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Revision 0

CALCULATION OF UPPER CONFIDENCE LIMITS FOR RCRA MONITORING AT THE 183-H SOLAR EVAPORATION BASINS TO SUPPORT THE JANUARY - JUNE 2020 SEMIANNUAL REPORT

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

Contractor for the U.S. Department of Energy
under Contract DE-AC06-08RL14788

CH2MHILL
Plateau Remediation Company

P.O. Box 1600
Richland, Washington 99352

Approved for Public Release;
Further Dissemination Unlimited

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By Lynn M. Ayers at 11:18 am, Sep 23, 2020

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ENVIRONMENTAL CALCULATION COVER PAGE

SECTION 1 - Completed by the Responsible Manager

Project: Soil and Groundwater Remediation Project

Date: 09/16/2020

Calculation Title and Description:
Calculation of Upper Confidence Limits for RCRA Monitoring at the 183-H Solar Evaporation Basins to Support the January - June 2020 Semiannual Report

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ENVIRONMENTAL CALCULATION COVER PAGE (Continued)

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SECTION 2 - Completed by Preparer

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ENVIRONMENTAL CALCULATION COVER PAGE (Continued)

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Terms

CERCLA	*Comprehensive Environmental Response, Compensation, and Liability Act*
CHPRC	CH2M HILL Plateau Remediation Company
ECF	environmental calculation file
GC/MS	gas chromatograph/mass spectrometer
HEIS	Hanford Environmental Information System
OU	operable unit
QC	quality control
RCRA	*Resource Conservation and Recovery Act of 1976*
RDL	required detection limit
UCL	upper confidence limit

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1 Purpose

This environmental calculation file (ECF) presents calculations of 95% upper confidence limits (UCLs) on the mean for filtered total chromium and nitrate (as NO_3) at the 183-H Solar Evaporation Basins *Resource Conservation and Recovery Act of 1976* (RCRA) site. The 95% UCLs are compared to the applicable concentration limits in WA7890008967, *Hanford Facility Resource Conservation and Recovery Act (RCRA) Permit, Dangerous Waste Portion for the Treatment, Storage, and Disposal of Dangerous Waste* (hereinafter referred to as the Hanford RCRA Permit). Calculations presented in this ECF were based on available results for groundwater samples collected through the end of June 2020.

2 Background

The 183-H Solar Evaporation Basins are located within the 100-H Area, overlying the 100-HR-3 Groundwater Operable Unit (OU) (Figure 1) and were used to evaporate various liquid waste streams from 300 Area fuel fabrication facilities. The final status groundwater monitoring plan was incorporated into the Hanford RCRA Permit, Revision 8c, on May 24, 2017. The new plan supersedes PNNL-11573, *Groundwater Monitoring Plan for the 183-H Solar Evaporation Basins*. The new corrective action monitoring plan requires calculation of the 95% UCLs on the mean for filtered total chromium and nitrate (as NO_3) based on the last 8 to 10 independent samples, and comparison of the 95% UCLs, or non-detect data, to the concentration limits established in the Hanford RCRA Permit. For this analysis, when available, data were limited to the last eight RCRA sampling events only.

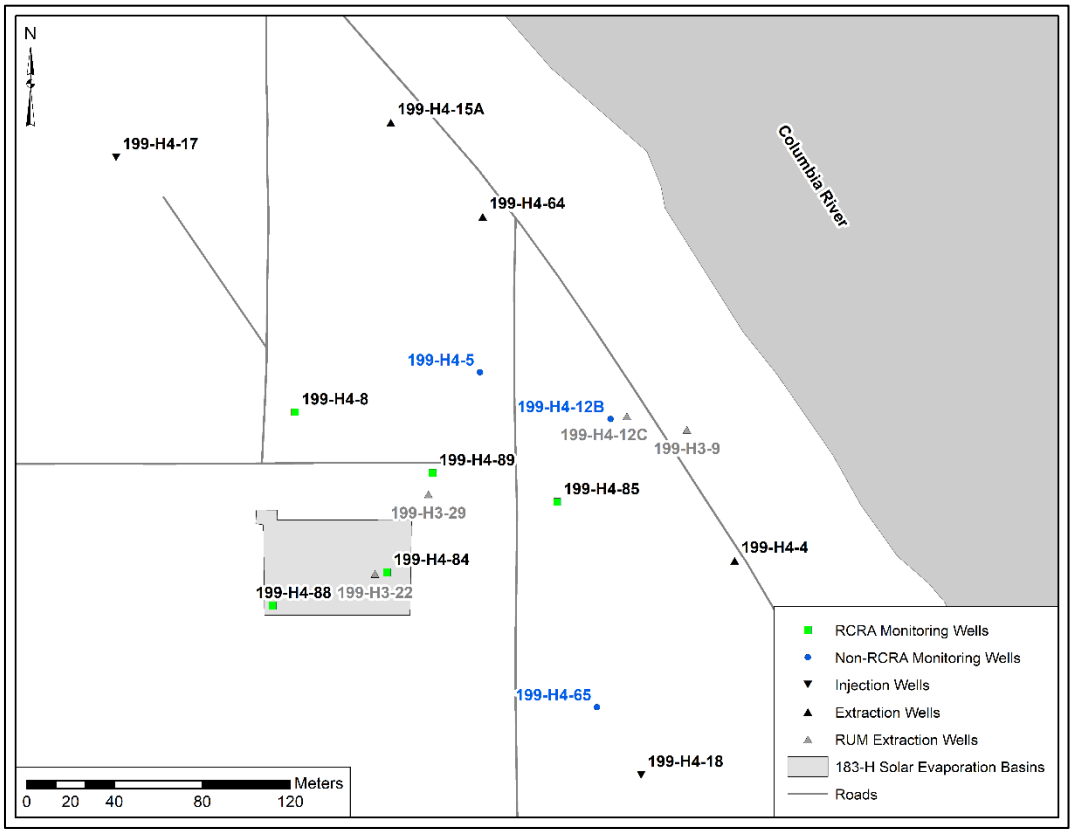

Figure 1. 183-H Solar Evaporation Basins and Associated Monitoring Wells

When all data are non-detects, all data are less than the concentration limits, or there are less than the required number of samples, calculation of the 95% UCL on the mean is not required and the data are evaluated visually to ensure compliance.

