Update to the 1999 Human Health Risk Assessment for the Frontier Fertilizer Superfund Site, Davis, California

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Introduction

Frontier Fertilizer (the Site) was initially developed in the 1950s and contained facilities that serviced the agricultural industry. The Site was listed on the U.S. Environmental Protection Agency's (EPA's) National Priorities List in 1994. The chemicals of concern (COCs) identified in the 1999 Risk Assessment at the Site are the pesticides 1,2-dibromoethane (EDB), 1,2-dibromo-3-chloropropane (DBCP), 1,2-dichloropropane (DCP), and 1,2,3-trichloropropane (TCP), which were used as soil fumigants. Carbon tetrachloride (CCl₄) also was used as a grain fumigant, and the source appears to be separate from the pesticides. The Site contains contaminated soil and a groundwater plume that extends in a northerly direction beyond the remainder parcel under residential housing.

The California Department of Toxic Substances Control (DTSC) installed a groundwater extraction and treatment system in 1993. EPA upgraded the system in 1995. A human health risk assessment (HHRA) was completed for the Site in April 1999 (Bechtel, 1999). The Site Record of Decision (ROD) (EPA, 2006), which was signed on September 28, 2006, presents the remedial action objectives (RAOs) and selected remedial actions for the entire Frontier Fertilizer Superfund Site. The in-situ thermal treatment remedial action for source area soil and groundwater was completed in 2012.

The First Five-Year Review Report (EPA, 2012) for the Site was completed in September 2012. One of the issues and recommendations from the 2012 Five-Year Review was that the toxicity value for TCP, which is one of the chemicals of concern (COCs) at the Site, had changed such that the current ROD cleanup goal may not be protective for future beneficial use of groundwater. The purpose of this technical memorandum (TM) is as follows:

- To evaluate the impact of the updated toxicity value on the current ROD cleanup level for TCP (as well as to evaluate changes to toxicity values for other COCs).
- To update the 1999 risk assessment with soil and groundwater data collected after the completion of the source area thermal treatment.
- To evaluate potential groundwater exposure pathways in the remainder parcel.
- To incorporate recent soil vapor characterization results sampled in 2015.
- To provide information for EPA to determine whether building restrictions or institutional controls are required.

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Current and Potential Future Site and Resource Uses

The former operations at the Site were abandoned in 1987. In 2000, EPA removed the warehouses, shops, the "pole barn," a labor camp complex, a tomato grading station, aboveground storage tanks, and underground storage tanks. The warehouse containing the groundwater treatment system is the only building left on-site. The site is securely fenced to prevent access. The Site is in an area zoned for light industrial/business park at the eastern edge of Davis. The nearest residence is approximately 600 feet north of the property boundary.

There are no drinking water wells installed in the S-1, S-2, or A-1 aquifer zones within the plumes contaminated by Site COCs. At present, these zones are not used for drinking water because of their generally low yield (S-1 and S-2) and high total dissolved solids (TDS) (S-1, S-2, and A-1). Even though the shallow groundwater is not currently used for drinking water, shallow groundwater at the Site is designated as having the beneficial use of potentially providing municipal and domestic water supply pursuant to the Water Quality Control Plan for the Sacramento River and San Joaquin River Basins, Fourth Edition (Basin Plan) (Regional Water Quality Control Board, 1998). This drinking water pathway is hypothetical, but is evaluated as if an on-site future resident installed a private drinking water well and use the water for drinking, showering, and washing. As such, drinking water standards were identified as RAOs in the ROD. The RAOs developed for Site groundwater are intended to protect potential future beneficial uses. Groundwater currently used for the public water supply comes from the A-2 aquifer found at depths greater than 180 feet below ground surface (bgs). This aquifer does not contain Site contaminants. The nearest drinking water supply well (CD32) is located southwest of the Site and withdraws water from depths greater than 700 feet bgs.

Data Included in the HHRA Update

A list of the soil, off-site groundwater, and on-site and remainder parcel groundwater sample locations used in this HHRA update is provided in Tables 1 through 3 and Figures 1 through 3. These data include the following:

- One soil exposure area (AOC 1) soil collected after thermal treatment (at eight locations, 19 soil samples were collected from depths between 1 and 13 feet below ground surface).
- Groundwater data collected from December 2012 through September 2013 were included in the HHRA update from two groundwater exposure areas:
 - On-site source area (post-thermal treatment samples) and remainder parcel
 - Off-site (quarterly groundwater monitoring events)

In addition, soil gas data from samples collected between July 6 and 9, 2015, at 14 locations were used to evaluate the vapor intrusion pathway for the on-site and remainder parcel. The locations are shown on Figure 3-1 of the Soil Gas Investigation Results Frontier Fertilizer Superfund Site Report (CH2M HILL, 2015).

Data Processing Procedures

The following rules were used to identify data for use in the post-thermal treatment HHRA:

- Estimated values (flagged with a "J" qualifier) were treated as detected concentrations.
- Data qualified as rejected (flagged "R") were not used in the HHRA.
- For duplicate samples, the following procedures were applied:
 - If there were two detections, the maximum of the two concentrations was used.
 - If there was one detection and one nondetection, the detected value was used.
 - If there were two nondetects, the minimum of the two concentrations was used.

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Exposure Pathways Evaluated

Based on the current and potential future land uses, the 1999 HHRA identified the following exposure scenarios and also computed associated risks for the following:

- Off-site current residents in the Mace Ranch residential area: The only potential exposure pathway identified in the 1999 HHRA for this scenario was indoor air vapor intrusion. Groundwater samples from the S-1 aguifer zone were used to evaluate the indoor air pathway.
- Hypothetical on-site future residents living at the source area: Within the 11.43-acre parcel, potential exposure pathways evaluated include indoor air vapor inhalation, outdoor vapor inhalation, direct contact with soils/dust, home gardening exposure, and domestic use of groundwater (i.e., drinking, showering, and washing activities). Groundwater samples from the S-2 aquifer zone were used to evaluate hypothetical domestic use of groundwater exposure.
- Hypothetical on-site future workers: Potential exposure pathways evaluated include indoor air vapor inhalation, outdoor vapor inhalation, and direct contact with soils/dust (includes soil ingestion, dust inhalation, and dermal contact).

These same exposure scenarios were evaluated in this HHRA update. The remainder parcel, which is an additional exposure area that was not included in the 1999 HHRA, was evaluated for indoor vapor intrusion and domestic use of groundwater in this HHRA update.

Exposure Point Concentrations

For soil and groundwater, the 95 percent upper confidence limits (95 UCLs) on the mean concentrations were used as the site-specific exposure point concentrations (EPCs). The 95 UCLs were calculated using EPA's ProUCL (Version 5.0.00) software tool (EPA, 2013) for soil in the on-site exposure area and for groundwater in each of the two groundwater exposure areas. For the groundwater direct contact exposure pathway (i.e., domestic use of groundwater), data from the S-2 aquifer zone within each exposure area were used. To account for variation in concentration over the last year and differences in frequency of sampling, average concentrations over the last four quarters in each well were calculated for each chemical of potential concern (COPC) before the 95 UCLs for that exposure area were generated.

Some chemicals such as aldrin and dieldrin were not analyzed for in the post-treatment sampling data; therefore, the EPCs for these COCs from the 1999 HHRA were used. This conservatively assumes that the levels of these persistent organic pesticides in soil have not changed over time.

For the vapor intrusion pathway, EPCs were estimated directly from the 2015 soil vapor sampling data for the on-site and remainder parcel, and EPCs were estimated from groundwater data from the S-1 (shallowest) aquifer zone for the off-site exposure area. Maximum groundwater concentrations from the off-site exposure area were used as EPCs to evaluate vapor intrusion instead of aggregating the data. Because the S-1 aquifer near the post-thermal treatment area was still exhibiting decreasing groundwater concentrations as a result of residual heating, only the third quarter 2013 results were used for wells AW-2A, MW-7A, MW-7B, X-1A, and X-6A. For evaluation of the vapor intrusion pathway at the on-site and remainder parcel, location-specific risks were estimated for each of the 14 locations sampled, using data from the shallow monitoring probes, where samples were collected at a depth of 6 feet bgs. For the 10 sample locations where split soil gas samples were taken, results from the most sensitive analyses by American Analytics using Low-Level TO-15 SIM were considered most reliable and preferentially used for estimation of risks.

Summary statistics for soil, S-1 aquifer zone wells, and S-2 aquifer zone wells are provided in Tables 4 through 6, respectively. Location-specific soil gas data collected from 6 feet bgs are provided in Table 7.

Calculation of Vapors into Buildings

The COCs evaluated in the 1999 Risk Assessment for vapor intrusion include EDB, DCP, TCP, and CCl₄; these VOCs evaporate at a relatively fast rate. If they are present in groundwater, the vapor produced upon evaporation may rise through the soil and eventually reach the atmosphere above the soil. If a building is located over the contaminated groundwater, then the vapors may collect under the building floor and move laterally until they reach the edge of the floor. The vapors may then move vertically toward the ground surface and enter the atmosphere, if the vapors are not impeded by other barriers. If there are cracks in the floor, the vapors may enter the building through the cracks. The rate of evaporation depends on the vapor pressure of the compound and the temperature of the groundwater. The rate that the vapor moves up through the soil depends on several factors, including the size of the spaces between the soil particles (porosity) and the moisture content of the soil. The amount of vapor entering and remaining in the building depends on several factors, including the distance between the chemical source and the building floor, the area and thickness of the floor, the width of the cracks in the floor, and the building ventilation rate.

For the off-site exposure area, DTSC's Screening-Level Model for Groundwater Contamination (updated in December 2014), a modified version of EPA's Johnson and Ettinger (J&E) vapor intrusion model, was used to calculate the potential concentration of a chemical vapor in a building using maximum concentrations in groundwater from this exposure area. DBCP was not detected in the shallow groundwater (S-1 aquifer zone); therefore, it was not included in the off-site exposure area vapor intrusion evaluation.

For the on-site and remainder parcel, DTSC's Screening-Level Model for Soil Gas Contamination (updated in December 2014) was used to calculate indoor air concentrations using location-specific soil gas concentration data from 6 feet bgs. The J&E input information from the baseline risk assessment, including soil type (silty clay) and depth to the water table (21 feet), were used. The J&E input information is identified in Table 8.

Toxicity Assessment

The EPA Regional Screening Levels (RSLs) were used in conjunction with the DTSC-modified values presented in HHRA Note 3, Table 1 and Table 3 (DTSC, 2015). In some cases, the DTSC alternative screening levels are more conservative than the RSLs. For those chemicals, the DTSC-modified values were used. In addition, consistent with Office of Human and Ecological Risk Overview (HERO) recommendation, route-to-route extrapolation between the oral and inhalation exposure pathways was applied where no toxicity value is available for the inhalation route of exposure but where an oral toxicity value is available. Toxicity values are provided in Table 9.

Risk Characterization

For this screening level risk assessment update, the sum of ratios approach as described in the RSL User's Guide was used (EPA, 2015). For cancer risk estimates, the site-specific EPC (as represented by the 95 UCL) for each detected COPC was divided by the corresponding risk-based concentration (RBC). This ratio was then multiplied by the target risk level associated with the RBC to give a chemical-specific excess lifetime cancer risk (ELCR).

Although synergistic or antagonistic interactions might occur between cancer-causing chemicals and other chemicals, information is generally lacking in the toxicological literature to predict quantitatively the effects of these potential interactions. Therefore, cancer risks are treated as additive within an exposure route in this assessment. This approach is consistent with the EPA guidelines on chemical mixtures (EPA, 1986).

