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Revision 0

Calculation of Critical Means for Calendar Year 2017 RCRA Groundwater Monitoring

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

ch2m

P.O. Box 1600
Richland, Washington 99352

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CH2M HILL Plateau Remediation Company

Date Published
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Terms

CM	critical mean
CR	critical range
CRAN	Comprehensive R Archive Network
CSV	comma-separated values (refers to an ASCII text file format)
CV	coefficient of variation
CY	calendar year
HEIS	Hanford Environmental Information System
LERF	Liquid Effluent Retention Facility
LLWMA	Low-Level Waste Management Area
LOQ	limit of quantitation
NA	not applicable or not available
NADA	Nondetects and Data Analysis
NRDWL	Nonradioactive Dangerous Waste Landfill
RCRA	*Resource Conservation and Recovery Act of 1976*
ROS	Regression on Order Statistics
su	standard unit
TOC	total organic carbon
TOX	total organic halides
TXT	text (refers to an ASCII text file format)

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1 Purpose

This calculation derives the statistical criteria (critical means [CMs]) for indicator parameters used in *Resource Conservation and Recovery Act of 1976* (RCRA) indicator parameter evaluation (interim status) and detection (final status) monitoring for calendar year (CY) 2017.

2 Background

The Hanford Site is a U.S. Department of Energy facility located in central Washington State along the Columbia River. The site operated as a nuclear production facility starting in the 1940s, and the last reactor was decommissioned in the late 1980s. During operation, many chemicals that can potentially migrate to groundwater were used. Since decommissioning, operations at the Hanford Site have changed to demolition and restoration, including remediation of known groundwater contamination under the *Comprehensive Environmental Response, Compensation, and Liability Act of 1980* and monitoring for new and existing facility impact to groundwater under RCRA. Hanford Site facilities that could create new impacts to groundwater are subject to WAC 173-303, "Dangerous Waste Regulations," which incorporate RCRA regulations for interim status (40 CFR 265, "Interim Status Standards for Owners and Operators of Hazardous Waste Treatment, Storage, and Disposal Facilities") and final status (40 CFR 264, "Standards for Owners and Operators of Hazardous Waste Treatment, Storage, and Disposal Facilities").

As established in WAC 173-303-400, "Interim Status Facility Standards," the facility is required by 40 CFR 265.92(b)(3), "Sampling and Analysis," to monitor pH, specific conductance, total organic carbon (TOC), and total organic halides (TOX) as indicator parameters for groundwater contamination. These parameters are to be measured in four replicate measurements, and a composite measurement should be calculated based on the mean of these four replicates. Monitoring for these parameters is also required by WA7890008967, *Hanford Facility Resource Conservation and Recovery Act Permit, Dangerous Waste Portion, Revision 8C, for the Treatment, Storage, and Disposal of Dangerous Waste* (hereafter referred to as the RCRA Permit), for detection monitoring at certain final-status sites. Samples collected at downgradient wells (compliance wells) are compared to upgradient wells (background wells) to identify potential impacts to groundwater from the facility. If concentrations in the compliance wells are significantly different from CM concentrations in background wells, there is evidence of facility impact to groundwater.

CMs are calculated for the 15 RCRA sites listed in Table 1.

Table 1. RCRA Sites for Indicator Parameter Statistical Comparisons

RCRA Site	Operable Unit
116-N-3 (1325-N) Facility	100-NR-2
116-N-1 (1301-N) Facility	100-NR-2
120-N-1 and 120-N-2 (1324-N/NA) Facilities	100-NR-2
216-A-29 Ditch	200-PO-1
216-A-36B Crib	200-PO-1
216-A-37-1 Crib	200-PO-1
216-B-3 Pond	200-PO-1
216-B-63 Trench	200-BP-5

Table 1. RCRA Sites for Indicator Parameter Statistical Comparisons

RCRA Site	Operable Unit
216-S-10 Pond and Ditch	200-UP-1
Liquid Effluent Retention Facility (LERF)	200-BP-5
Low-Level Waste Management Area-1 (LLWMA-1)	200-BP-5
Low-Level Waste Management Area-2 (LLWMA-2)	200-BP-5
Low-Level Waste Management Area-3 (LLWMA-3)	200-ZP-1
Low-Level Waste Management Area-4 (LLWMA-4)	200-ZP-1
Nonradioactive Dangerous Waste Landfill	200-PO-1

Reference: *Resource Conservation and Recovery Act of 1976*, 42 USC 6901, et seq.

This document describes the approach for calculating CMs for statistical comparisons. The calculated CMs will be compared with data collected during CY 2017 to determine if any exceedances (compliance well concentrations higher than the calculated CMs) have occurred. These comparisons will occur in quarterly RCRA monitoring reports and are beyond the scope of this document. CMs are calculated once for each CY unless sampling changes warrant recalculation.

2.1 Derivation of and Calculation of Critical Means as Prediction Limits

As established in WAC 173-303-400, the facility is required by 40 CFR 265.92(b)(3) to monitor pH, specific conductance, TOC, and TOX as indicator parameters for groundwater contamination. At each sampling event, these parameters are usually measured in four replicate samples. A composite measurement is calculated as the average of the replicates (its aliquot measurements). The methodology for identifying nondetects was established in ECF-Hanford-13-0013, *Calculation of Critical Means for Calendar Year 2013 RCRA Groundwater Monitoring*. When all of the aliquots are nondetects, the sample is treated as a nondetect in the subsequent analysis and its reporting limit is set to the smallest of the aliquot reporting limits. If the proportion of the nondetects is less than 1, the composite measurement is treated as a detected value in the subsequent analysis.

All statistical procedures are carried out separately for each RCRA unit and analyte. The unit-wide false-positive rate is controlled at $\alpha = 1\%$ by means of a Bonferroni adjustment based on the number of compliance decisions anticipated during each monitoring event to which these procedures will apply.

A set of reference (background) data is created for each analyte at each RCRA unit. In most cases, these data are obtained at designated upgradient wells during a specified (recent) period. The reference data, which consist of replicate samples obtained at each well during each sampling event, are composited into one value per well per sampling event. This background dataset is used to compute CMs (or for pH, a critical range [CR]). These are prediction limits (or intervals, respectively) for data that will be obtained at downgradient (compliance) wells during any single monitoring event. Composite measurements from those downgradient wells will be compared to CMs and CRs. Any downgradient composite result that exceeds its CMs (or lies outside its CRs, in the case of pH) will be considered statistically significant evidence that the groundwater it represents differs from conditions represented by the reference dataset. Such a determination is called a positive result.

CMs and CRs are derived from the test statistic for the Average Replicate t-test and calculated using the following formulas:

Critical mean $$CM = m + t_{df,k,\alpha}\, s\sqrt{1+\frac{1}{n}}$$ (Equation 2.1)

Critical range $$CR = m \pm t_{df,k,\alpha/2}\, s\sqrt{1+\frac{1}{n}}$$ (Equation 2.2)

where:

m = estimates the background mean

s = estimates the background standard deviation

n = the count of data used to compute the mean m

α = the minimum unit-wide false-positive rate for any single (future) monitoring event; set at 1%

k = the number of comparisons (counting all analytes) that have the potential to create a positive result within a RCRA unit during any single monitoring event

$t_{df,k,\alpha}$ = the upper 100% – α/k quantile of Student's t distribution with df degrees of freedom

$t_{df,k,\alpha/2}$ = the upper 100% – α/(2k) quantile of Student's t distribution with df degrees of freedom

df = the degrees of freedom (equal to $n - 1$ for the interwell tests)

The Student t quantiles have been generically referred to as "t_{crit}". The quantities α/k and $\alpha/(2k)$ have been referred to as the "adjusted" α or $\alpha_{adjusted}$. These terms are used in the tabulated results appearing in Chapter 7. The Student t-test was used in accordance with 40 CFR 265.93, "Preparation, Evaluation, and Response."

Typically, k will equal the number of upgradient and downgradient wells multiplied by the number of analytical parameters being tested (always equal to 4).

According to ECF-Hanford-13-0013, CMs (and CRs) are recalculated annually or if the number of comparisons changes. Annual recalculation, using a sliding period for selecting the background data, is intended to account for changing background conditions. Changes in the number of comparisons are usually the result of changes in monitoring well networks (i.e., wells are added or deleted). If changes occur in a monitoring well network, CMs and CRs for that facility are recalculated for subsequent sampling events using the new well network.

2.2 Counting Comparisons for the Bonferroni Adjustment

For comparability with previous calculations, as set forth in ECF-Hanford-13-0013, the number of comparisons for this analysis includes both upgradient and downgradient wells. Under 40 CFR 265.93(b), the comparison must consider individually each of the wells in the monitoring system. As such, at each RCRA unit, the number of analytes is multiplied by the total number of wells, including background wells, to accommodate planned testing of future results at upgradient wells.

3 Methodology

CMs were calculated using the interwell approach following procedures outlined in EPA 530/R-09-007, *Statistical Analysis of Groundwater Monitoring Data at RCRA Facilities Unified Guidance*, to set limits based on data from an upgradient well that is assumed to be unimpacted by activities at the monitored site.

3.1 Background and Compliance Wells

At each RCRA site, background wells are identified as wells that were hydraulically upgradient of the facility. Compliance wells are identified as wells that were hydraulically downgradient of the facility. A list of wells and well locations based on RCRA sites is presented in Appendix A.

3.2 Data Acquisition

Groundwater chemistry data are downloaded from the Hanford Environmental Information System (HEIS), which is maintained by CH2M HILL Plateau Remediation Company, and exported into a Microsoft® Access® database (HEIS_Chem1_01122017.accdb and HEIS_Chem2_01122017.accdb). Data for this analysis were downloaded from the HEIS database on January 12, 2017. The HEIS database contains one table (HEIS2_ADM_PNLGW_STD_RESULT_MV_1 and HEIS2_ADM_PNLGW_STD_RESULT_MV_2, respectively), which contains information on groundwater chemistry samples, including lab and review data qualifiers, sample medium, sample collection purpose, analytical method, and reporting limits. Fields extracted from the HEIS database for use in the CM calculations are presented in Table 2.

Table 2. HEIS Database Fields

Field Extracted	Definition
WELL_NAME	Location ID
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	Lab Data Qualifier
REVIEW_QUALIFIER	Review Data Qualifier[a]
COLLECTION_PURPOSE	Primary Reason for Sample Collection[b]

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Table 2. HEIS Database Fields

Field Extracted	Definition
VALIDATION_QUALIFIER	Validation Qualifier

a. Review Data Qualifier codes are as follows:

- F = The result is undergoing further review.
- G = Record has been reviewed and determined to be correct, or the record has been modified to make it correct.
- H = Laboratory holding time exceeded before the sample was analyzed.
- P = Potential problem. Collection/analysis circumstances make value questionable.
- Q = Associated quality control sample is out of limits.
- R = Do not use. Further review indicates the result is not valid. These points are not included in outputs or downloads.
- Y = Result suspect. Review – insufficient evidence to show result valid or invalid.
- Z = Miscellaneous circumstances exist. Additional information may be found in the RESULT_COMMENT field for this record.

b. Sample collection purpose codes are as follows:

C =	Characterization	T =	Transportation
IH =	Industrial Hygiene	TS =	Time Series
IP =	In Process	VER =	Verification
R =	Routine	VP =	Vertical Profile
S =	Special Studies	WM =	Waste Management

The RCRA parameter data (pH, specific conductance, TOC, and TOX) from the HEIS database are exported into two text (TXT) files named qryChemHeis1.txt and qryChemHeis2.txt.

3.3 Review Qualifiers

Data are removed from the dataset prior to calculation of CMs based on their review qualifiers (Table 3). This step was conducted for each individual sample prior to compiling composite samples.

Table 3. Review Qualifiers for Data Removal

Review Qualifier	Definition
Y	Result is suspect. Review had insufficient evidence to show result valid or invalid.
R	Do not use. Further review indicates the result is not valid.
F	Result is undergoing further review.
Q	Associated quality control sample is out of limits.

3.4 Collection Purpose

Data for the calculation of CMs are limited to data that were collected for routine purposes or verification (i.e., COLLECTION_PURPOSE = "R" or "VER"). This step was conducted for each individual sample prior to compiling composite samples.

3.5 Outliers

Based on visual inspection of the data, obvious outliers were removed prior to analysis (Table 4). Additional outlier testing was performed on composite samples (see Section 3.12) to identify any other potential outliers.

Table 4. Outliers Removed from Analysis

Well	Contaminant of Concern	Sample Date	Basis
699-26-38	Total organic carbon	10/17/2016	An order of magnitude higher than all other measured concentrations at this location

3.6 Nonroutine Samples

Several samples collected in December 2016 were identified in the HEIS database with COLLECTION_PURPOSE = "R". However, the samples were collected for a one-time, nonroutine analysis and were not included in the CM calculations (Table 5).

Table 5. Nonroutine Samples Collected in December

Well Name	Sample Date
199-N-105A	12/19/2016
199-N-2	12/19/2016
199-N-3	12/19/2016
199-N-34	12/14/2016
199-N-34	12/21/2016
199-N-57	12/14/2016
199-N-28	12/14/2016
199-N-32	12/14/2016
199-N-41	12/14/2016
199-N-81	12/14/2016
199-N-165	12/12/2016
199-N-71	12/12/2016
199-N-72	12/13/2016
199-N-73	12/12/2016
199-N-74	12/12/2016
199-N-77	12/13/2016

3.7 Calculation of Composite Results

At each RCRA site and for each well and analyte, composite results are calculated as the average of the replicates (its *aliquot* measurements). When none of the aliquots in the composite (also referred to as a "composite sample" to emphasize the composite nature of the measurements) are classified as a nondetect, the following statistics are calculated to characterize the background conditions and to support the CM/CR calculations:

Estimated background mean for composite sample

$$m_c = \frac{1}{n_c}\sum_{i=1}^{n_c} x_i \qquad \text{(Equation 3.1)}$$

Estimated standard deviation for composite sample

$$s_c = \sqrt{\frac{1}{n_c - 1}\sum_{i=1}^{n_c}(x_i - m_c)^2} \qquad \text{(Equation 3.2)}$$

where:

m_c = the composite sample mean

n_c = the number of aliquots in the composite sample

x_i = the aliquot measurement

s_c = the composite sample standard deviation

When one or more values in the dataset are nondetects, the procedures described in Section 3.10.1 (treatment of nondetects for computing statistics of composite samples) are used to compute m_c and s_c.

3.8 Identifying Background Data

CMs for each RCRA site are calculated from measurements at wells identified as being upgradient of the RCRA site (i.e., background wells). Classification of well location (upgradient versus downgradient) is presented in Appendix A. Several RCRA site groundwater monitoring plans have been or are in the process of being revised to modify the monitoring well networks because of changes in groundwater flow in the Central Plateau area. Table 6 presents the background well networks used for previous (2016) CM calculations and the new revised (or proposed) RCRA site groundwater monitoring networks. CMs are calculated for both the previous (2016) and new networks. For RCRA areas not presented in Table 6, no changes were made to the well networks.

Table 6. RCRA Areas with Multiple Calculated CMs/CRs

RCRA Area	Network	Background Wells
216-A-29 Ditch	Wells used in 2016 critical mean calculations	299-E26-12 299-E26-13 699-43-45
	New	299-E25-34 299-E25-43 299-E25-47 299-E26-13

Table 6. RCRA Areas with Multiple Calculated CMs/CRs

RCRA Area	Network	Background Wells
216-A-36B Crib	Wells used in 2016 critical mean calculations	299-E17-19
	New	299-E17-1 299-E17-19
216-A-37-1 Crib	Wells used in 2016 critical mean calculations	299-E25-47 299-E25-48
	New	299-E25-35 299-E25-47
216-B-3 Pond	Wells used in 2016 critical mean calculations	699-44-39B 699-45-42
	New	699-44-39B 699-45-42 New well (to be drilled)
LLWMA-1	Wells used in 2016 critical mean calculations	299-E32-10 299-E32-3 299-E32-5 299-E32-6 299-E32-7 299-E32-8 299-E32-9 299-E33-34
	New	299-E32-3 299-E33-266
LLWMA-4	Wells used in 2016 critical mean calculations	299-W18-21
	New	299-W17-1

3.9 Determination of Date Range

EPA 530/R-09-007 (pg. 5-3) recommends at least "8 to 10 independent background observations be collected before running most statistical tests." To ensure this, the number of composite measurements for each analyte at each RCRA site is counted over a minimum 2-year period covering 2015 and 2016 and adjusted, as necessary, to provide an adequate background dataset. Whenever this count is less than eight for any analyte at a RCRA site, the date range is expanded backwards in time until all analytes have at least eight samples. This common date range is used to estimate background conditions for the CR/CM calculations at that site.