3 Methodology

This section discusses the data and methods used to complete the calculations presented in this document. Section 3.1 discusses the data acquisition and processing and Section 3.2 discusses the 95% UCL calculations on the mean.

3.1 Data Acquisition and Processing

This section discusses the acquisition and processing of data prior to the 95% UCL calculations.

3.1.1 Chemistry Data Acquisition

Groundwater chemistry data were downloaded from the Hanford Environmental Information System (HEIS) database, which is maintained by CH2M HILL Plateau Remediation Company (CHPRC), and exported into a Microsoft Access® database (named HEIS_CHEM_08102020.accdb). The data for this analysis were downloaded from the HEIS database on August 10, 2020. The HEIS database contains a table (HEIS_ADM_PNLGW_STD_RESULT_MV), which comprises information on groundwater samples, including laboratory and review data qualifiers, sample medium, sample collection purpose, analytical method, and reporting limits. The fields extracted from the HEIS database for use in calculations described in this document are presented in Table 1.

Table 1. HEIS Database Fields for Chemistry 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
MEDIA	Sample Medium

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Table 1. HEIS Database Fields for Chemistry Data

Field Extracted*	Definition
METHOD_NAME	Analytical Method
REPORTING_LIMIT	Reporting Limit

*Field codes are defined in HNF-38155, *HEIS Sample, Result, and Sampling Site Data Dictionary*.
HEIS = Hanford Environmental Information System

3.1.2 Daily Averaging

A daily average was calculated for chemistry data with multiple measurements on the same day. When all measurements on the same day were non-detect, the highest detection limit was used for the daily value. For daily duplicates where only one of the samples was non-detect, the detected value was used for the daily value. Duplicate daily measurements and the calculated daily average within the last 8 samples dataset are presented in Table 2.

Table 2. Duplicate Daily Measurements and Calculated Daily Averages

Well Name	Constituent	Sample Date	Measured Concentration	Calculated Daily Average
199-H4-88	Filtered Total Chromium	5/1/2019	10.1 µg/L 10.2 µg/L	10.15 µg/L
199-H4-88	Nitrate (as NO_3)	5/1/2019	47.8 mg/L 47.8 mg/L	47.8 mg/L

µg/L = micrograms per liter
mg/L = milligrams per liter

3.1.3 Data Qualifiers

Non-detects in the chemistry data set were identified using the laboratory qualifier (LAB_QUALIFIER = U or any other qualifier that includes “U”). The method detection limit was substituted for concentration measurements when identified as a non-detect based on the laboratory qualifier. All estimated data (LAB_QUALIFIER = B or J) were treated as detected values. Data with laboratory qualifiers C (the analyte was detected in both the sample and the associated quality control (QC) blank, and the sample concentration was ≥ 5X the blank), D (analyte was reported at a secondary dilution factor (DF), typically DF > 1), N (all (except gas chromatograph/mass spectrometer (GC/MS) based analysis) - spike and/or spike duplicated sample recovery is outside control limits) and X (recommended holding time exceeded) were included in this analysis.

3.1.4 Wells and Constituents

The list of wells and constituents for this analysis was based on the groundwater monitoring plan incorporated on May 24, 2017, into the Hanford RCRA Permit (WA7890008967), as listed in Table 3.

Table 3. Wells and Constituents

Well Name	Constituent
199-H4-8	Filtered Total Chromium, Nitrate (as NO_3)
199-H4-84	Filtered Total Chromium, Nitrate (as NO_3)
199-H4-85	Filtered Total Chromium, Nitrate (as NO_3)
199-H4-88	Filtered Total Chromium, Nitrate (as NO_3)
199-H4-89	Filtered Total Chromium, Nitrate (as NO_3)

3.1.5 Time Period of Analysis

Due to the limited number of available RCRA sampling events, previous ECF calculations of the 95% UCLs on the mean for filtered total chromium and nitrate (as NO_3) at the 183-H Solar Evaporation Basins contained the last ten samples, regardless of sampling program (ECF-HANFORD-19-0092, *Calculation of Upper Confidence Limits for RCRA Monitoring at the 183-H Solar Evaporation Basins to Support the January – June 2019 Semi-Annual Report*). Due to the increase in the number of available RCRA sampling events, datasets for the current analysis were limited to RCRA sampling events only, when available (Table 4). Data for monitoring wells 199-H4-8, 199-H4-84, 199-H4-88 and 199-H4-89 were limited to samples collected under the RCRA sampling program. Data for monitoring well 199-H4-85 included samples collected under the RCRA sampling program and the *Comprehensive Environmental Response, Compensation, and Liability Act* (CERCLA) sampling program. The last eight independent samples (i.e., eight samples collected on different dates) scheduled to be collected through the end of June 2020 were included in the datasets if available.

Table 4. Sampling Data

Well Name	Analyte	Sampling Date Range	Number of Samples
199-H4-8	Filtered Total Chromium	11/15/2016 – 06/16/2020[a]	8
199-H4-84	Filtered Total Chromium	02/08/2017 – 06/17/2020 [a]	8
199-H4-85	Filtered Total Chromium	02/10/2016 – 06/17/2020	8[b]
199-H4-88	Filtered Total Chromium	08/16/2018 – 06/17/2020	8
199-H4-89	Filtered Total Chromium	02/12/2018 – 06/17/2020[c]	8
199-H4-8	Nitrate (as NO_3)	11/15/2016 –06/16/2020[a]	8
199-H4-84	Nitrate (as NO_3)	02/08/2017– 06/17/2020 [a]	8
199-H4-85	Nitrate (as NO_3)	05/17/2018 – 06/17/2020	8[b]
199-H4-88	Nitrate (as NO_3)	08/16/2018 – 06/17/2020	8

Table 4. Sampling Data

Well Name	Analyte	Sampling Date Range	Number of Samples
199-H4-89	Nitrate (as NO_3)	02/12/2018 – 06/17/2020[c]	8

a. RCRA sampling scheduled for the fourth quarter of 2019 was unsuccessful due to dry wells associated with low river stage.

b. Dataset contains both RCRA and CERCLA samples.

c. No RCRA sample was collected during the 12/30/2019 sampling event due to limited water availability in the well.