The cumulative ELCR for multiple COPCs was computed as the sum of the chemical-specific ELCRs, as shown in the following equation:

$$ELCR = \left[\left(\frac{conc_x}{RBC_x} \times TR_x \right) + \left(\frac{conc_y}{RBC_y} \times TR_y \right) + \left(\frac{conc_z}{RBC_z} \times TR_z \right) \right]$$

Where:

ELCR = cumulative excess lifetime cancer risk

 $Conc_{x..z} = UCL concentration of chemical x..z (milligrams per kilogram [mg/kg])$

 $RBC_{x..z}$ = risk-based concentration of chemical x..z in soil (mg/kg)

 $TR_{x..z}$ = target risk corresponding to $RBC_{x..z}$

For noncancer effects, the likelihood that a receptor will develop an adverse effect is estimated by comparing the predicted level of exposure for a particular chemical (in this case, conservatively represented as the UCL soil concentration) with the highest level of exposure that is considered protective (represented as the RBC). This ratio is termed the hazard quotient (HQ), and the sum of HQs is termed the hazard index (HI).

This evaluation estimates the noncancer HI using the following equation:

$$HI = \left[\left(\frac{conc_x}{RBC_x} \right) + \left(\frac{conc_y}{RBC_y} \right) + \left(\frac{conc_z}{RBC_z} \right) \right]$$

Where:

HI = noncancer hazard index

 $Conc_{x..z}$ = UCL concentration of chemical x..z (mg/kg)

 $RBC_{x..z}$ = risk-based concentration of chemical x..z in soil (mg/kg)

For this cumulative risk evaluation for soil, groundwater, and soil gas, RBCs are represented by EPA industrial and residential RSLs (EPA, 2015) and DTSC HHRA Note 3 (DTSC, 2015) values.

For the purposes of this evaluation, the potential for unacceptable human health risks is identified using the following risk thresholds:

- In interpreting estimates of ELCRs, the EPA under the Superfund program generally considers action to be warranted when the multi-chemical aggregate cancer risk for all exposure routes within a specific exposure scenario exceeds 1×10^{-4} . Action generally is not required for risks falling within 1×10^{-6} and 1×10^{-4} ; however, this is judged on a case-by-case basis (EPA, 1991). Under state guidance, DTSC considers a cancer risk exceeding 1×10^{-6} as a regulatory point of departure value.
- Under both EPA and state guidance, unacceptable noncancer hazard exists if the multi-chemical aggregate noncancer hazard for all exposure routes within a specific exposure scenario exceeds a target noncancer HI of 1.

Tables 10 through 14 provide summaries of the risk and hazard results for both the residential and industrial receptor groups for exposure to soil, groundwater, and soil gas. The risk characterization results are summarized below. Attachment A provides chemical-specific risk and hazard results.

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Residential Risk and Hazard Results

Direct Contact with Soil and Ingestion of Homegrown Produce

Potential exposures to on-site soil are evaluated for a hypothetical resident. Potential routes of exposure to COPCs in soil include incidental ingestion, dermal contact, inhalation of ambient dust and vapors, and ingestion of homegrown vegetables.

The potential cancer risk for a hypothetical future resident exposure to COCs in soil (Table 10) is 7×10^{-6} , which is within EPA's target risk range but exceeds the DTSC point of departure. The noncancer HI is 0.06, which does not exceed the noncancer threshold of 1. The soil exposure pathway that contributes most to the total soil cancer risk estimate is ingestion of homegrown produce, and the primary contributors are aldrin and dieldrin. The estimated risks from exposure to these compounds may be overestimated because the EPCs from the 1999 HHRA were used in the calculations (new data were not available). The post-treatment sampling did not analyze for aldrin and dieldrin due to the low frequency of detection (aldrin was detected seven out of 169 samples, and dieldrin was detected 11 out of 169 samples) during the RI.

The post-treatment risk from soil exposure is an order of magnitude lower than the risk calculated in the baseline risk assessment (9×10^{-5}) for the hypothetical future residential exposure scenario, primarily because of the substantial reduction of VOC levels from the thermal treatment.

Tap Water Exposure

Potential exposures to groundwater are evaluated for hypothetical future residents who may use groundwater for domestic purposes. Potential routes of exposure to COPCs in groundwater include ingestion, dermal contact while showering or bathing, and inhalation of vapors while performing household chores (e.g., washing dishes). Although use of groundwater for domestic purposes is evaluated, it is considered highly unlikely. Contaminant levels vary significantly between three groundwater zones. The shallow zone, called the S-1, extends to approximately 60 feet bgs. The S-2 zone extends from approximately 60 to 90 feet bgs. The A-1 aquifer extends from approximately 90 to 140 feet bgs. Data from wells screened in the S-2 zone were conservatively used to evaluate groundwater used for domestic purposes in this assessment. The drinking water supply for the City of Davis comes from a deeper A-2 aquifer that begins at approximately 180 feet bgs. No contaminants above drinking water standards have been detected in the A-2 aquifer.

Off-site Exposure Area

Potential risk from exposure to groundwater use for hypothetical domestic purposes for the off-site exposure area (Table 11) is 3×10^{-3} , which exceeds both EPA's target range and the DTSC point of departure. The primary contributor to risk is TCP, which contributes 70 percent of the total risk. In the off-site wells, TCP was detected in 3 of 11 samples with a maximum detected concentration of 5.8 micrograms per liter (µg/L) (in well X-7B). The HI for the off-site exposure area is 13, which exceeds the noncancer threshold of 1. The primary contributor is DCP, which contributes 49 percent of the total HI. DCP was detected in three of 11 samples with a maximum concentration of 180 µg/L (in well X-7B).

On-site and Remainder Parcel Exposure Area

Potential risk from exposure to groundwater used for hypothetical domestic purposes for the on-site and remainder parcel (Table 11) is 1×10^{-2} , which exceeds both EPA's target range and the DTSC point of departure. The primary contributor to risk is TCP, which contributes 91 percent of the total risk. In the on-site and remainder parcel wells, TCP was detected in 25 of 32 samples with a maximum detected concentration of 26.3 μ g/L (in well MW-8B). The risk has decreased by more than an order of magnitude since the baseline risk assessment was conducted when the risk was estimated at 8×10^{-1} . The HI for the on-site and remainder

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REVISED FINAL HHRA UPDATE TM ES042914223851SAC/385112 parcel area is 64, which exceeds the noncancer threshold of 1. The primary contributor is DCP, which contributes 71 percent of the total HI. DCP was detected in 22 of 32 samples with a maximum concentration of 1,065 μ g/L (in well MW-8B). The HI has significantly decreased since the baseline risk assessment (HI=11,000).

Vapor Intrusion Exposure

Vapor intrusion is the general term given to the migration of volatile chemicals from subsurface contaminated soils and groundwater into the indoor air spaces of overlying buildings through openings in the building foundation. For the off-site exposure area, groundwater data from wells screened in the S-1 aquifer zone (which extends to a depth of approximately 60 feet bgs) and the DTSC modified J&E groundwater model were used. For the on-site and remainder parcel, DTSC's modified J&E soil gas model was used to calculate indoor air concentrations using location-specific soil gas concentration data from 6 feet bgs. The J&E soil model is no longer endorsed by DTSC or EPA so soil to indoor air was not evaluated in this assessment.

Off-site Exposure Area

Potential risk from residential vapor intrusion exposure for the off-site exposure area (Table 12) is 7×10^{-8} , which is below both EPA's target range and the DTSC point of departure. The risk from vapor intrusion is similar to when the baseline risk assessment was conducted (risk = 6×10^{-7}). The off-site groundwater concentrations for all of the COPCs are currently lower than they were when the baseline risk assessment was conducted. The HI for the off-site exposure area is well below the noncancer threshold of 1.

On-site and Remainder Parcel Exposure Area

The location-specific risks and hazards from potential vapor intrusion exposure for the on-site and remainder parcel for each of the 14 locations sampled are provided in Table 13. The results indicate that none of the 14 locations have risk estimates exceeding EPA's target risk range, and risk at two locations are slightly above the DTSC point of departure. The primary contributor to risk at locations CH-027 and CH-036 is TCP, which contributes 99 percent to the total risk. The calculated risk from vapor intrusion has substantially decreased since the baseline risk assessment was conducted (risk = 3×10^{-4}). The on-site and remainder parcel groundwater concentrations are lower than they were in 1999 when the baseline risk assessment was conducted. The residential HI estimates for the on-site and remainder parcel are well below the noncancer threshold of 1. The HI has significantly decreased since the baseline risk assessment was conducted (HI = 24).

Industrial Risk and Hazard Results

Soil Exposure - Direct Contact

Potential exposures to soil (1 to 13 feet bgs) are evaluated for an industrial worker. Potential routes of exposure to COPCs in soil include incidental ingestion, dermal contact, and inhalation of ambient dust and vapors.

The potential cancer risk for an industrial worker (Table 10) is 5×10^{-7} , which is below both EPA's target risk range and the DTSC point of departure. The post-treatment risk from exposure to soil is much lower than the baseline risk of 3.5×10^{-6} . The noncancer HI is 0.002, which does not exceed the noncancer threshold of 1.

Groundwater Exposure - Vapor Intrusion - Off-site Area

Potential vapor intrusion exposure under an industrial scenario for the off-site area (Table 12) is 1×10^{-8} , which is below both EPA's target range and the DTSC point of departure. The HI for the off-site area is well below the noncancer threshold of 1.

Groundwater Exposure - Vapor Intrusion - On-site and Remainder Parcel

The location-specific risks and hazards from potential vapor intrusion exposure for the on-site and remainder parcel for each of the 14 locations sampled are provided in Table 14. The results indicate that none of the 14 locations have risk estimates exceeding EPA's target risk range or the DTSC point of departure. The calculated risk from vapor intrusion has decreased by more than two orders of magnitude since the baseline risk assessment was conducted (risk = 1×10^{-4}). The HI estimates for the on-site and remainder parcel wells are well below the noncancer threshold of 1. The HI has decreased by more than several orders of magnitude since the baseline risk assessment was conducted (HI = 0.9).

Uncertainties

The estimates of risks and hazards are based on a large number of assumptions about exposure and toxicity. It is important to identify and discuss the uncertainties to put the estimates of risk and hazard in proper perspective. This section addresses the uncertainties associated with the identification of COPCs, development of exposure assumptions, exposure pathways and conditions, and risk characterization.

Uncertainties in the Identification of COPCs

The nature and extent of contamination at the Site was estimated by collecting soil, groundwater, and soil gas samples and analyzing them for chemical substances known to have been released (or suspected of having been released) to the environment by human activities that occurred on the Site. Six investigations have been performed to characterize the nature and extent of contamination of the Site and surrounding area. Three of the investigations focused on groundwater, two focused on both soil and groundwater, and one focused on soil gas. Each investigation sought to fill the data gaps left by the previous investigation. From the beginning, pesticides were the target of the investigations; however, chemical analyses of VOCs, semivolatile organic compounds, pesticides, and metals were also performed. Together, these investigations were comprehensive and reduced the uncertainty that the major site-related contaminants were identified.

There are technological limits to the detection of some COPCs, most notably for the detection of 1,2,3-trichloropropane. Since the start of the Remedial Investigation / Feasibility Study, the advancement in sensitivity of commercial 1,2,3-trichloropropane detection in groundwater has improved the detection capability about two orders of magnitude (from 0.5 to 0.005 µg/L) and has now become widely acceptable. Low level detection methods for 1,2,3-trichloropropane in vapor are less developed than for groundwater, and the reporting limits necessary to achieve some health-conservative risk-based action levels are not commercially available; the most recent sample event used the most sensitive method currently available.

Uncertainties Associated with the Exposure Assessment

Future soil EPCs were assumed to be equal to existing concentrations. This assumption does not account for fate and transport processes likely to occur in the future. Because some of the COPCs are VOCs, the volatiles will likely be released from soil over time; therefore, risk estimates are likely to be overestimated for future exposure scenarios.

