Wilson Hilferty (WH) Approx. Gamma UPL	22617	90% Percentile	22194
95% Hawkins Wixley (HW) Approx. Gamma UPL	22625	95% Percentile	22573
95% WH Approx. Gamma UTL with 95% Coverage	23350	99% Percentile	23293
95% HW Approx. Gamma UTL with 95% Coverage	23366		
95% WH USL	23195	95% HW USL	23209

Lognormal GOF Test

Shapiro Wilk Test Statistic	0.887	Shapiro Wilk Lognormal GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.213	Lilliefors Lognormal GOF Test
5% Lilliefors Critical Value	0.22	Data appear Lognormal at 5% Significance Level

Data appear Lognormal at 5% Significance Level

Background Statistics assuming Lognormal Distribution

95% UTL with 95% Coverage	23416	90% Percentile (z)	22116
95% UPL (t)	22651	95% Percentile (z)	22476
95% USL	23253	99% Percentile (z)	23168

Nonparametric Distribution Free Background Statistics

Data appear Normal at 5% Significance Level

Nonparametric Upper Limits for Background Threshold Values

Order of Statistic, r	15	95% UTL with 95% Coverage	22100
Approx, f used to compute achieved CC	0.789	Approximate Actual Confidence Coefficient achieved by UTL	0.537
		Approximate Sample Size needed to achieve specified CC	59
95% Percentile Bootstrap UTL with 95% Coverage	22100	95% BCA Bootstrap UTL with 95% Coverage	22100
95% UPL	22100	90% Percentile	21780
90% Chebyshev UPL	23712	95% Percentile	21960
95% Chebyshev UPL	24981	99% Percentile	22072
95% USL	22100		

Note: The use of USL tends to yield a conservative estimate of BTV, especially when the sample size starts exceeding 20.

Therefore, one may use USL to estimate a BTV only when the data set represents a background data set free of outliers and consists of observations collected from clean unimpacted locations.

The use of USL tends to provide a balance between false positives and false negatives provided the data represents a background data set and when many onsite observations need to be compared with the BTV.

VAL (nitrate)

General Statistics

Total Number of Observations	15	Number of Distinct Observations	9
Minimum	12400	First Quartile	13225
Second Largest	14200	Median	13500
Maximum	14200	Third Quartile	13800
Mean	13517	SD	512.6
Coefficient of Variation	0.0379	Skewness	-0.451
Mean of logged Data	9.511	SD of logged Data	0.0383

Critical Values for Background Threshold Values (BTVs)

Tolerance Factor K (For UTL)	2.566	d2max (for USL)	2.409
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Normal GOF Test

Shapiro Wilk Test Statistic	0.951	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Normal at 5% Significance Level
Lilliefors Test Statistic	0.109	Lilliefors GOF Test
5% Lilliefors Critical Value	0.22	Data appear Normal at 5% Significance Level

Data appear Normal at 5% Significance Level

Background Statistics Assuming Normal Distribution

95% UTL with 95% Coverage	14832	90% Percentile (z)	14174
95% UPL (t)	14449	95% Percentile (z)	14360
95% USL	14751	99% Percentile (z)	14709

Gamma GOF Test

A-D Test Statistic	0.274	Anderson-Darling Gamma GOF Test
5% A-D Critical Value	0.734	Detected data appear Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.114	Kolmogorov-Smirnov Gamma GOF Test
5% K-S Critical Value	0.221	Detected data appear Gamma Distributed at 5% Significance Level

Detected data appear Gamma Distributed at 5% Significance Level

Gamma Statistics

k hat (MLE)	736.5	k star (bias corrected MLE)	589.3
Theta hat (MLE)	18.35	Theta star (bias corrected MLE)	22.94
nu hat (MLE)	22096	nu star (bias corrected)	17678
MLE Mean (bias corrected)	13517	MLE Sd (bias corrected)	556.8

Background Statistics Assuming Gamma Distribution

95% Wilson Hilferty (WH) Approx. Gamma UPL	14470	90% Percentile	14235
95% Hawkins Wixley (HW) Approx. Gamma UPL	14473	95% Percentile	14445
95% WH Approx. Gamma UTL with 95% Coverage	14877	99% Percentile	14846
95% HW Approx. Gamma UTL with 95% Coverage	14883		
95% WH USL	14791	95% HW USL	14796

Lognormal GOF Test

Shapiro Wilk Test Statistic	0.947	Shapiro Wilk Lognormal GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.111	Lilliefors Lognormal GOF Test
5% Lilliefors Critical Value	0.22	Data appear Lognormal at 5% Significance Level

Data appear Lognormal at 5% Significance Level

Background Statistics assuming Lognormal Distribution

95% UTL with 95% Coverage	14901	90% Percentile (z)	14186
95% UPL (t)	14481	95% Percentile (z)	14385
95% USL	14812	99% Percentile (z)	14765

Nonparametric Distribution Free Background Statistics

Data appear Normal at 5% Significance Level

Nonparametric Upper Limits for Background Threshold Values

Order of Statistic, r	15	95% UTL with 95% Coverage	14200
Approx, f used to compute achieved CC	0.789	Approximate Actual Confidence Coefficient achieved by UTL	0.537
		Approximate Sample Size needed to achieve specified CC	59
95% Percentile Bootstrap UTL with 95% Coverage	14200	95% BCA Bootstrap UTL with 95% Coverage	14200
95% UPL	14200	90% Percentile	14200
90% Chebyshev UPL	15105	95% Percentile	14200
95% Chebyshev UPL	15824	99% Percentile	14200
95% USL	14200		

Note: The use of USL tends to yield a conservative estimate of BTV, especially when the sample size starts exceeding 20. Therefore, one may use USL to estimate a BTV only when the data set represents a background data set free of outliers

and consists of observations collected from clean unimpacted locations.

The use of USL tends to provide a balance between false positives and false negatives provided the data represents a background data set and when many onsite observations need to be compared with the BTV.

VAL (ph measurement)

General Statistics

Total Number of Observations	15	Number of Distinct Observations	10
Minimum	7.53	First Quartile	7.61
Second Largest	7.77	Median	7.65
Maximum	7.85	Third Quartile	7.755
Mean	7.669	SD	0.0907
Coefficient of Variation	0.0118	Skewness	0.406
Mean of logged Data	2.037	SD of logged Data	0.0118

Critical Values for Background Threshold Values (BTVs)

Tolerance Factor K (For UTL)	2.566	d2max (for USL)	2.409
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Normal GOF Test

Shapiro Wilk Test Statistic	0.952	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Normal at 5% Significance Level
Lilliefors Test Statistic	0.164	Lilliefors GOF Test
5% Lilliefors Critical Value	0.22	Data appear Normal at 5% Significance Level

Data appear Normal at 5% Significance Level

Background Statistics Assuming Normal Distribution

95% UTL with 95% Coverage	7.902	90% Percentile (z)	7.786
95% UPL (t)	7.834	95% Percentile (z)	7.819
95% USL	7.888	99% Percentile (z)	7.88

Gamma GOF Test

A-D Test Statistic	0.93	Anderson-Darling Gamma GOF Test
5% A-D Critical Value	0.734	Data Not Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.289	Kolmogorov-Smirnov Gamma GOF Test
5% K-S Critical Value	0.221	Data Not Gamma Distributed at 5% Significance Level