The following exceptions apply to this rule:

- 216-S-10 Pond and Ditch: Sample size is restricted to four due to documented spatial variability in specific conductance (ECF-200UP1-12-0055, *Analysis of Spatial Variability of Specific Conductance in Groundwater at the 216-S-10 Pond & Ditch*). To maintain a sample size of four for pH, specific conductance, TOC, and TOX, a start date of analysis for CM calculations was set at May 5, 2015.
- Liquid Effluent Retention Facility (LERF): The Welch's t-test was performed for this RCRA site to calculate CMs (Section 3.13). Sample size is limited due to lack of data at the upgradient well before September 2011.
- Low-Level Waste Management Area-3 (LLWMA-3): The start date for analysis was changed to June 12, 2013 due to suspect drilling oil contamination in earlier samples. CMs are also calculated using an intrawell method (see Section 3.14).
- Nonradioactive Dangerous Waste Landfill (NRDWL): As described in 01-GWVZ-025, "Results of Assessment at the Non-Radioactive Dangerous Waste Landfill (NRDWL)," elevated levels of calcium, bicarbonate, magnesium, and sulfate from the Solid Waste Landfill impacts the specific conductance measurements in the NRDWL downgradient monitoring wells. To account for the spatial variability caused by the elevated levels of the nonregulated constituents from the Solid Waste Landfill, the background dataset size is restricted to 1 year of samples, but may be adjusted as needed to maintain at least a minimum of a sample size of four. To maintain the restricted sample size, the start date for analysis was set at January 1, 2016.

3.10 Handling Nondetects

Processing of nondetects proceeds through two stages. In the first stage, raw data are combined into composite measurements. Each composite is flagged according to the detectability of the data contributing to its value. These composites are grouped into reference datasets for each analyte at each RCRA unit. At the second stage, estimates of the means (m) and standard deviations (s) required for the CM/CR calculations are computed, depending on what proportion of the reference dataset consists of nondetects.

3.10.1 Stage 1: Computing Composite Values

All decisions in this monitoring program are based on composite measurements. That is, when four measurements are available at one monitoring event for an analyte at a well, these measurements are called replicates and are combined into a single value called a composite measurement for that event-analyte-well combination. The replicate measurements become the aliquots of the resulting composite measurement.

At the outset, beginning with the data selected as described in Sections 3.2 through 3.8, the following summary statistics are computed for each composite, c. The individual aliquot values are denoted x_i with indexes ranging from 1 through n_c. When replicate i is not detected, x_i equals the reporting limit associated with that sample.

Number of nondetects	$n_{c,0}$	(Equation 3.3)
Proportion of nondetects	$\frac{n_{c,0}}{n_c}$	(Equation 3.4)
Minimum detection limit[1]	min (x_i | result i not detected)	(Equation 3.5)
Maximum detected value[2]	max(x_i)	(Equation 3.6)
Mean of all values	$m_c = \frac{1}{n_c}\sum_{i=1}^{n_c} x_i$	(Equation 3.7)
Coefficient of variation (CV) (calculated when all aliquots of a composite sample are detected values)	$\frac{s_{c,d}}{m_{c,d}}$	(Equation 3.8)

where:

$s_{c,d}$ = the standard deviation of the composite sample when all aliquots are detected (i.e., no nondetects)

$m_{c,d}$ = the mean of the composite sample when all aliquots are detected (i.e., no nondetects)

The composite measurement is taken to be the mean of all values (m_c), and the composite measurement standard deviation is s_c. Multiple reporting limits were not present for composite sample aliquots (i.e., all aliquots of any composite sample had the same reporting limit).

The reporting limit is substituted for aliquots with measurements below the reporting limit. When all of the aliquots are nondetects, the sample is treated as a nondetect in the subsequent analysis and its reporting limit is set to the smallest of the aliquot reporting limits. If the proportion of the nondetects is less than 1, the composite measurement is treated as a detected value in the subsequent analysis.

3.10.2 Stage 2: Treatment of Nondetects for Computing Statistics of Reference Datasets

3.10.2.1 Datasets with Less Than 10 Percent Nondetects

EPA 530/R-09-007 (pg. 15-5) indicates that t-tests and prediction limits (and therefore the CM/CR calculations that are derived from them) are not significantly affected by substitution of half the reporting limit when the proportion of nondetects is no more than 10 percent to 15 percent of the total sample. Therefore, this substitution method is employed here for datasets where up to 10 percent of the composite samples are identified as nondetects. Equations 3.1 and 3.2 are then applied as if all values were actually quantified.

3.10.2.2 Datasets with between 10 Percent and 50 Percent Nondetects

Regression on Order Statistics (ROS) is used to account for nondetects in datasets where between 10 percent and 50 percent of the composite samples are identified as nondetects. The ROS method imputes values for nondetects based on an assumed distribution of the underlying data.
EPA 530/R-09-007 provides a detailed description of the ROS method (pg. 15-13). The calculations are

[1] Defined as detection limit in ECF-Hanford-13-0013.
[2] When all aliquots of a composite sample are nondetects, the maximum detected value is equal to the maximum reporting limit.

carried out using the Nondetects and Data Analysis (NADA) (Helsel, 2005, *Nondetects and Data Analysis: Statistics for Censored Environmental Data*) package in R (see Chapter 5 of this document). These calculations produce estimates of the background mean and standard deviation, replacing those in Equations 3.1 and 3.2.

3.10.2.3 Datasets with Greater Than 50 Percent Nondetects

Consistent with methodology set forth in ECF-Hanford-13-0013, dataset statistics and CM values are not calculated for datasets where (strictly) more than 50 percent of the composite samples are identified as nondetects. For RCRA sites 216-A-29 Ditch (original and new), 216-A37-1 PUREX Plant Crib (new), 216-B-3 Pond (original and new), 216-B-63 (original), LLWMA-1 (original), and the NRDWL, CMs for TOX could not be calculated because the percent nondetects of the composite samples exceeded 50 percent. The CM of TOC for RCRA sites 216-S-10 Pond and Ditch, LLWMA-1 (original), LLWMA-2, and LLWMA-4 (new) could not be calculated because the percent nondetects of the composite samples exceeded 50 percent.

3.11 Test for Normality

The background datasets are tested at the $\alpha = 0.05$ level using the Shapiro-Wilk test to evaluate the null hypothesis that the data are normally distributed. EPA 530/R-09-007 (pg. 10-13) provides a detailed description of the Shapiro-Wilk test. It is conducted using the "stats" package in R (see Chapter 5 of this document). CMs and CRs calculated from datasets that show evidence of departing from normal distributions are flagged in the tabulated results presented in Chapter 7. The Shapiro-Wilk test was also used to evaluate the null hypothesis that the data are log-normally distributed.

3.12 Test for Outliers

The background datasets are tested using the Grubbs test at the $\alpha = 0.001$ level to identify outliers, consistent with ECF-Hanford-13-0013. This test is useful for identifying exactly one outlier in a dataset (Grubbs, 1969, "Procedures for Detecting Outlying Observations in Samples") using composite measurements. The Grubbs test is conducted using the "outliers" package in R (see Chapter 5 of this document). Outliers were removed at the discretion of project scientists. No additional outliers to those listed in Table 3-3 were removed for the CY 2017 CM calculations based on the Grubbs test results.

3.13 Welch's T-Test

The statistical method for calculating CMs for the LERF RCRA site is outlined in Section D3.9.3 of DOE/RL-2013-46, *Groundwater Monitoring Plan for the Liquid Effluent Retention Facility*. This method is used for the LERF RCRA site only, in lieu of the previously described method. Since data are unavailable for the upgradient well prior to September 2011, data from both the upgradient and downgradient wells are used in the calculation of CMs. First, summary statistics (mean, standard deviation, and variance) are calculated for the pooled upgradient and compliance well datasets. Next, the degree of freedom (*df*) is calculated using the following equation:

$$df = \left[\frac{s_{BG}^2}{n_{BG}} + \frac{s_C^2}{n_C}\right]^2 \Bigg/ \left[\frac{\left(s_{BG}^2/n_{BG}\right)^2}{n_{BG}-1} + \frac{\left(s_C^2/n_C\right)^2}{n_C-1}\right] \qquad \text{(Equation 3.9)}$$

where s^2 is the variance for the pooled dataset, n is the number of samples in the pooled dataset, and the subscripts BG and C indicate the background dataset and the compliance well datasets, respectively.

The calculated degrees of freedom are used to determine the critical value using Table 16-1 of Appendix D of EPA 530/R-09-007.

3.14 Intrawell Method

There are three sites where an intrawell test was determined to be more appropriate than an interwell test: 1324-N/NA, 1325-N, and LLWMA-3. Specific conductance at sites 1324-N/NA and 1325-N compliance wells is affected by historical discharges of nonregulated sulfate. The LLWMA-3 compliance monitoring wells may be affected by injection of treated effluent from the 200 West Pump and Treat, which is injected downgradient of the upgradient well used for establishing background at LLWMA-3.

For upgradient-to-downgradient well comparisons, a crucial detection monitoring assumption is that downgradient well changes in groundwater quality are only caused by onsite releases of regulated constituents. The influence of the nonregulated releases and the injection of treated effluent result in spatial variability potentially leading to large numbers of false-positive detections at the compliance wells based on CMs calculated by the interwell method. Intrawell testing is identified in EPA 530/R-09-007 as a method to eliminate the problem of natural spatial variability.

Interim status monitoring regulations applicable to LLWMA-3 do not provide for intrawell testing; however, CMs are calculated using the intrawell method and provided for comparison in Chapter 7.

Intrawell limit methods use previous results collected in a monitoring well to set a limit that determines whether future samples in the same well represent an adverse change in groundwater quality. A statistically significant ("positive") result is interpreted as evidence of a real difference between the previous results and the future measurement.

The initial steps for obtaining and subsetting data for the intrawell method are the same as described in Sections 3.2. through 3.8. The method for handling nondetects and assessing normality in the intrawell method are the same as described in Sections 3.9 and 3.10. Calculations specific to the intrawell method are described in the following subsections.

The wells evaluated using the intrawell test are presented in Table 7.

Table 7. RCRA Sites and Wells Evaluated Using the Intrawell Test

RCRA Area	Wells
1324-NA (120-N-1) Percolation Pond and 1324-N (120-N-2) Surface Impoundment	199-N-72 199-N-73 199-N-165
1325-N (116-N-3) Liquid Waste Disposal Facility	199-N-32 199-N-41 199-N-81
Low-Level Waste Management Area 3 (LLWMA-3)	299-W10-29 299-W10-30 299-W10-31

3.14.1 Test for Homogeneity of Variance

By default, the variances in the logarithms of the composite indicator parameter results are assumed to be the same in each well. This assumption is tested using Levene's test (adjusted for nondetects). EPA 530/R-09-007 (pg. 11-4) provides a detailed description of Levene's test. Levene's test is conducted using the "lawstat" package in R (see Chapter 5 of this document) at an $\alpha = 1\%$ level. CMs and CRs calculated from datasets that show evidence of departing from the assumption of having the same variance are flagged in the tabulated results presented in Chapter 7. Individual well means together with a single pooled standard deviation are used for computing the CMs.

3.14.2 Calculation of Test Statistics and Critical Means

As established in ECF-HANFORD-13-0013, Rev.1, the CM is calculated as in Equations 2.1 and 2.2, but based on a pooled standard deviation (s_{ij}) estimated from all the compliance wells in the RCRA unit. The wells, which will be indexed by $j = 1, 2, 3$, contribute three reference datasets (x_{ij}) where j (which indexes the individual composite results) ranges from 1 through n_j (the amount of reference data available at each well). The total count of reference data is written n. For specific conductance, TOC, and TOX, let $y_{ij} = \ln(x_{ij})$ and for pH, let $y_{ij} = x_{ij}$. Let n_w be the number of wells in the pooled dataset (in this case, 3).

Individual well log means

$$m_j = \frac{1}{n_j}\sum_{i=1}^{n_j} y_{ij} \qquad \text{(Equation 3.10)}$$

Individual well log variance

$$s_j^2 = \frac{1}{n_j - 1}\sum_{i=1}^{n_j}\left(y_{ij} - m_j\right)^2 \qquad \text{(Equation 3.11)}$$

Pooled log variance

$$s^2 = \frac{1}{\sum_{j=1}^{n_w}\left(n_j - 1\right)}\sum_{j=1}^{n_w}\left(n_j - 1\right)s_j^2 = \frac{1}{n-3}\sum_{j=1}^{3}\left(n_j - 1\right)s_j^2 \qquad \text{(Equation 3.12)}$$

Pooled well standard deviation

$$s = \sqrt{s^2} \qquad \text{(Equation 3.13)}$$

Pooled degrees of freedom

$$df_{pooled} = n - n_w \qquad \text{(Equation 3.14)}$$

Individual well critical means

$$CM_j = \exp\left(m_j + t_{df_{pooled},k,\alpha}\, s\sqrt{1 + \frac{1}{n_j}}\right) \qquad \text{(Equation 3.15)}$$

Individual well critical range

$$CM_j = m_j \pm t_{df_{pooled},k,\alpha}\, s\sqrt{1 + \frac{1}{n_j}} \qquad \text{(Equation 3.16)}$$

The value of k is set, as in all other cases, to the total number of analytes (four).

4 Assumptions and Inputs

The following assumptions are made in the CMs analysis:

1. Reference data from upgradient wells are assumed to represent natural groundwater or background conditions.
2. Unless otherwise noted, it is assumed that the mean and variance of each analytical parameter exhibit no spatial variation within each region represented by the upgradient wells at any RCRA unit.
3. Time series of results are assumed stationary, which implies they have no trend. While it is recognized that groundwater quality may naturally change with time, accounting for trends is deliberately avoided by choosing a relative short period of records and periodically recalculating CMs.
4. The Student's t-test, from which the CM and CR limits are derived, assumes the sampling distribution of the mean follows a normal distribution and the sampling distribution of the variance independently is proportional to a chi-squared distribution with the assumed degrees of freedom. A large coefficient of variation (CV) can be an indication of non-normality of the mean (Equation 3.8). As a diagnostic adjunct to the Shapiro-Wilk test of normality, the CV is calculated each time a CM is calculated.
5. It is assumed that no seasonal fluctuations occur in the data.
6. Datasets with large numbers of nondetects (where data are censored below the detection limits) will result in unreliable CMs. Typically, CMs will be close to the detection limits but less than quantitation limits (which are approximately three times the detection limits). Therefore, when more than 50 percent of the reference (composite) results are nondetects, the limit of quantitation (LOQ) is used as the comparison value for detecting facility effect (in place of a CM). LOQ calculations and comparisons are made elsewhere.

Table 8 summarizes the number of data used in the calculation of CMs/CRs, including the number of data removed by each data processing step.

Table 8. Summary of Data used for Calculation of CMs/CRs

	Number of Samples	Percent of Total
Number of Total Aliquots from HEIS Database		
Total Number of Data from HEIS	**128,524**	
pH	51,874	40.4%
Specific conductance	51,814	40.3%
TOC	13,820	10.8%
TOX	11,016	8.6%
Number of Total Aliquots for Upgradient Wells		
Total Number of Data for Upgradient Wells	**16,428**	
pH	4,173	25.4%
Specific conductance	4,196	25.5%
TOC	4,118	25.1%

Table 8. Summary of Data used for Calculation of CMs/CRs

	Number of Samples	Percent of Total
TOX	3,941	24.0%
Number of Samples Removed Based on Review Qualifiers	**449**	**2.7%**
pH	0	0%
Specific conductance	5	0.1%
TOC	169	4.1%
TOX	275	7.0%
Number of Samples Removed Based on Collection Purpose	**168**	**1.0%**
pH	41	1.0%
Specific conductance	43	1.0%
TOC	52	1.3%
TOX	32	0.8%
Number of Aliquots	**15,811**	**96.2%**
Number of Nondetects	**3,824**	**23.3%**
pH	0	0%
Specific conductance	0	0%
TOC	1,566	38.0%
TOX	2,258	57.3%
Number of Composite Samples for Upgradient Wells		
Number of Event-Analyte-Well Combinations	**4,383**	
pH	1,198	28.7%
Specific conductance	1,213	28.9%
TOC	1,042	25.3%
TOX	930	23.6%

5 Software Applications

CMs were calculated using the public domain computing platform R (version 3.1.3 published 9/3/2015). R provides data manipulation, calculation, and graphical display capabilities to support data analysis (Venables et al., 2010, *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 (UNIX, Windows, and Mac OS). The base installation of R contains statistical and plotting functions and many more are available for download through the Comprehensive R Archive Network (CRAN). Several R packages are used for calculating CMs. The packages were downloaded from the CRAN and are listed in Table 9.