CERCLA = *Comprehensive Environmental Response, Compensation, and Liability Act.*

RCRA = *Resource Conservation and Recovery Act of 1976.*

3.1.6 Outliers

The data sets were evaluated for outliers through visual inspection of timeseries plots. No outliers were identified in the datasets used in this analysis.

3.2 Calculated 95% UCLs on the Mean

A statistical software package, ProUCL version 5.1, was used to calculate the 95% UCL on the mean, in accordance with the new corrective action groundwater monitoring plan. ProUCL is available through the U.S. Environmental Protection Agency and provides statistical methods and graphical tools that are commonly used in environmental assessments. ProUCL is capable of working with datasets where non-detects are present. There are several methods available in ProUCL for calculating 95% UCLs on the mean. These methods account for the underlying distribution of the data and the presence of non-detects. For datasets with non-detects, ProUCL uses the Kaplan-Meier method, a non-parametric method for calculating the mean and standard deviation. ProUCL highlights a recommended UCL calculation method 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 95% UCL calculations were performed on datasets with a minimum of eight samples available and with at least one sample above the concentration limit. As shown in Table 5 below, only four datasets met these criteria. Calculation of 95% UCLs for the other datasets was not required.

Table 5. Dataset Summary and Criteria to Calculate 95% UCL

Analyte	Concentration Limit	Well Name	Number of Samples	Percent Non-Detect	Number of Samples Exceeding Concentration Limit	95% UCL Calculation Required
Filtered total chromium	48 µg/L	199-H4-8	8	0%	0	No
		199-H4-84	8	0%	2	**Yes**
		199-H4-85	8	13%	0	No

Table 5. Dataset Summary and Criteria to Calculate 95% UCL

Analyte	Concentration Limit	Well Name	Number of Samples	Percent Non-Detect	Number of Samples Exceeding Concentration Limit	95% UCL Calculation Required
		199-H4-88	8	0%	0	No
		199-H4-89	8	13%	0	No
Nitrate (as NO_3)	45 mg/L	199-H4-8	8	0%	0	No
		199-H4-84	8	0%	5	**Yes**
		199-H4-85	8	0%	0	No
		199-H4-88	8	0%	8	**Yes**
		199-H4-89	8	0%	2	**Yes**

UCL = upper confidence limit

4 Assumptions

Given the number of samples required by the permit, UCL calculations assume that:

- Concentrations observed at a well are not significantly affected by active remediation activities at the site for the period over which calculations are made.
- There are no concentration trends with time for the datasets used to calculate 95% UCLs. ProUCL does not explicitly test for concentration trends when calculating 95% UCLs. In the presence of a concentration trend, ProUCL will calculate a wider confidence interval on the mean.
- In addition, all of the data for a well/analyte pair are from the same statistical distribution. ProUCL tests the data distribution prior to calculating 95% UCLs and ProUCL highlights a recommended 95% UCL method based on the data distribution.

5 Software Applications

95% UCL calculations were performed using ProUCL version 5.1.

6 Calculation

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

- *qryChemHeis1.txt* and *qryChemHeis2.txt*: Concentration data from the HEIS database
- *ProUCL_Datasets_08102020.xlsx*: datasets for use in ProUCL

Datasets were imported into the ProUCL software and 95% UCLs were calculated using all available methods and accounting for the presence of non-detects. The reported 95% UCL was selected based on the ProUCL results, including evaluation of the data distribution and sample size.

7 Results

The datasets evaluated for 95% UCL calculation and the output files from ProUCL are presented in Appendix A, and the 95% UCL results are presented in Table 6. Results for nitrate (as NO_3) were converted to milligrams per liter (mg/L) prior to processing with ProUCL. Timeseries plots for all wells and constituents are presented in Appendix B.

Table 6. Calculated 95% UCLs

Well Name	Analyte	Concentration Limit	95% UCL	95% UCL Result Evaluation
199-H4-84	Chromium	48 µg/L	185.7[a] µg/L	Above Concentration Limit
199-H4-84	Nitrate (as NO_3)	45 mg/L	92.78[b] mg/L	Above Concentration Limit
199-H4-88	Nitrate (as NO_3)	45 mg/L	73.65[b] mg/L	Above Concentration Limit
199-H4-89	Nitrate (as NO_3)	45 mg/L	41.59[b] mg/L	Below Concentration Limit

a. ProUCL method: 95% Adjusted Gamma UCL

b. ProUCL method: 95% Student's-t UCL

UCL = upper confidence limit

8 References

Comprehensive Environmental Response, Compensation, and Liability Act of 1980, 42 USC 9601, et seq., Pub. L. 107-377, December 31, 2002. Available at: https://www.csu.edu/cerc/researchreports/documents/CERCLASummary1980.pdf.

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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.

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Resource Conservation and Recovery Act of 1976, 42 USC 6901, et seq. Available at: https://elr.info/sites/default/files/docs/statutes/full/rcra.pdf.

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Appendix A

Upper Confidence Limit (UCL) Datasets and ProUCL Output Results

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Table A-1. Dataset for 183-H Solar Evaporation Basins