Data Not Gamma Distributed at 5% Significance Level

Gamma Statistics

k hat (MLE)	7673	k star (bias corrected MLE)	6138
Theta hat (MLE)	9.9954E-4	Theta star (bias corrected MLE)	0.00125

nu hat (MLE) 230185	nu star (bias corrected) 184149
MLE Mean (bias corrected) 7.669	MLE Sd (bias corrected) 0.0979

Background Statistics Assuming Gamma Distribution

95% Wilson Hilferty (WH) Approx. Gamma UPL	7.835	90% Percentile	7.795
95% Hawkins Wixley (HW) Approx. Gamma UPL	7.835	95% Percentile	7.831
95% WH Approx. Gamma UTL with 95% Coverage	7.904	99% Percentile	7.899
95% HW Approx. Gamma UTL with 95% Coverage	7.904		
95% WH USL	7.889	95% HW USL	7.89

Lognormal GOF Test

Shapiro Wilk Test Statistic	0.953	Shapiro Wilk Lognormal GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.162	Lilliefors Lognormal GOF Test
5% Lilliefors Critical Value	0.22	Data appear Lognormal at 5% Significance Level

Data appear Lognormal at 5% Significance Level

Background Statistics assuming Lognormal Distribution

95% UTL with 95% Coverage	7.905	90% Percentile (z)	7.786
95% UPL (t)	7.835	95% Percentile (z)	7.819
95% USL	7.89	99% Percentile (z)	7.882

Nonparametric Distribution Free Background Statistics

Data appear Normal at 5% Significance Level

Nonparametric Upper Limits for Background Threshold Values

Order of Statistic, r	15	95% UTL with 95% Coverage	7.85
Approx, f used to compute achieved CC	0.789	Approximate Actual Confidence Coefficient achieved by UTL	0.537
		Approximate Sample Size needed to achieve specified CC	59
95% Percentile Bootstrap UTL with 95% Coverage	7.85	95% BCA Bootstrap UTL with 95% Coverage	7.85
95% UPL	7.85	90% Percentile	7.766
90% Chebyshev UPL	7.951	95% Percentile	7.794
95% Chebyshev UPL	8.078	99% Percentile	7.839
95% USL	7.85		

Note: The use of USL tends to yield a conservative estimate of BTV, especially when the sample size starts exceeding 20. Therefore, one may use USL to estimate a BTV only when the data set represents a background data set free of outliers and consists of observations collected from clean unimpacted locations.

The use of USL tends to provide a balance between false positives and false negatives provided the data represents a background data set and when many onsite observations need to be compared with the BTV.

VAL (specific conductance)

General Statistics

Total Number of Observations	15	Number of Distinct Observations	13
Minimum	245	First Quartile	429
Second Largest	450	Median	438
Maximum	450	Third Quartile	443.5
Mean	425.1	SD	50.56
Coefficient of Variation	0.119	Skewness	-3.679
Mean of logged Data	6.043	SD of logged Data	0.151

Critical Values for Background Threshold Values (BTVs)

Tolerance Factor K (For UTL)	2.566	d2max (for USL)	2.409
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Normal GOF Test

Shapiro Wilk Test Statistic	0.442	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.881	Data Not Normal at 5% Significance Level
Lilliefors Test Statistic	0.409	Lilliefors GOF Test
5% Lilliefors Critical Value	0.22	Data Not Normal at 5% Significance Level

Data Not Normal at 5% Significance Level

Background Statistics Assuming Normal Distribution

95% UTL with 95% Coverage	554.8	90% Percentile (z)	489.9
95% UPL (t)	517	95% Percentile (z)	508.2
95% USL	546.9	99% Percentile (z)	542.7

Gamma GOF Test

A-D Test Statistic	3.668	Anderson-Darling Gamma GOF Test
5% A-D Critical Value	0.734	Data Not Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.43	Kolmogorov-Smirnov Gamma GOF Test
5% K-S Critical Value	0.221	Data Not Gamma Distributed at 5% Significance Level

Data Not Gamma Distributed at 5% Significance Level

Gamma Statistics

k hat (MLE)	55.15	k star (bias corrected MLE)	44.16
Theta hat (MLE)	7.708	Theta star (bias corrected MLE)	9.625
nu hat (MLE)	1654	nu star (bias corrected)	1325
MLE Mean (bias corrected)	425.1	MLE Sd (bias corrected)	63.96

Background Statistics Assuming Gamma Distribution

95% Wilson Hilferty (WH) Approx. Gamma UPL	539.1	90% Percentile	508.8
95% Hawkins Wixley (HW) Approx. Gamma UPL	542.6	95% Percentile	535.5
95% WH Approx. Gamma UTL with 95% Coverage	592.5	99% Percentile	587.8
95% HW Approx. Gamma UTL with 95% Coverage	598.8		
95% WH USL	581	95% HW USL	586.7

Lognormal GOF Test

Shapiro Wilk Test Statistic	0.404	Shapiro Wilk Lognormal GOF Test
5% Shapiro Wilk Critical Value	0.881	Data Not Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.438	Lilliefors Lognormal GOF Test
5% Lilliefors Critical Value	0.22	Data Not Lognormal at 5% Significance Level

Data Not Lognormal at 5% Significance Level**Background Statistics assuming Lognormal Distribution**

95% UTL with 95% Coverage	620.9	90% Percentile (z)	511.3
95% UPL (t)	554.6	95% Percentile (z)	540.2
95% USL	606.3	99% Percentile (z)	598.8

Nonparametric Distribution Free Background Statistics**Data do not follow a Discernible Distribution (0.05)****Nonparametric Upper Limits for Background Threshold Values**

Order of Statistic, r	15	95% UTL with 95% Coverage	450
Approx, f used to compute achieved CC	0.789	Approximate Actual Confidence Coefficient achieved by UTL	0.537
		Approximate Sample Size needed to achieve specified CC	59
95% Percentile Bootstrap UTL with 95% Coverage	450	95% BCA Bootstrap UTL with 95% Coverage	450
95% UPL	450	90% Percentile	448.8
90% Chebyshev UPL	581.7	95% Percentile	450
95% Chebyshev UPL	652.7	99% Percentile	450
95% USL	450		

Note: The use of USL tends to yield a conservative estimate of BTV, especially when the sample size starts exceeding 20.

Therefore, one may use USL to estimate a BTV only when the data set represents a background data set free of outliers and consists of observations collected from clean unimpacted locations.

The use of USL tends to provide a balance between false positives and false negatives provided the data represents a background data set and when many onsite observations need to be compared with the BTV.