For the vapor intrusion evaluation of the off-site exposure area, there is some uncertainty associated with the chemical-specific groundwater-to-indoor air attenuation factors as recommended outputs by EPA's J&E vapor intrusion model. Exposure to indoor air was also evaluated using chemical-specific attenuation factors from the DTSC's modified version of EPA's J&E vapor intrusion model (DTSC, 2014) for residents and industrial workers. If DTSC's more conservative default attenuation factors are used in the calculations, then the results indicate the following:

Potential residential vapor intrusion exposure for the off-site exposure area is 9 x 10⁻⁶, which is within the risk management range but exceeds the point of departure. The HI is 0.01, which does not exceed the noncancer threshold.

REVISED FINAL HHRA UPDATE TM ES042914223851SAC/385112 8 • Potential vapor intrusion exposure under an industrial scenario for the off-site area is 9×10^{-7} , which is below both EPA's target range and the point of departure. The HI of 0.002 for the off-site area is well below the noncancer threshold of 1.

Derivation of chemical concentrations in produce grown for consumption in contaminated soil adds additional uncertainty because limited studies on this transport pathway have been performed. Consequently, exposure point concentrations in produce for the hypothetical future resident may be underor overestimated. In addition, because aldrin and dieldrin data were not available after thermal treatment, pre-treatment data for these compounds were used. Any attenuation of these compounds would result in a reduction in exposure and risk.

It is not certain whether people who work on-site after the industrial park is developed will be exposed in the manner assumed in the risk assessment. For example, if the industrial park is covered with buildings, paved areas, and landscaping consisting of well-maintained grassy areas bordered by shrubs and trees, exposure of people who work at the site will be limited to chemical vapors released from the soil into the indoor and outdoor air. Exposure by soil ingestion, dermal contact with soil, and inhalation of dust will be minimal or nonexistent.

Uncertainties Associated with Risk Characterization

In the risk characterization, the assumption was made that the total risk of developing cancer from exposure to site contaminants is the sum of the risk attributed to each individual contaminant. Likewise, the potential for the development of noncancer adverse effects is the sum of the noncarcinogenic risks estimated for exposure to each individual contaminant. This approach is consistent with EPA guidance; however, the approach does not account for the possibility that constituents act synergistically or antagonistically. Therefore, there is uncertainty associated with the estimated cumulative risks for carcinogens and HIs for noncarcinogens.

For this evaluation, the noncarcinogenic risks from all COPCs were summed to obtain the HI. The HQs for individual chemicals were not segregated based on target organs; therefore, the HI could overestimate the potential for one type of noncancer effect because all COPCs do not affect the same target organ. However, because individual chemical HQs exceeded unity, this uncertainty is considered minimal.

The risk estimates for the indoor air pathway using the 2015 soil vapor sampling data for the on-site and remainder parcel are considered superior when compared to the previous approach in the 1999 HHRA, where this pathway was evaluated using groundwater data. However, there is still some uncertainty associated with the risk characterization for soil vapor (e.g., spatial and temporal variability of concentrations and use of a default soil vapor-to-indoor air attenuation factor). To provide an additional line of evidence supporting the conclusions for the indoor air pathway for the on-site and remainder parcel, the 2015 results were also evaluated using EPA's Vapor Intrusion Screening Level (VISL) Calculator (EPA, 2014). This approach reflects EPA's most current methodology for screening site vapor risks. All default assumptions were retained in the calculator with the exception of the toxicity values for CCl₄, where the more conservative DTSC values were used.

The location-specific results of the VISL screening evaluation of soil vapor concentrations for the on-site and remainder parcel are provided in Table A-9 of Attachment A. The results indicate that none of the 14 locations have residential risk estimates exceeding EPA's target risk range or the DTSC point of departure, and the residential HI estimates are well below the noncancer threshold of 1. This uncertainty evaluation supports the conclusions provided in the risk characterization for soil vapor.

Summary

Reduced concentrations of COPCs in soil indicate that the thermal treatment has been successful. Risks for both residential and industrial receptors have been significantly lowered. However, risks from exposure to groundwater continue to be above both EPA and DTSC target levels. Even though the shallow groundwater

is not currently used for drinking water, hypothetical domestic use exposure to groundwater exceeds target levels in the on-site and remainder parcel and off-site exposure areas. Potential risks from vapor intrusion exposure are below or within the EPA target risk range and below the noncancer threshold in both the off-site exposure area and the on-site and remainder parcel exposure area. Risk at two of 14 soil gas sample locations slightly exceeds the DTSC point of departure in the on-site and remainder parcel exposure area. Due to risks exceeding the point of departure, as well as uncertainty surrounding both historic property use and analytical methods, restrictions consisting of institutional controls to prevent future residential, day care, and hospital use are recommended. Therefore, institutional controls (restricting the on-site and remainder parcel exposure area to industrial site use, including building requirements) are justified.

References

Bechtel. 1999. Baseline Risk Assessment Report, Frontier Fertilizer Superfund Site.

California Department of Toxic Substances Control (DTSC). 2014. *Screening Level Model for Groundwater Contamination*. http://www.dtsc.ca.gov/SiteCleanup/Vapor Intrusion.cfm

California Department of Toxic Substances Control (DTSC). 2015. HHRA Note 3. DTSC recommended methodology for use of U.S. EPA Regional Screening Levels (RSLs) in the Human Health Risk Assessment process at hazardous waste sites and permitted facilities. http://www.dtsc.ca.gov/assessingrisk/humanrisk2.cfm

California Regional Water Quality Control Board Central Valley Region. 1998. Water Quality Control Plan for the Sacramento River and San Joaquin River Basins. Fourth Edition. September.

CH2M HILL. 2015. Soil Gas Investigation Results, Frontier Fertilizer Superfund Site Report.

- U.S. Environmental Protection Agency (EPA). 2015. *Regional Screening Levels (RSLs) for Chemical Contaminants at Superfund Sites*. June. http://www.epa.gov/region09/superfund/prg/index.html U.S. Environmental Protection Agency (EPA). 2014. Vapor Intrusion Screening Level (VISL) Calculator, User's Guide. Currently available online at: http://www.epa.gov/vaporintrusion/vapor-intrusion-screening-level-calculator-user-guide
- U.S. Environmental Protection Agency (EPA). 2013. *Software for Calculating Upper Confidence Limits (UCLs) ProUCL Version 5.0* [Online] http://www.epa.gov/osp/hstl/tsc/software.htm#
- U.S. Environmental Protection Agency (EPA). 2012. First Five-Year Review Report for Frontier Fertilizer Superfund Site. Yolo County, California. September.
- U.S. Environmental Protection Agency (EPA). 2006. *Record of Decision, Soil and Groundwater Frontier Fertilizer Superfund Site*. September.
- U.S. Environmental Protection Agency (EPA). 1991. *Role of the Baseline Risk Assessment in Superfund Remedy Selection Decisions*. OSWER Directive 9355.0-30. April 22.
- U.S. Environmental Protection Agency (EPA). 1986. *Guidelines for the Health Risk Assessment of Chemical Mixtures*. Federal Register Vol. 51 34014-34041. September 24, 1986.



TABLE 1
Soil Samples Used in the Risk Assessment Update
Update to the 1999 Human Health Risk Assessment for the Frontier Fertilizer Superfund Site, Davis, California

Location ID	Sample ID	Sample Date	Sample Type	Top Depth (feet)
SB-06	SB06-A655-02	9/9/2013	N	1
	SB06-A655-04	9/9/2013	N	4
	SB06-A655-10	9/9/2013	N	1
SB-07	SB07-A655-02	8/26/2013	N	4
	SB07-A655-05	8/26/2013	N	9
SB-08	SB08-A655-02	9/5/2013	N	1
	SB08-B655-06	9/5/2013	FD	1
	SB08-A655-06	9/5/2013	N	4
	SB08-A655-10	9/5/2013	N	9
SB-09	SB09-A655-02	8/28/2013	N	5
	SB09-A655-05	8/28/2013	N	1
	SB09-A655-10	8/28/2013	N	5
SB-10	SB10-A655-02	9/6/2013	N	9
	SB10-A655-04	9/6/2013	N	1
	SB10-A655-10	9/6/2013	N	9
SB-11	SB11-A655-10	9/10/2013	N	4
	SB12-B655-02	8/30/2013	FD	1
	SB12-A655-02	8/30/2013	N	4
	SB12-A655-05	8/30/2013	N	9
	SB12-A655-10	8/30/2013	N	10
SB-15	SB15-A655-11	9/9/2013	N	9

FD = field duplicate N = normal sample

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TABLE 2
S-1 Groundwater Samples Used for the Indoor Air Pathway
Update to the 1999 Human Health Risk Assessment for the Frontier Fertilizer Superfund Site, Davis, California

Exposure Area	Zone Code	Location ID	Sample ID	Sample Date	Sample Type
Off-site	S-1	OW-11A	OW11A-A412	12/11/2012	N
			OW11A-A113	3/8/2013	N
			OW11A-A213	6/7/2013	N
			OW11A-A313	9/17/2013	N
Off-site	S-1	OW-12A	OW12A-A412	12/14/2012	N
			OW12A-A113	3/21/2013	N
			OW12A-A213	6/19/2013	N
			OW12A-A313	9/20/2013	N
Off-site	S-1	OW-14A	OW14A-A313	9/10/2013	N
Off-site	S-1	OW-15A	OW15A-A313	9/11/2013	N
Off-site	S-1	OW-16A	OW16A-A313	9/10/2013	N
Off-site	S-1	OW-5A	OW5A-A412	12/10/2012	N
			OW5A-A113	3/12/2013	N
			OW5A-A213	6/18/2013	N
			OW5A-A313	9/13/2013	N
Off-site	S-1	OW-6A	OW6A-A412	12/19/2012	N
			OW6A-A113	3/11/2013	N
			OW6A-A213	6/18/2013	N
			OW6A-A313	9/9/2013	N
Off-site	S-1	OW-7A	OW7A-A412	12/10/2012	N
			OW7A-A113	3/13/2013	N
			OW7A-A213	6/17/2013	N
			OW7A-A313	9/13/2013	N
Off-site	S-1	OW-9A	OW9A-A412	12/18/2012	N
			OW9A-B412	12/18/2012	FD
			OW9A-A113	3/20/2013	N
			OW9A-B113	3/20/2013	FD
			OW9A-A213	6/18/2013	N
			OW9A-A313	9/16/2013	N
Off-site	S-1	X-5A	X5A-A412	12/7/2012	N
			X5A-A113	3/11/2013	N
			X5A-A213	6/11/2013	N
			X5A-A313	9/26/2013	N

^{*}Data not used for vapor intrusion EPC.