Table 9. R Packages Used for Critical Means Calculations

[R] Package	Package Description	Version
data.table	Enhanced data processing	1.9.4
lawstat	Tools for biostatistics, public policy, and law	2.5
NADA	Handling nondetects	1.5-6
outliers	Tests for outliers	0.14
plyr	Tools for splitting, applying, and combining data	1.8.1
reshape2	Restructure and aggregate data	1.4

6 Calculation

The R code used to process the data and calculate CMs for each site is included in Appendix B. The text files (qryChemHeis1.txt and qryChemHeis2.txt) contain the data downloaded from the HEIS database (see Section 3.2), the csv file (usr438ext30879.csv) contains January 2017 data for well 699-26-38, and the csv file (ClosureSamples_01302017.csv) contains the list of closure samples to be excluded from the analysis. In addition, a csv file containing information on well location for each RCRA site is used in the R code (2016_Updated_RCRA_GW_Monitoring_Well_List_Modified_02022016 - recieved from ALee - 1-24-2017.csv).

Output information is written to the files:

1. HANFORD-CRITICAL_MEANS-2017-(date of analysis).csv – Contains CMs calculated using the Interwell Method
2. Hanford-1324-N_1325-N-CM-2017-(date of analysis).csv – Contains CMs for 1324-N/NA and 1325-N calculated using the Intrawell Method
3. Hanford-LLWMA3-CM-2017-(date of analysis).csv – Contains CMs for LLWMA-3 calculated using the Intrawell Method
4. Data_Removed-(date of analysis).txt – Contains all of the data removed based on review qualifiers
5. LERF_Data_Removed-(date of analysis).txt – Contains all of the data removed based on review qualifiers for the LERF dataset
6. Totals_1-(date of analysis).txt – Contains a summary of total number of data in the dataset
7. Totals_UP-(date of analysis).txt – Contains a summary of the total number of samples for upgradient wells
8. Totals_Removed_Qualifier-(date of analysis).txt – Contains a summary of the total number of samples removed based on the review qualifier
9. Totals_Removed_Collection-(date of analysis).txt – Contains a summary of the total number of samples removed based on the collection purpose
10. Totals_Aliquots-(date of analysis).txt – Contains a summary of the total number of aliquots in the final dataset

11. Totals_NDs-(date of analysis).txt – Contains a summary of the total number of nondetects in the final dataset

12. Totals_Composite-(date of analysis).txt – Contains a summary of the total number of composite samples in the final dataset

This information has been formatted to produce the tables presented in the results section of this report as well as in the annual groundwater monitoring report.

7 Results

Results are listed in Tables 10 through 33.

Table 10. Critical Means for the 1301-N (116-N-1) Liquid Waste Disposal Facility for CY 2017 Comparisons

Statistic	Specific Conductance	Total Organic Carbon	Total Organic Halides	pH Measurement
Number of Upgradient Wells	2			
Date Range for Data	9/16/2014 – 12/31/2016			
Number of Composite Samples	10	10	9	10
% Nondetects	0%	50%	0%	0%
Mean	738 µS/cm	538 µg/L	9.10 µg/L	7.76 su
Median	740 µS/cm	411 µg/L	8.16 µg/L	7.78 su
Standard Deviation	207 µS/cm	299 µg/L	3.76 µg/L	0.31 su
Coefficient of Variation	0.280	0.556	0.413	0.040
Maximum	1031 µS/cm	1103 µg/L	14.93 µg/L	8.17 su
Number of Comparisons	20	20	20	20
alpha per comp ($\alpha_{adjusted}$)	5.00E-04	5.00E-04	5.00E-04	2.50E-04
$t_{crit,i}$	4.78	4.78	5.04	5.29
Critical Mean	1773 µS/cm	2038[a] µg/L	29.06 µg/L	9.50 su
Lower Critical Range				6.02 su

a. Dataset not log normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

Table 11. Critical Means for the 1325-N (116-N-3) Liquid Waste Disposal Facility for CY 2017 Comparisons

Statistic	Specific Conductance	Total Organic Carbon	Total Organic Halides	pH Measurement
Number of Upgradient Wells	Intrawell limits; see Table 12	1		
Date Range for Data		9/4/2012 – 12/31/2016		
Number of Composite Samples		11	8	11
% Nondetects		27%	13%	0%
Mean		339 µg/L	6.00 µg/L	8.05 su
Median		330 µg/L	6.09 µg/L	8.05 su
Standard Deviation		161 µg/L	1.01 µg/L	0.09 su
Coefficient of Variation		0.476	0.169	0.011
Maximum		628 µg/L	7.60 µg/L	8.19 su
Number of Comparisons		16	16	16
alpha per comp ($\alpha_{adjusted}$)		6.25E-04	6.25E-04	3.13E-04
$t_{crit,i}$		4.44	5.20	4.90
Critical Mean		1087 µg/L	11.59 µg/L	8.50 su
Lower Critical Range				7.59 su

su = standard unit

Table 12. Intrawell Critical Means for the 1325-N (116-N-3) Liquid Waste Disposal Facility for CY 2017 Comparisons

Statistic	199-N-32	199-N-41	199-N-81
Specific Conductance Intrawell Critical Means			
Mean	485 µS/cm	602 µS/cm	506 µS/cm
Standard Deviation	36 µS/cm	42 µS/cm	19 µS/cm
Number of Composite Samples	12	11	13
Levene test p-value	0.094	0.094	0.094
Pooled Standard Deviation (log scale)	0.062	0.062	0.062
Pooled Sample Size	36	36	36
alpha	0.01	0.01	0.01
df_{pooled}	33	33	33
$t_{crit,i}$	3.01	3.01	3.01
Critical Mean	588 µS/cm	731 µS/cm	613 µS/cm

Table 13. Critical Means for the 1324-NA (120-N-1) Percolation Pond and 1324-N (120-N-2) Surface Impoundment for CY 2017 Comparisons

Statistic	Specific Conductance	Total Organic Carbon	Total Organic Halides	pH Measurement
Number of Upgradient Wells	Intrawell limits; see Table 14	1		
Date Range for Data		3/7/2013 – 12/31/2016		
Number of Composite Samples		10	8	17
% Nondetects		40%	0%	0%
Mean		386 µg/L	9.49 µg/L	8.05 su
Median		307 µg/L	8.00 µg/L	8.09 su
Standard Deviation		139 µg/L	4.06 µg/L	0.15 su
Coefficient of Variation		0.361	0.428	0.019
Maximum		610 µg/L	14.43 µg/L	8.21 su
Number of Comparisons		16	16	16
alpha per comp ($\alpha_{adjusted}$)		6.25E-04	6.25E-04	3.13E-04
$t_{crit,i}$		4.62	5.20	4.24
Critical Mean		1061 µg/L	31.90[a] µg/L	8.72[a,b] su
Lower Critical Range				7.37[a,b] su

a. Dataset not normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

b. Dataset not log normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

su = standard unit

Table 14. Intrawell Critical Means for the 1324-NA (120-N-1) Percolation Pond and 1324-N (120-N-2) Surface Impoundment for CY 2017 Comparisons

Statistic	199-N-165	199-N-72	199-N-73
Specific Conductance Intrawell Critical Means			
Mean	700 µS/cm	875 µS/cm	708 µS/cm
Standard Deviation	73 µS/cm	75 µS/cm	129 µS/cm
Number of Composite Samples	21	13	13
Levene test p-value	0.015	0.015	0.015
Pooled Standard Deviation (log scale)	0.127	0.127	0.127
Pooled Sample size	47	47	47
alpha	0.01	0.01	0.01
df_{pooled}	44	44	44
$t_{crit,i}$	2.96	2.96	2.96
Critical mean	1028 µS/cm	1292 µS/cm	1045 µS/cm

Table 15. Critical Means for the 216-A-29 Ditch for CY 2017 Comparisons

Statistic	Specific Conductance	Total Organic Carbon	Total Organic Halides	pH Measurement
Number of Upgradient Wells	3			
Date Range for Data	1/9/2015 – 12/31/2016	4/1/2015 – 12/31/2016	1/9/2015 – 12/31/2016	
Number of Composite Samples	21	18	17	21
% Nondetects	0%	39%	65%	0%
Mean	294 µS/cm	378 µg/L	NA	8.22 su
Median	287 µS/cm	330 µg/L	NA	8.24 su
Standard Deviation	29 µS/cm	197 µg/L	NA	0.18 su
Coefficient of Variation	0.099	0.521	NA	0.022
Maximum	350 µS/cm	815 µg/L	15.93[c] µg/L	8.63 su
Number of Comparisons	32	32	NA	32
alpha per comp ($\alpha_{adjusted}$)	3.13E-04	3.13E-04	NA	1.56E-04
$t_{crit,i}$	4.05	4.18	NA	4.35
Critical Mean	415[a] µS/cm	1225[a,b] µg/L	NA	9.02 su
Lower Critical Range				7.42 su

a. Dataset not normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

b. Dataset not log normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

c. Percent nondetects too high to calculate critical mean. Maximum of background used as a qualitative comparison.

NA = not applicable or not available

su = standard unit

Table 16. Critical Means for the 216-A-29 Ditch - NEW for CY 2017 Comparisons

Statistic	Specific Conductance	Total Organic Carbon	Total Organic Halides	pH Measurement
Number of Upgradient Wells	4			
Date Range for Data	1/9/2015 – 12/31/2016	4/1/2015 – 12/31/2016	1/9/2015 – 12/31/2016	
Number of Composite Samples	19	15	14	19
% Nondetects	0%	27%	79%	0%
Mean	348 µS/cm	360 µg/L	NA	8.22 su
Median	340 µS/cm	367 µg/L	NA	8.23 su
Standard Deviation	88 µS/cm	89 µg/L	NA	0.21 su
Coefficient of Variation	0.254	0.246	NA	0.026
Maximum	489 µS/cm	521 µg/L	7.70[b] µg/L	8.75 su
Number of Comparisons	28	28	NA	28
alpha per comp ($\alpha_{adjusted}$)	3.57E-04	3.57E-04	NA	1.79E-04
$t_{crit,i}$	4.07	4.31	NA	4.38
Critical Mean	717[a] µS/cm	756[a] µg/L	NA	9.18 su
Lower Critical Range				7.27 su

a. Dataset not log normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

b. Percent nondetects too high to calculate critical mean. Maximum of background used as a qualitative comparison.

NA = not applicable or not available

su = standard unit

Table 17. Critical Means for the 216-A-36B PUREX Plant Crib for CY 2017 Comparisons

Statistic	Specific Conductance	Total Organic Carbon	Total Organic Halides	pH Measurement
Number of Upgradient Wells	1			
Date Range for Data	1/14/2013 – 12/31/2016			
Number of Composite Samples	9	8	8	9
% Nondetects	0%	38%	38%	0%
Mean	710 µS/cm	294 µg/L	5.36 µg/L	7.85 su
Median	714 µS/cm	281 µg/L	4.06 µg/L	7.82 su
Standard Deviation	25 µS/cm	86 µg/L	5.13 µg/L	0.11 su
Coefficient of Variation	0.035	0.294	0.958	0.014
Maximum	756 µS/cm	459 µg/L	17.43 µg/L	8.10 su
Number of comparisons	16	16	16	16
alpha per comp ($\alpha_{adjusted}$)	6.25E-04	6.25E-04	6.25E-04	3.13E-04
$t_{crit,i}$	4.86	5.20	5.20	5.43
Critical Mean	836 µS/cm	770 µg/L	33.69[a,b] µg/L	8.49 su
Lower Critical Range				7.20 su

a. Dataset not normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

b. Dataset not log normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

su = standard unit

Table 18. Critical Means for the 216-A-36B PUREX Plant Crib - NEW for CY 2017 Comparisons

Statistic	Specific Conductance	Total Organic Carbon	Total Organic Halides	pH Measurement
Number of Upgradient Wells	2			
Date Range for Data	1/14/2013 – 12/31/2016			
Number of Composite Samples	12	8	8	12
% Nondetects	0%	38%	38%	0%
Mean	664 µS/cm	294 µg/L	5.36 µg/L	7.89 su
Median	705 µS/cm	281 µg/L	4.06 µg/L	7.83 su
Standard Deviation	85 µS/cm	86 µg/L	5.13 µg/L	0.15 su
Coefficient of Variation	0.128	0.294	0.958	0.019
Maximum	756 µS/cm	459 µg/L	17.43 µg/L	8.16 su
Number of comparisons	24	24	24	24
alpha per comp ($\alpha_{adjusted}$)	4.17E-04	4.17E-04	4.17E-04	2.08E-04
$t_{crit,i}$	4.55	5.58	5.58	4.98
Critical Mean	1066[a,b] µS/cm	804 µg/L	35.75[a,b] µg/L	8.67[a,b] su
Lower Critical Range				7.12[a,b] su

a. Dataset not normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

b. Dataset not log normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

su = standard unit

Table 19. Critical Means for the 216-A-37-1 PUREX Plant Crib for CY 2017 Comparisons

Statistic	Specific Conductance	Total Organic Carbon	Total Organic Halides	pH Measurement
Number of Upgradient Wells	2			
Date Range for Data	7/7/2014 – 12/31/2016			
Number of composite samples	12	10	8	12
% Nondetects	0%	50%	38%	0%
Mean	512 µS/cm	348 µg/L	5.00 µg/L	8.20 su
Median	578 µS/cm	337 µg/L	4.64 µg/L	8.07 su
Standard Deviation	104 µS/cm	86 µg/L	1.69 µg/L	0.28 su
Coefficient of Variation	0.204	0.246	0.338	0.035
Maximum	623 µS/cm	521 µg/L	8.35 µg/L	8.75 su
Number of Comparisons	20	20	20	20
alpha per comp ($\alpha_{adjusted}$)	5.00E-04	5.00E-04	5.00E-04	2.50E-04
$t_{crit,i}$	4.44	4.78	5.41	4.86
Critical Mean	993[a,b] µS/cm	777[a] µg/L	14.69 µg/L	9.64 su
Lower Critical Range				6.77 su

a. Dataset not normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

b. Dataset not log normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

su = standard unit

Table 20. Critical Means for the 216-A-37-1 PUREX Plant Crib - NEW for CY 2017 Comparisons

Statistic	Specific Conductance	Total Organic Carbon	Total Organic Halides	pH Measurement
Number of Upgradient Wells	2			
Date Range for Data	1/9/2015 – 12/31/2016	4/1/2015 – 12/31/2016	1/9/2015 – 12/31/2016	
Number of composite samples	11	9	8	11
% Nondetects	0%	44%	63%	0%
Mean	465 µS/cm	338 µg/L	NA	8.32 su
Median	497 µS/cm	345 µg/L	NA	8.33 su
Standard Deviation	57 µS/cm	90 µg/L	NA	0.22 su
Coefficient of Variation	0.123	0.266	NA	0.026
Maximum	523 µS/cm	521 µg/L	4.78[c] µg/L	8.75 su
Number of comparisons	20	20	NA	20
alpha per comp ($\alpha_{adjusted}$)	5.00E-04	5.00E-04	NA	2.50E-04
$t_{crit,i}$	4.59	5.04	NA	5.05
Critical mean	739[a,b] µS/cm	817[a,b] µg/L	NA	9.46 su
Lower critical range				7.18 su

a. Dataset not normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

b. Dataset not log normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

c. Percent nondetects too high to calculate critical mean. Maximum of background used as a qualitative comparison.

NA = not applicable or not available

su = standard unit

Table 21. Critical Means for the 216-B-3 Pond for CY 2017 Comparisons

Statistic	Specific Conductance	Total Organic Carbon	Total Organic Halides	pH Measurement
Number of Upgradient Wells	2			
Date Range for Data	2/6/2014 – 12/31/2016			
Number of composite samples	13	11	8	13
% Nondetects	0%	27%	88%	0%
Mean	287 µS/cm	517 µg/L	NA	8.04 su
Median	285 µS/cm	416 µg/L	NA	8.09 su
Standard Deviation	31 µS/cm	423 µg/L	NA	0.19 su
Coefficient of Variation	0.109	0.818	NA	0.024
Maximum	336 µS/cm	1510 µg/L	5.00[c] µg/L	8.25 su
Number of comparisons	20	20	NA	20
alpha per comp ($\alpha_{adjusted}$)	5.00E-04	5.00E-04	NA	2.50E-04
$t_{crit,i}$	4.32	4.59	NA	4.72
Critical mean	428 µS/cm	2543[a] µg/L	NA	8.98[b] su
Lower critical range				7.09[b] su

a. Dataset not normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

b. Dataset not log normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

c. Percent nondetects too high to calculate critical mean. Maximum of background used as a qualitative comparison.