VAL (sulfate)**General Statistics**

Total Number of Observations	15	Number of Distinct Observations	13
Minimum	40200	First Quartile	41800
Second Largest	46000	Median	44000
Maximum	47000	Third Quartile	44700
Mean	43363	SD	1991
Coefficient of Variation	0.0459	Skewness	0.109
Mean of logged Data	10.68	SD of logged Data	0.0459

Critical Values for Background Threshold Values (BTVs)

Tolerance Factor K (For UTL)	2.566	d2max (for USL)	2.409
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Normal GOF Test

Shapiro Wilk Test Statistic	0.963	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Normal at 5% Significance Level
Lilliefors Test Statistic	0.159	Lilliefors GOF Test
5% Lilliefors Critical Value	0.22	Data appear Normal at 5% Significance Level

Data appear Normal at 5% Significance Level**Background Statistics Assuming Normal Distribution**

95% UTL with 95% Coverage	48472	90% Percentile (z)	45915
95% UPL (t)	46985	95% Percentile (z)	46638
95% USL	48160	99% Percentile (z)	47995

Gamma GOF Test

A-D Test Statistic	0.312	Anderson-Darling Gamma GOF Test
5% A-D Critical Value	0.734	Detected data appear Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.168	Kolmogorov-Smimov Gamma GOF Test
5% K-S Critical Value	0.221	Detected data appear Gamma Distributed at 5% Significance Level

Detected data appear Gamma Distributed at 5% Significance Level**Gamma Statistics**

k hat (MLE)	508.9	k star (bias corrected MLE)	407.2
Theta hat (MLE)	85.21	Theta star (bias corrected MLE)	106.5
nu hat (MLE)	15268	nu star (bias corrected)	12216
MLE Mean (bias corrected)	43363	MLE Sd (bias corrected)	2149

Background Statistics Assuming Gamma Distribution

95% Wilson Hilferty (WH) Approx. Gamma UPL	47054	90% Percentile	46139
95% Hawkins Wixley (HW) Approx. Gamma UPL	47064	95% Percentile	46958
95% WH Approx. Gamma UTL with Coverage	95% 48641	99% Percentile	48519
95% HW Approx. Gamma UTL with Coverage	95% 48664		
95% WH USL	48305	95% HW USL	48324

Lognormal GOF Test

Shapiro Wilk Test Statistic	0.963	Shapiro Wilk Lognormal GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.166	Lilliefors Lognormal GOF Test
5% Lilliefors Critical Value	0.22	Data appear Lognormal at 5% Significance Level

Data appear Lognormal at 5% Significance Level**Background Statistics assuming Lognormal Distribution**

95% UTL with Coverage	95% 48734	90% Percentile (z)	45944
95% UPL (t)	47092	95% Percentile (z)	46717
95% USL	48384	99% Percentile (z)	48201

Nonparametric Distribution Free Background Statistics**Data appear Normal at 5% Significance Level****Nonparametric Upper Limits for Background Threshold Values**

Order of Statistic, r	15	95% UTL with Coverage	47000
Approx, f used to compute achieved CC	0.789	Approximate Actual Confidence Coefficient achieved by UTL	0.537
		Approximate Sample Size needed to achieve specified CC	59
95% Percentile Bootstrap UTL with Coverage	95% 47000	95% BCA Bootstrap UTL with Coverage	47000
95% UPL	47000	90% Percentile	45600
90% Chebyshev UPL	49532	95% Percentile	46300
95% Chebyshev UPL	52326	99% Percentile	46860
95% USL	47000		

Note: The use of USL tends to yield a conservative estimate of BTV, especially when the sample size starts exceeding 20.

Therefore, one may use USL to estimate a BTV only when the data set represents a background data set free of outliers and consists of observations collected from clean unimpacted locations.

The use of USL tends to provide a balance between false positives and false negatives provided the data represents a background data set and when many onsite observations need to be compared with the BTV.

VAL (temperature)**General Statistics**

Total Number of Observations	15	Number of Distinct Observations	10
Minimum	17.8	First Quartile	18.35
Second Largest	19.2	Median	18.5
Maximum	19.6	Third Quartile	18.7
Mean	18.57	SD	0.448
Coefficient of Variation	0.0241	Skewness	0.802
Mean of logged Data	2.921	SD of logged Data	0.0239

Critical Values for Background Threshold Values (BTVs)

Tolerance Factor K (For UTL)	2.566	d2max (for USL)	2.409
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Normal GOF Test

Shapiro Wilk Test Statistic	0.934	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Normal at 5% Significance Level
Lilliefors Test Statistic	0.189	Lilliefors GOF Test
5% Lilliefors Critical Value	0.22	Data appear Normal at 5% Significance Level

Data appear Normal at 5% Significance Level**Background Statistics Assuming Normal Distribution**

95% UTL with 95% Coverage	19.72	90% Percentile (z)	19.15
95% UPL (t)	19.39	95% Percentile (z)	19.31
95% USL	19.65	99% Percentile (z)	19.62

Gamma GOF Test

A-D Test Statistic	0.52	Anderson-Darling Gamma GOF Test
5% A-D Critical Value	0.734	Detected data appear Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.182	Kolmogorov-Smirnov Gamma GOF Test
5% K-S Critical Value	0.221	Detected data appear Gamma Distributed at 5% Significance Level

Detected data appear Gamma Distributed at 5% Significance Level**Gamma Statistics**

k hat (MLE)	1861	k star (bias corrected MLE)	1489
Theta hat (MLE)	0.00998	Theta star (bias corrected MLE)	0.0125
nu hat (MLE)	55837	nu star (bias corrected)	44671
MLE Mean (bias corrected)	18.57	MLE Sd (bias corrected)	0.481

Background Statistics Assuming Gamma Distribution

95% Wilson Hilferty (WH) Approx. Gamma UPL	19.39	90% Percentile	19.19
95% Hawkins Wixley (HW) Approx. Gamma UPL	19.39	95% Percentile	19.37
95% WH Approx. Gamma UTL with 95% Coverage	19.74	99% Percentile	19.71
95% HW Approx. Gamma UTL with 95% Coverage	19.74		
95% WH USL	19.66	95% HW USL	19.67

Lognormal GOF Test

Shapiro Wilk Test Statistic	0.939	Shapiro Wilk Lognormal GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.184	Lilliefors Lognormal GOF Test
5% Lilliefors Critical Value	0.22	Data appear Lognormal at 5% Significance Level

Data appear Lognormal at 5% Significance Level**Background Statistics assuming Lognormal Distribution**

95% UTL with 95% Coverage	19.74	90% Percentile (z)	19.15
95% UPL (t)	19.39	95% Percentile (z)	19.31
95% USL	19.67	99% Percentile (z)	19.63

Nonparametric Distribution Free Background Statistics**Data appear Normal at 5% Significance Level****Nonparametric Upper Limits for Background Threshold Values**

Order of Statistic, r	15	95% UTL with 95% Coverage	19.6
Approx, f used to compute achieved CC	0.789	Approximate Actual Confidence Coefficient achieved by UTL	0.537
		Approximate Sample Size needed to achieve specified CC	59
95% Percentile Bootstrap UTL with 95% Coverage	19.6	95% BCA Bootstrap UTL with 95% Coverage	19.6
95% UPL	19.6	90% Percentile	19.16
90% Chebyshev UPL	19.96	95% Percentile	19.32
95% Chebyshev UPL	20.59	99% Percentile	19.54
95% USL	19.6		

Note: The use of USL tends to yield a conservative estimate of BTV, especially when the sample size starts exceeding 20.

Therefore, one may use USL to estimate a BTV only when the data set represents a background data set free of outliers and consists of observations collected from clean unimpacted locations.

The use of USL tends to provide a balance between false positives and false negatives provided the data represents a background data set and when many onsite observations need to be compared with the BTV.