FD = field duplicate N = normal sample

TABLE 3
S-2 Groundwater Samples Used for the Drinking Water Pathway
Update to the 1999 Human Health Risk Assessment for the Frontier Fertilizer Superfund Site, Davis, California

Exposure Area	Zone Code	Location ID	Sample ID	Sample Date	Sample Type
Off-site	S-2	OW-11B	OW11B-A412	12/11/2012	N
		OW-11B	OW11B-A113	3/8/2013	N
		OW-11B	OW11B-A213	6/7/2013	N
		OW-11B	OW11B-A313	9/17/2013	N
Off-site	S-2	OW-12B	OW12B-A412	12/14/2012	N
		OW-12B	OW12B-A113	3/21/2013	N
		OW-12B	OW12B-A213	6/19/2013	N
		OW-12B	OW12B-A313	9/20/2013	N
Off-site	S-2	OW-13B	OW13B-A313	9/20/2013	N
Off-site	S-2	OW-14B	OW14A-A313	9/10/2013	N
Off-site	S-2	OW-15B	OW15B-A313	9/11/2013	N
Off-site	S-2	OW-16B	OW16B-A313	9/10/2013	N
Off-site	S-2	OW-20B	OW20B-A412	12/12/2012	N
			OW20B-A113	3/15/2013	N
			OW20B-A213	6/19/2013	N
			OW20B-B213	6/19/2013	FD
			OW20B-A313	9/24/2013	N
			OW20B-B313	9/24/2013	FD
Off-site	S-2	OW-5B	OW5B-A412	12/10/2012	N
			OW5B-A113	3/12/2013	N
			OW5B-A213	6/18/2013	N
			OW5B-A313	9/26/2013	N
Off-site	S-2	OW-7B	OW7B-A412	12/10/2012	N
			OW7B-A113	3/13/2013	N
			OW7B-A213	6/17/2013	N
			OW7B-A313	9/13/2013	N
Off-site	S-2	OW-9B	OW9B-A412	12/18/2012	N
			MW9B-A113	3/12/2013	N
			OW9B-A213	6/18/2013	N
			OW9B-B213	6/18/2013	FD
			OW9B-A313	9/16/2013	N
Off-site	S-2	X-7B	X7B-A412	12/11/2012	N
Remainder	S-2	AW-2B	AW2B-A412	12/17/2012	N
			AW2B-A113	3/21/2013	N
			AW2B-A213	6/14/2013	N
			AW2B-A313	9/30/2013	N

TABLE 3
S-2 Groundwater Samples Used for the Drinking Water Pathway
Update to the 1999 Human Health Risk Assessment for the Frontier Fertilizer Superfund Site, Davis, California

Exposure Area	Zone Code	Location ID	Sample ID	Sample Date	Sample Type
On-site	S-2	BB-1	BB1-A654	8/23/2013	N
			BB1-B654	8/23/2013	FD
On-site	S-2	BB-2	BB2-A654	8/23/2013	N
On-site	S-2	BB-3	BB3-A654	8/23/2013	N
On-site	S-2	CC-1	CC1-A654	8/22/2013	N
On-site	S-2	CC-4	CC4-A654	8/21/2013	N
On-site	S-2	DD-1	DD1-A654	8/21/2013	N
			DD1-B654	8/21/2013	FD
On-site	S-2	DD-4	DD4-A654	8/21/2013	N
On-site	S-2	DD-5	DD5-A654	9/12/2013	N
On-site	S-2	EE-2	EE2-A654	8/23/2013	N
On-site	S-2	EE-4	EE4-A654	8/23/2013	N
On-site	S-2	EE-5	EE5-A654	8/23/2013	N
Remainder	S-2	FF-2	FF2-A654	8/22/2013	N
Remainder	S-2	GG-1	GG1-A654	9/13/2013	N
Remainder	S-2	GG-2	GG2-A654	9/12/2013	N
Remainder	S-2	GG-4	GG4-A654	9/13/2013	N
On-site	S-2	MW-3B	MW3B-A313	9/20/2013	N
On-site	S-2	MW-5C	MW5C-A113	3/19/2013	N
Remainder	S-2	MW-11B	MW11A-A412	12/14/2012	N
			MW11B-B412	12/14/2012	FD
			MW11A-A113	3/15/2013	N
			MW11B-A113	3/15/2013	FD
			MW11A-B213	6/21/2013	N
			MW11B-B213	6/21/2013	FD
			MW11B-A313	9/19/2013	N
			MW11B-B313	9/19/2013	FD
Remainder	S-2	MW-12B	MW12B-A412	12/12/2012	N
			MW12B-A113	3/12/2013	N
			MW12B-A213	6/19/2013	N
			MW12A-A313	9/19/2013	N
Remainder	S-2	MW-8B	MW8B-A412	12/11/2012	N
			MW8B-A113	3/12/2013	N
			MW8B-A213	6/21/2013	N
			MW8B-A313	9/17/2013	N

TABLE 3
S-2 Groundwater Samples Used for the Drinking Water Pathway
Update to the 1999 Human Health Risk Assessment for the Frontier Fertilizer Superfund Site, Davis, California

Exposure Area	Zone Code	Location ID	Sample ID	Sample Date	Sample Type
Remainder	S-2	MW-9B	MW9B-A113	3/12/2013	N
			MW9B-A313	9/25/2013	N
Remainder	S-2	OW-3B	OW3B-A412	12/13/2012	N
			OW3B-A113	3/14/2013	N
			OW3B-A213	6/20/2013	N
			OW3B-A313	9/19/2013	N
Remainder	S-2	OW-4B	OW4B-A412	12/13/2012	N
			OW4B-A113	3/14/2013	N
			OW4B-A213	6/20/2013	N
			OW4B-A313	9/18/2013	N
			OW4B-B313	9/18/2013	FD
On-site	S-2	PC-2B	PC2B-A412	12/18/2012	N
			PC2B-A113	3/19/2013	N
			PC2B-A213	6/5/2013	N
			PC2B-A313	9/18/2013	N
Remainder	S-2	X-10B	X10B-A412	12/19/2012	N
			X10B-A113	3/14/2013	N
			X10B-A213	6/21/2013	N
			X10B-A313	9/18/2013	N
			X10B-B313	9/18/2013	FD
Remainder	S-2	X-1B	X1B-A412	12/18/2012	N
			X1B-A113	3/20/2013	N
			X1B-A213	6/14/2013	N
			X1B-A313	9/23/2013	N
Remainder	S-2	X-2B	X2B-A412	12/19/2012	N
			X2B-A113	3/21/2013	N
			X2B-A213	6/21/2013	N
			X2B-A313	9/17/2013	N
Remainder	S-2	X-3B	X3B-A412	12/13/2012	N
			X3B-A113	3/21/2013	N
			X3B-A213	6/21/2013	N
			X3B-A313	9/18/2013	N
Remainder	S-2	X-4B	X4B-A412	12/19/2012	N
			X4B-A113	3/21/2013	N
			X4B-A213	6/21/2013	N
			X4B-A313	9/25/2013	N
			X4B-B313	9/25/2013	FD

TABLE 3
S-2 Groundwater Samples Used for the Drinking Water Pathway
Update to the 1999 Human Health Risk Assessment for the Frontier Fertilizer Superfund Site, Davis, California

Exposure Area	Zone Code	Location ID	Sample ID	Sample Date	Sample Type
Remainder	S-2	X-6B	X6B-A412	12/17/2012	N
			X6B-A113	3/20/2013	N
			X6B-A213	6/14/2013	N
			X6B-B213	6/14/2013	FD
			X6B-A313	9/26/2013	N
			X6B-B313	9/26/2013	FD
			X7B-A113	3/8/2013	N
			X7B-A213	6/7/2013	N
			X7B-A313	9/17/2013	N
Remainder	S-2	X-8B	X8B-A412	12/13/2012	N
			X8B-A113	3/14/2013	N
			X8B-A213	6/17/2013	N
			X8B-A313	9/19/2013	N

TABLE 4
Summary Statistics and Exposure Point Concentrations for Soil Samples Used in the Post-removal Human Health Risk Assessment Update
Update to the 1999 Human Health Risk Assessment for the Frontier Fertilizer Superfund Site, Davis, California

СОРС	Number of Samples	Number of Detects	Percent Detected	Minimum Detected Concentration (μg/kg)	Maximum Detected Concentration (μg/kg)	Mean (μg/kg)	Median (μg/kg)	95% UCL (μg/kg)	EPC (μg/kg)	EPC Basis
1,2,3-Trichloropropane	19	4	21.05%	0.11	0.57	0.26	0.18	0.159	0.159	95% KM (t) UCL
1,2-Dibromoethane	19	2	10.53%	0.028	0.034	0.031	0.031	0.0298	0.0298	95% KM (t) UCL
1,2-Dichloropropane	19	1	5.26%	7	7	7	7	N/A	7	Maximum

μg/kg = microgram(s) per kilogram

COPC = chemical of potential concern

EPC = exposure point concentration

KM = Kaplan Meier

UCL = upper confidence limit on the mean

TABLE 5
Summary Statistics and Exposure Point Concentrations for S-1 Aquifer Zone Groundwater Samples Used in the Post-removal Human Health Risk Assessment Update
Update to the 1999 Human Health Risk Assessment for the Frontier Fertilizer Superfund Site, Davis, California

Exposure Area	СОРС	Number of Samples	Number of Detects	Percent Detected	Minimum Detected Concentration (μg/L)	Maximum Detected Concentration (µg/L)
On-site and	1,2,3-Trichloropropane	62	38	61.29%	0.003	160 (33) ^a
Remainder Parcel	1,2-Dibromoethane	71	24	33.80%	0.004	53 (8.6) a
	1,2-Dichloropropane	71	40	56.34%	0.059	890 (230) ^a
	Carbon tetrachloride	71	15	21.13%	0.058	1.9
Off-site	1,2,3-Trichloropropane	31	8	25.81%	0.003	0.019
	1,2-Dibromoethane	31	3	9.68%	0.003	0.039
	1,2-Dichloropropane	31	1	3.23%	0.085	0.085
	Carbon tetrachloride	31	4	12.90%	0.085	0.6

^{*}Concentrations in parentheses were used for the vapor intrusion pathway. Because the S-1 aquifer near the post-thermal treatment area was still exhibiting decreasing groundwater concentrations as a result of residual heating, only the third quarter 2013 results were used for wells AW-2A, MW-7A, MW-7B, X-1A, and X-6A.

μg/L = microgram(s) per liter

COPC = chemical of potential concern

TABLE 6
Summary Statistics and Exposure Point Concentrations for S-2 Aquifer Zone Groundwater Samples Used in the Post-removal Human Health Risk Assessment Update
Update to the 1999 Human Health Risk Assessment for the Frontier Fertilizer Superfund Site, Davis, California

Exposure Area	сорс	Number of Samples	Number of Detects	Percent Detected	Minimum Detected Concentration (µg/L)	Maximum Detected Concentration (μg/L)	Mean (μg/L)	Median (μg/L)	95% UCL (μg/L)	EPC (μg/L)	EPC Basis
On-site and	1,1,2,2-Tetrachloroethane	32	0	0.00%	N/A	N/A	N/A	N/A	N/A	N/A	N/A
Remainder Parcel	1,1-Dichloroethylene	32	0	0.00%	N/A	N/A	N/A	N/A	N/A	N/A	N/A
Parcei	1,2,3-Trichloropropane	32	25	78.13%	0.003	26.3	1.62	0.055	9.627	9.627	99% KM (Chebyshev) UCL
	1,2-Dibromo-3-chloropropane	32	7	21.88%	0.006	0.5	0.17	0.053	0.0819	0.0819	95% KM (percentile bootstrap) UCL
	1,2-Dibromoethane	32	5	15.63%	0.00275	13.27	2.703	0.081	0.97	0.97	95% GROS adjusted gamma UCL
	1,2-Dichloroethane	32	9	28.13%	0.07	2.133	0.634	0.24	0.428	0.428	95% KM (t) UCL
	1,2-Dichloropropane	32	22	68.75%	0.1	1065	64.69	0.965	378.2	378.2	99% KM (Chebyshev) UCL
	1,3-Dichloropropane	32	6	18.75%	0.06	1.537	0.454	0.272	0.386	0.386	95% KM (t) UCL
	Benzene	32	12	37.50%	0.083	93	16.53	1.7	12.24	12.24	95% KM (t) UCL
	Carbon tetrachloride	32	12	37.50%	0.11	13.4	3.94	1.22	2.637	2.637	95% KM (t) UCL
	Chloroform	32	15	46.88%	0.089	24	2.231	0.61	2.671	2.671	95% KM (BCA) UCL
	cis-1,3-Dichloropropene	32	3	9.38%	0.22	0.5	0.327	0.26	0.282	0.282	95% KM (t) UCL
	trans-1,3-Dichloropropene	32	0	0.00%	N/A	N/A	N/A	N/A	N/A	N/A	N/A
	Vinyl chloride	32	6	18.75%	0.098	0.25	0.15	0.105	0.2	0.2	95% KM (% bootstrap) UCL
Off-site	1,1,2,2-Tetrachloroethane	11	0	0.00%	N/A	N/A	N/A	N/A	N/A	N/A	N/A
	1,1-Dichloroethylene	11	0	0.00%	N/A	N/A	N/A	N/A	N/A	N/A	N/A
	1,2,3-Trichloropropane	11	3	27.27%	0.017	5.833	2.167	0.65	1.709	1.709	95% KM (t) UCL
	1,2-Dibromo-3-chloropropane	11	0	0.00%	N/A	N/A	N/A	N/A	N/A	N/A	N/A
	1,2-Dibromoethane	11	2	18.18%	1.11	6.075	3.593	3.593	6.075	6.075	Maximum
	1,2-Dichloroethane	11	1	9.09%	0.325	0.325	0.325	0.325	0.325	0.325	Maximum
	1,2-Dichloropropane	11	3	27.27%	0.187	180	63.32	9.775	51.87	51.87	95% KM (t) UCL
	1,3-Dichloropropane	11	1	9.09%	0.47	0.47	0.47	0.47	0.47	0.47	Maximum
	Benzene	11	0	0.00%	N/A	N/A	N/A	N/A	N/A	N/A	N/A
	Carbon tetrachloride	11	2	18.18%	0.2	3.243	1.721	1.721	2.806	2.806	97.5% KM (Chebyshev) UCL
	Chloroform	11	1	9.09%	1.45	1.45	1.45	1.45	1.45	1.45	Maximum