NA = not applicable or not available

su = standard unit

Table 22. Critical Means for the 216-B-3 Pond - NEW for CY 2017 Comparisons

Statistic	Specific Conductance	Total Organic Carbon	Total Organic Halides	pH Measurement
Number of Upgradient Wells	2			
Date Range for Data	2/6/2014 – 12/31/2016			
Number of composite samples	13	11	8	13
% Nondetects	0%	27%	88%	0%
Mean	287 µS/cm	517 µg/L	NA	8.04 su
Median	285 µS/cm	416 µg/L	NA	8.09 su
Standard Deviation	31 µS/cm	423 µg/L	NA	0.19 su
Coefficient of Variation	0.109	0.818	NA	0.024
Maximum	336 µS/cm	1510 µg/L	5.00[c] µg/L	8.25 su
Number of comparisons	20	20	NA	20
alpha per comp ($\alpha_{adjusted}$)	5.00E-04	5.00E-04	NA	2.50E-04
$t_{crit,i}$	4.32	4.59	NA	4.72
Critical mean	428 µS/cm	2543[a] µg/L	NA	8.98[b] su
Lower critical range				7.09[b] su

a. Dataset not normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

b. Dataset not log normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

c. Percent nondetects too high to calculate critical mean. Maximum of background used as a qualitative comparison.

NA = not applicable or not available

su = standard unit

Table 23. Critical Means for the 216-B-63 Trench for CY 2017 Comparisons

Statistic	Specific Conductance	Total Organic Carbon	Total Organic Halides	pH Measurement
Number of Upgradient Wells	3			
Date Range for Data	4/3/2015 – 12/31/2016			
Number of composite samples	13	13	8	13
% Nondetects	0%	38%	63%	0%
Mean	611 µS/cm	313 µg/L	NA	8.12 su
Median	645 µS/cm	306 µg/L	NA	8.10 su
Standard Deviation	74 µS/cm	76 µg/L	NA	0.09 su
Coefficient of Variation	0.122	0.242	NA	0.011
Maximum	685 µS/cm	430 µg/L	7.70[c] µg/L	8.24 su
Number of comparisons	24	24	NA	24
alpha per comp ($\alpha_{adjusted}$)	4.17E-04	4.17E-04	NA	2.08E-04
$t_{crit,i}$	4.42	4.42	NA	4.82
Critical mean	951[a,b] µS/cm	659 [a,b] µg/L	NA	8.56 su
Lower critical range				7.68 su

a. Dataset not normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

b. Dataset not log normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

c. Percent nondetects too high to calculate critical mean. Maximum of background used as a qualitative comparison.

NA = not applicable or not available

su = standard unit

Table 24. Critical Means for the 216-S-10 Pond and Ditch for CY 2017 Comparisons

Statistic	Specific Conductance	Total Organic Carbon	Total Organic Halides	pH Measurement
Number of Upgradient Wells	1			
Date Range for Data	5/5/2015 – 12/31/2016			
Number of composite samples	4	4	4	4
% Nondetects	0%	100%	25%	0%
Mean	299 µS/cm	NA	7.38 µg/L	7.68 su
Median	300 µS/cm	NA	6.71 µg/L	7.68 su
Standard Deviation	7 µS/cm	NA	2.43 µg/L	0.18 su
Coefficient of Variation	0.023	NA	0.329	0.024
Maximum	306 µS/cm	720[a] µg/L	10.63 µg/L	7.85 su
Number of comparisons	20	NA	20	20
alpha per comp ($\alpha_{adjusted}$)	5.00E-04	NA	5.00E-04	2.50E-04
$t_{crit,i}$	12.92	NA	12.92	16.33
Critical mean	398 µS/cm	NA	42.44 µg/L	11.04 su
Lower critical range				4.31 su

a. Percent nondetects too high to calculate critical mean. Maximum of background used as a qualitative comparison.

NA = not applicable or not available

su = standard unit

Table 25. Critical Means for the Liquid Effluent Retention Facility for CY 2017 Comparisons

Statistic	Specific Conductance	Total Organic Carbon	Total Organic Halides	pH Measurement
Number of Upgradient Wells	1			
Number of compliance wells	2			
Date Range for Data	9/11/2011 – 12/31/2016			
Number of composite samples	30	25	27	31
% Nondetects	0%	0%	19%	0%
Mean	752 µS/cm	1288 µg/L	5.98 µg/L	7.92 su
Median	764 µS/cm	741 µg/L	5.03 µg/L	7.92 su
Standard Deviation	57 µS/cm	1071 µg/L	2.54 µg/L	0.14 su
Coefficient of Variation	0.076	0.832	0.424	0.017
Maximum	834 µS/cm	4900 µg/L	10.40 µg/L	8.15 su
Number of comparisons	12	12	12	12
alpha per comp ($\alpha_{adjusted}$)	8.33E-03	8.33E-03	8.33E-03	4.17E-04
$t_{crit,i}$	3.48	4.37	3.59	3.90
Critical mean	838 µS/cm	3920[a,b] µg/L	10.33 [a,b] µg/L	8.08 su
Lower critical range				7.68 su

a. Dataset not normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

b. Dataset not log normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

su = standard unit

Table 26. Critical Means for Low-Level Waste Management Area 1 for CY 2017 Comparisons

Statistic	Specific Conductance	Total Organic Carbon	Total Organic Halides	pH Measurement
Number of Upgradient Wells	8			
Date Range for Data	1/13/2015 – 12/31/2016			
Number of composite samples	33	33	28	33
% Nondetects	0%	61%	71%	0%
Mean	526 µS/cm	NA	NA	8.06 su
Median	503 µS/cm	NA	NA	8.08 su
Standard Deviation	99 µS/cm	NA	NA	0.12 su
Coefficient of Variation	0.189	NA	NA	0.015
Maximum	739 µS/cm	720[c] µg/L	6.21[c] µg/L	8.26 su
Number of comparisons	52	NA	NA	52
alpha per comp ($\alpha_{adjusted}$)	1.92E-04	NA	NA	9.62E-05
$t_{crit,i}$	3.97	NA	NA	4.21
Critical mean	926[a,b] µS/cm	NA	NA	8.58[a,b] su
Lower critical range				7.54[a,b] su

a. Dataset not normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

b. Dataset not log normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

c. Percent nondetects too high to calculate critical mean. Maximum of background used as a qualitative comparison.

NA = not applicable or not available

su = standard unit

Table 27. Critical Means for Low-Level Waste Management Area 1 - NEW for CY 2017 Comparisons

Statistic	Specific Conductance	Total Organic Carbon	Total Organic Halides	pH Measurement
Number of Upgradient Wells	2			
Date Range for Data	7/30/2014 – 12/31/2016			
Number of composite samples	9	9	8	9
% Nondetects	0%	44%	38%	0%
Mean	444 µS/cm	363 µg/L	2.86 µg/L	7.98 su
Median	453 µS/cm	360 µg/L	2.51 µg/L	8.03 su
Standard Deviation	26 µS/cm	179 µg/L	0.92 µg/L	0.14 su
Coefficient of Variation	0.059	0.493	0.321	0.017
Maximum	477 µS/cm	725 µg/L	4.54 µg/L	8.17 su
Number of comparisons	28	28	28	28
alpha per comp ($\alpha_{adjusted}$)	3.57E-04	3.57E-04	3.57E-04	1.79E-04
$t_{crit,i}$	5.32	5.32	5.73	5.91
Critical mean	592 µS/cm	1366[a,b] µg/L	8.43 µg/L	8.84 su
Lower critical range				7.12 su

a. Dataset not normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

b. Dataset not log normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

su = standard unit

Table 28. Critical Means for Low-Level Waste Management Area 2 for CY 2017 Comparisons

Statistic	Specific Conductance	Total Organic Carbon	Total Organic Halides	pH Measurement
Number of Upgradient Wells	1			
Date Range for Data	10/15/2012 – 12/31/2015			
Number of composite samples	9	9	8	9
% Nondetects	0%	56%	13%	0%
Mean	554 µS/cm	NA	7.52 µg/L	8.06 su
Median	557 µS/cm	NA	6.84 µg/L	8.07 su
Standard Deviation	15 µS/cm	NA	2.81 µg/L	0.07 su
Coefficient of Variation	0.027	NA	0.373	0.009
Maximum	578 µS/cm	720[a] µg/L	12.20 µg/L	8.16 su
Number of comparisons	36	NA	36	36
alpha per comp ($\alpha_{adjusted}$)	2.78E-04	NA	2.78E-04	1.39E-04
$t_{crit,i}$	5.53	NA	5.98	6.14
Critical mean	642 µS/cm	NA	25.31 µg/L	8.53 su
Lower critical range				7.59 su

a. Percent nondetects too high to calculate critical mean. Maximum of background used as a qualitative comparison.

NA = not applicable or not available

su = standard unit

Table 29. Critical Means for Low-Level Waste Management Area 3 for CY 2017 Comparisons

Statistic	Specific Conductance	Total Organic Carbon	Total Organic Halides	pH Measurement
Number of Upgradient Wells	1			
Date Range for Data	6/12/2013 – 12/31/2016			
Number of composite samples	8	8	7	8
% Nondetects	0%	13%	43%	0%
Mean	389 µS/cm	443 µg/L	5.16 µg/L	8.03 su
Median	385 µS/cm	376 µg/L	5.13 µg/L	8.00 su
Standard Deviation	13 µS/cm	176 µg/L	0.68 µg/L	0.10 su
Coefficient of Variation	0.034	0.397	0.132	0.012
Maximum	406 µS/cm	702 µg/L	6.09 µg/L	8.18 su
Number of comparisons	16	16	16	16
alpha per comp ($\alpha_{adjusted}$)	6.25E-04	6.25E-04	6.25E-04	3.13E-04
$t_{crit,i}$	5.20	5.20	5.71	5.86
Critical mean	462 µS/cm	1413 µg/L	9.32[a,b] µg/L	8.63 su
Lower critical range				7.43 su

a. Dataset not normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

b. Dataset not log normally distributed based on Shapiro-Wilk Test ($p < 0.05$).

su = standard unit

Table 30. Intrawell Critical Means for Low-Level Waste Management Area 3 for CY 2017 Comparisons

Statistic	299-W10-29	299-W10-30	299-W10-31
Specific Conductance Intrawell Critical Means			
Mean	395 µS/cm	416 µS/cm	526 µS/cm
Standard Deviation	11 µS/cm	25 µS/cm	69 µS/cm
Number of composite samples	9	10	10
Levene test p-value	0.002	0.002	0.002
Pooled standard Deviation (log scale)	0.082	0.082	0.082
Pooled sample size	0.01	0.01	0.01
alpha	26	26	26
df_{pooled}	3.07	3.07	3.07
$t_{crit,i}$	516	543	686
Critical mean	395[a] µS/cm	416[a] µS/cm	526[a] µS/cm
Total Organic Carbon Intrawell Critical Means			
Mean	266 µg/L	445 µg/L	402 µg/L
Standard Deviation	163 µg/L	258 µg/L	154 µg/L
Number of composite samples	8	9	10
Levene test p-value	0.092	0.092	0.092
Pooled standard Deviation (log scale)	0.477	0.477	0.477
Pooled sample size	0.01	0.01	0.01
alpha	24	24	24
df_{pooled}	3.09	3.09	3.09
$t_{crit,i}$	1268	2105	1886
Critical mean	266 µg/L	445 µg/L	402 µg/L
Total Organic Halides Intrawell Critical Means			
Mean	8.10 µg/L	10.72 µg/L	18.22 µg/L
Standard Deviation	3.36 µg/L	5.56 µg/L	3.20 µg/L
Number of composite samples	7	8	8
Levene test p-value	0.045	0.045	0.045
Pooled Standard Deviation (log scale)	0.396	0.396	0.396
Pooled sample size	0.01	0.01	0.01
alpha	20	20	20
df_{pooled}	3.15	3.15	3.15
$t_{crit,i}$	30.80	40.33	68.57
Critical mean	8.10[a] µg/L	10.72[a] µg/L	18.22[a] µg/L

Table 30. Intrawell Critical Means for Low-Level Waste Management Area 3 for CY 2017 Comparisons

Statistic	299-W10-29	299-W10-30	299-W10-31
pH Measurement Intrawell Critical Means			
Mean	7.95 su	7.88 su	7.85 su
Standard Deviation	0.09 su	0.13 su	0.16 su
Number of composite samples	9	10	10
Levene test p-value	0.754	0.754	0.754
Pooled standard Deviation	0.130	0.130	0.130
Pooled sample size	0.01	0.01	0.01
alpha	26	26	26
df_{pooled}	3.07	3.07	3.07
$t_{crit,i}$	8.37	8.30	8.27
Upper critical range	7.53 su	7.46 su	7.43 su
Lower critical range	7.95 su	7.88 su	7.85 su

a. Dataset indicates evidence of heteroscedasticity (Levene Test $p < 0.05$).

su = standard unit

Table 31. Critical Means for Low-Level Waste Management Area 4 for CY 2017 Comparisons

Statistic	Specific Conductance	Total Organic Carbon	Total Organic Halides	pH Measurement
Number of Upgradient Wells	1			
Date Range for Data	2/10/2010 – 12/31/2016			
Number of composite samples	11	8	7	11
% Nondetects	0%	38%	14%	0%
Mean	553 µS/cm	346 µg/L	11.15 µg/L	7.88 su
Median	547 µS/cm	256 µg/L	12.90 µg/L	7.89 su
Standard Deviation	35 µS/cm	267 µg/L	6.98 µg/L	0.18 su
Coefficient of Variation	0.063	0.773	0.626	0.022
Maximum	602 µS/cm	968 µg/L	22.10 µg/L	8.27 su
Number of comparisons	24	24	24	24
alpha per comp ($\alpha_{adjusted}$)	4.17E-04	4.17E-04	4.17E-04	2.08E-04
$t_{crit,i}$	4.71	5.58	6.17	5.17
Critical mean	725 µS/cm	1926 µg/L	57.18 µg/L	8.83 su
Lower critical range				6.94 su

su = standard unit

Table 32. Critical Means for Low-Level Waste Management Area 4 – NEW for CY 2017 Comparisons

Statistic	Specific Conductance	Total Organic Carbon	Total Organic Halides	pH Measurement
Number of Upgradient Wells	1			
Date Range for Data	5/12/2004 – 12/31/2016	1/13/2016 – 12/31/2016		5/12/2004 – 12/31/2016
Number of composite samples	22	3	3	22
% Nondetects	0%	100%	0%	0%
Mean	388 µS/cm	NA	9.40 µg/L	7.71 su
Median	389 µS/cm	NA	9.00 µg/L	7.72 su
Standard Deviation	11 µS/cm	NA	0.78 µg/L	0.10 su
Coefficient of Variation	0.028	NA	0.083	0.012
Maximum	410 µS/cm	720[a] µg/L	10.30 µg/L	7.91 su
Number of comparisons	28	NA	28	28
alpha per comp ($\alpha_{adjusted}$)	3.57E-04	NA	3.57E-04	1.79E-04
$t_{crit,i}$	3.96	NA	37.40	4.25
Critical mean	432 µS/cm	NA	43.13 µg/L	8.13 su
Lower critical range				7.29 su

a. Percent nondetects too high to calculate critical mean. Maximum of background used as a qualitative comparison.

NA = not applicable or not available

su = standard unit

Table 33. Critical Means for Nonradioactive Dangerous Waste Landfill for CY 2017 Comparisons

Statistic	Specific Conductance	Total Organic Carbon	Total Organic Halides	pH Measurement
Number of Upgradient Wells	3			
Date Range for Data	1/21/2016 – 12/31/2016		4/13/2016	1/21/2016 – 12/31/2016
Number of composite samples	9	8	7	9
% Nondetects	0%	13%	100%	0%
Mean	504 µS/cm	350 µg/L	NA	7.38 su
Median	511 µS/cm	380 µg/L	NA	7.39 su
Standard Deviation	21 µS/cm	116 µg/L	NA	0.09 su
Coefficient of Variation	0.042	0.332	NA	0.012
Maximum	532 µS/cm	482 µg/L	7.70[a] µg/L	7.56 su
Number of comparisons	32	32	NA	32
alpha per comp ($\alpha_{adjusted}$)	3.13E-04	3.13E-04	NA	1.56E-04
$t_{crit,i}$	5.43	5.86	NA	6.03
Critical mean	625 µS/cm	1072 µg/L	NA	7.92 su
Lower critical range				6.83 su

a. Percent nondetects too high to calculate critical mean. Maximum of background used as a qualitative comparison.

NA = not applicable or not available

su = standard unit

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Appendix A

List of Upgradient and Downgradient Wells by Site

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A1 List of Upgradient and Downgradient Wells by Site

Table A-1 presents the list of RCRA Site upgradient and downgradient wells used for the critical mean calculations.