VAL (total arsenic)

General Statistics

Total Number of Observations	14	Number of Missing Observations	0
Number of Distinct Observations	10		
Number of Detects	8	Number of Non-Detects	6
Number of Distinct Detects	7	Number of Distinct Non-Detects	3
Minimum Detect	3.7	Minimum Non-Detect	4.4
Maximum Detect	9.9	Maximum Non-Detect	14
Variance Detected	5.958	Percent Non-Detects	42.86%
Mean Detected	5.913	SD Detected	2.441
Mean of Detected Logged Data	1.707	SD of Detected Logged Data	0.392

Critical Values for Background Threshold Values (BTVs)

Tolerance Factor K (For UTL)	d2max (for USL)	2.372
2.614		

Normal GOF Test on Detects Only

Shapiro Wilk Test Statistic	0.813	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.818	Data Not Normal at 5% Significance Level
Lilliefors Test Statistic	0.33	Lilliefors GOF Test
5% Lilliefors Critical Value	0.283	Data Not Normal at 5% Significance Level

Data Not Normal at 5% Significance Level

Kaplan Meier (KM) Background Statistics Assuming Normal Distribution

KM Mean	KM SD	2.017
5.195		
95% UTL95% Coverage	95% KM UPL (t)	8.893
10.47		
90% KM Percentile (z)	95% KM Percentile (z)	8.513
7.78		
99% KM Percentile (z)	95% KM USL	9.979
9.888		

DL/2 Substitution Background Statistics Assuming Normal Distribution

Mean	SD	2.569
4.729		
95% UTL95% Coverage	95% UPL (t)	9.437
11.44		
90% Percentile (z)	95% Percentile (z)	8.954
8.02		
99% Percentile (z)	95% USL	10.82
10.7		

DL/2 is not a recommended method. DL/2 provided for comparisons and historical reasons

Gamma GOF Tests on Detected Observations Only

A-D Test Statistic	Anderson-Darling GOF Test
0.761	

5% A-D Critical Value	0.717	Data Not Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.325	Kolmogorov-Smirnov GOF
5% K-S Critical Value	0.295	Data Not Gamma Distributed at 5% Significance Level

Data Not Gamma Distributed at 5% Significance Level

Gamma Statistics on Detected Data Only

k hat (MLE)	7.313	k star (bias corrected MLE)	4.654
Theta hat (MLE)	0.808	Theta star (bias corrected MLE)	1.27
nu hat (MLE)	117	nu star (bias corrected)	74.47
MLE Mean (bias corrected)	5.913		
MLE Sd (bias corrected)	2.741	95% Percentile of Chisquare (2kstar)	17.35

Gamma ROS Statistics using Imputed Non-Detects

GROS may not be used when data set has > 50% NDs with many tied observations at multiple DLs

GROS may not be used when kstar of detects is small such as <1.0, especially when the sample size is small (e.g., <15-20)

For such situations, GROS method may yield incorrect values of UCLs and BTVs

This is especially true when the sample size is small.

For gamma distributed detected data, BTVs and UCLs may be computed using gamma distribution on KM estimates

Minimum	3.05	Mean	5.152
Maximum	9.9	Median	4.426
SD	2.091	CV	0.406
k hat (MLE)	7.902	k star (bias corrected MLE)	6.256
Theta hat (MLE)	0.652	Theta star (bias corrected MLE)	0.823
nu hat (MLE)	221.3	nu star (bias corrected)	175.2
MLE Mean (bias corrected)	5.152	MLE Sd (bias corrected)	2.06
95% Percentile of Chisquare (2kstar)	21.71	90% Percentile	7.905
95% Percentile	8.94	99% Percentile	11.11

The following statistics are computed using Gamma ROS Statistics on Imputed Data

Upper Limits using Wilson Hilferty (WH) and Hawkins Wixley (HW) Methods

	WH	HW		WH	HW
95% Approx. Gamma UTL with 95% Coverage	11.51	11.68	95% Approx. Gamma UPL	9.151	9.186
95% Gamma USL	10.74	10.86			

Estimates of Gamma Parameters using KM Estimates

Mean (KM)	5.195	SD (KM)	2.017
Variance (KM)	4.069	SE of Mean (KM)	0.603
k hat (KM)	6.633	k star (KM)	5.259
nu hat (KM)	185.7	nu star (KM)	147.3

theta hat (KM)	0.783	theta star (KM)	0.988
80% gamma percentile (KM)	6.944	90% gamma percentile (KM)	8.227
95% gamma percentile (KM)	9.394	99% gamma percentile (KM)	11.85

The following statistics are computed using gamma distribution and KM estimates

Upper Limits using Wilson Hilferty (WH) and Hawkins Wixley (HW) Methods

	WH	HW		WH	HW
95% Approx. Gamma UTL with 95% Coverage	11.06	11.17	95% Approx. Gamma UPL	8.907	8.912
95% KM Gamma Percentile	8.432	8.423	95% Gamma USL	10.36	10.43

Lognormal GOF Test on Detected Observations Only

Shapiro Wilk Test Statistic	0.837	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.818	Detected Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.303	Lilliefors GOF Test
5% Lilliefors Critical Value	0.283	Data Not Lognormal at 5% Significance Level

Detected Data appear Approximate Lognormal at 5% Significance Level

Background Lognormal ROS Statistics Assuming Lognormal Distribution Using Imputed Non-Detects

Mean in Original Scale	5.196	Mean in Log Scale	1.589
SD in Original Scale	2.038	SD in Log Scale	0.339
95% UTL95% Coverage	11.88	95% BCA UTL95% Coverage	9.9
95% Bootstrap (%) UTL95% Coverage	9.9	95% UPL (t)	9.116
90% Percentile (z)	7.563	95% Percentile (z)	8.553
99% Percentile (z)	10.77	95% USL	10.94

Statistics using KM estimates on Logged Data and Assuming Lognormal Distribution

KM Mean of Logged Data	1.587	95% KM UTL (Lognormal)95% Coverage	11.55
KM SD of Logged Data	0.329	95% KM UPL (Lognormal)	8.933
95% KM Percentile Lognormal (z)	8.397	95% KM USL (Lognormal)	10.66

Background DL/2 Statistics Assuming Lognormal Distribution

Mean in Original Scale	4.729	Mean in Log Scale	1.423
SD in Original Scale	2.569	SD in Log Scale	0.524
95% UTL95% Coverage	16.34	95% UPL (t)	10.85
90% Percentile (z)	8.127	95% Percentile (z)	9.832
99% Percentile (z)	14.05	95% USL	14.39

DL/2 is not a Recommended Method. DL/2 provided for comparisons and historical reasons.

Nonparametric Distribution Free Background Statistics**Data appear to follow a Discernible Distribution at 5% Significance Level****Nonparametric Upper Limits for BTVs(no distinction made between detects and nondetects)**

Order of Statistic, r	14	95% UTL with 95% Coverage	14
Approx, f used to compute achieved CC	0.737	Approximate Actual Confidence Coefficient achieved by UTL	0.512
Approximate Sample Size needed to achieve specified CC	59	95% UPL	14
95% USL	14	95% KM Chebyshev UPL	14.3

Note: The use of USL tends to yield a conservative estimate of BTV, especially when the sample size starts exceeding 20.

Therefore, one may use USL to estimate a BTV only when the data set represents a background data set free of outliers and consists of observations collected from clean unimpacted locations.

The use of USL tends to provide a balance between false positives and false negatives provided the data represents a background data set and when many onsite observations need to be compared with the BTV.