TABLE 6
Summary Statistics and Exposure Point Concentrations for S-2 Aquifer Zone Groundwater Samples Used in the Post-removal Human Health Risk Assessment Update
Update to the 1999 Human Health Risk Assessment for the Frontier Fertilizer Superfund Site, Davis, California

Exposure Area	СОРС	Number of Samples	Number of Detects	Percent Detected	Minimum Detected Concentration (μg/L)	Maximum Detected Concentration (μg/L)	Mean (μg/L)	Median (μg/L)	95% UCL (μg/L)	EPC (μg/L)		EPC Basis
Off-site	cis-1,3-Dichloropropene	11	0	0.00%	N/A	N/A	N/A	N/A	N/A	N/A	N/A	
(continued)	trans-1,3-Dichloropropene	11	0	0.00%	N/A	N/A	N/A	N/A	N/A	N/A	N/A	
	Vinyl chloride	11	1	9.09%	0.04	0.04	0.04	0.04	0.04	0.04	Maximum	

μg/L = microgram(s) per liter

COPC = chemical of potential concern

EPC = exposure point concentration

KM = Kaplan Meier

UCL = upper confidence limit on the mean

TABLE 7

Soil Gas Data to Evaluate Vapor Intrusion Exposure – On-site/Remainder Parcel

Update to the 1999 Human Health Risk Assessment for the Frontier Fertilizer Superfund Site, Davis, California

Analy Location	ysis Method: Analyte: CAS No.: Units:	TO15 1,2,3-Trichloropropane 96-18-4 µg/m³	TO15 1,2-Dibromo-3-chloropropane 96-12-8 μg/m³	TO15 1,2-Dibromoethane (EDB) 106-93-4 μg/m³	TO15 1,2-Dichloropropane 78-87-5 µg/m³	TO15 Carbon Tetrachloride 56-23-5 μg/m³
CH-011-S		0.054 J	0.05 U	0.01 U	0.05 U	0.08 U
CH-011-S		0.15 U	0.24 U	0.19 U	0.11 U	0.16 U
CH-011-S		0.1 =	0.05 U	0.01 U	0.05 U	0.08 U
CH-014-S		0.18 J	0.05 U	0.01 U	0.05 U	0.08 U
CH-014-S		0.15 U	0.24 U	0.19 U	0.11 U	0.16 U
CH-014-S		0.15 U	0.24 U	0.19 U	0.11 U	0.16 U
CH-017-S		0.13 J	0.05 U	0.01 U	0.05 U	0.85 =
CH-017-S		0.21 J	0.24 U	0.19 U	0.11 U	1.2 =
CH-019-S		0.13 J	0.05 U	0.01 U	0.05 U	0.17 =
CH-019-S		0.15 U	0.24 U	0.19 U	0.11 U	0.24 J
CH-019-S		0.16 J	0.24 U	0.19 U	0.11 U	0.26 J
CH-021-S		0.069 J	0.05 UJ	0.01 UJ	0.05 UJ	0.08 UJ
CH-021-S		0.15 U	0.24 U	0.19 U	0.11 U	0.16 U
CH-027-S		0.84 =	0.24 U	0.19 U	9.6 =	0.26 J
CH-027-S		1.3 =	0.24 U	0.19 U	11 =	0.33 =
CH-028-S		0.15 U	0.24 U	0.19 U	0.11 U	0.16 U
CH-029-S		0.41 =	0.24 U	0.19 U	0.11 U	0.16 U
CH-030-S		0.15 U	0.24 U	0.19 U	0.11 U	0.16 U
CH-031-S		0.15 U	0.24 U	0.19 U	0.11 U	3.3 =
CH-032-S		0.24 J	0.24 U	0.19 U	0.11 U	0.18 J
CH-035-S		0.45 =	0.24 U	0.19 U	0.13 J	0.16 U
CH-036-S		1.8 =	0.24 U	0.19 U	0.11 U	0.22 J
CH-037-S		0.15 U	0.24 U	0.19 U	0.11 U	0.23 J

 $\mu g/m^3$ = microgram(s) per cubic meter CAS = Chemical Abstracts Service

EDB = ethylene dibromide

TABLE 8 Input Information, Johnson and Ettinger Screening Models Update to the 1999 Human Health Risk Assessment for the Frontier Fertilizer Superfund Site, Davis, California

Description	Input Value	Units	Source
Contaminant concentration in groundwater	Chemical-specific	μg/L	Site-specific
Depth below grade to bottom of floor	15	cm	Default
Depth below grade to water table	660	cm	Site-specific
Soil type directly above water table	Silty clay	none	Site-specific
Average soil/groundwater temperature	17	degrees centigrade	Site-specific
Vadose zone dry bulk density	1.38	g/cm³	Default for silty clay
Vadose zone total soil porosity	0.481	unitless	Default for silty clay
Vadose zone water-filled soil porosity	0.216	unitless	Default for silty clay

 $\mu g/L$ = microgram(s) per liter g/cm³ = gram(s) per cubic centimeter

TABLE 9 **Toxicity Factors**Update to the 1999 Human Health Risk Assessment for the Frontier Fertilizer Superfund Site, Davis, California

Analyte	Oral Slope Factor (mg/kg-day) ⁻¹	Reference	Inhalation Unit Risk (µg/m³)	Reference	Chronic Oral Reference Dose (mg/kg-day)	Reference	Chronic Inhalation Reference Concentration (mg/m³)	Reference
1,1,2,2-Tetrachloroethane	0.2	I	0.000058	C	0.02	I	0.08	С
1,1-Dichloroethylene		С		С	0.05	Р	0.07	С
1,2,3-Trichloropropane	30	1	0.0075	С	0.004	1	0.0003	1
1,2-Dibromo-3-chloropropane	0.8	Р	0.006	Р	0.0002	Р	0.0002	1
1,2-Dibromoethane (EDB)	2	1	0.0006	1	0.009	1	0.0008	С
1,2-Dichloroethane	0.091	1	0.000026	1	0.006	Х	0.007	Р
1,2-Dichloropropane	0.036	С	0.00001	С	0.09	Α	0.004	I
1,3-Dichloropropane					0.02	Р	0.08	С
Benzene	0.1	С	0.000029	С	0.004	1	0.003	С
Carbon tetrachloride	0.15	С	0.000042	С	0.004	1	0.04	С
Chloroform	0.031	С	0.000023	1	0.01	1	0.098	Α
cis-1,3-Dichloropropene	0.1	1	0.000016	С	0.03	1	0.02	I
trans-1,3-Dichloropropene	0.1	1	0.000016	С	0.03	1	0.02	1
Vinyl chloride	0.72	1	0.000078	1	0.003	1	0.1	1

 $\mu g = microgram(s)$

EDB = ethylene dibromide

 m^3 = cubic meter(s)

mg/kg-day = milligram(s) per kilogram per day

Reference codes:

A= Agency for Toxic Substances and Disease Registry minimal risk levels

C = California Environmental Protection Agency Office of Environmental Health Hazard Assessment's Chronic Exposure Levels

H = Health Effects Assessment Summary Table

I = EPA's Integrated Risk Information System

P = Provisional Peer Reviewed Toxicity Values

S = See RSL User's Guide for Special Considerations (Section 5)

X = Provisional Peer Reviewed Toxicity Values Appendix

TABLE 10
Summary of Risks and Hazards from Soil Exposure
Update to the 1999 Human Health Risk Assessment for the Frontier Fertilizer Superfund Site, Davis, California

Scenario	Exposure Area	Exposure Medium	Risk	Primary Contributors	Hazard
Residential	On-site	Soil (1 to 13 feet bgs)	2E-06	Dieldrin (76% of risk)	0.02
		Homegrown produce	<u>5E-06</u>	Dieldrin (59% of risk)	<u>0.04</u>
		Total	7E-06		0.06
Industrial	On-site	Soil (1 to 13 feet bgs)	5E-07	None	0.002

TABLE 11
Summary of Risks and Hazards from Groundwater Exposure

Update to the 1999 Human Health Risk Assessment for the Frontier Fertilizer Superfund Site, Davis, California

Scenario	Exposure Area	Exposure Medium	Risk	Primary Contributors	Hazard	Primary Contributors	
Residential	On-site/remainder parcel	Tap water	1E-02	TCP (91%), DCP (6%)	62	DCP (74%), TCP (25%)	
	Off-site	Tap water	3E-03	TCP (71%), DCP (25%)	9	DCP (66%), TCP (29%)	

Notes:

DCP = 1,2-dichloropropane

TCP = 1,2,3-trichloropropane

TABLE 12
Summary of Risks and Hazards from Vapor Intrusion Exposure – Off-Site Exposure Area
Update to the 1999 Human Health Risk Assessment for the Frontier Fertilizer Superfund Site, Davis, California

Scenario	Exposure Area	Exposure Medium	Risk	Primary Contributors	Hazard	Primary Contributors
Residential	Off-site	Indoor air	7E-08		0.00007	
Industrial	Off-site	Indoor air	1E-08		0.00002	

TABLE 13
Summary of Residential Risks and Hazards from Vapor Intrusion Exposure – On-site/Remainder Parcel
Update to the 1999 Human Health Risk Assessment for the Frontier Fertilizer Superfund Site, Davis, California

Sample Location	Cancer Risk	Primary Contributors*	н	Primary Contributors*
CH-011-S	1E-07		0.0001	
CH-014-S	2E-07		0.0003	
CH-017-S	2E-07		0.0002	
CH-019-S	2E-07		0.0002	
CH-021-S	8E-08		0.0001	
CH-027-S	2E-06	TCP (99%)	0.003	
CH-028-S	ND		ND	
CH-029-S	5E-07		0.0006	
CH-030-S	ND		ND	
CH-031-S	2E-08		0.00003	
CH-032-S	3E-07		0.0003	
CH-035-S	5E-07		0.0006	
CH-036-S	2E-06	TCP (>99%)	0.003	
CH-037-S	1E-09		0.000002	

^{*} Primary contributors to the total risk are listed when $> 10^{-6}$. Primary contributors to the HI are listed when HI > 1.