Well Name	Sample Date	Analyte	Reported Value	Units	Qualifier	ProUCL Non-detect Identification*
199-H4-8	11/15/2016	Chromium	7.4	µg/L	B	1
199-H4-8	5/3/2017	Chromium	3.3	µg/L		1
199-H4-8	11/10/2017	Chromium	3	µg/L	BC	1
199-H4-8	2/12/2018	Chromium	2.8	µg/L		1
199-H4-8	5/17/2018	Chromium	4.2	µg/L	BC	1
199-H4-8	11/13/2018	Chromium	3.6	µg/L		1
199-H4-8	5/1/2019	Chromium	5.5	µg/L		1
199-H4-8	6/16/2020	Chromium	4	µg/L	UD	0
199-H4-84	2/8/2017	Chromium	33	µg/L		1
199-H4-84	5/3/2017	Chromium	8.1	µg/L		1
199-H4-84	11/10/2017	Chromium	2.9	µg/L	BC	1
199-H4-84	2/12/2018	Chromium	83.9	µg/L	D	1
199-H4-84	5/17/2018	Chromium	8	µg/L	BC	1
199-H4-84	11/13/2018	Chromium	20	µg/L		1
199-H4-84	5/1/2019	Chromium	30	µg/L		1
199-H4-84	6/17/2020	Chromium	220	µg/L		1
199-H4-85	2/10/2016	Chromium	16.1	µg/L		1
199-H4-85	5/22/2016	Chromium	6.76	µg/L	B	1
199-H4-85	2/12/2018	Chromium	4.4	µg/L	B	1
199-H4-85	5/17/2018	Chromium	5.8	µg/L	BC	1
199-H4-85	11/13/2018	Chromium	6.58	µg/L	B	1
199-H4-85	5/1/2019	Chromium	5	µg/L	N	1
199-H4-85	12/30/2019	Chromium	5.74	µg/L	B	1
199-H4-85	6/17/2020	Chromium	3	µg/L	U	0
199-H4-88	8/16/2018	Chromium	17	µg/L		1
199-H4-88	11/13/2018	Chromium	12.1	µg/L		1
199-H4-88	3/7/2019	Chromium	11.5	µg/L		1
199-H4-88	5/1/2019	Chromium	10.15	µg/L	N	1
199-H4-88	8/5/2019	Chromium	7.82	µg/L	B	1
199-H4-88	11/8/2019	Chromium	10	µg/L		1
199-H4-88	12/30/2019	Chromium	8.8	µg/L	B	1
199-H4-88	6/17/2020	Chromium	8.67	µg/L	B	1
199-H4-89	2/12/2018	Chromium	3.6	µg/L	B	1
199-H4-89	5/17/2018	Chromium	3.9	µg/L	BC	1
199-H4-89	8/16/2018	Chromium	3.77	µg/L	B	1
199-H4-89	11/13/2018	Chromium	7.1	µg/L	BD	1

Table A-1. Dataset for 183-H Solar Evaporation Basins

Well Name	Sample Date	Analyte	Reported Value	Units	Qualifier	ProUCL Non-detect Identification*
199-H4-89	3/7/2019	Chromium	4.3	µg/L	BD	1
199-H4-89	5/2/2019	Chromium	4.4	µg/L	BD	1
199-H4-89	8/5/2019	Chromium	4.92	µg/L	B	1
199-H4-89	6/17/2020	Chromium	3	µg/L	U	0
199-H4-8	11/15/2016	Nitrate	9.3	mg/L	D	1
199-H4-8	5/3/2017	Nitrate	12.4	mg/L		1
199-H4-8	11/10/2017	Nitrate	11.1	mg/L	D	1
199-H4-8	2/12/2018	Nitrate	12.2	mg/L		1
199-H4-8	5/17/2018	Nitrate	11.1	mg/L	D	1
199-H4-8	11/13/2018	Nitrate	13.3	mg/L	D	1
199-H4-8	5/1/2019	Nitrate	11.5	mg/L	D	1
199-H4-8	6/16/2020	Nitrate	20.5	mg/L		1
199-H4-84	2/8/2017	Nitrate	75.3	mg/L	D	1
199-H4-84	5/3/2017	Nitrate	13.1	mg/L	D	1
199-H4-84	11/10/2017	Nitrate	30.5	mg/L	D	1
199-H4-84	2/12/2018	Nitrate	100	mg/L	D	1
199-H4-84	5/17/2018	Nitrate	25.2	mg/L	D	1
199-H4-84	11/13/2018	Nitrate	70.8	mg/L	D	1
199-H4-84	5/1/2019	Nitrate	55.8	mg/L	D	1
199-H4-84	6/17/2020	Nitrate	142	mg/L	D	1
199-H4-85	5/17/2018	Nitrate	10.2	mg/L	D	1
199-H4-85	11/13/2018	Nitrate	28.8	mg/L	D	1
199-H4-85	3/7/2019	Nitrate	7.53	mg/L		1
199-H4-85	5/1/2019	Nitrate	5.31	mg/L	D	1
199-H4-85	8/6/2019	Nitrate	3.53	mg/L		1
199-H4-85	12/30/2019	Nitrate	1.7	mg/L		1
199-H4-85	2/24/2020	Nitrate	1.96	mg/L		1
199-H4-85	6/17/2020	Nitrate	4.03	mg/L		1
199-H4-88	8/16/2018	Nitrate	79.7	mg/L	D	1
199-H4-88	11/13/2018	Nitrate	53.1	mg/L	D	1
199-H4-88	3/7/2019	Nitrate	53.1	mg/L	D	1
199-H4-88	5/1/2019	Nitrate	47.8	mg/L	D	1
199-H4-88	8/5/2019	Nitrate	45.2	mg/L	DX	1
199-H4-88	11/8/2019	Nitrate	66.4	mg/L		1
199-H4-88	12/30/2019	Nitrate	70.8	mg/L	D	1
199-H4-88	6/17/2020	Nitrate	88.5	mg/L	D	1

Table A-1. Dataset for 183-H Solar Evaporation Basins

Well Name	Sample Date	Analyte	Reported Value	Units	Qualifier	ProUCL Non-detect Identification*
199-H4-89	2/12/2018	Nitrate	22.5	mg/L	DX	1
199-H4-89	5/17/2018	Nitrate	19.9	mg/L	D	1
199-H4-89	8/16/2018	Nitrate	22.1	mg/L	D	1
199-H4-89	11/13/2018	Nitrate	57.5	mg/L	D	1
199-H4-89	3/7/2019	Nitrate	19.9	mg/L	D	1
199-H4-89	5/2/2019	Nitrate	21.3	mg/L		1
199-H4-89	8/5/2019	Nitrate	37.6	mg/L	D	1
199-H4-89	6/17/2020	Nitrate	50.5	mg/L	D	1

*Value used in ProUCL to identify non-detects (0) and detected values (1).

DF = dilution factor

GC/MS = gas chromatograph/mass spectrometer

IDL = instrument detection limit

MDL = method detection limit

QC = quality control

RDL = required detection limit

Qualifier Definitions:

B = The analyte was detected at a value less than the contract RDL, but greater than or equal to the IDL/MDL (as appropriate).

C = The analyte was detected in both the same and the associated QC blank, and the sample concentration was ≥ 5X the blank.

D = Analyte was reported at a secondary dilution factor, typically DF > 1.

N = All (except GC/MS based analysis) - Spike and/or spike duplicated sample recovery is outside control limits.

X = Recommended holding time exceeded.