VAL (total calcium)**General Statistics**

Total Number of Observations	15	Number of Distinct Observations	15
Minimum	46700	First Quartile	49350
Second Largest	55100	Median	50200
Maximum	55500	Third Quartile	51600
Mean	50687	SD	2362
Coefficient of Variation	0.0466	Skewness	0.765
Mean of logged Data	10.83	SD of logged Data	0.046

Critical Values for Background Threshold Values (BTVs)

Tolerance Factor K (For UTL)	2.566	d2max (for USL)	2.409
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Normal GOF Test

Shapiro Wilk Test Statistic	0.93	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Normal at 5% Significance Level
Lilliefors Test Statistic	0.181	Lilliefors GOF Test
5% Lilliefors Critical Value	0.22	Data appear Normal at 5% Significance Level

Data appear Normal at 5% Significance Level

Background Statistics Assuming Normal Distribution

95% UTL with 95% Coverage	56748	90% Percentile (z)	53714
95% UPL (t)	54984	95% Percentile (z)	54572
95% USL	56377	99% Percentile (z)	56182

Gamma GOF Test

A-D Test Statistic	0.467	Anderson-Darling Gamma GOF Test	
5% A-D Critical Value	0.734	Detected data appear Gamma Distributed at 5% Significance Level	
K-S Test Statistic	0.172	Kolmogorov-Smirnov Gamma GOF Test	
5% K-S Critical Value	0.221	Detected data appear Gamma Distributed at 5% Significance Level	
Detected data appear Gamma Distributed at 5% Significance Level			

Gamma Statistics

k hat (MLE)	502.4	k star (bias corrected MLE)	401.9
Theta hat (MLE)	100.9	Theta star (bias corrected MLE)	126.1
nu hat (MLE)	15071	nu star (bias corrected)	12058
MLE Mean (bias corrected)	50687	MLE Sd (bias corrected)	2528

Background Statistics Assuming Gamma Distribution

95% Wilson Hilferty (WH) Approx. Gamma UPL	55030	90% Percentile	53953
95% Hawkins Wixley (HW) Approx. Gamma UPL	55036	95% Percentile	54916
95% WH Approx. Gamma UTL with 95% Coverage	56897	99% Percentile	56753
95% HW Approx. Gamma UTL with 95% Coverage	56917		
95% WH USL	56501	95% HW USL	56518

Lognormal GOF Test

Shapiro Wilk Test Statistic	0.94	Shapiro Wilk Lognormal GOF Test	
5% Shapiro Wilk Critical Value	0.881	Data appear Lognormal at 5% Significance Level	
Lilliefors Test Statistic	0.171	Lilliefors Lognormal GOF Test	
5% Lilliefors Critical Value	0.22	Data appear Lognormal at 5% Significance Level	
Data appear Lognormal at 5% Significance Level			

Background Statistics assuming Lognormal Distribution

95% UTL with 95% Coverage	56979	90% Percentile (z)	53711
95% UPL (t)	55055	95% Percentile (z)	54616
95% USL	56569	99% Percentile (z)	56355

Nonparametric Distribution Free Background Statistics

Data appear Normal at 5% Significance Level

Nonparametric Upper Limits for Background Threshold Values

Order of Statistic, r	15	95% UTL with 95% Coverage	55500
Approx, f used to compute achieved CC	0.789	Approximate Actual Confidence Coefficient achieved by UTL	0.537
		Approximate Sample Size needed to achieve specified CC	59
95% Percentile Bootstrap UTL with 95% Coverage	55500	95% BCA Bootstrap UTL with 95% Coverage	55500
95% UPL	55500	90% Percentile	54100
90% Chebyshev UPL	58006	95% Percentile	55220
95% Chebyshev UPL	61321	99% Percentile	55444
95% USL	55500		

Note: The use of USL tends to yield a conservative estimate of BTV, especially when the sample size starts exceeding 20.

Therefore, one may use USL to estimate a BTV only when the data set represents a background data set free of outliers and consists of observations collected from clean unimpacted locations.

The use of USL tends to provide a balance between false positives and false negatives provided the data represents a background data set and when many onsite observations need to be compared with the BTV.

VAL (total dissolved solids)**General Statistics**

Total Number of Observations	2	Number of Distinct Observations	2
Minimum	271000	First Quartile	279000
Second Largest	271000	Median	287000
Maximum	303000	Third Quartile	295000
Mean	287000	SD	22627
Coefficient of Variation	0.0788	Skewness	N/A

Warning: This data set only has 2 observations!

Data set is too small to compute reliable and meaningful statistics and estimates!

The data set for variable VAL (total dissolved solids) was not processed!

It is suggested to collect at least 8 to 10 observations before using these statistical methods!

If possible, compute and collect Data Quality Objectives (DQO) based sample size and analytical results.

VAL (total iron)**General Statistics**

Total Number of Observations	15	Number of Missing Observations	0
Number of Distinct Observations	5		

Number of Detects	1	Number of Non-Detects	14
Number of Distinct Detects	1	Number of Distinct Non-Detects	4
Minimum Detect	37	Minimum Non-Detect	22
Maximum Detect	37	Maximum Non-Detect	53
Variance Detected	N/A	Percent Non-Detects	93.33%
Mean Detected	37	SD Detected	N/A
Mean of Detected Logged Data	3.611	SD of Detected Logged Data	N/A

Warning: Only one distinct data value was detected! ProUCL (or any other software) should not be used on such a data set!
It is suggested to use alternative site specific values determined by the Project Team to estimate environmental parameters (e.g., EPC, BTV).

The data set for variable VAL (total iron) was not processed!

VAL (total magnesium)

General Statistics

Total Number of Observations	15	Number of Distinct Observations	11
Minimum	12000	First Quartile	12250
Second Largest	13900	Median	12750
Maximum	14300	Third Quartile	12850
Mean	12743	SD	651.1
Coefficient of Variation	0.0511	Skewness	1.178
Mean of logged Data	9.452	SD of logged Data	0.0499

Critical Values for Background Threshold Values (BTVs)

Tolerance Factor K (For UTL)	d2max (for USL)
2.566	2.409

Normal GOF Test

Shapiro Wilk Test Statistic	0.863
5% Shapiro Wilk Critical Value	0.881
Lilliefors Test Statistic	0.213
5% Lilliefors Critical Value	0.22

Shapiro Wilk GOF Test

Data Not Normal at 5% Significance Level

Lilliefors GOF Test

Data appear Normal at 5% Significance Level

Data appear Approximate Normal at 5% Significance Level

Background Statistics Assuming Normal Distribution

95% UTL with 95% Coverage	14414	90% Percentile (z)	13578
95% UPL (t)	13928	95% Percentile (z)	13814
95% USL	14312	99% Percentile (z)	14258

Gamma GOF Test

A-D Test Statistic	0.75	Anderson-Darling Gamma GOF Test
5% A-D Critical Value	0.734	Data Not Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.201	Kolmogorov-Smirnov Gamma GOF Test
5% K-S Critical Value	0.221	Detected data appear Gamma Distributed at 5% Significance Level
Detected data follow Appr. Gamma Distribution at 5% Significance Level		

Gamma Statistics

k hat (MLE)	423.6	k star (bias corrected MLE)	338.9
Theta hat (MLE)	30.08	Theta star (bias corrected MLE)	37.6
nu hat (MLE)	12708	nu star (bias corrected)	10168
MLE Mean (bias corrected)	12743	MLE Sd (bias corrected)	692.2