HI = hazard index

ND = no detects

TCP = 1,2,3-trichloropropane

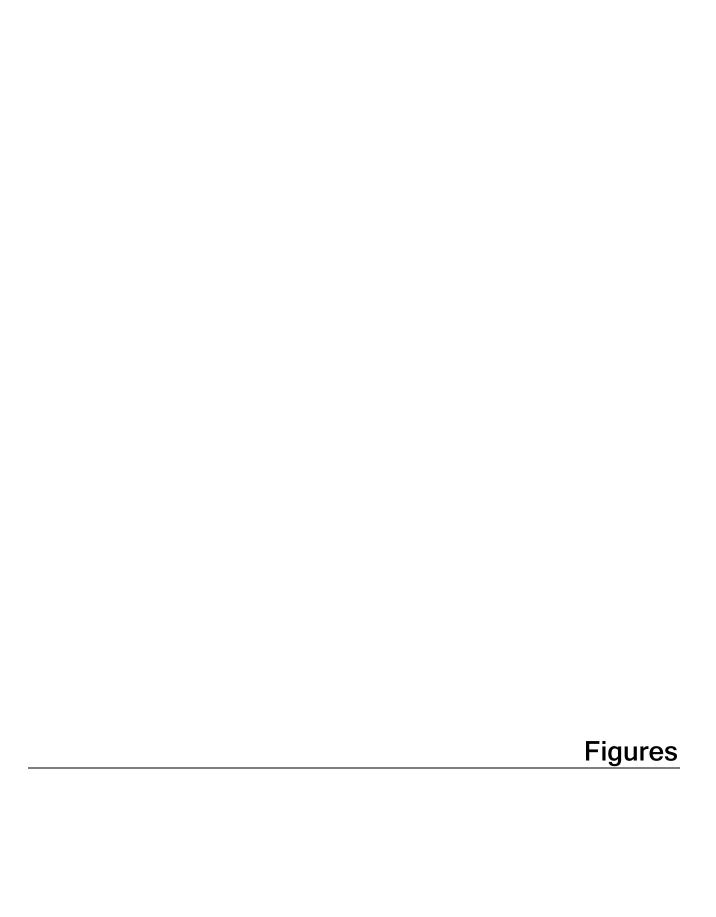
TABLE 14
Summary of Industrial Risks and Hazards from Vapor Intrusion Exposure - On-site/Remainder Parcel
Update to the 1999 Human Health Risk Assessment for the Frontier Fertilizer Superfund Site, Davis, California

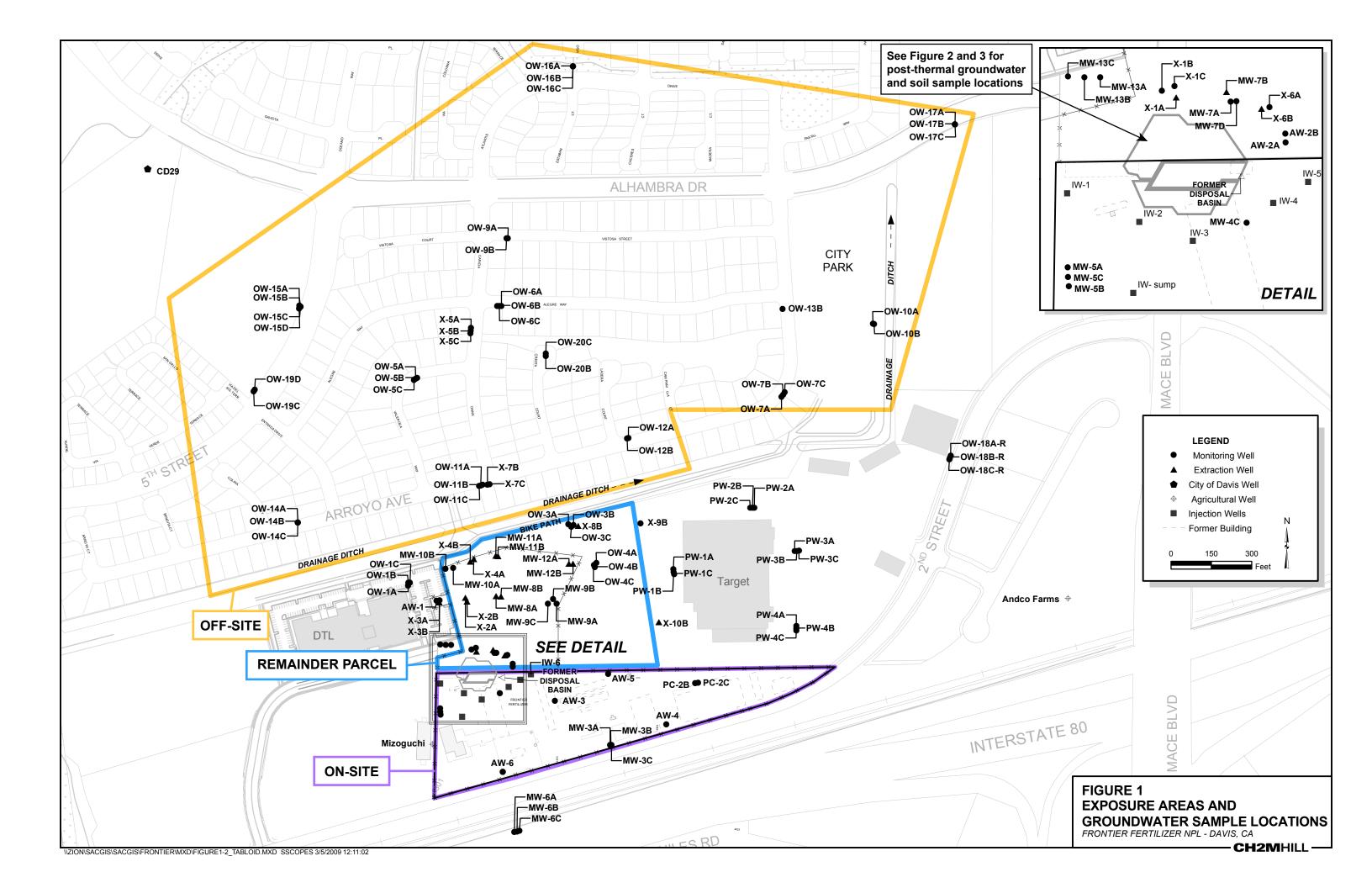
Sample Location	Cancer Risk	Primary Contributors*	н	Primary Contributors*
CH-011-S	1E-08		0.00002	
CH-014-S	2E-08		0.00003	
CH-017-S	2E-08		0.00002	
CH-019-S	2E-08		0.00002	
CH-021-S	9E-09		0.00001	
CH-027-S	2E-07		0.0004	
CH-028-S	ND		ND	
CH-029-S	5E-08		0.00007	
CH-030-S	ND		ND	
CH-031-S	2E-09		0.00004	
CH-032-S	3E-08		0.00004	
CH-035-S	6E-08		0.00008	
CH-036-S	2E-07		0.0003	
CH-037-S	2E-10		0.0000003	

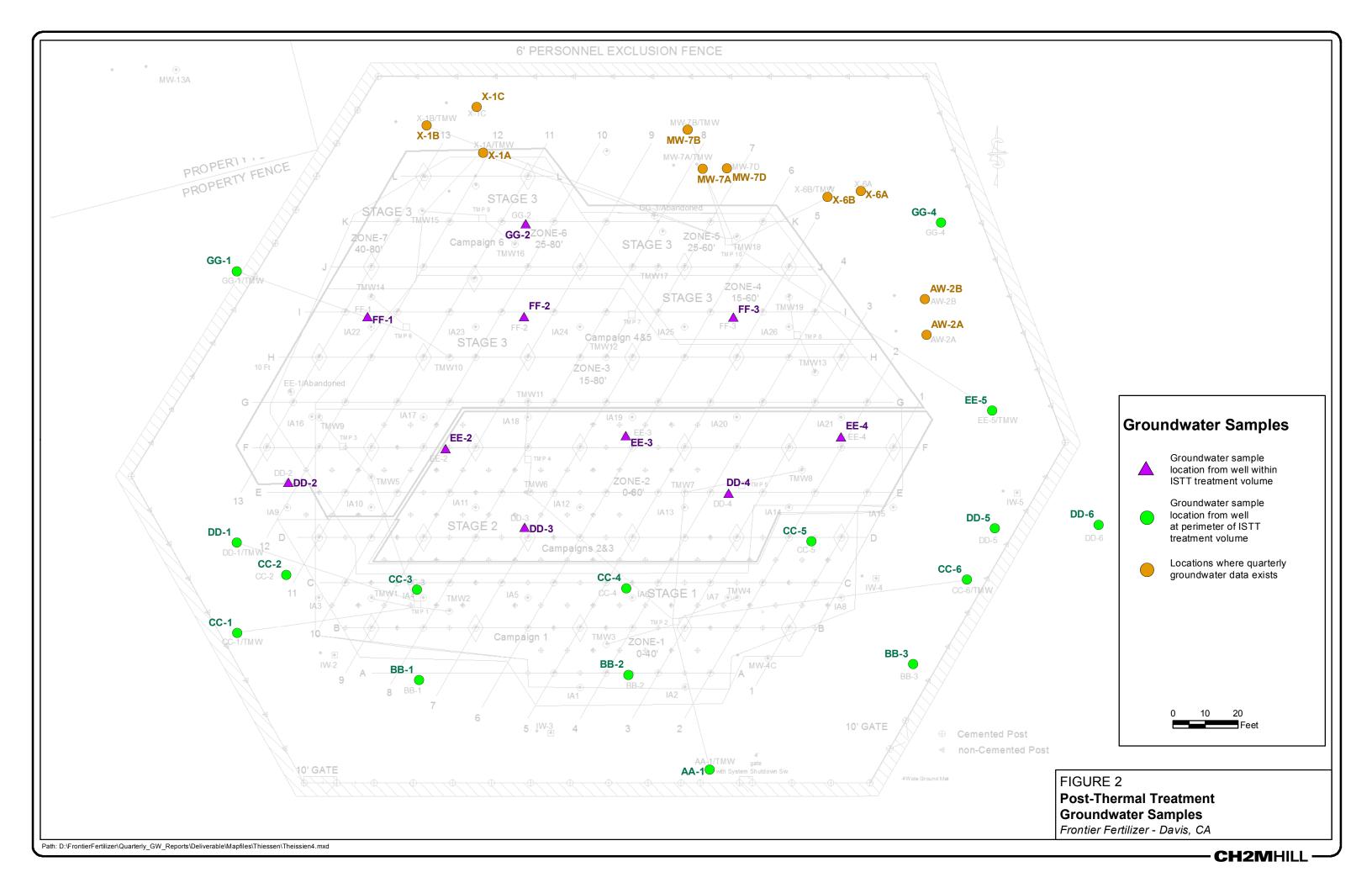
^{*} Primary contributors to the total risk are listed when $> 10^{-6}$. Primary contributors to the HI are listed when HI > 1.