Table A-1. List of Wells by Site

Site[a]	Location[b]	Well Name[c]	Use
116-N-1 (1301-N)	DOWN	199-N-105A	TRUE
116-N-1 (1301-N)	DOWN	199-N-2	TRUE
116-N-1 (1301-N)	DOWN	199-N-3	TRUE
116-N-1 (1301-N)	UP	199-N-34	TRUE
116-N-1 (1301-N)	UP	199-N-57	TRUE
116-N-3 (1325-N)	DOWN	199-N-32	TRUE
116-N-3 (1325-N)	DOWN	199-N-41	TRUE
116-N-3 (1325-N)	UP	199-N-74	TRUE
116-N-3 (1325-N)	DOWN	199-N-81	TRUE
120-N-1 and 120-N-2 (1324-N/NA)	DOWN	199-N-165	TRUE
120-N-1 and 120-N-2 (1324-N/NA)	UP	199-N-71	TRUE
120-N-1 and 120-N-2 (1324-N/NA)	DOWN	199-N-72	TRUE
120-N-1 and 120-N-2 (1324-N/NA)	DOWN	199-N-73	TRUE
216-A-29 Ditch	DOWN	299-E25-26	TRUE
216-A-29 Ditch	DOWN	299-E25-32P	TRUE
216-A-29 Ditch	DOWN	299-E25-34	TRUE
216-A-29 Ditch	DOWN	299-E25-35	TRUE
216-A-29 Ditch	DOWN	299-E25-48	TRUE
216-A-29 Ditch	UP	299-E26-12	TRUE
216-A-29 Ditch	UP	299-E26-13	TRUE
216-A-29 Ditch	UP	699-43-45	TRUE
216-A-29 Ditch-NEW	DOWN	299-E25-26	TRUE
216-A-29 Ditch-NEW	DOWN	299-E25-32P	TRUE
216-A-29 Ditch-NEW	UP	299-E25-34	TRUE
216-A-29 Ditch-NEW	DOWN	299-E25-35	TRUE
216-A-29 Ditch-NEW	UP	299-E25-43	TRUE
216-A-29 Ditch-NEW	UP	299-E25-47	TRUE
216-A-29 Ditch-NEW	UP	299-E26-13	TRUE
216-A-36B Crib	DOWN	299-E17-14	TRUE

Table A-1. List of Wells by Site

Site[a]	Location[b]	Well Name[c]	Use
216-A-36B Crib	DOWN	299-E17-16	TRUE
216-A-36B Crib	DOWN	299-E17-18	TRUE
216-A-36B Crib	UP	299-E17-19	TRUE
216-A-36B Crib-NEW	UP	299-E17-1	TRUE
216-A-36B Crib-NEW	DOWN	299-E17-14	TRUE
216-A-36B Crib-NEW	DOWN	299-E17-15	TRUE
216-A-36B Crib-NEW	DOWN	299-E17-16	TRUE
216-A-36B Crib-NEW	DOWN	299-E17-18	TRUE
216-A-36B Crib-NEW	UP	299-E17-19	TRUE
216-A-37-1 Crib	DOWN	299-E25-17	TRUE
216-A-37-1 Crib	DOWN	299-E25-19	TRUE
216-A-37-1 Crib	DOWN	299-E25-20	TRUE
216-A-37-1 Crib	UP	299-E25-47	TRUE
216-A-37-1 Crib	UP	299-E25-48	TRUE
216-A-37-1 Crib-NEW	DOWN	299-E25-17	TRUE
216-A-37-1 Crib-NEW	DOWN	299-E25-19	TRUE
216-A-37-1 Crib-NEW	DOWN	299-E25-20	TRUE
216-A-37-1 Crib-NEW	UP	299-E25-35	TRUE
216-A-37-1 Crib-NEW	UP	299-E25-47	TRUE
216-B-3 Pond	DOWN	699-42-42B	TRUE
216-B-3 Pond	DOWN	699-43-44	TRUE
216-B-3 Pond	DOWN	699-43-45	TRUE
216-B-3 Pond	UP	699-44-39B	TRUE
216-B-3 Pond	UP	699-45-42	TRUE
216-B-3 Pond-NEW	DOWN	699-42-42B	TRUE
216-B-3 Pond-NEW	DOWN	699-43-44	TRUE
216-B-3 Pond-NEW	DOWN	699-43-45	TRUE
216-B-3 Pond-NEW	UP	699-44-39B	TRUE
216-B-3 Pond-NEW	UP	699-45-42	TRUE
216-B-63	DOWN	299-E27-16	TRUE
216-B-63	DOWN	299-E27-18	TRUE
216-B-63	DOWN	299-E27-19	TRUE

Table A-1. List of Wells by Site

Site[a]	Location[b]	Well Name[c]	Use
216-B-63	UP	299-E33-33	TRUE
216-B-63	UP	299-E34-12	TRUE
216-B-63	UP	299-E34-8	TRUE
216-S-10 Pond and Ditch	DOWN	299-W26-13	TRUE
216-S-10 Pond and Ditch	DOWN	299-W26-14	TRUE
216-S-10 Pond and Ditch	DOWN	699-32-76	TRUE
216-S-10 Pond and Ditch	DOWN	699-33-75	TRUE
216-S-10 Pond and Ditch	UP	699-33-76	TRUE
LERF	UP	299-E26-14	TRUE
LERF	DOWN	299-E26-15	TRUE
LERF	DOWN	299-E26-79	TRUE
LLWMA-1	DOWN	299-E28-26	TRUE
LLWMA-1	DOWN	299-E28-27	TRUE
LLWMA-1	DOWN	299-E28-28	TRUE
LLWMA-1	UP	299-E32-10	TRUE
LLWMA-1	UP	299-E32-3	TRUE
LLWMA-1	UP	299-E32-5	TRUE
LLWMA-1	UP	299-E32-6	TRUE
LLWMA-1	UP	299-E32-7	TRUE
LLWMA-1	UP	299-E32-8	TRUE
LLWMA-1	UP	299-E32-9	TRUE
LLWMA-1	DOWN	299-E33-28	TRUE
LLWMA-1	DOWN	299-E33-29	TRUE
LLWMA-1	UP	299-E33-34	TRUE
LLWMA-1-New	DOWN	299-E28-26	TRUE
LLWMA-1-New	DOWN	299-E28-27	TRUE
LLWMA-1-New	DOWN	299-E28-28	TRUE
LLWMA-1-New	UP	299-E32-3	TRUE
LLWMA-1-New	UP	299-E33-266	TRUE
LLWMA-1-New	DOWN	299-E33-28	TRUE
LLWMA-1-New	DOWN	299-E33-29	TRUE
LLWMA-2	DOWN	299-E27-10	TRUE

Table A-1. List of Wells by Site

Site[a]	Location[b]	Well Name[c]	Use
LLWMA-2	DOWN	299-E27-11	TRUE
LLWMA-2	DOWN	299-E27-17	TRUE
LLWMA-2	DOWN	299-E27-8	TRUE
LLWMA-2	DOWN	299-E27-9	TRUE
LLWMA-2	DOWN	299-E34-10	TRUE
LLWMA-2	DOWN	299-E34-12	TRUE
LLWMA-2	UP	299-E34-2	TRUE
LLWMA-2	DOWN	299-E34-9	TRUE
LLWMA-2-New	DOWN	299-E27-10	TRUE
LLWMA-2-New	DOWN	299-E27-8	TRUE
LLWMA-2-New	DOWN	299-E27-9	TRUE
LLWMA-2-New	UP	299-E34-2	TRUE
LLWMA-3	DOWN	299-W10-29	TRUE
LLWMA-3	DOWN	299-W10-30	TRUE
LLWMA-3	DOWN	299-W10-31	TRUE
LLWMA-3	UP	299-W9-2	TRUE
LLWMA-4	DOWN	299-W15-152	TRUE
LLWMA-4	DOWN	299-W15-224	TRUE
LLWMA-4	DOWN	299-W15-30	TRUE
LLWMA-4	DOWN	299-W15-83	TRUE
LLWMA-4	DOWN	299-W15-94	TRUE
LLWMA-4	UP	299-W18-21	TRUE
LLWMA-4-NEW	DOWN	299-W15-152	TRUE
LLWMA-4-NEW	DOWN	299-W15-224	TRUE
LLWMA-4-NEW	DOWN	299-W15-30	TRUE
LLWMA-4-NEW	DOWN	299-W15-83	TRUE
LLWMA-4-NEW	DOWN	299-W15-94	TRUE
LLWMA-4-NEW	UP	299-W17-1	TRUE
LLWMA-4-NEW	DOWN	299-W18-40	TRUE
NRDWL	DOWN	699-25-34B	TRUE
NRDWL	DOWN	699-25-34D	TRUE
NRDWL	DOWN	699-25-34F	TRUE

Table A-1. List of Wells by Site

Site[a]	Location[b]	Well Name[c]	Use
NRDWL	DOWN	699-26-33A	TRUE
NRDWL	UP	699-26-34A	TRUE
NRDWL	DOWN	699-26-34B	TRUE
NRDWL	UP	699-26-35A	TRUE
NRDWL	UP	699-26-38	TRUE

a. Site is the *Resource Conservation and Recovery Act of 1976* (RCRA) site.

b. Location is the specified location (upgradient or downgradient) of the well from the RCRA site.

c. Well name is the name of the well.

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Appendix B

Critical Means Analysis R Code

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B1 Critical Means Analysis R Code

Appendix B includes the R code used to process the data and calculate critical means for each site.

```
#-----------------------------------------------------------#
#--This script calculates the Critical Means for Hanford RCRA Areas for CY2017
#--Script written by: E. DiFilippo (SSP&A): modified from ECF-HANFORD-13-0013, REV. 0
#--R Version: 3.1.3
#--Package data.table version: 1.9.4
#--Package NADA version: 1.5-6
#--Package reshape2 version: 1.4
#--Package plyr version: 1.8.1
#--Package outliers version: 0.14
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Set working directory--#
setwd("Z:/1393_HANFORD_FY2017/094 - RCRA CRITICAL MEANS")
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Load Libraries--#
library(data.table) # used for data storage
library(NADA)       # used for non-detect analysis
library(outliers)   # used for grubbs test for outliers
library(plyr)               # used to provide efficient aggregation functions
library(reshape2)   # used to reformat data
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Import User-Defined Functions--#
source('R_Functions/readCHEMHEIS.R')
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Date of Run for File Exporting--#
DATE <- as.character(Sys.Date())
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Assign any variables--#
ALPHA <- 0.01                           # site-wide error rate
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Read in Data from Text file Downloads from Hanford Databases--#
DATA1 <- readCHEMHEIS('Data/Data Pull - 01122017/qryChemHEIS1.txt')
DATA2 <- readCHEMHEIS('Data/Data Pull - 01122017/qryChemHEIS2.txt')
DATA <- rbind(DATA1,DATA2)
RCRASITES <- fread("Data/2016_Updated_RCRA_GW_Monitoring_Well_List_Modified_02022016 - recieved from ALee - 1-24-2017.csv",
header=TRUE)
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Format Sample Dates--#
DATA[,EVENT := as.POSIXct(EVENT,format='%m/%d/%Y %H:%M:%S',tz='UTC')]
DATA[,EVENT := as.Date(EVENT,format='%Y-%m-%d')]
DATA <- subset(DATA,DATA$EVENT >= as.Date(ISOdate(2004,01,01)))
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Subset by Analyte--#
AN <- c('pH Measurement','Specific Conductance','Total organic halides','Total organic carbon')
DATA <- subset(DATA,DATA$ANALYTE %in% AN)
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Import RCRA Site Closure Samples--#
CLOS <- fread('Data/ClosureSamples_01302017.csv')
CLOS[,EVENT := as.POSIXct(Date_Collected,format='%m/%d/%Y',tz='UTC')]
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Import New Data for 699-26-38--#
```

```
NEW <- fread('Data/usr438ext30879.csv')
NEW$EVENT <- as.Date(ISOdate(2017,01,05))
NEW$DIL <- 1
NEW$COLLECTION_PURPOSE <- 'VER'
NEW$OWNER_ID <- NA
NEW$DEPTH <- NA
NEW <- subset(NEW,select=c('WELL_NAME','EVENT','FILTERED_FLAG','STD_CON_LONG_NAME','STD_VALUE_RPTD',
                'STD_ANAL_UNITS_RPTD','LAB_QUALIFIER','REVIEW_QUALIFIER',
                'VALIDATION_QUALIFIER','DIL','MEDIA','COLLECTION_PURPOSE',
                'OWNER_ID','METHOD_NAME','ReviewDate','DEPTH','STD_REPORTING_LIMIT'))
setnames(NEW,names(NEW),names(DATA))
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Add New Data--#
DATA <- rbind(DATA,NEW)
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Remove Closure Samples--#
ROW <- which(DATA$NAME %in% CLOS$Well & month(DATA$EVENT) == 12 & year(DATA$EVENT) == 2016)
DATA <- DATA[!ROW,]
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Remove TOC OUtlier--#
ROW <- which(DATA$NAME == '699-26-38' & DATA$ANALYTE == 'Total organic carbon' & DATA$EVENT ==
as.Date(ISOdate(2016,10,17)))
DATA <- DATA[!ROW,]
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Drop wells identified but not used--#
RCRASITES <- subset(RCRASITES, Use == TRUE )
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Export Summary of Total Number of Samples--#
TOTALS1 = data.table(ROWS=c('Total No. Samples',
                'Total No. pH Samples',
                'Total No. SC Samples',
                'Total No. TOC Samples',
                'Total No. TOX Samples'),
            TOTALS=c(nrow(DATA),
                nrow(DATA[ANALYTE=='pH Measurement']),
                nrow(DATA[ANALYTE=='Specific Conductance']),
                nrow(DATA[ANALYTE=='Total organic carbon']),
                nrow(DATA[ANALYTE=='Total organic halides'])))

TOTALS1[,PERCENT := (TOTALS/TOTALS[1])*100]
write.table(TOTALS1,paste0('Output/Totals_1_',DATE,'.txt'),sep='|',row.names=FALSE)
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Subset LERF Data. Evaluated using Different Method--#
LERFSITES <- subset(RCRASITES,Site == 'LERF')
LERF <- subset(DATA,NAME %in% LERFSITES$WELL_NAME)
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--subset data from upgradient wells. note that some wells serve as both up
#--and down gradient wells--#
DATA <- subset(DATA,DATA$NAME %in% unique(subset(RCRASITES, LOC == "UP")$WELL_NAME ))
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Merge Sample Data and Well Info Data--#
setkey(DATA,NAME)
setkey(RCRASITES,WELL_NAME)
DATA <- RCRASITES[DATA,allow.cartesian=TRUE]
```

```
DATA <- DATA[LOC=='UP']
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Export Summary of Total Number of Samples for Upgradient Wells--#
TOTALS2 <- data.table(ROWS=c('Total No. Samples',
                    'Total No. pH Samples',
                    'Total No. SC Samples',
                    'Total No. TOC Samples',
                    'Total No. TOX Samples'),
                TOTALS=c(nrow(DATA),
                      nrow(DATA[ANALYTE=='pH Measurement']),
                      nrow(DATA[ANALYTE=='Specific Conductance']),
                      nrow(DATA[ANALYTE=='Total organic carbon']),
                      nrow(DATA[ANALYTE=='Total organic halides'])))

TOTALS2[,PERCENT := (TOTALS/TOTALS[1])*100]
write.table(TOTALS2,paste0('Output/Totals_UP_',DATE,'.txt'),sep='|',row.names=FALSE)
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Check units consistancy--#
TEMP <- aggregate(DATA$UNIT, by=list(DATA$ANALYTE),
            function(x){length(unique(x))})
if(max(TEMP$x) > 1)stop("Different units - check")
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Identify nonDetects; TRUE indicates nondetect--#
DATA[,NDS := FALSE]
DATA[grep("U",LABQ),NDS := TRUE]
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Based on discussions censoring will be done base on review_qualifiers
#--indicate samples to be dropped because of review qualifiers--#
ROW <- which(DATA$REVIEWQ %like% 'Y' | DATA$REVIEWQ %like% 'R' | DATA$REVIEWQ %like% 'F' | DATA$REVIEWQ %like%
'Q')
REMOVED <- DATA[ROW,]
DATA <- DATA[!ROW,]
write.table(REMOVED,paste0('Output/Data_Removed_',DATE,'.txt'),sep='|',row.names=FALSE)
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Export Summary of Total Number of Samples Removed based on Review Qualifier--#
TOTALS3 <- data.table(ROWS=c('Total No. Samples',
                    'Total No. pH Samples',
                    'Total No. SC Samples',
                    'Total No. TOC Samples',
                    'Total No. TOX Samples'),
                TOTALS3=c(nrow(REMOVED),
                      nrow(REMOVED[ANALYTE=='pH Measurement']),
                      nrow(REMOVED[ANALYTE=='Specific Conductance']),
                      nrow(REMOVED[ANALYTE=='Total organic carbon']),
                      nrow(REMOVED[ANALYTE=='Total organic halides'])))
setkey(TOTALS2,ROWS)
setkey(TOTALS3,ROWS)
TOTALS3 <- TOTALS2[TOTALS3]

TOTALS3[,PERCENT := (TOTALS3/TOTALS)*100]
TOTALS3 <- subset(TOTALS3,select=c('ROWS','TOTALS3','PERCENT'))
write.table(TOTALS3,paste0('Output/Totals_Removed_Qualifier_',DATE,'.txt'),sep='|',row.names=FALSE)
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--use only data from 'routine' or verification collection purpose--#
REMOVED2 <- DATA[!COLLECTION_PURPOSE %in% c("R",'VER')]
DATA <- DATA[DATA$COLLECTION_PURPOSE %in% c("R",'VER'),]
#-----------------------------------------------------------------#
```

```
#-----------------------------------------------------------------#
#--Export Summary of Total Number of Samples Removed based on Collection Purpose--#
TOTALS4 = data.table(ROWS=c('Total No. Samples',
                    'Total No. pH Samples',
                    'Total No. SC Samples',
                    'Total No. TOC Samples',
                    'Total No. TOX Samples'),
               TOTALS4=c(nrow(REMOVED2),
                    nrow(REMOVED2[ANALYTE=='pH Measurement']),
                    nrow(REMOVED2[ANALYTE=='Specific Conductance']),
                    nrow(REMOVED2[ANALYTE=='Total organic carbon']),
                    nrow(REMOVED2[ANALYTE=='Total organic halides'])))
setkey(TOTALS2,ROWS)
setkey(TOTALS4,ROWS)
TOTALS4 = TOTALS2[TOTALS4]

TOTALS4[,PERCENT := (TOTALS4/TOTALS)*100]
TOTALS4 = subset(TOTALS4,select=c('ROWS','TOTALS4','PERCENT'))
write.table(TOTALS4,paste0('Output/Totals_Removed_Collection_',DATE,'.txt'),sep='|',row.names=FALSE)
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Export Summary of Total Number of Aliquots--#
TOTALS5 = data.table(ROWS='Total No. Samples',
               TOTALS=nrow(DATA))

TOTALS5[,PERCENT := (TOTALS/TOTALS2[ROWS=='Total No. Samples']$TOTALS)*100]
write.table(TOTALS5,paste0('Output/Totals_Aliquots_',DATE,'.txt'),sep='|',row.names=FALSE)
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Export Summary of Total Number of Non-Detects--#
NDS_TOT = DATA[NDS=='TRUE']
TOTALS6 = data.table(ROWS=c('Total No. Samples',
                    'Total No. pH Samples',
                    'Total No. SC Samples',
                    'Total No. TOC Samples',
                    'Total No. TOX Samples'),
               TOTALS6=c(nrow(NDS_TOT),
                    nrow(NDS_TOT[ANALYTE=='pH Measurement']),
                    nrow(NDS_TOT[ANALYTE=='Specific Conductance']),
                    nrow(NDS_TOT[ANALYTE=='Total organic carbon']),
                    nrow(NDS_TOT[ANALYTE=='Total organic halides'])))

setkey(TOTALS2,ROWS)
setkey(TOTALS6,ROWS)
TOTALS6 = TOTALS2[TOTALS6]

TOTALS6[,PERCENT := (TOTALS6/TOTALS)*100]
TOTALS6 = subset(TOTALS6,select=c('ROWS','TOTALS6','PERCENT'))
write.table(TOTALS6,paste0('Output/Totals_NDs_',DATE,'.txt'),sep='|',row.names=FALSE)
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Calculate the number of comparison made at each site--#
NCOMP <- data.table(as.data.frame(table(RCRASITES$Site)))
setnames(NCOMP,colnames(NCOMP),c("Site","NCOMP"))
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Create lists of sites and analyte names--#
SITES <- sort(unique(DATA$Site))
ANALYTES <- unique(DATA$ANALYTE)
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Remove LERF Site.  Evaluated using different Methodlogy--#
SITES = SITES[!SITES %in% c('LERF')]
#-----------------------------------------------------------------#
```

```
#-----------------------------------------------------------------#
#--summarize number of records per event-well location case is a unique id
#--for each well--#
DATA[,CASE := paste0(EVENT,WELL_NAME)]
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Calculating Summary Statistics for each Well by Sample Date
#--(1 sample per well per sample date, taking the mean of all measurements)--#
DATA_SUM <- data.table(DATA)[,list(N_NDS=sum(NDS),
                        N_SAMPLE=length(NDS),
                        PROPND=sum(NDS)/length(NDS),
                        MEAN_REPORTED=mean(VAL),
                        DETLIMIT=min(VAL),
                        MEAN_DETECTS=mean(VAL[!NDS]),
                        SD_DETECTS=sd(VAL[!NDS]),
                        CV_DETECTS=sd(VAL[!NDS])/mean(VAL[!NDS])),
                        by=c("Site","LOC","WELL_NAME","EVENT","ANALYTE","CASE")]
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Export Summary of Total Number of Composite Samples--#
TOTALS7 = data.table(ROWS=c('Total No. Samples',
                    'Total No. pH Samples',
                    'Total No. SC Samples',
                    'Total No. TOC Samples',
                    'Total No. TOX Samples'),
                TOTALS7=c(nrow(DATA_SUM),
                    nrow(DATA_SUM[ANALYTE=='pH Measurement']),
                    nrow(DATA_SUM[ANALYTE=='Specific Conductance']),
                    nrow(DATA_SUM[ANALYTE=='Total organic carbon']),
                    nrow(DATA_SUM[ANALYTE=='Total organic halides'])))

setkey(TOTALS2,ROWS)
setkey(TOTALS7,ROWS)
TOTALS7 = TOTALS2[TOTALS7]

TOTALS7[,PERCENT := (TOTALS7/TOTALS)*100]
TOTALS7 = subset(TOTALS7,select=c('ROWS','TOTALS7','PERCENT'))
write.table(TOTALS7,paste0('Output/Totals_Composite_',DATE,'.txt'),sep='|',row.names=FALSE)
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Identify nonDetects; TRUE indicates nondetect for Summary Dataset--#
DATA_SUM[,NDS := PROPND==1]
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Creating a Column of adjusted values for handling NDs--#
DATA_SUM[,ADJVAL := MEAN_REPORTED]
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Calculate Summary Statistics for Each Site including NDs--#
DATA_SUM_COUNTS <- data.table(DATA_SUM)[,list(ALL_NDS=sum(PROPND==1),
                        N_SAMPLES=length(PROPND),
                        PROPNDALL=round(100*sum(PROPND==1)/length(PROPND))),
                        by=c("ANALYTE","Site")]
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Creating data frame to place results for exporting--#
OUT <- NULL
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Loop through all Sites--#
for(i in 1:length(SITES)) {

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