Background Statistics Assuming Gamma Distribution

95% Wilson Hilferty (WH) Approx. Gamma UPL	13934	90% Percentile	13638
95% Hawkins Wixley (HW) Approx. Gamma UPL	13935	95% Percentile	13903
95% WH Approx. Gamma UTL with 95% Coverage	14449	99% Percentile	14409
95% HW Approx. Gamma UTL with 95% Coverage	14453		
95% WH USL	14340	95% HW USL	14343

Lognormal GOF Test

Shapiro Wilk Test Statistic	0.876	Shapiro Wilk Lognormal GOF Test
5% Shapiro Wilk Critical Value	0.881	Data Not Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.203	Lilliefors Lognormal GOF Test
5% Lilliefors Critical Value	0.22	Data appear Lognormal at 5% Significance Level
Data appear Approximate Lognormal at 5% Significance Level		

Background Statistics assuming Lognormal Distribution

95% UTL with 95% Coverage	14468	90% Percentile (z)	13569
95% UPL (t)	13938	95% Percentile (z)	13818
95% USL	14355	99% Percentile (z)	14296

Nonparametric Distribution Free Background Statistics

Data appear Approximate Normal at 5% Significance Level

Nonparametric Upper Limits for Background Threshold Values

Order of Statistic, r	15	95% UTL with 95% Coverage	14300
Approx, f used to compute achieved CC	0.789	Approximate Actual Confidence Coefficient achieved by UTL	0.537

Approximate Sample Size needed to achieve specified CC				59
95% Percentile Bootstrap UTL with 95% Coverage	14300	95% BCA Bootstrap UTL with 95% Coverage	14300	
95% UPL	14300	90% Percentile	13540	
90% Chebyshev UPL	14761	95% Percentile	14020	
95% Chebyshev UPL	15674	99% Percentile	14244	
95% USL	14300			

Note: The use of USL tends to yield a conservative estimate of BTV, especially when the sample size starts exceeding 20.

Therefore, one may use USL to estimate a BTV only when the data set represents a background data set free of outliers and consists of observations collected from clean unimpacted locations.

The use of USL tends to provide a balance between false positives and false negatives provided the data represents a background data set and when many onsite observations need to be compared with the BTV.

VAL (total manganese)

General Statistics			
Total Number of Observations	15	Number of Missing Observations	0
Number of Distinct Observations	13		
Number of Detects	6	Number of Non-Detects	9
Number of Distinct Detects	6	Number of Distinct Non-Detects	7
Minimum Detect	0.31	Minimum Non-Detect	0.26
Maximum Detect	2.97	Maximum Non-Detect	4
Variance Detected	1.066	Percent Non-Detects	60%
Mean Detected	1.02	SD Detected	1.032
Mean of Detected Logged Data	-0.325	SD of Detected Logged Data	0.856

Critical Values for Background Threshold Values (BTVs)

Tolerance Factor K (For UTL)	d2max (for USL)	2.409
2.566		

Normal GOF Test on Detects Only

Shapiro Wilk Test Statistic	0.736	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.788	Data Not Normal at 5% Significance Level
Lilliefors Test Statistic	0.356	Lilliefors GOF Test
5% Lilliefors Critical Value	0.325	Data Not Normal at 5% Significance Level

Data Not Normal at 5% Significance Level

Kaplan Meier (KM) Background Statistics Assuming Normal Distribution

KM Mean	0.731	KM SD	0.733
95% UTL95% Coverage	2.613	95% KM UPL (t)	2.065

90% KM Percentile (z)	1.671	95% KM Percentile (z)	1.938
99% KM Percentile (z)	2.437	95% KM USL	2.498

DL/2 Substitution Background Statistics Assuming Normal Distribution

Mean	1.035	SD	0.782
95% UTL95% Coverage	3.042	95% UPL (t)	2.458
90% Percentile (z)	2.037	95% Percentile (z)	2.322
99% Percentile (z)	2.855	95% USL	2.92

DL/2 is not a recommended method. DL/2 provided for comparisons and historical reasons

Gamma GOF Tests on Detected Observations Only

A-D Test Statistic	0.644	Anderson-Darling GOF Test	
5% A-D Critical Value	0.707	Detected data appear Gamma Distributed at 5% Significance Level	
K-S Test Statistic	0.36	Kolmogorov-Smirnov GOF	
5% K-S Critical Value	0.337	Data Not Gamma Distributed at 5% Significance Level	

Detected data follow Appr. Gamma Distribution at 5% Significance Level

Gamma Statistics on Detected Data Only

k hat (MLE)	1.595	k star (bias corrected MLE)	0.909
Theta hat (MLE)	0.64	Theta star (bias corrected MLE)	1.123
nu hat (MLE)	19.14	nu star (bias corrected)	10.9
MLE Mean (bias corrected)	1.02		
MLE Sd (bias corrected)	1.07	95% Percentile of Chisquare (2kstar)	5.632

Gamma ROS Statistics using Imputed Non-Detects

GROS may not be used when data set has > 50% NDs with many tied observations at multiple DLs

GROS may not be used when kstar of detects is small such as <1.0, especially when the sample size is small (e.g., <15-20)

For such situations, GROS method may yield incorrect values of UCLs and BTVs

This is especially true when the sample size is small.

For gamma distributed detected data, BTVs and UCLs may be computed using gamma distribution on KM estimates

Minimum	0.01	Mean	0.626
Maximum	2.97	Median	0.384
SD	0.732	CV	1.17
k hat (MLE)	1.037	k star (bias corrected MLE)	0.874
Theta hat (MLE)	0.603	Theta star (bias corrected MLE)	0.715
nu hat (MLE)	31.12	nu star (bias corrected)	26.23
MLE Mean (bias corrected)	0.626	MLE Sd (bias corrected)	0.669
95% Percentile of Chisquare (2kstar)	5.495	90% Percentile	1.489

95% Percentile	99% Percentile	3.084
1.966		

The following statistics are computed using Gamma ROS Statistics on Imputed Data

Upper Limits using Wilson Hilferty (WH) and Hawkins Wixley (HW) Methods

	WH	HW		WH	HW
95% Approx. Gamma UTL with 95% Coverage	3.261	3.712	95% Approx. Gamma UPL	2.068	2.209
95% Gamma USL	2.98	3.346			

Estimates of Gamma Parameters using KM Estimates

Mean (KM)	SD (KM)	0.733
0.731		
Variance (KM)	SE of Mean (KM)	0.24
0.538		
k hat (KM)	k star (KM)	0.839
0.994		
nu hat (KM)	nu star (KM)	25.18
29.81		
theta hat (KM)	theta star (KM)	0.871
0.736		
80% gamma percentile (KM)	90% gamma percentile (KM)	1.757
1.192		
95% gamma percentile (KM)	99% gamma percentile (KM)	3.682
2.331		

The following statistics are computed using gamma distribution and KM estimates

Upper Limits using Wilson Hilferty (WH) and Hawkins Wixley (HW) Methods

	WH	HW		WH	HW
95% Approx. Gamma UTL with 95% Coverage	2.812	2.878	95% Approx. Gamma UPL	1.927	1.918
95% KM Gamma Percentile	1.752	1.734	95% Gamma USL	2.608	2.652