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ProUCL Results for Filtered Total Chromium

UCL Statistics for Data Sets with Non-Detects

User Selected Options	
Date/Time of Computation	ProUCL 5.18/17/2020 11:06:06 AM
From File	ProUCL_Datasets_03052020_a.xls
Full Precision	OFF
Confidence Coefficient	95%
Number of Bootstrap Operations	2000

VAL (199-h4-84)

General Statistics

Total Number of Observations	8	Number of Distinct Observations	8
		Number of Missing Observations	0
Minimum	2.9	Mean	50.74
Maximum	220	Median	25
SD	73.07	Std. Error of Mean	25.83
Coefficient of Variation	1.44	Skewness	2.235

Note: Sample size is small (e.g., <10), if data are collected using ISM approach, you should use guidance provided in ITRC Tech Reg Guide on ISM (ITRC, 2012) to compute statistics of interest. For example, you may want to use Chebyshev UCL to estimate EPC (ITRC, 2012). Chebyshev UCL can be computed using the Nonparametric and All UCL Options of ProUCL 5.1

Normal GOF Test

Shapiro Wilk Test Statistic	0.688	**Shapiro Wilk GOF Test**
5% Shapiro Wilk Critical Value	0.818	Data Not Normal at 5% Significance Level
Lilliefors Test Statistic	0.346	**Lilliefors GOF Test**
5% Lilliefors Critical Value	0.283	Data Not Normal at 5% Significance Level

Data Not Normal at 5% Significance Level

Assuming Normal Distribution

95% Normal UCL		**95% UCLs (Adjusted for Skewness)**	
95% Student's-t UCL	99.68	95% Adjusted-CLT UCL (Chen-1995)	115
		95% Modified-t UCL (Johnson-1978)	103.1

Gamma GOF Test

A-D Test Statistic	0.36	**Anderson-Darling Gamma GOF Test**
5% A-D Critical Value	0.746	Detected data appear Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.228	**Kolmogorov-Smirnov Gamma GOF Test**
5% K-S Critical Value	0.304	Detected data appear Gamma Distributed at 5% Significance Level

Detected data appear Gamma Distributed at 5% Significance Level

Gamma Statistics

k hat (MLE)	0.742	k star (bias corrected MLE)	0.547
Theta hat (MLE)	68.35	Theta star (bias corrected MLE)	92.71
nu hat (MLE)	11.88	nu star (bias corrected)	8.756
MLE Mean (bias corrected)	50.74	MLE Sd (bias corrected)	68.58
		Approximate Chi Square Value (0.05)	3.181
Adjusted Level of Significance	0.0195	Adjusted Chi Square Value	2.393

Assuming Gamma Distribution

95% Approximate Gamma UCL (use when n>=50)	139.7	95% Adjusted Gamma UCL (use when n<50)	185.7

Lognormal GOF Test

Shapiro Wilk Test Statistic	0.978	**Shapiro Wilk Lognormal GOF Test**
5% Shapiro Wilk Critical Value	0.818	Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.145	**Lilliefors Lognormal GOF Test**
5% Lilliefors Critical Value	0.283	Data appear Lognormal at 5% Significance Level

Data appear Lognormal at 5% Significance Level

Lognormal Statistics

Minimum of Logged Data	1.065	Mean of logged Data	3.119
Maximum of Logged Data	5.394	SD of logged Data	1.388

Assuming Lognormal Distribution

95% H-UCL	607.4	90% Chebyshev (MVUE) UCL	122.5
95% Chebyshev (MVUE) UCL	155.8	97.5% Chebyshev (MVUE) UCL	201.9
99% Chebyshev (MVUE) UCL	292.4		

Nonparametric Distribution Free UCL Statistics

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

Nonparametric Distribution Free UCLs

95% CLT UCL	93.23	95% Jackknife UCL	99.68
95% Standard Bootstrap UCL	90.4	95% Bootstrap-t UCL	249
95% Hall's Bootstrap UCL	305.9	95% Percentile Bootstrap UCL	95.86
95% BCA Bootstrap UCL	118.3		
90% Chebyshev(Mean, Sd) UCL	128.2	95% Chebyshev(Mean, Sd) UCL	163.3
97.5% Chebyshev(Mean, Sd) UCL	212.1	99% Chebyshev(Mean, Sd) UCL	307.8

Suggested UCL to Use

95% Adjusted Gamma UCL	185.7

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.
Recommendations are based upon data size, data distribution, and skewness.

These recommendations are based upon the results of the simulation studies summarized in Singh, Maichle, and Lee (2006).
However, simulations results will not cover all Real World data sets; for additional insight the user may want to consult a statistician.

ProUCL Results for Nitrate

UCL Statistics for Data Sets with Non-Detects

User Selected Options	
Date/Time of Computation	ProUCL 5.18/17/2020 11:06:40 AM
From File	ProUCL_Datasets_03052020_b.xls
Full Precision	OFF
Confidence Coefficient	95%
Number of Bootstrap Operations	2000

VAL (199-h4-84)

General Statistics

Total Number of Observations	8	Number of Distinct Observations	8
		Number of Missing Observations	0
Minimum	13.1	Mean	64.09
Maximum	142	Median	63.3
SD	42.83	Std. Error of Mean	15.14
Coefficient of Variation	0.668	Skewness	0.706

Note: Sample size is small (e.g., <10), if data are collected using ISM approach, you should use guidance provided in ITRC Tech Reg Guide on ISM (ITRC, 2012) to compute statistics of interest. For example, you may want to use Chebyshev UCL to estimate EPC (ITRC, 2012). Chebyshev UCL can be computed using the Nonparametric and All UCL Options of ProUCL 5.1

Normal GOF Test

Shapiro Wilk Test Statistic	0.948	**Shapiro Wilk GOF Test**
5% Shapiro Wilk Critical Value	0.818	Data appear Normal at 5% Significance Level
Lilliefors Test Statistic	0.159	**Lilliefors GOF Test**
5% Lilliefors Critical Value	0.283	Data appear Normal at 5% Significance Level

Data appear Normal at 5% Significance Level

Assuming Normal Distribution

95% Normal UCL		95% UCLs (Adjusted for Skewness)	
95% Student's-t UCL	92.78	95% Adjusted-CLT UCL (Chen-1995)	93.03
		95% Modified-t UCL (Johnson-1978)	93.41