```
#--Subsetting dataset by Site--#
DATA_SUM_SUB <- DATA_SUM[Site == SITES[i] & LOC == "UP",]
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Number of comparisons--#
NCOMP_SUB <- subset(NCOMP,Site == SITES[i])$NCOMP * length(ANALYTES)
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Setting Minimum Sample Numbers Required for Analysis--#
if(SITES[i]=="216-S-10 Pond and Ditch") {MINSAMPN <-4} else {MINSAMPN <-8}
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--determine whether the data collection window needs to be expanded beyond two years.
CHECK <- aggregate(DATA_SUM_SUB$MEAN_REPORTED, by=list(DATE=DATA_SUM_SUB$EVENT,
                   ANALYTE=DATA_SUM_SUB$ANALYTE,
                   CASE=DATA_SUM_SUB$CASE),mean)
CHECK <- dcast(melt(as.data.frame(table(CHECK$DATE,CHECK$ANALYTE)),id=c("Var1","Var2")),formula=Var1~Var2)
CHECK <- data.table(CHECK[order(CHECK[,1],decreasing=TRUE),])
setnames(CHECK,'Var1','DATE')

for(k in 1:length(ANALYTES)){CHECK[,k+1] <- cumsum(CHECK[,k+1,with=FALSE])}

 #--Check to see number of data points exist after 1/1/2015--#
        COMP_DATE_ROW = match(FALSE, as.POSIXct(CHECK$DATE) > ISOdate(2015,1,1)) - 1
         if(is.na(COMP_DATE_ROW)) COMP_DATE_ROW <- nrow(CHECK)

        #--Determine the row which satisfies the minimum sample number--#
        COMP_SAMP_ROW = max(min(which(CHECK[,2,with=FALSE] >= MINSAMPN)),
   min(which(CHECK[,3,with=FALSE] >= MINSAMPN)),
   min(which(CHECK[,4,with=FALSE] >= MINSAMPN)),
   min(which(CHECK[,5,with=FALSE] >= MINSAMPN)))
                 if (COMP_SAMP_ROW == Inf) {COMP_SAMP_ROW = nrow(CHECK)}

        #--Choose start date--#
        STARTDATE = max(COMP_DATE_ROW,COMP_SAMP_ROW)
 STARTDATE = as.Date(CHECK[STARTDATE,DATE],format='%Y-%m-%d')

        #--hard coded and needs to change next year--#
        if(SITES[i]=="216-S-10 Pond and Ditch") {STARTDATE <- as.Date(ISOdate(2015,05,05))}
 # if(SITES[i]=="216-A-29 Ditch") {STARTDATE <- as.Date(ISOdate(2014,01,01))}
 # if(SITES[i]=="216-A-29 Ditch-NEW") {STARTDATE <- as.Date(ISOdate(2014,01,01))}
 # if(SITES[i]=="216-B-63") {STARTDATE <- as.Date(ISOdate(2015,01,01))}
 # if(SITES[i]=="LLWMA-1") {STARTDATE <- as.Date(ISOdate(2015,01,01))}
 # if(SITES[i]=="LLWMA-1-New") {STARTDATE <- as.Date(ISOdate(2015,01,01))}
 if(SITES[i]=="LLWMA-3") {STARTDATE <- as.Date(ISOdate(2013,06,12))}
 if(SITES[i]=="LLWMA-4") {STARTDATE <- as.Date(ISOdate(2009,08,01))}
 if(SITES[i]=="NRDWL") {STARTDATE <- as.Date(ISOdate(2016,01,01))}
 # if(SITES[i]=="NRDWL-NEW") {STARTDATE <- as.Date(ISOdate(2016,01,01))}
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Subset data by start date--#
DATA_SUM_SUB <- subset(DATA_SUM_SUB,EVENT >= STARTDATE)
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Analyte Loop--#
for(j in 1:length(ANALYTES)){

#-----------------------------------------------------------#
#--Subset Data by Analyte--#
        DATA_ANALYTE_SUB <- DATA_SUM_SUB[DATA_SUM_SUB$ANALYTE == ANALYTES[j], ]
        #-----------------------------------------------------------#