Lognormal GOF Test on Detected Observations Only

Shapiro Wilk Test Statistic	0.862	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.788	Detected Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.324	Lilliefors GOF Test
5% Lilliefors Critical Value	0.325	Detected Data appear Lognormal at 5% Significance Level

Detected Data appear Lognormal at 5% Significance Level

Background Lognormal ROS Statistics Assuming Lognormal Distribution Using Imputed Non-Detects

Mean in Original Scale	Mean in Log Scale	-0.713
0.659		
SD in Original Scale	SD in Log Scale	0.721
0.701		
95% UTL95% Coverage	95% BCA UTL95% Coverage	2.97
3.121		
95% Bootstrap (%) UTL95% Coverage	95% UPL (t)	1.821
2.97		
90% Percentile (z)	95% Percentile (z)	1.606
1.236		
99% Percentile (z)	95% USL	2.787
2.626		

Statistics using KM estimates on Logged Data and Assuming Lognormal Distribution

KM Mean of Logged Data	-0.619	95% KM UTL (Lognormal)	95% Coverage	3.211
KM SD of Logged Data	0.696	95% KM UPL (Lognormal)		1.909
95% KM Percentile Lognormal (z)	1.691	95% KM USL (Lognormal)		2.879

Background DL/2 Statistics Assuming Lognormal Distribution

Mean in Original Scale	1.035	Mean in Log Scale	-0.25
SD in Original Scale	0.782	SD in Log Scale	0.828
95% UTL	6.509	95% UPL (t)	3.508
90% Percentile (z)	2.248	95% Percentile (z)	3.037
99% Percentile (z)	5.338	95% USL	5.716

DL/2 is not a Recommended Method. DL/2 provided for comparisons and historical reasons.

Nonparametric Distribution Free Background Statistics

Data appear to follow a Discernible Distribution at 5% Significance Level

Nonparametric Upper Limits for BTVs (no distinction made between detects and nondetects)

Order of Statistic, r	15	95% UTL with 95% Coverage	4
Approx, f used to compute achieved CC	0.789	Approximate Actual Confidence Coefficient achieved by UTL	0.537
Approximate Sample Size needed to achieve specified CC	59	95% UPL	4
95% USL	4	95% KM Chebyshev UPL	4.033

Note: The use of USL tends to yield a conservative estimate of BTV, especially when the sample size starts exceeding 20.

Therefore, one may use USL to estimate a BTV only when the data set represents a background data set free of outliers and consists of observations collected from clean unimpacted locations.

The use of USL tends to provide a balance between false positives and false negatives provided the data represents a background data set and when many onsite observations need to be compared with the BTV.

VAL (total organic carbon)**General Statistics**

Total Number of Observations	2	Number of Missing Observations	0
Number of Distinct Observations	1		
Number of Detects	0	Number of Non-Detects	2
Number of Distinct Detects	0	Number of Distinct Non-Detects	1
Minimum Detect	N/A	Minimum Non-Detect	330
Maximum Detect	N/A	Maximum Non-Detect	330
Variance Detected	N/A	Percent Non-Detects	100%
Mean Detected	N/A	SD Detected	N/A

Mean of Detected Logged Data N/A

SD of Detected Logged Data N/A

Warning: This data set only has 2 observations!**Data set is too small to compute reliable and meaningful statistics and estimates!****The data set for variable VAL (total organic carbon) was not processed!****It is suggested to collect at least 8 to 10 observations before using these statistical methods!****If possible, compute and collect Data Quality Objectives (DQO) based sample size and analytical results.****VAL (total potassium)****General Statistics**

Total Number of Observations	15	Number of Distinct Observations	14
Minimum	6030	First Quartile	6470
Second Largest	7400	Median	6630
Maximum	7900	Third Quartile	7005
Mean	6765	SD	498.3
Coefficient of Variation	0.0737	Skewness	0.659
Mean of logged Data	8.817	SD of logged Data	0.0725

Critical Values for Background Threshold Values (BTVs)

Tolerance Factor K (For UTL)	d2max (for USL)
2.566	2.409

Normal GOF Test

Shapiro Wilk Test Statistic	0.95	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Normal at 5% Significance Level
Lilliefors Test Statistic	0.159	Lilliefors GOF Test
5% Lilliefors Critical Value	0.22	Data appear Normal at 5% Significance Level

Data appear Normal at 5% Significance Level**Background Statistics Assuming Normal Distribution**

95% UTL with 95% Coverage	8044	90% Percentile (z)	7404
95% UPL (t)	7671	95% Percentile (z)	7585
95% USL	7965	99% Percentile (z)	7924

Gamma GOF Test

A-D Test Statistic	0.324	Anderson-Darling Gamma GOF Test
5% A-D Critical Value	0.734	Detected data appear Gamma Distributed at 5% Significance Level

K-S Test Statistic	0.161	Kolmogorov-Smirnov Gamma GOF Test
5% K-S Critical Value	0.221	Detected data appear Gamma Distributed at 5% Significance Level
Detected data appear Gamma Distributed at 5% Significance Level		

Gamma Statistics

k hat (MLE)	201.9	k star (bias corrected MLE)	161.6
Theta hat (MLE)	33.51	Theta star (bias corrected MLE)	41.87
nu hat (MLE)	6057	nu star (bias corrected)	4847
MLE Mean (bias corrected)	6765	MLE Sd (bias corrected)	532.2

Background Statistics Assuming Gamma Distribution

95% Wilson Hilferty (WH) Approx. Gamma UPL	7689	90% Percentile	7455
95% Hawkins Wixley (HW) Approx. Gamma UPL	7692	95% Percentile	7664
95% WH Approx. Gamma UTL with 95% Coverage	8097	99% Percentile	8064
95% HW Approx. Gamma UTL with 95% Coverage	8105		
95% WH USL	8011	95% HW USL	8017

Lognormal GOF Test

Shapiro Wilk Test Statistic	0.959	Shapiro Wilk Lognormal GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.153	Lilliefors Lognormal GOF Test
5% Lilliefors Critical Value	0.22	Data appear Lognormal at 5% Significance Level

Data appear Lognormal at 5% Significance Level**Background Statistics assuming Lognormal Distribution**

95% UTL with 95% Coverage	8129	90% Percentile (z)	7406
95% UPL (t)	7700	95% Percentile (z)	7603
95% USL	8037	99% Percentile (z)	7989

Nonparametric Distribution Free Background Statistics**Data appear Normal at 5% Significance Level****Nonparametric Upper Limits for Background Threshold Values**

Order of Statistic, r	15	95% UTL with 95% Coverage	7900
Approx, f used to compute achieved CC	0.789	Approximate Actual Confidence Coefficient achieved by UTL	0.537
		Approximate Sample Size needed to achieve specified CC	59
95% Percentile Bootstrap UTL with 95% Coverage	7900	95% BCA Bootstrap UTL with 95% Coverage	7900
95% UPL	7900	90% Percentile	7308
90% Chebyshev UPL	8309	95% Percentile	7550

95% Chebyshev UPL 9008

99% Percentile 7830

95% USL 7900

Note: The use of USL tends to yield a conservative estimate of BTV, especially when the sample size starts exceeding 20.

Therefore, one may use USL to estimate a BTV only when the data set represents a background data set free of outliers and consists of observations collected from clean unimpacted locations.

The use of USL tends to provide a balance between false positives and false negatives provided the data represents a background data set and when many onsite observations need to be compared with the BTV.