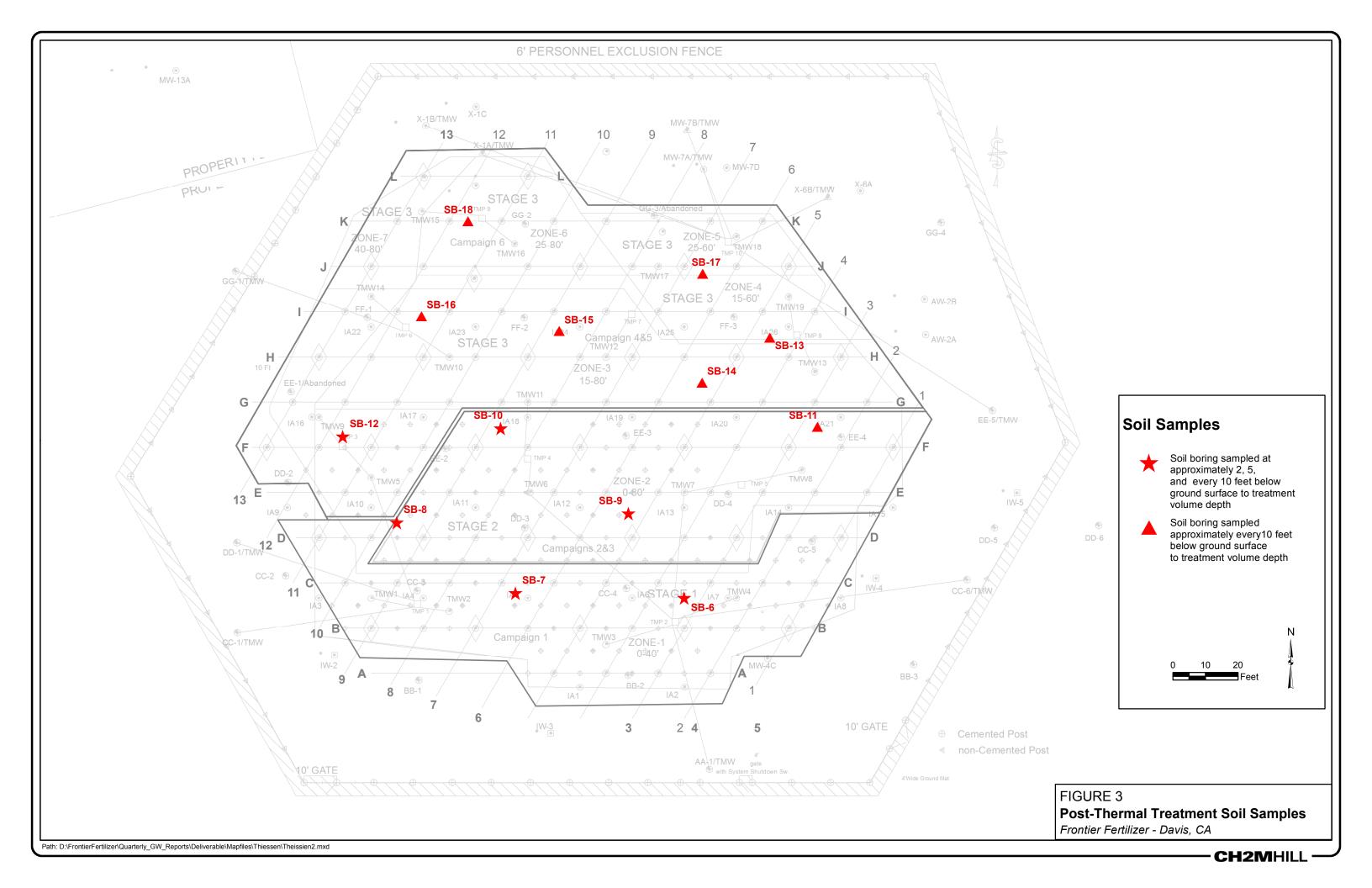
HI = hazard index

ND = no detects









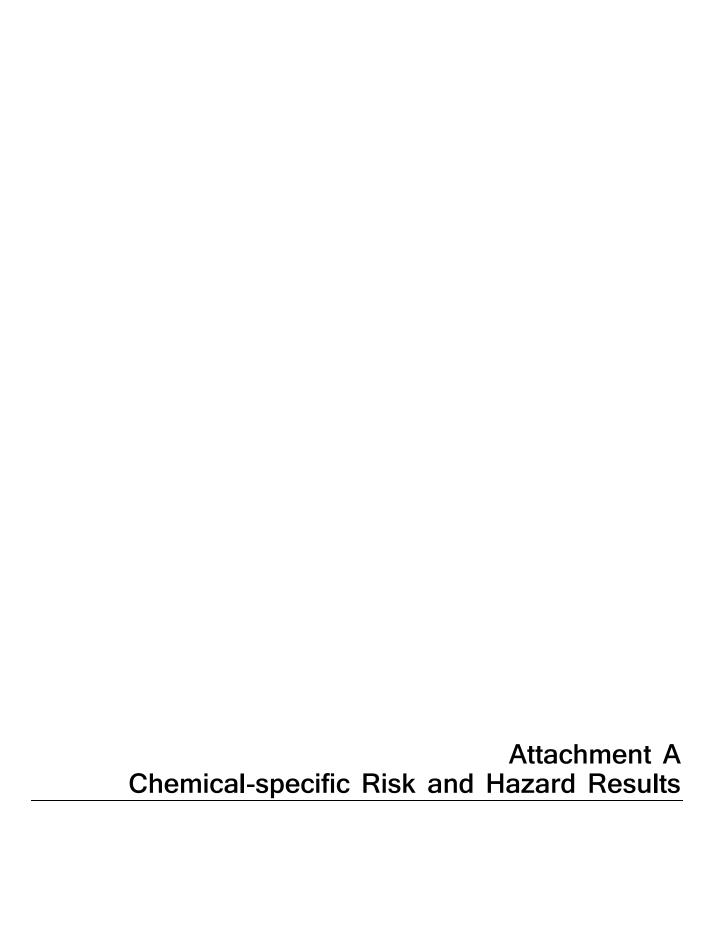


TABLE A-1 Risk Characterization Summary – Residential Scenario

Update to the 1999 Human Health Risk Assessment for the Frontier Fertilizer Superfund Site, Davis, California

Scenario Timeframe:FutureReceptor Population:ResidentReceptor Age:Adult + Child

Exposure Medium	Chemical of Concern	EPC	Units	Res Soil RSL Cancer	Res Soil RSL Non-cancer	Risk	Risk Percent Contribution	Hazard Quotient	Hazard Percent Contribution
Soil	Aldrin	0.014	mg/kg	0.029	1.8	5E-07	25.09%	0.008	35.21%
	1,2-Dibromoethane (EDB)	0.0000298	mg/kg	0.034	7.2	9E-10	0.05%	0.0000041	0.02%
	Dichloropropane	0.007	mg/kg	1	16	7E-09	0.36%	0.0004	1.98%
	Dieldrin	0.043	mg/kg	0.03	3.1	1E-06	74.50%	0.014	62.79%
	Subtotal					2E-06		0.02	
Homegrown Vegetables*	Aldrin	0.014	mg/kg			2E-06	41.40%	0.02	53.05%
	Dieldrin	0.043	mg/kg			3E-06	58.60%	0.02	46.95%
	Subtotal					5E-06		0.04	
	Cumulative Risk/Hazard Inc	dex				7E-06		0.06	

^{*}Homegrown Vegetable Consumption results from the 1999 HHRA.

Notes:

EDB = ethylene dibromide

EPC = Exposure Point Concentration

RSL = Regional Screening Level

TABLE A-2 Risk Characterization Summary – Industrial Scenario

Update to the 1999 Human Health Risk Assessment for the Frontier Fertilizer Superfund Site, Davis, California

Scenario Timeframe: Future

Industrial worker

Receptor Population: Industria Receptor Age: Adult

Exposure Medium	Chemical of Concern	EPC	Units	Ind Soil RSL Cancer	Ind Soil RSL Non-cancer	Risk	Risk Percent Contribution	Hazard Quotient	Hazard Percent Contribution
Soil	Aldrin	0.014	mg/kg	0.1	18	1E-07	26.28%	0.0008	34.23%
	1,2-Dibromoethane (EDB)	0.0000298	mg/kg	0.17	31	2E-10	0.03%	0.00000096	0.042%
	Dichloropropane	0.007	mg/kg	4.4	66	2E-09	0.30%	0.0001	4.67%
	Dieldrin	0.043	mg/kg	0.11	31	4E-07	73.39%	0.0014	61.05%
	Cumulative Risk/Hazard Inc	dex				5E-07		0.002	

Notes:

EDB = ethylene dibromide

EPC = Exposure Point Concentration

RSL = Regional Screening Level

TABLE A-3
Risk Characterization Summary – Tap Water (Off-site Parcel)

Scenario Timeframe: Future
Receptor Population: Resident
Receptor Age: Adult + Child

Medium	Exposure Point	Chemical of Concern	Groundwater EPC	Units	RSL Cancer	RSL Non-cancer	Risk	Risk Percent Contribution	Hazard Quotient	Hazard Percent Contribution
Off-site Groundwater	S-2 Water-bearing Zone – tap water	Carbon tetrachloride	2.806	mg/L	0.11	49	3E-05	0.79%	0.06	0.45%
	S-2 Water-bearing Zone – tap water	Chloroform	1.45	mg/L	0.22	97	7E-06	0.20%	0.015	0.12%
	S-2 Water-bearing Zone – tap water	1,2-Dibromoethane (EDB)	6.075	mg/L	0.0075	1.7	8E-04	24.98%	3.57	28.19%
	S-2 Water-bearing Zone – tap water	1,2-Dichloroethane	0.325	mg/L	0.17	13	2E-06	0.06%	0.03	0.20%
	S-2 Water-bearing Zone – tap water	1,2-Dichloropropane	51.87	mg/L	0.44	8.3	1E-04	3.64%	6	49.30%
	S-2 Water-bearing Zone – tap water	1,2,3-Trichloropropane	1.709	mg/L	0.00075	0.62	2E-03	70.27%	3	21.74%
	S-2 Water-bearing Zone – tap water	Vinyl chloride	0.04	mg/L	0.019	44	2E-06	0.06%	0.001	0.01%
	Cumulative Risk/Hazard Index						3E-03		13	

Notes:

EDB = ethylene dibromide

EPC = Exposure Point Concentration

TABLE A-4
Risk Characterization Summary – Tap Water (On-site and Remainder Parcel)

Scenario Timeframe: Future
Receptor Population: Resident
Receptor Age: Adult + Child

								Risk		Hazard
			Groundwater		RSL	RSL		Percent	Hazard	Percent
Medium	Exposure Point	Chemical of Concern	EPC	Units	Cancer	Non-cancer	Risk	Contribution	Quotient	Contribution
On-site and	S-2 Water-bearing Zone – tap water	Benzene	12.24	mg/L	0.45	5.7	3E-05	0.19%	2.15	3.35%
Remainder Parcel Groundwater	S-2 Water-bearing Zone – tap water	Carbon tetrachloride	2.637	mg/L	0.11	49	2E-05	0.17%	0.05	0.08%
Groundwater	S-2 Water-bearing Zone – tap water	Chloroform	2.671	mg/L	0.22	97	1E-05	0.09%	0.028	0.04%
	S-2 Water-bearing Zone – tap water	1,2-Dibromoethane (EDB)	0.97	mg/L	0.0075	1.7	1E-04	0.91%	0.57	0.89%
	S-2 Water-bearing Zone – tap water	1,2-Dibromo-3-Chloroprop	0.0819	mg/L	0.00033	0.37	2E-04	1.73%	0.2	0.34%
	S-2 Water-bearing Zone – tap water	1,2-Dichloroethane	0.428	mg/L	0.17	13	3E-06	0.02%	0.03	0.05%
	S-2 Water-bearing Zone – tap water	1,2-Dichloropropane	378.2	mg/L	0.44	8.3	9E-04	6.08%	46	71.02%
	S-2 Water-bearing Zone – tap water	1,3-Dichloropropane	0.386	mg/L	N/A	110	N/A	N/A	0.0035	0.0055%
	S-2 Water-bearing Zone – tap water	cis-1,3-Dichloropropene	0.282	mg/L	0.47	39	6E-07	0.00%	0.007	0.01%
	S-2 Water-bearing Zone – tap water	1,2,3-Trichloropropane	9.627	mg/L	0.00075	0.62	1E-02	90.73%	16	24.20%
	S-2 Water-bearing Zone – tap water	Vinyl chloride	0.2	mg/L	0.019	44	1E-05	0.07%	0.005	0.01%
	Cumulative Risk/Hazard Index						1E-02		64	

Notes:

EDB = ethylene dibromide

EPC = Exposure Point Concentration

TABLE A-5
Risk Characterization Summary – Indoor Air – Off-site Exposure Area Residential Scenario

Scenario Timeframe: Future
Receptor Population: Resident
Receptor Age: Adult

							Soil Gas	Indoor Air	Res Air	Res Air		Risk		Hazard
	Exposure			Groundwater		Attenuation	EPC	EPC	RSL	RSL		Percent	Hazard	Percent
Medium	Medium	Exposure Point	Chemical of Concern	EPC	Units	Factor	(mg/m ³)	(mg/m ³)	Cancer	Non-cancer	Risk	Contribution	Quotient	Contribution
Groundwater	Indoor Air	Indoor Air – Off-site	Dibromoethane (EDB)	0.039	mg/L	2.13671E-05	6.65E-01	1.42E-05	0.0047	0.83	3.0E-09	4.49%	0.0000171	20.21%
		Indoor Air – Off-site	1,2-Dichloropropane	0.085	mg/L	7.62151E-06	6.76E+00	5.15E-05	0.28	4.2	1.8E-10	0.27%	0.000012	14.49%
		Indoor Air – Off-site	1,2,3-Trichloropropane	0.019	mg/L	3.50649E-05	1.64E-01	5.75E-06	0.00014	0.31	4.1E-08	61.04%	0.000019	21.92%
		Indoor Air – Off-site	Carbon tetrachloride	0.6	mg/L	3.18696E-06	4.84E+02	1.54E-03	0.067	42	2.3E-08	34.20%	0.000037	43.38%
	•	Cumulative Risk/Ha	zard Index						•		7E-08		0.00008	

Notes:

Groundwater data were used to determine soil gas concentrations, attenuation factors, and indoor air concentrations using the HERD groundwater screening model.