Gamma GOF Test

A-D Test Statistic	0.192	**Anderson-Darling Gamma GOF Test**
5% A-D Critical Value	0.723	Detected data appear Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.151	**Kolmogorov-Smirnov Gamma GOF Test**
5% K-S Critical Value	0.297	Detected data appear Gamma Distributed at 5% Significance Level

Detected data appear Gamma Distributed at 5% Significance Level

Gamma Statistics

k hat (MLE)	2.257	k star (bias corrected MLE)	1.494
Theta hat (MLE)	28.39	Theta star (bias corrected MLE)	42.9
nu hat (MLE)	36.11	nu star (bias corrected)	23.9
MLE Mean (bias corrected)	64.09	MLE Sd (bias corrected)	52.43
		Approximate Chi Square Value (0.05)	13.78
Adjusted Level of Significance	0.0195	Adjusted Chi Square Value	11.88

Assuming Gamma Distribution

95% Approximate Gamma UCL (use when n>=50))	111.2	95% Adjusted Gamma UCL (use when n<50)	129

Lognormal GOF Test

Shapiro Wilk Test Statistic	0.959	**Shapiro Wilk Lognormal GOF Test**
5% Shapiro Wilk Critical Value	0.818	Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.175	**Lilliefors Lognormal GOF Test**
5% Lilliefors Critical Value	0.283	Data appear Lognormal at 5% Significance Level

Data appear Lognormal at 5% Significance Level

Lognormal Statistics

Minimum of Logged Data	2.573	Mean of logged Data	3.923
Maximum of Logged Data	4.956	SD of logged Data	0.791

Assuming Lognormal Distribution

95% H-UCL	165.9	90% Chebyshev (MVUE) UCL	122.2
95% Chebyshev (MVUE) UCL	147.7	97.5% Chebyshev (MVUE) UCL	183.1
99% Chebyshev (MVUE) UCL	252.7		

Nonparametric Distribution Free UCL Statistics

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

Nonparametric Distribution Free UCLs

95% CLT UCL	88.99	95% Jackknife UCL	92.78
95% Standard Bootstrap UCL	87.46	95% Bootstrap-t UCL	99.05
95% Hall's Bootstrap UCL	102.9	95% Percentile Bootstrap UCL	88.33
95% BCA Bootstrap UCL	90.98		
90% Chebyshev(Mean, Sd) UCL	109.5	95% Chebyshev(Mean, Sd) UCL	130.1
97.5% Chebyshev(Mean, Sd) UCL	158.6	99% Chebyshev(Mean, Sd) UCL	214.7

Suggested UCL to Use

95% Student's-t UCL	92.78

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.
Recommendations are based upon data size, data distribution, and skewness.

These recommendations are based upon the results of the simulation studies summarized in Singh, Maichle, and Lee (2006).
However, simulations results will not cover all Real World data sets; for additional insight the user may want to consult a statistician.

VAL (199-h4-88)

General Statistics

Total Number of Observations	8	Number of Distinct Observations	7
		Number of Missing Observations	0
Minimum	45.2	Mean	63.08
Maximum	88.5	Median	59.75
SD	15.79	Std. Error of Mean	5.583
Coefficient of Variation	0.25	Skewness	0.497

Note: Sample size is small (e.g., <10), if data are collected using ISM approach, you should use guidance provided in ITRC Tech Reg Guide on ISM (ITRC, 2012) to compute statistics of interest.
For example, you may want to use Chebyshev UCL to estimate EPC (ITRC, 2012).
Chebyshev UCL can be computed using the Nonparametric and All UCL Options of ProUCL 5.1

Normal GOF Test

Shapiro Wilk Test Statistic	0.923	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.818	Data appear Normal at 5% Significance Level
Lilliefors Test Statistic	0.236	Lilliefors GOF Test
5% Lilliefors Critical Value	0.283	Data appear Normal at 5% Significance Level

Data appear Normal at 5% Significance Level

Assuming Normal Distribution

95% Normal UCL		95% UCLs (Adjusted for Skewness)	
95% Student's-t UCL	73.65	95% Adjusted-CLT UCL (Chen-1995)	73.31
		95% Modified-t UCL (Johnson-1978)	73.82

Gamma GOF Test

A-D Test Statistic	0.334	Anderson-Darling Gamma GOF Test
5% A-D Critical Value	0.716	Detected data appear Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.241	Kolmogorov-Smirnov Gamma GOF Test
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

k hat (MLE)	18.74	k star (bias corrected MLE)	11.8
Theta hat (MLE)	3.365	Theta star (bias corrected MLE)	5.346
nu hat (MLE)	299.9	nu star (bias corrected)	188.8
MLE Mean (bias corrected)	63.08	MLE Sd (bias corrected)	18.36
		Approximate Chi Square Value (0.05)	158
Adjusted Level of Significance	0.0195	Adjusted Chi Square Value	150.9

Assuming Gamma Distribution

95% Approximate Gamma UCL (use when n>=50))	75.36	95% Adjusted Gamma UCL (use when n<50)	78.93

Lognormal GOF Test

Shapiro Wilk Test Statistic	0.933	**Shapiro Wilk Lognormal GOF Test**
5% Shapiro Wilk Critical Value	0.818	Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.222	**Lilliefors Lognormal GOF Test**
5% Lilliefors Critical Value	0.283	Data appear Lognormal at 5% Significance Level

Data appear Lognormal at 5% Significance Level

Lognormal Statistics

Minimum of Logged Data	3.811	Mean of logged Data	4.117
Maximum of Logged Data	4.483	SD of logged Data	0.247

Assuming Lognormal Distribution

95% H-UCL	76.25	90% Chebyshev (MVUE) UCL	79.62
95% Chebyshev (MVUE) UCL	87.12	97.5% Chebyshev (MVUE) UCL	97.53
99% Chebyshev (MVUE) UCL	118		

Nonparametric Distribution Free UCL Statistics

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

Nonparametric Distribution Free UCLs

95% CLT UCL	72.26	95% Jackknife UCL	73.65
95% Standard Bootstrap UCL	71.85	95% Bootstrap-t UCL	74.8
95% Hall's Bootstrap UCL	72.56	95% Percentile Bootstrap UCL	72.36
95% BCA Bootstrap UCL	72.03		
90% Chebyshev(Mean, Sd) UCL	79.82	95% Chebyshev(Mean, Sd) UCL	87.41
97.5% Chebyshev(Mean, Sd) UCL	97.94	99% Chebyshev(Mean, Sd) UCL	118.6

Suggested UCL to Use

95% Student's-t UCL	73.65

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.
Recommendations are based upon data size, data distribution, and skewness.