        #-----------------------------------------------------------#
        #--Change Start Date for 216-S-10 Pond and Ditch TOC Measurements--#
        STARTDATE = min(DATA_ANALYTE_SUB$EVENT)
```

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

#-----------------------------------------------------------------#
#--Handling Non-detects--#

        #--If more than 50% of the values are NDs, than do not use results
        if(mean(DATA_ANALYTE_SUB$NDS) > 0.5){
                OUTPUT_SUM <- data.frame(table = unique(DATA_ANALYTE_SUB$Site),
                                                        ANALYTE = ANALYTES[j],
                                                        N = nrow(DATA_ANALYTE_SUB),
                                                        PROP_ND =
mean(DATA_ANALYTE_SUB$NDS),
                                                        MEAN = NA,
                                                        MEDIAN = NA,
                                                        SD = NA,
                                                        MAX =
max(DATA_ANALYTE_SUB$ADJVAL),
                                                        SHAPIRO_NORM = NA,
                                                        SHAPIRO_LOG = NA,
                                                        CV = NA,
                                                        GRUBBS = NA,
                                                        GRUBBSLOG = NA,
                                                        GRUBBS_OUT = NA,
                                                        GRUBBSLOG_OUT = NA,
                                                        ND_METHOD = "None",
                                                        START_DATE = STARTDATE,
                                                        ACRIT = NA,
                                                        TCRIT = NA,
                                                        CMDW = NA,
                                                        CMUP = NA,
                                                        NCOMP = NA)

        #--If less than 10% of the samples are Non-detects, use the subsitution
        #--method (1/2 DL), otherwise wus Regression on Order Statistics--#
        } else if(mean(DATA_ANALYTE_SUB$NDS) <= 0.1){
                ND_METHOD <- "HALF.RL"
                DATA_ANALYTE_SUB$ADJVAL[DATA_ANALYTE_SUB$NDS] <-
                DATA_ANALYTE_SUB$MEAN_REPORTED[DATA_ANALYTE_SUB$NDS]/2
        } else {
                ND_METHOD <- "ROS"
                DATA_ROS =
ros(obs=DATA_ANALYTE_SUB$ADJVAL,censored=DATA_ANALYTE_SUB$NDS)
                DATA_ANALYTE_SUB = DATA_ANALYTE_SUB[order(DATA_ANALYTE_SUB$ADJVAL),]
                DATA_ANALYTE_SUB$ADJVAL = DATA_ROS[14]
        }
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Determining Critical Values for Student t-Test--#
 if(ANALYTES[j] == 'pH Measurement'){
  ALPHA_CRIT <- (ALPHA/NCOMP_SUB)/2
 }      else {
  ALPHA_CRIT <- ALPHA/NCOMP_SUB
 }
        MN <- mean(DATA_ANALYTE_SUB$ADJVAL)
        SD <- sd(DATA_ANALYTE_SUB$ADJVAL)
        N <- nrow(DATA_ANALYTE_SUB)
        TCRIT <- qt(ALPHA_CRIT,df=N-1,lower.tail=FALSE,log=FALSE)
        CMUP <- MN + TCRIT *SD * sqrt(1 + 1/N)
        CMDW <- MN - TCRIT *SD * sqrt(1 + 1/N)
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--testing for Normality--#
        SHAPIRO_NORM <- try(shapiro.test(DATA_ANALYTE_SUB$MEAN_REPORTED)$p.value,
silent=TRUE)
        SHAPIRO_LOG <- try(shapiro.test(log(DATA_ANALYTE_SUB$MEAN_REPORTED))$p.value,
silent=TRUE)

        #--Returns dummy value if test is an error--#
```

```
                    if(class(SHAPIRO_NORM) =="try-error") SHAPIRO_NORM <- -999
                    if(class(SHAPIRO_LOG) =="try-error") SHAPIRO_LOG <- -999
        #-----------------------------------------------------#

        #-----------------------------------------------------#
        #--Outliers Analysis--#
                GRUBBS <- grubbs.test(DATA_ANALYTE_SUB$MEAN_REPORTED, type=10, opposite=FALSE,
two.sided=FALSE)
                GRUBBSLOG <- grubbs.test(log(DATA_ANALYTE_SUB$MEAN_REPORTED), type=10,
opposite=FALSE, two.sided=FALSE)
                GRUBBS_OUT = GRUBBS$alt
                GRUBBSLOG_OUT = GRUBBSLOG$alt
        #-----------------------------------------------------#

        #-----------------------------------------------------#
        #--Summary of Analysis--#
        OUTPUT_SUM <- data.frame(table = unique(DATA_ANALYTE_SUB$Site),
                ANALYTE = ANALYTES[j],
                                                N = N,
                                                PROP_ND = mean(DATA_ANALYTE_SUB$NDS),
                                                MEAN = mean(DATA_ANALYTE_SUB$ADJVAL),
                                                MEDIAN =
median(DATA_ANALYTE_SUB$ADJVAL),
                                                SD = sd(DATA_ANALYTE_SUB$ADJVAL),
                                                MAX = max(DATA_ANALYTE_SUB$ADJVAL),
                                                SHAPIRO_NORM = SHAPIRO_NORM,
                                                SHAPIRO_LOG = SHAPIRO_LOG,
                                                CV =
sd(DATA_ANALYTE_SUB$ADJVAL)/mean(DATA_ANALYTE_SUB$ADJVAL),
                                                GRUBBS = GRUBBS$p.value,
                                                GRUBBSLOG = GRUBBSLOG$p.value,
                                                GRUBBS_OUT = GRUBBS_OUT,
                                                GRUBBSLOG_OUT = GRUBBSLOG_OUT,
                                                ND_METHOD = ND_METHOD,
                                                START_DATE = STARTDATE,
                                                        ACRIT = ALPHA_CRIT,
                                                TCRIT = TCRIT,
                                                CMDW = CMDW,
                                                CMUP = CMUP,
                                                NCOMP = NCOMP_SUB)
        #-----------------------------------------------------#

        #-----------------------------------------------------#
        #--Output Matrix--#
                OUT  <- rbind(OUT, OUTPUT_SUM)
        #-----------------------------------------------------#
    }
    #-----------------------------------------------------#
}
#-----------------------------------------------------#

#-----------------------------------------------------#
#--LERF Critical Means Method--#
#-----------------------------------------------------#

 #-----------------------------------------------------#
 #--Check units consistancy--#
 TEMP <- aggregate(LERF$UNITS, by=list(LERF$ANALYTE),
        function(x){length(unique(x))})
 if(max(TEMP$x) > 1)stop("Different units - check")
 #-----------------------------------------------------#

 #-----------------------------------------------------#
 #--Identify nonDetects; TRUE indicates nondetect--#
 LERF[,NDS := FALSE]
 LERF[grep("U",LABQ),NDS := TRUE]
 #-----------------------------------------------------#

 #-----------------------------------------------------#
 #--Based on discussions censoring will be done base on review_qualifiers
```

```
#--indicate samples to be dropped because of review qualifiers--#
LERF_REMOVED <- subset(LERF,REVIEWQ %in% c('Y','R','F','Q','QH'))
LERF <- subset(LERF,!REVIEWQ %in% c('Y','R','F','Q','QH'))
write.table(LERF_REMOVED,paste0('Output/LERF_Data_Removed_',DATE,'.txt'),sep='|',row.names=FALSE)
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--use only data from 'routine' collection purpose--#
LERF <- LERF[LERF$COLLECTION_PURPOSE %in% c('R','C','VER'),]
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Calculate the number of comparison made at each site--#
LERF_DOWN <- subset(LERFSITES,LOC == 'DOWN')
LERF_NCOMP <- length(sort(unique(LERF$NAME)))
LERF_NCOMP <- LERF_NCOMP * length(ANALYTES)
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Merge Sample Data and Well Info Data--#
setkey(LERF,NAME)
setkey(LERFSITES,WELL_NAME)
LERF <- LERFSITES[LERF,allow.cartesian=TRUE]
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--summarize number of records per event-well location case is a unique id
#--for each well--#
LERF[,CASE := paste0(EVENT,WELL_NAME)]
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Calculating Summary Statistics for each Well by Sample Date
#--(1 sample per well per sample date, taking the mean of all measurements)--#
LERF_SUM <- data.table(LERF)[,list(N_NDS=sum(NDS),
                    N_SAMPLE=length(NDS),
                    PROPND=sum(NDS)/length(NDS),
                    MEAN_REPORTED=mean(VAL),
                    DETLIMIT=min(VAL),
                    MEAN_DETECTS=mean(VAL[!NDS]),
                    SD_DETECTS=sd(VAL[!NDS]),
                    CV_DETECTS=sd(VAL[!NDS])/mean(VAL[!NDS])),
                 by=c("WELL_NAME",'Site','LOC','Use','EVENT','ANALYTE','CASE')]
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Subsetting Downgradient Data to Time Frame of Upgradient Data--#
MINDATE <- LERF_SUM[LOC=='UP']
MINDATE <- min(year(MINDATE$EVENT))
LERF_SUM <- subset(LERF_SUM,year(EVENT) >= MINDATE)
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Identify nonDetects; TRUE indicates nondetect for Summary Dataset--#
LERF_SUM[,NDS := PROPND==1]
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Creating a Column of adjusted values for handling NDs--#
LERF_SUM[,ADJVAL := MEAN_REPORTED]
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Calculate Summary Statistics for Each Site including NDs--#
LERF_SUM_COUNTS <- data.table(LERF_SUM)[,list(ALL_NDS=sum(PROPND==1),
                        N_SAMPLES=length(PROPND),
                        PROPNDALL=round(100*sum(PROPND==1)/length(PROPND))),
                     by=c("ANALYTE","Site")]
#-----------------------------------------------------------------#
```

```
#-----------------------------------------------------------#
#--Analyte Loop--#
for(k in 1:length(ANALYTES)){

 #-----------------------------------------------------------#
 #--Subset Data by Analyte--#
 LERF_SUB <- LERF_SUM[ANALYTE == ANALYTES[k]]
 #-----------------------------------------------------------#

 #-----------------------------------------------------------#
 #--Determine Start Date--#
 LERF_STARTDATE <- as.Date(ISOdate(2011,09,11))
 #-----------------------------------------------------------#

 #-----------------------------------------------------------#
 #--Handling Non-detects--#

 #--If more than 50% of the values are NDs, than do not use results
 if(mean(LERF_SUB$NDS) > 0.5){
  OUTPUT_SUM <- data.frame(table = 'LERF',
                ANALYTE = ANALYTES[k],
                N = nrow(LERF_SUB),
                PROP_ND = mean(LERF_SUB$NDS),
                MEAN = NA,
                MEDIAN = NA,
                SD = NA,
                MAX = max(LERF_SUB$ADJVAL),
                SHAPIRO_NORM = NA,
                SHAPIRO_LOG = NA,
                CV = NA,
                GRUBBS = NA,
                GRUBBSLOG = NA,
                GRUBBS_OUT = NA,
                GRUBBSLOG_OUT = NA,
                ND_METHOD = "None",
                START_DATE = LERF_STARTDATE,
                ACRIT = NA,
                TCRIT = NA,
                CMDW = NA,
                CMUP = NA,
                NCOMP = NA)

  #--If less than 10% of the samples are Non-detects, use the subsitution
  #--method (1/2 DL), otherwise wus Regression on Order Statistics--#
 } else if(mean(LERF_SUB$NDS) <= 0.1){
  ND_METHOD <- "HALF.RL"
 } else {
  ND_METHOD <- "ROS"
 }

 #--Substitution Method (1/2 DL)--#
 if(ND_METHOD == "HALF.RL"){
  LERF_SUB$ADJVAL[LERF_SUB$NDS] <- LERF_SUB$MEAN_REPORTED[LERF_SUB$NDS]/2
 }

 #--Regression on Order Statistics (ROS) Method--#
 if(ND_METHOD == "ROS"){
  LERF_ROS <- ros(obs=LERF_SUB$ADJVAL,censored=LERF_SUB$NDS)
  LERF_SUB <- LERF_SUB[order(LERF_SUB$ADJVAL),]
  LERF_SUB$ADJVAL = LERF_ROS[14]
 }
 #-----------------------------------------------------------#

 #-----------------------------------------------------------#
 #--Determining Critical Values for Welch's t-Test--#
 if(ANALYTES[k] == 'pH Measurement'){
  ALPHA_CRIT_LERF <- (ALPHA/LERF_NCOMP)/2
 }        else {
  ALPHA_CRIT_LERF <- ALPHA/LERF_NCOMP
 }
```

```
  LERF_STATS <- data.table(LERF_SUB)[,list(N=length(NDS),
                    MEAN=mean(ADJVAL),
                    SD=sd(ADJVAL),
                    VAR=var(ADJVAL)),
                 by=c('LOC')]

  COMP <- LERF_STATS[LOC=='DOWN']
  BG <- LERF_STATS[LOC=='UP']
  TSTAT = (COMP$MEAN - BG$MEAN)/(sqrt((BG$VAR/BG$N) + (COMP$VAR/COMP$N)))
  DF <- (((BG$VAR/BG$N)+(COMP$VAR/COMP$N))^2)/(((BG$VAR/BG$N)^2)/(BG$N-1) + ((COMP$VAR/COMP$N)^2)/(COMP$N-1))
  TCRIT <- qt(ALPHA_CRIT_LERF,df=DF,lower.tail=FALSE,log=FALSE)
  CMUP <- BG$MEAN + TCRIT * sqrt((BG$VAR/BG$N)+(COMP$VAR/COMP$N))
  CMDW <- BG$MEAN - TCRIT * sqrt((BG$VAR/BG$N)+(COMP$VAR/COMP$N))
  #-----------------------------------------------------------#

  #-----------------------------------------------------------#
  #--testing for Normality--#
  SHAPIRO_NORM <- try(shapiro.test(LERF_SUB$MEAN_REPORTED)$p.value, silent=TRUE)
  SHAPIRO_LOG <- try(shapiro.test(log(LERF_SUB$MEAN_REPORTED))$p.value, silent=TRUE)

  #--Returns dummy value if test is an error--#
  if(class(SHAPIRO_NORM) =="try-error") SHAPIRO_NORM <- -999
  if(class(SHAPIRO_LOG) =="try-error") SHAPIRO_LOG <- -999
  #-----------------------------------------------------------#

  #-----------------------------------------------------------#
  #--Outliers Analysis--#
  GRUBBS <- grubbs.test(LERF_SUB$MEAN_REPORTED, type=10, opposite=FALSE, two.sided=FALSE)
  GRUBBSLOG <- grubbs.test(log(LERF_SUB$MEAN_REPORTED), type=10, opposite=FALSE, two.sided=FALSE)
  GRUBBS_OUT <- GRUBBS$alt
  GRUBBSLOG_OUT <- GRUBBSLOG$alt
  #-----------------------------------------------------------#

  #-----------------------------------------------------------#
  #--Summary of Analysis--#
  OUTPUT_SUM <- data.frame(table = "LERF",
              ANALYTE = ANALYTES[k],
              N = nrow(LERF_SUB),
              PROP_ND = mean(LERF_SUB$NDS),
              MEAN = mean(LERF_SUB$ADJVAL),
              MEDIAN = median(LERF_SUB$ADJVAL),
              SD = sd(LERF_SUB$ADJVAL),
              MAX = max(LERF_SUB$ADJVAL),
              SHAPIRO_NORM = SHAPIRO_NORM,
              SHAPIRO_LOG = SHAPIRO_LOG,
              CV = sd(LERF_SUB$ADJVAL)/mean(LERF_SUB$ADJVAL),
              GRUBBS = GRUBBS$p.value,
              GRUBBSLOG = GRUBBSLOG$p.value,
              GRUBBS_OUT = GRUBBS_OUT,
              GRUBBSLOG_OUT = GRUBBSLOG_OUT,
              ND_METHOD = ND_METHOD,
              START_DATE = LERF_STARTDATE,
              ACRIT = ALPHA_CRIT_LERF,
              TCRIT = TCRIT,
              CMDW = CMDW,
              CMUP = CMUP,
              NCOMP = LERF_NCOMP)
  #-----------------------------------------------------------#

  #-----------------------------------------------------------#
  #--Output Matrix--#
  OUT  <- rbind(OUT, OUTPUT_SUM)
  #-----------------------------------------------------------#
 }
 #-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Export output matrix--#
FILE <- paste0('Output/HANFORD-CRITICAL_MEANS-2017_',DATE,'.csv')
```

```
write.table(OUT,FILE, sep = ",", row.names = FALSE)
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--This script calculates the Intrawell TOC Limits for Hanford RCRA Area 1324-N/A & 1325-N for CY2017
#--Script written by: Erica DiFilippo (SSP&A) - modified from ECF-HANFORD-13-0013, REV. 0
#--R Version: 3.1.3
#--Package NADA version: 1.5-6
#--Package data.table version: 1.8.10
#--Package lawstat version: 2.5
#--Package outliers version: 0.14
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Set working directory--#
setwd("Z:/1393_HANFORD_FY2017/094 - RCRA CRITICAL MEANS")
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Load Libraries--#
library(data.table)
library(lawstat)
library(NADA)
library(outliers)
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Import User-Defined Functions--#
source('R_Functions/readCHEMHEIS.R')
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Read in Data from Text file Downloads from Hanford Databases--#
DATA1 <- readCHEMHEIS('Data/Data Pull - 01122017/qryChemHEIS1.txt')
DATA2 <- readCHEMHEIS('Data/Data Pull - 01122017/qryChemHEIS2.txt')
DATA <- rbind(DATA1,DATA2)
RCRASITES <- fread("Data/2016_Updated_RCRA_GW_Monitoring_Well_List_Modified_02022016 - recieved from ALee - 1-24-2017.csv",
header=TRUE)
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Format Sample Dates--#
DATA[,EVENT := as.POSIXct(EVENT,format='%m/%d/%Y %H:%M',tz='UTC')]
DATA[,EVENT := as.Date(EVENT,format='%Y-%m-%d')]
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Subset by Analyte--#
AN <- c('pH Measurement','Specific Conductance','Total organic halides','Total organic carbon')
DATA <- subset(DATA,DATA$ANALYTE %in% AN)
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Import RCRA Site Closure Samples--#
CLOS <- fread('Data/ClosureSamples_01302017.csv')
CLOS[,EVENT := as.POSIXct(Date_Collected,format='%m/%d/%Y',tz='UTC')]
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Import New Data for 699-26-38--#
NEW <- fread('Data/usr438ext30879.csv')
NEW$EVENT <- as.Date(ISOdate(2017,01,05))
NEW$DIL <- 1
NEW$COLLECTION_PURPOSE <- 'VER'
NEW$OWNER_ID <- NA
NEW$DEPTH <- NA
NEW <- subset(NEW,select=c('WELL_NAME','EVENT','FILTERED_FLAG','STD_CON_LONG_NAME','STD_VALUE_RPTD',
              'STD_ANAL_UNITS_RPTD','LAB_QUALIFIER','REVIEW_QUALIFIER',