VAL (total sodium)**General Statistics**

Total Number of Observations	15	Number of Distinct Observations	12
Minimum	18400	First Quartile	20150
Second Largest	22200	Median	21000
Maximum	23800	Third Quartile	21600
Mean	20860	SD	1350
Coefficient of Variation		Skewness	0.0614
	0.0647	SD of logged Data	0.065
Mean of logged Data	9.944		

Critical Values for Background Threshold Values (BTVs)

Tolerance Factor K (For UTL)	d2max (for USL)	2.409
2.566		

Normal GOF Test

Shapiro Wilk Test Statistic	0.954	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Normal at 5% Significance Level
Lilliefors Test Statistic	0.153	Lilliefors GOF Test
5% Lilliefors Critical Value	0.22	Data appear Normal at 5% Significance Level

Data appear Normal at 5% Significance Level

Background Statistics Assuming Normal Distribution

95% UTL with 95% Coverage	24324	90% Percentile (z)	22590
95% UPL (t)	23316	95% Percentile (z)	23081
95% USL	24112	99% Percentile (z)	24001

Gamma GOF Test

A-D Test Statistic	0.371	Anderson-Darling Gamma GOF Test
5% A-D Critical Value	0.734	Detected data appear Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.152	Kolmogorov-Smirnov Gamma GOF Test

5% K-S Critical Value 0.221 Detected data appear Gamma Distributed at 5% Significance Level

Detected data appear Gamma Distributed at 5% Significance Level

Gamma Statistics

k hat (MLE)	254.9	k star (bias corrected MLE)	204
Theta hat (MLE)	81.83	Theta star (bias corrected MLE)	102.3
nu hat (MLE)	7648	nu star (bias corrected)	6120
MLE Mean (bias corrected)	20860	MLE Sd (bias corrected)	1461

Background Statistics Assuming Gamma Distribution

95% Wilson Hilferty (WH) Approx. Gamma UPL	23389	90% Percentile	22752
95% Hawkins Wixley (HW) Approx. Gamma UPL	23399	95% Percentile	23319
95% WH Approx. Gamma UTL with 95% Coverage	24496	99% Percentile	24407
95% HW Approx. Gamma UTL with 95% Coverage	24520		
95% WH USL	24260	95% HW USL	24281

Lognormal GOF Test

Shapiro Wilk Test Statistic	0.952	Shapiro Wilk Lognormal GOF Test
5% Shapiro Wilk Critical Value	0.881	Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.161	Lilliefors Lognormal GOF Test
5% Lilliefors Critical Value	0.22	Data appear Lognormal at 5% Significance Level

Data appear Lognormal at 5% Significance Level

Background Statistics assuming Lognormal Distribution

95% UTL with 95% Coverage	24595	90% Percentile (z)	22626
95% UPL (t)	23430	95% Percentile (z)	23167
95% USL	24345	99% Percentile (z)	24215

Nonparametric Distribution Free Background Statistics

Data appear Normal at 5% Significance Level

Nonparametric Upper Limits for Background Threshold Values

Order of Statistic, r	15	95% UTL with 95% Coverage	23800
Approx, f used to compute achieved CC	0.789	Approximate Actual Confidence Coefficient achieved by UTL	0.537
		Approximate Sample Size needed to achieve specified CC	59
95% Percentile Bootstrap UTL with 95% Coverage	23800	95% BCA Bootstrap UTL with 95% Coverage	23800
95% UPL	23800	90% Percentile	22040
90% Chebyshev UPL	25043	95% Percentile	22680
95% Chebyshev UPL	26938	99% Percentile	23576

95% USL 23800

Note: The use of USL tends to yield a conservative estimate of BTV, especially when the sample size starts exceeding 20. Therefore, one may use USL to estimate a BTV only when the data set represents a background data set free of outliers and consists of observations collected from clean unimpacted locations.

The use of USL tends to provide a balance between false positives and false negatives provided the data represents a background data set and when many onsite observations need to be compared with the BTV.

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Appendix D

Software Installation and Checkout Form

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SOFTWARE INSTALLATION AND CHECKOUT FORM	
Software Owner Instructions: Complete Fields 1-13, then run test cases in Field 14. Compare test case results listed in Field 15 to corresponding Test Report outputs. If results are the same, sign and date Field 19. If not, resolve differences and repeat above steps.	
Software Subject Matter Expert Instructions: Assign test personnel. Approve the installation of the code by signing and dating Field 21, then maintain form as part of the software support documentation.	
GENERAL INFORMATION	
1. Software Name: ProUCL	Version No.: 5.1
EXECUTABLE INFORMATION	
2. Executable Name (include path): Following executable files in directory: [DIRECTORY]	
3. Executable Size (bytes): MD5 signatures above uniquely identify each executable file	
COMPILATION INFORMATION	
4. Hardware System (i.e., property number or ID): Acquired software; compile by vendor (EPA)	
5. Operating System (include version number): Acquired software; compile by vendor (EPA)	
INSTALLATION AND CHECKOUT INFORMATION	
6. Hardware System (i.e., property number or ID): 00905	
7. Operating System (include version number): Windows 10 Pro V.10.0.19043	
8. Open Problem Report? ☐ Yes ☒ No PR/CR No.: _____	
TEST CASE INFORMATION	
9. Directory/Path: RiskModeling\software-management	
10. Procedures: CHPRC-01270, ProUCL Software Management Plan	
11. Libraries: N/A	
12. Input Files: ProUCL InstallationTestCase.xls	
13. Output Files: to screen	
14. Test Cases: ITC-ProUCL-1, Installation Test Problem	
15. Test Case Results: Pass	
16. Test Performed By: Corey Brumbaugh	
17. Test Results: ☒ Satisfactory, Accepted for Use ☐ Unsatisfactory	
18. Disposition (include HISI update):	

SOFTWARE INSTALLATION AND CHECKOUT FORM (Continued)	
19. Prepared By (Software Owner): <i>Print First and Last Name</i>	CHRISTOPHER FARROW (Affiliate) Digitally signed by CHRISTOPHER FARROW (Affiliate) DN: cn=US, o=U.S. Government, ou=Department of Energy, c=US, email=christopher.farrow@nrc.gov, o=U.S. Government, ou=Department of Energy, cn=CHRISTOPHER FARROW (Affiliate) Reason: I have reviewed this document Location: your signing location here Date: 2022.03.03 11:05:27-0800 Foxit Reader Version: 10.1.6 <i>Signature / Date</i>
20. Test Personnel: Title: Ecological Risk Assessor <i>Print First and Last Name</i>	Corey Brumbaugh Digitally signed by Corey Brumbaugh DN: cn=US, ou=Ecological Risk Assessment, o=INTERA Incorporated, cn=Corey Brumbaugh, email=brumbaugh@intera.com, c=US, ou=Ecological Risk Assessment, o=INTERA Incorporated, cn=Corey Brumbaugh Reason: I am the author of this document Location: West Richland, WA Date: 2022.03.03 08:22:34-0800 Foxit Reader Version: 10.1.6 <i>Signature / Date</i>
Title: <i>Print First and Last Name</i>	<i>Signature / Date</i>
Title: <i>Print First and Last Name</i>	<i>Signature / Date</i>
21. Approved By (Software SME): <i>Print First and Last Name</i>	<i>Signature / Date</i>