These recommendations are based upon the results of the simulation studies summarized in Singh, Maichle, and Lee (2006).
However, simulations results will not cover all Real World data sets; for additional insight the user may want to consult a statistician.

VAL (199-h4-89)

General Statistics

Total Number of Observations	8	Number of Distinct Observations	7
		Number of Missing Observations	0
Minimum	19.9	Mean	31.41
Maximum	57.5	Median	22.3
SD	15.2	Std. Error of Mean	5.373
Coefficient of Variation	0.484	Skewness	1.05

Note: Sample size is small (e.g., <10), if data are collected using ISM approach, you should use guidance provided in ITRC Tech Reg Guide on ISM (ITRC, 2012) to compute statistics of interest.
For example, you may want to use Chebyshev UCL to estimate EPC (ITRC, 2012).
Chebyshev UCL can be computed using the Nonparametric and All UCL Options of ProUCL 5.1

Normal GOF Test

Shapiro Wilk Test Statistic	0.771	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.818	Data Not Normal at 5% Significance Level
Lilliefors Test Statistic	0.346	Lilliefors GOF Test
5% Lilliefors Critical Value	0.283	Data Not Normal at 5% Significance Level

Data Not Normal at 5% Significance Level

Assuming Normal Distribution

95% Normal UCL		95% UCLs (Adjusted for Skewness)	
95% Student's-t UCL	41.59	95% Adjusted-CLT UCL (Chen-1995)	42.38
		95% Modified-t UCL (Johnson-1978)	41.92

Gamma GOF Test

A-D Test Statistic	0.899	Anderson-Darling Gamma GOF Test
5% A-D Critical Value	0.719	Data Not Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.353	Kolmogorov-Smirnov Gamma GOF Test
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

k hat (MLE)	5.659	k star (bias corrected MLE)	3.62

Theta hat (MLE)	5.551	Theta star (bias corrected MLE)	8.678
nu hat (MLE)	90.54	nu star (bias corrected)	57.92
MLE Mean (bias corrected)	31.41	MLE Sd (bias corrected)	16.51
		Approximate Chi Square Value (0.05)	41.42
Adjusted Level of Significance	0.0195	Adjusted Chi Square Value	37.92

Assuming Gamma Distribution

95% Approximate Gamma UCL (use when n>=50))	43.92	95% Adjusted Gamma UCL (use when n<50)	47.98

Lognormal GOF Test

Shapiro Wilk Test Statistic	0.791	**Shapiro Wilk Lognormal GOF Test**
5% Shapiro Wilk Critical Value	0.818	Data Not Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.334	**Lilliefors Lognormal GOF Test**
5% Lilliefors Critical Value	0.283	Data Not Lognormal at 5% Significance Level

Data Not Lognormal at 5% Significance Level

Lognormal Statistics

Minimum of Logged Data	2.991	Mean of logged Data	3.356
Maximum of Logged Data	4.052	SD of logged Data	0.441

Assuming Lognormal Distribution

95% H-UCL	46.03	90% Chebyshev (MVUE) UCL	45.91
95% Chebyshev (MVUE) UCL	52.57	97.5% Chebyshev (MVUE) UCL	61.81
99% Chebyshev (MVUE) UCL	79.97		

Nonparametric Distribution Free UCL Statistics

Data do not follow a Discernible Distribution (0.05)

Nonparametric Distribution Free UCLs

95% CLT UCL	40.25	95% Jackknife UCL	41.59
95% Standard Bootstrap UCL	39.79	95% Bootstrap-t UCL	52.17
95% Hall's Bootstrap UCL	39.83	95% Percentile Bootstrap UCL	40.54
95% BCA Bootstrap UCL	41.33		
90% Chebyshev(Mean, Sd) UCL	47.53	95% Chebyshev(Mean, Sd) UCL	54.83
97.5% Chebyshev(Mean, Sd) UCL	64.97	99% Chebyshev(Mean, Sd) UCL	84.87

Suggested UCL to Use

95% Student's-t UCL	41.59	or 95% Modified-t UCL	41.92

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.
Recommendations are based upon data size, data distribution, and skewness.

These recommendations are based upon the results of the simulation studies summarized in Singh, Maichle, and Lee (2006).
However, simulations results will not cover all Real World data sets; for additional insight the user may want to consult a statistician.