              'VALIDATION_QUALIFIER','DIL','MEDIA','COLLECTION_PURPOSE',
              'OWNER_ID','METHOD_NAME','ReviewDate','DEPTH','STD_REPORTING_LIMIT'))
```

```
setnames(NEW,names(NEW),names(DATA))
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Add New Data--#
DATA <- rbind(DATA,NEW)
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Remove Closure Samples--#
DATA$MATCH <- paste0(DATA$NAME,'-',DATA$EVENT)
CLOS$MATCH <- paste0(CLOS$Well,'-',CLOS$EVENT)
DATA <- subset(DATA,!DATA$MATCH %in% CLOS$MATCH)
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Drop wells identified but not used--#
RCRASITES <- subset(RCRASITES, Use == TRUE )
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Merge Sample Data and Well Info Data--#
setkey(DATA,NAME)
setkey(RCRASITES,WELL_NAME)
DATA <- RCRASITES[DATA,allow.cartesian=TRUE]
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Subset Data for LLWMA-3 Only--#
DATA <- subset(DATA,Site %in% c('116-N-3 (1325-N)','120-N-1 and 120-N-2 (1324-N/NA)') & LOC == 'DOWN')
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Identify nonDetects; TRUE indicates nondetect--#
DATA[,NDS := FALSE]
DATA[grep("U",LABQ),NDS := TRUE]
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Based on discussions censoring will be done base on review_qualifiers indicate samples
#--to be dropped because of review qualifiers--#
DATA <- subset(DATA,!REVIEWQ %in% c("Y","R","F","Q","QH"))
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--use only data from 'routine' collection purpose--#
DATA <- DATA[DATA$COLLECTION_PURPOSE %in% c("R","VER"),]
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Calculating Summary Statistics for each Well by Sample Date (1 sample per well per
#--sample date, taking the mean of all measurements)--#
DATA_SUM <- data.table(DATA)[,list(N_NDS=sum(NDS),
                        N_SAMPLE=length(NDS),
                        PROPND=sum(NDS)/length(NDS),
                        MEAN_REPORTED=mean(VAL),
                        DETLIMIT=min(VAL),
                        MEAN_DETECTS=mean(VAL[!NDS]),
                        SD_DETECTS=sd(VAL[!NDS]),
                        CV_DETECTS=sd(VAL[!NDS])/mean(VAL[!NDS])),
                    by=c("Site","LOC","WELL_NAME","EVENT","ANALYTE")]
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Identify nonDetects; TRUE indicates nondetect for Summary Dataset--#
DATA_SUM[,NDS := PROPND==1]
#-----------------------------------------------------------------#

#-----------------------------------------------------------------#
#--Creating a Column of adjusted values for handling NDs--#
```

```
DATA_SUM[,ADJVAL := MEAN_REPORTED]
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Set Start Date of Analysis--#
DATA_SUM <- DATA_SUM[EVENT >= as.Date(ISOdate(2012,07,01))]
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Creating data frame to place results for exporting--#
OUT <- NULL
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Loop through all Analytes--#
ANALYTES <- sort(unique(DATA_SUM$ANALYTE))
SITES <- sort(unique(DATA$Site))
for(j in 1:length(SITES)){

 SUB <- DATA_SUM[Site == SITES[j]]

 for(i in 1:length(ANALYTES)) {

 #-----------------------------------------------------------#
 #--Subsetting dataset by Site--#
 DATA_SUM_SUB <- SUB[ANALYTE==ANALYTES[i]]
 #-----------------------------------------------------------#

 #-----------------------------------------------------------#
 #--Determine Methodology for Handling Non-Detects--#
 if(mean(DATA_SUM_SUB$PROPND) <= 0.1){ND_METHOD <- "HALF.RL"} else {ND_METHOD <- "ROS"}

  #--Substitution Method (1/2 DL)--#
  if(ND_METHOD == "HALF.RL"){
   DATA_SUM_SUB[,ADJVAL := MEAN_REPORTED]
   DATA_SUM_SUB$ADJVAL[DATA_SUM_SUB$PROPND==1] <-
DATA_SUM_SUB$MEAN_REPORTED[DATA_SUM_SUB$PROPND==1]/2}

  #--Regression on Order Statistics (ROS) Method--#
  if(ND_METHOD == "ROS"){
   DATA_SUM_SUB[,ADJVAL := MEAN_REPORTED]
   DATA_ROS <- ros(obs=DATA_SUM_SUB$ADJVAL,censored=DATA_SUM_SUB$PROPND==1,forwardT="log",reverseT="exp")
   DATA_SUM_SUB <- DATA_SUM_SUB[order(DATA_SUM_SUB$ADJVAL),]
   DATA_SUM_SUB$ADJVAL = DATA_ROS[14]}
 #-----------------------------------------------------------#

 #-----------------------------------------------------------#
 #--Calculate Normality for the Pooled Dataset--#
 if (ANALYTES[i] == 'pH Measurement'){
  SHAPIRO <- try(shapiro.test(DATA_SUM_SUB$MEAN_REPORTED)$p.value, silent=TRUE)
 } else {
  SHAPIRO <- try(shapiro.test(log(DATA_SUM_SUB$MEAN_REPORTED))$p.value, silent=TRUE)
 }
 #-----------------------------------------------------------#

 #-----------------------------------------------------------#
 #--Levene's Test--#
 if (ANALYTES[i] == 'pH Measurement'){
  LEVENE <- lawstat::levene.test(DATA_SUM_SUB$ADJVAL,DATA_SUM_SUB$WELL_NAME,location="mean")
  LEVENE <- LEVENE$p.value
 } else {
  LEVENE <- lawstat::levene.test(log(DATA_SUM_SUB$ADJVAL),DATA_SUM_SUB$WELL_NAME,location="mean")
  LEVENE <- LEVENE$p.value
 }
 #-----------------------------------------------------------#

 #-----------------------------------------------------------#
 #--Anova Test--#
 if (ANALYTES[i] == 'pH Measurement'){
  ANOVA <- anova(lm(ADJVAL~WELL_NAME,DATA_SUM_SUB))[1,5]
```

```
} else {
 ANOVA <- anova(lm(log(ADJVAL)~WELL_NAME,DATA_SUM_SUB))[1,5]
}
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Pooled Variance--#
if (ANALYTES[i] == 'pH Measurement'){
 SD <- data.table(DATA_SUM_SUB)[,list(VAR=var(ADJVAL),
                        SD=sd(ADJVAL),
                        N=length(ADJVAL)),
                    by=c("WELL_NAME",'ANALYTE')]
} else {
 SD <- data.table(DATA_SUM_SUB)[,list(VAR=var(log(ADJVAL)),
                        SD=sd(log(ADJVAL)),
                        N=length(ADJVAL)),
                    by=c("WELL_NAME",'ANALYTE')]
}

SD[,VAR2 := (N-1)*VAR]
VAR_POOLED <- sum(SD$VAR2)/(nrow(DATA_SUM_SUB)-length(unique(DATA_SUM_SUB$WELL_NAME)))
SD_POOLED <- sqrt(VAR_POOLED)
N_POOLED <- length(DATA_SUM_SUB$ADJVAL)
DF_POOLED <- N_POOLED-length(unique(DATA_SUM_SUB$WELL_NAME))
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Outlier Test--#
if (ANALYTES[i] == 'pH Measurement'){
 GRUBBS <- grubbs.test(DATA_SUM_SUB$ADJVAL, type=10, opposite=FALSE, two.sided=FALSE)
} else {
 GRUBBS <- grubbs.test(log(DATA_SUM_SUB$ADJVAL), type=10, opposite=FALSE, two.sided=FALSE)
}
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Summary Statistics--#
STATS <-  data.table(DATA_SUM_SUB)[,list(MEAN=mean(ADJVAL),
                        VAR=var(ADJVAL),
                        SD=sd(ADJVAL),
                        POOLED_SD=SD_POOLED,
                        N=length(ADJVAL),
                        POOLED_N=N_POOLED,
                        LEVENE=LEVENE,
                        SHAPIRO=SHAPIRO,
                        ANOVA=ANOVA,
                        GRUBBS=GRUBBS$p.value,
                        ALPHA=0.01,
                        DF_POOLED=DF_POOLED),
                    by=c('Site',"WELL_NAME",'ANALYTE')]
STATS[,TCRIT := qt(1-0.01/(length(ANALYTES)),df=DF_POOLED)]

if (ANALYTES[i] == 'pH Measurement'){

 STATS[,CMUP_LOG := NA]
 STATS[,CMDW_LOG := NA]
 STATS[,CMUP := MEAN + TCRIT * SD_POOLED * sqrt(1 + 1/N)]
 STATS[,CMDW := MEAN - TCRIT * SD_POOLED * sqrt(1 + 1/N)]

} else {

 STATS[,CMUP_LOG := log(MEAN) + TCRIT * SD_POOLED * sqrt(1 + 1/N)]
 STATS[,CMDW_LOG := NA]
 STATS[,CMUP := exp(CMUP_LOG)]
 STATS[,CMDW := exp(CMDW_LOG)]

}
OUT <- rbind(OUT,STATS)
#-----------------------------------------------------------#
}
```

```
}
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Export Tables--#
DATE <- as.character(Sys.Date())
FILE <- paste0('Output/Hanford-1324-N_1325-N-CM-2017-',DATE,'.csv')
write.table(OUT,FILE,sep=',',row.names=FALSE)
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--This script calculates the Intrawell TOC Limits for Hanford RCRA Area LLWMA-3 for CY2017
#--Script written by: Erica DiFilippo (SSP&A) - modified from ECF-HANFORD-13-0013, REV. 0
#--R Version: 3.1.3
#--Package NADA version: 1.5-6
#--Package data.table version: 1.8.10
#--Package lawstat version: 2.5
#--Package outliers version: 0.14
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Set working directory--#
setwd("Z:/1393_HANFORD_FY2017/094 - RCRA CRITICAL MEANS")
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Load Libraries--#
library(data.table)
library(lawstat)
library(NADA)
library(outliers)
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Import User-Defined Functions--#
source('R_Functions/readCHEMHEIS.R')
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Date of Run for File Exporting--#
DATE <- as.character(Sys.Date())
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Assign any variables--#
ALPHA <- 0.01                          # site-wide error rate
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Read in Data from Text file Downloads from Hanford Databases--#
DATA1 <- readCHEMHEIS('Data/Data Pull - 01122017/qryChemHEIS1.txt')
DATA2 <- readCHEMHEIS('Data/Data Pull - 01122017/qryChemHEIS2.txt')
DATA <- rbind(DATA1,DATA2)
RCRASITES <- fread("Data/2016_Updated_RCRA_GW_Monitoring_Well_List_Modified_02022016 - recieved from ALee - 1-24-2017.csv",
header=TRUE)
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Format Sample Dates--#
DATA[,EVENT := as.POSIXct(EVENT,format='%m/%d/%Y %H:%M:%S',tz='UTC')]
DATA[,EVENT := as.Date(EVENT,format='%Y-%m-%d')]
DATA <- subset(DATA,DATA$EVENT >= as.Date(ISOdate(2004,01,01)))
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Subset by Analyte--#
AN <- c('pH Measurement','Specific Conductance','Total organic halides','Total organic carbon')
DATA <- subset(DATA,DATA$ANALYTE %in% AN)
#-----------------------------------------------------------#
```

```
#-----------------------------------------------------------#
#--Import RCRA Site Closure Samples--#
CLOS <- fread('Data/ClosureSamples_01302017.csv')
CLOS[,EVENT := as.POSIXct(Date_Collected,format='%m/%d/%Y',tz='UTC')]
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Import New Data for 699-26-38--#
NEW <- fread('Data/usr438ext30879.csv')
NEW$EVENT <- as.Date(ISOdate(2017,01,05))
NEW$DIL <- 1
NEW$COLLECTION_PURPOSE <- 'VER'
NEW$OWNER_ID <- NA
NEW$DEPTH <- NA
NEW <- subset(NEW,select=c('WELL_NAME','EVENT','FILTERED_FLAG','STD_CON_LONG_NAME','STD_VALUE_RPTD',
              'STD_ANAL_UNITS_RPTD','LAB_QUALIFIER','REVIEW_QUALIFIER',
              'VALIDATION_QUALIFIER','DIL','MEDIA','COLLECTION_PURPOSE',
              'OWNER_ID','METHOD_NAME','ReviewDate','DEPTH','STD_REPORTING_LIMIT'))
setnames(NEW,names(NEW),names(DATA))
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Add New Data--#
DATA <- rbind(DATA,NEW)
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Remove Closure Samples--#
DATA$MATCH <- paste0(DATA$NAME,'-',DATA$EVENT)
CLOS$MATCH <- paste0(CLOS$Well,'-',CLOS$EVENT)
DATA <- subset(DATA,!DATA$MATCH %in% CLOS$MATCH)
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Drop wells identified but not used--#
RCRASITES <- subset(RCRASITES, Use == TRUE )
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Merge Sample Data and Well Info Data--#
setkey(DATA,NAME)
setkey(RCRASITES,WELL_NAME)
DATA <- RCRASITES[DATA,allow.cartesian=TRUE]
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Subset Data for LLWMA-3 Only--#
DATA <- subset(DATA,Site == 'LLWMA-3' & LOC == 'DOWN')
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Identify nonDetects; TRUE indicates nondetect--#
DATA[,NDS := FALSE]
DATA[grep("U",LABQ),NDS := TRUE]
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Based on discussions censoring will be done base on review_qualifiers indicate samples
#--to be dropped because of review qualifiers--#
DATA <- subset(DATA,!REVIEWQ %in% c("Y","R","F","Q","QH"))
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--use only data from 'routine' collection purpose--#
DATA <- DATA[DATA$COLLECTION_PURPOSE %in% c("R","VER"),]
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Calculating Summary Statistics for each Well by Sample Date (1 sample per well per
#--sample date, taking the mean of all measurements)--#
```

```
DATA_SUM <- data.table(DATA)[,list(N_NDS=sum(NDS),
                    N_SAMPLE=length(NDS),
                    PROPND=sum(NDS)/length(NDS),
                    MEAN_REPORTED=mean(VAL),
                    DETLIMIT=min(VAL),
                    MEAN_DETECTS=mean(VAL[!NDS]),
                    SD_DETECTS=sd(VAL[!NDS]),
                    CV_DETECTS=sd(VAL[!NDS])/mean(VAL[!NDS])),
                  by=c("Site","LOC","WELL_NAME","EVENT","ANALYTE")]
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Identify nonDetects; TRUE indicates nondetect for Summary Dataset--#
DATA_SUM[,NDS := PROPND==1]
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Creating a Column of adjusted values for handling NDs--#
DATA_SUM[,ADJVAL := MEAN_REPORTED]
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Set Start Date of Analysis--#
DATA_SUM <- DATA_SUM[EVENT >= as.Date(ISOdate(2012,07,01))]
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Creating data frame to place results for exporting--#
OUT <- NULL
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Loop through all Analytes--#
ANALYTES <- sort(unique(DATA_SUM$ANALYTE))
for(i in 1:length(ANALYTES)) {

 #-----------------------------------------------------------#
 #--Subsetting dataset by Site--#
 DATA_SUM_SUB <- DATA_SUM[ANALYTE==ANALYTES[i]]
 #-----------------------------------------------------------#

 #-----------------------------------------------------------#
 #--Determine Methodology for Handling Non-Detects--#
 if(mean(DATA_SUM_SUB$PROPND) <= 0.1){ND_METHOD <- "HALF.RL"} else {ND_METHOD <- "ROS"}

  #--Substitution Method (1/2 DL)--#
  if(ND_METHOD == "HALF.RL"){
   DATA_SUM_SUB[,ADJVAL := MEAN_REPORTED]
   DATA_SUM_SUB$ADJVAL[DATA_SUM_SUB$PROPND==1] <-
DATA_SUM_SUB$MEAN_REPORTED[DATA_SUM_SUB$PROPND==1]/2}

  #--Regression on Order Statistics (ROS) Method--#
  if(ND_METHOD == "ROS"){
   DATA_SUM_SUB[,ADJVAL := MEAN_REPORTED]
   DATA_ROS <- ros(obs=DATA_SUM_SUB$ADJVAL,censored=DATA_SUM_SUB$PROPND==1,forwardT="log",reverseT="exp")
   DATA_SUM_SUB <- DATA_SUM_SUB[order(DATA_SUM_SUB$ADJVAL),]
   DATA_SUM_SUB$ADJVAL = DATA_ROS[14]}
 #-----------------------------------------------------------#

 #-----------------------------------------------------------#
 #--Calculate Normality for the Pooled Dataset--#
 if (ANALYTES[i] == 'pH Measurement'){
  SHAPIRO <- try(shapiro.test(DATA_SUM_SUB$MEAN_REPORTED)$p.value, silent=TRUE)
 } else {
  SHAPIRO <- try(shapiro.test(log(DATA_SUM_SUB$MEAN_REPORTED))$p.value, silent=TRUE)
 }
 #-----------------------------------------------------------#

 #-----------------------------------------------------------#
 #--Levene's Test--#
```

```
if (ANALYTES[i] == 'pH Measurement'){
 LEVENE <- lawstat::levene.test(DATA_SUM_SUB$ADJVAL,DATA_SUM_SUB$WELL_NAME,location="mean")
 LEVENE <- LEVENE$p.value
} else {
 LEVENE <- lawstat::levene.test(log(DATA_SUM_SUB$ADJVAL),DATA_SUM_SUB$WELL_NAME,location="mean")
 LEVENE <- LEVENE$p.value
}
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Pooled Variance--#
if (ANALYTES[i] == 'pH Measurement'){
 SD <- data.table(DATA_SUM_SUB)[,list(VAR=var(ADJVAL),
                          SD=sd(ADJVAL),
                          N=length(ADJVAL)),
                     by=c("WELL_NAME",'ANALYTE')]
} else {
 SD <- data.table(DATA_SUM_SUB)[,list(VAR=var(log(ADJVAL)),
                          SD=sd(log(ADJVAL)),
                          N=length(ADJVAL)),
                     by=c("WELL_NAME",'ANALYTE')]
}

SD[,VAR2 := (N-1)*VAR]
VAR_POOLED <- sum(SD$VAR2)/(nrow(DATA_SUM_SUB)-length(unique(DATA_SUM_SUB$WELL_NAME)))
SD_POOLED <- sqrt(VAR_POOLED)
N_POOLED <- length(DATA_SUM_SUB$ADJVAL)
DF_POOLED <- N_POOLED-length(unique(DATA_SUM_SUB$WELL_NAME))
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Outlier Test--#
if (ANALYTES[i] == 'pH Measurement'){
 GRUBBS <- grubbs.test(DATA_SUM_SUB$ADJVAL, type=10, opposite=FALSE, two.sided=FALSE)
} else {
 GRUBBS <- grubbs.test(log(DATA_SUM_SUB$ADJVAL), type=10, opposite=FALSE, two.sided=FALSE)
}
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Summary Statistics--#
STATS <-  data.table(DATA_SUM_SUB)[,list(MEAN=mean(ADJVAL),
                          VAR=var(ADJVAL),
                          SD=sd(ADJVAL),
                          POOLED_SD=SD_POOLED,
                          N=length(ADJVAL),
                          POOLED_N=N_POOLED,
                          LEVENE=LEVENE,
                          SHAPIRO=SHAPIRO,
                          GRUBBS=GRUBBS$p.value,
                          ALPHA=0.01,
                          DF_POOLED=DF_POOLED),
                     by=c("WELL_NAME",'ANALYTE')]
STATS[,TCRIT := qt(1-0.01/(length(ANALYTES)),df=DF_POOLED)]

if (ANALYTES[i] == 'pH Measurement'){

 STATS[,CMUP_LOG := NA]
 STATS[,CMDW_LOG := NA]
 STATS[,CMUP := MEAN + TCRIT * SD_POOLED * sqrt(1 + 1/N)]
 STATS[,CMDW := MEAN - TCRIT * SD_POOLED * sqrt(1 + 1/N)]

} else {

 STATS[,CMUP_LOG := log(MEAN) + TCRIT * SD_POOLED * sqrt(1 + 1/N)]
 STATS[,CMDW_LOG := NA]
 STATS[,CMUP := exp(CMUP_LOG)]
 STATS[,CMDW := exp(CMDW_LOG)]

}
```

```
 OUT <- rbind(OUT,STATS)
 #-----------------------------------------------------------#
}
#-----------------------------------------------------------#

#-----------------------------------------------------------#
#--Export Tables--#
DATE <- as.character(Sys.Date())
FILE <- paste0('Output/Hanford-LLWMA3-CM-2017-',DATE,'.csv')
write.table(OUT,FILE,sep='|',row.names=FALSE)
#-----------------------------------------------------------#
```

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