Appendix B

Timeseries Plots

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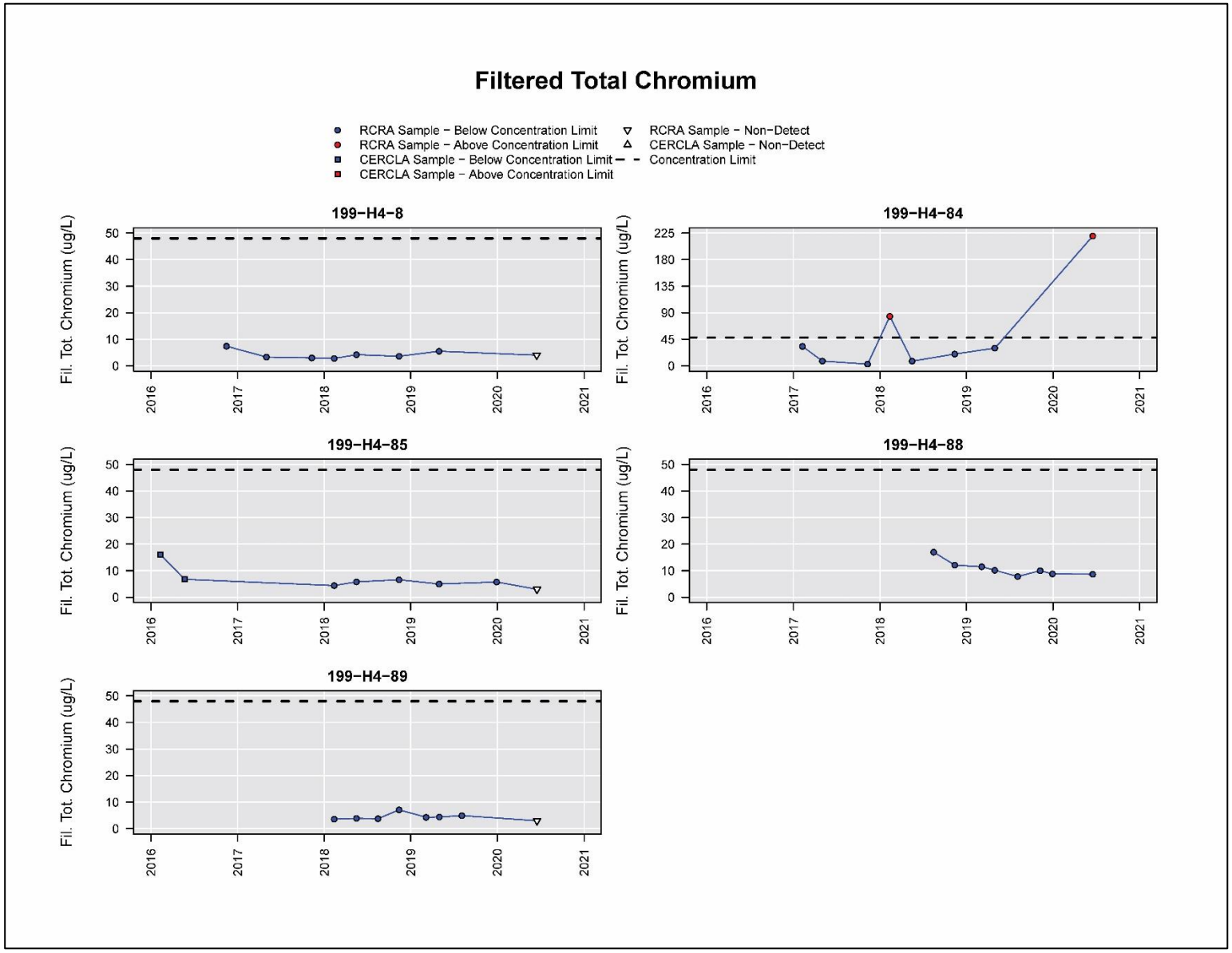

Figure B-1. Chromium Timeseries

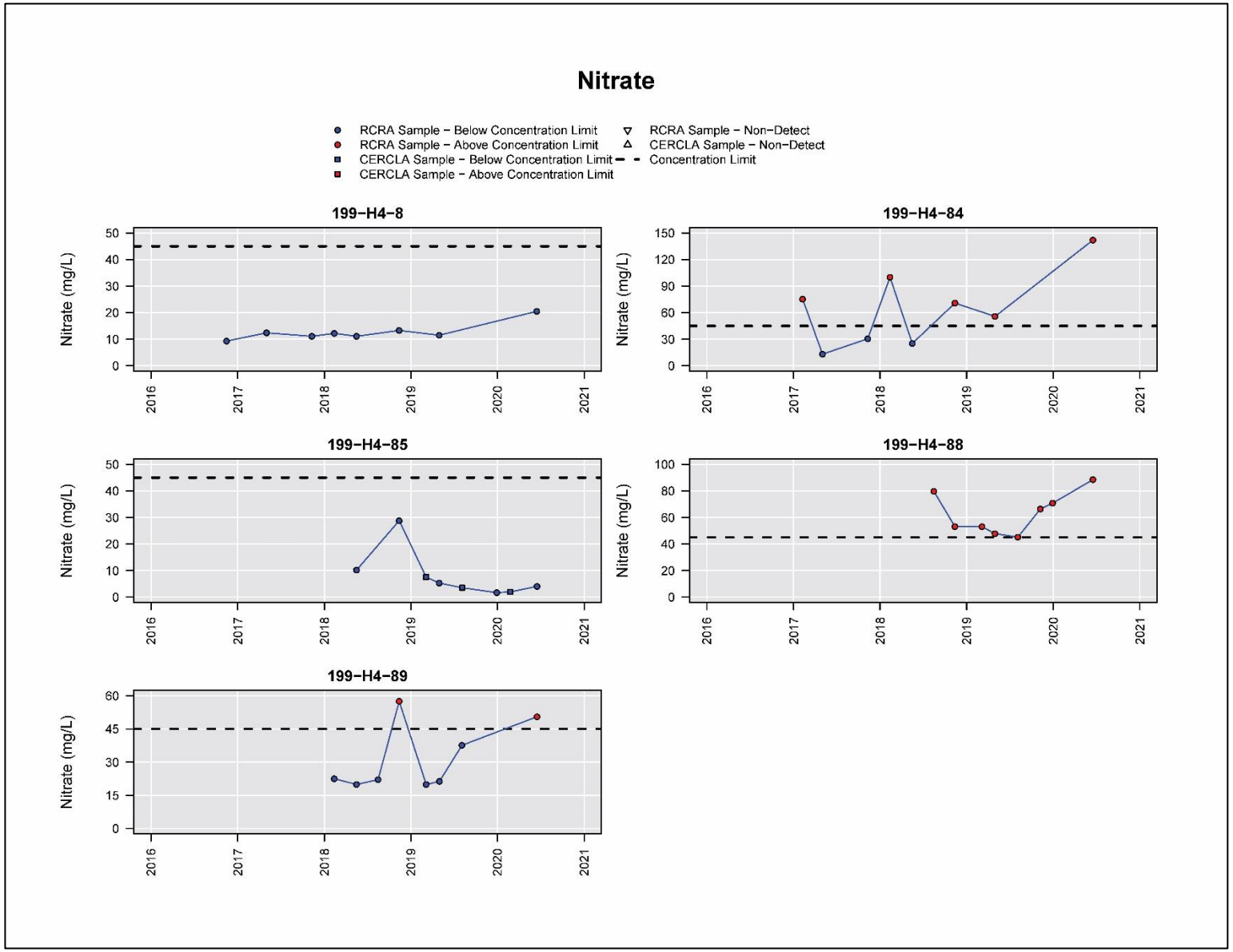

Figure B-2. Nitrate Timeseries