Inputs to the Johnson & Ettinger model are listed in Table 8.

EDB = ethylene dibromide

EPC = Exposure Point Concentration

HERD = Human and Ecological Risk Division

TABLE A-6
Risk Characterization Summary – Indoor Air – Off-site Exposure Area Industrial Scenario

Scenario Timeframe: Future
Receptor Population: Resident
Receptor Age: Adult

							Soil Gas	Indoor Air	Ind Air	Ind Air		Risk		Hazard
	Exposure			Groundwater		Attenuation	EPC	EPC	RSL	RSL		Percent	Hazard	Percent
Medium	Medium	Exposure Point	Chemical of Concern	EPC	Units	Factor	(mg/m ³)	(mg/m^3)	Cancer	Non-cancer	Risk	Contribution	Quotient	Contribution
Groundwater	Indoor Air	Indoor Air – Off-site	Dibromoethane (EDB)	0.039	mg/L	2.13671E-05	6.65E-01	1.42E-05	0.02	3.5	7.1E-10	7.37%	0.00000406	20.41%
		Indoor Air – Off-site	1,2-Dichloropropane	0.085	mg/L	7.62151E-06	6.76E+00	5.15E-05	1.2	18	4.3E-11	0.45%	0.0000029	14.40%
		Indoor Air – Off-site	1,2,3-Trichloropropane	0.019	mg/L	3.50649E-05	1.64E-01	5.75E-06	0.0016	1.3	3.6E-09	37.33%	0.0000044	22.09%
	_	Indoor Air – Off-site	Carbon tetrachloride	0.6	mg/L	3.18696E-06	4.84E+02	1.54E-03	0.29	180	5.3E-09	54.85%	0.0000086	43.10%
	•	Cumulative Risk/Haz	zard Index								1E-08		0.00002	

Notes:

Groundwater data were used to determine soil gas concentrations, attenuation factors, and indoor air concentrations using the HERD groundwater screening model.

Inputs to the Johnson & Ettinger model are listed in Table 8.

EDB = ethylene dibromide

EPC = Exposure Point Concentration

HERD = Human and Ecological Risk Division

TABLE A-7
Risk Characterization Summary – Indoor Air – On-site and Remainder Parcel Exposure Area Residential Scenario
Update to the 1999 Human Health Risk Assessment for the Frontier Fertilizer Superfund Site, Davis, California

		San	nple ID:		CH01:	1S-A657A		C	:H014S-A6	57A	(CH017S-A6	557A	C	:H019S-A6	557A	C	:H021S-A6	57A		CH027S-A	A657R		СН	028S-A657	R
Analysis	•						Non-cancer			Non-cancer			Non-cancer			Non-cancer			Non-cancer				Non-cancer			Non-cancer
Method	Analyte	CAS No.	Units	Result	Result	ELCR	HQ	Result	ELCR	HQ	Result	ELCR	HQ	Result	ELCR	HQ	Result	ELCR	HQ	Result	Result	ELCR	HQ	Result	ELCR	HQ
TO15	1,2,3-Trichloropropane	96-18-4	$\mu g/m^3$	0.054 J	0.1 =	1E-07	0.0001	0.18 J	2E-07	0.0003	0.13 J	2E-07	0.0002	0.13 J	2E-07	0.0002	0.069 J	8E-08	0.0001	0.84 =	1.3 =	2E-06	0.002	0.15 U		
TO15	1,2-Dibromo-3-chloropropane	96-12-8	$\mu g/m^3$	0.05 U	0.05 U			0.05 U			0.05 U			0.05 U			0.05 UJ			0.24 U	0.24 U			0.24 U		
TO15	1,2-Dibromoethane (EDB)	106-93-4	$\mu g/m^3$	0.01 U	0.01 U			0.01 U			0.01 U			0.01 U			0.01 UJ			0.19 U	0.19 U			0.19 U		
TO15	1,2-Dichloropropane	78-87-5	$\mu g/m^3$	0.05 U	0.05 U			0.05 U			0.05 U			0.05 U			0.05 UJ			9.6 =	11 =	2E-08	0.001	0.11 U		
TO15	Carbon tetrachloride	56-23-5	$\mu g/m^3$	0.08 U	0.08 U			0.08 U			0.85 =	5E-09	0.000009	0.17 =	1E-09	0.000002	0.08 UJ			0.26 J	0.33 =	2E-09	0.000003	0.16 U		
	Total Ri	isk or Hazard	d Index:			1E-07	0.0001		2E-07	0.0003		2E-07	0.0002		2E-07	0.0002		8E-08	0.0001			2E-06	0.003		0E+00	0.0000

(Table Continued)

		Sar	nple ID:	CF	1029S-A65	57R	CH	030S-A657I	R	СНО)31S-A657	R	СНО)32S-A657	7R	СНО)35S-A657	R		CH036S-A65	7R		CH037S-A6	57R
Analysis					ı	Non-cance	er	ľ	Non-cance	er	1	Non-cance	r		Non-cance	r	1	Non-cance	r		Non-cancer			Non-cancer
Method	Analyte	CAS No.	Units	Result	ELCR	HQ	Result	ELCR	HQ	Result	ELCR	HQ	Result	ELCR	HQ	Result	ELCR	HQ	Result	ELCR	HQ	Result	ELCR	HQ
TO15	1,2,3-Trichloropropane	96-18-4	μg/m³	0.41 =	5E-07	0.0006	0.15 U			0.15 U			0.24 J	3E-07	0.0003	0.45 =	5E-07	0.0006	1.8 =	2E-06	0.003	0.15 U		
TO15	1,2-Dibromo-3-chloropropane	96-12-8	$\mu g/m^3$	0.24 U			0.24 U			0.24 U			0.24 U			0.24 U			0.24 U			0.24 U		
TO15	1,2-Dibromoethane (EDB)	106-93-4	$\mu g/m^3$	0.19 U			0.19 U			0.19 U			0.19 U			0.19 U			0.19 U			0.19 U		
TO15	1,2-Dichloropropane	78-87-5	$\mu g/m^3$	0.11 U			0.11 U			0.11 U			0.11 U			0.13 J	2E-10	0.00002	0.11 U			0.11 U		
TO15	Carbon tetrachloride	56-23-5	$\mu g/m^3$	0.16 U			0.16 U			3.3 =	2E-08	0.00003	0.18 J	1E-09	#######	0.16 U			0.22 J	1E-09	0.000002	0.23 J	1E-09	0.000002
	Total Ri	sk or Hazar	d Index:		5E-07	0.0006		0E+00	0.0000		2E-08	0.00003		3E-07	0.0003		5E-07	0.0006		2E-06	0.003		1E-09	0.000002

Notes:

CH011 and CH027 show two results due to collection of a duplicate.

μg/m³ = microgram(s) per cubic meter

ELCR = excess lifetime cancer risk

HQ = hazard quotient

TABLE A-8
Risk Characterization Summary – Indoor Air – On-site and Remainder Parcel Exposure Area Industrial Scenario
Update to the 1999 Human Health Risk Assessment for the Frontier Fertilizer Superfund Site, Davis, California

		Sam	ple ID:		CH011	S-A657A			CH014S-A	657A	(CH017S-A6	557A		CH019S-A65	57A	(CH021S-A6	557A		CH027S-A	657R		СН0	28S-A657R	
Analysis	;						Non-cancer			Non-cancer			Non-cancer			Non-cancer			Non-cancer				Non-cancer	15190A		Non-cancer
Method	Analyte	CAS No.	Units	Result		ELCR	HQ	Result	ELCR	HQ	Result	ELCR	HQ	Result	ELCR	HQ	Result	ELCR	HQ	Result	Result	ELCR	HQ	Result	ELCR	HQ
TO15	1,2,3-Trichloropropane	96-18-4	μg/m³	0.054 J	0.1 =	1E-08	0.00002	0.18 J	2E-08	0.00003	0.13 J	2E-08	0.00002	0.13 J	2E-08	0.00002	0.069 J	9E-09	0.00001	0.84 =	1.3 =	2E-07	0.0002	0.15 U		
TO15	1,2-Dibromo-3-chloropropane	96-12-8	μg/m³	0.05 U	0.05 U			0.05 U			0.05 U			0.05 U			0.05 UJ			0.24 U	0.24 U			0.24 U		
TO15	1,2-Dibromoethane (EDB)	106-93-4	μg/m³	0.01 U	0.01 U			0.01 U			0.01 U			0.01 U			0.01 UJ			0.19 U	0.19 U			0.19 U		
TO15	1,2-Dichloropropane	78-87-5	μg/m³	0.05 U	0.05 U			0.05 U			0.05 U			0.05 U			0.05 UJ			9.6 =	11 =	2E-09	0.0002	0.11 U		
TO15	Carbon tetrachloride	56-23-5	μg/m³	0.08 U	0.08 U			0.08 U			0.85 =	6E-10	0.000001	0.17 =	1E-10	0.0000002	0.08 UJ			0.26 J	0.33 =	2E-10	0.0000004	0.16 U		
	Total Ris	k or Hazard	l Index:			1E-08	0.00002		2E-08	0.00003		2E-08	0.00002		2E-08	0.00002		9E-09	0.00001			2E-07	0.0004		0E+00	0.0000

(Table Continued)

		Sample ID:	Cl	1029S-A6	57R	CH0	30S-A657R	ł	CH	031S-A657	7R	(CH032S-A6	57R	CH	035S-A657	7R		CH036S-A65	57R		CH037S-A	.657R
Analysis					Non-cancer		N	on-cance	r		Non-cancer			Non-cancer			Non-cancer			Non-cancer			Non-cancer
Method	Analyte	CAS No. Units	Result	ELCR	HQ	Result	ELCR	HQ	Result	ELCR	HQ	Result	ELCR	HQ	Result	ELCR	HQ	Result	ELCR	HQ	Result	ELCR	HQ
TO15	1,2,3-Trichloropropane	96-18-4 μg/m ³	0.41 =	5E-08	0.00007	0.15 U			0.15 U			0.24 J	3E-08	0.00004	0.45 =	6E-08	0.00007	1.8 =	2E-07	0.0003	0.15 U		
TO15	1,2-Dibromo-3-chloropropane	96-12-8 μg/m ³	0.24 U			0.24 U			0.24 U			0.24 U			0.24 U			0.24 U			0.24 U		ļ
TO15	1,2-Dibromoethane (EDB)	106-93-4 μg/m ³	0.19 U			0.19 U			0.19 U			0.19 U			0.19 U			0.19 U			0.19 U		ļ
TO15	1,2-Dichloropropane	78-87-5 μg/m ³	0.11 U			0.11 U			0.11 U			0.11 U			0.13 J	3E-11	0.000002	0.11 U			0.11 U		ļ
TO15	Carbon tetrachloride	56-23-5 μg/m ³	0.16 U			0.16 U			3.3 =	2E-09	0.000004	0.18 J	1E-10	0.0000002	0.16 U			0.22 J	2E-10	0.0000003	0.23 J	2E-10	0.0000003
	Total R	isk or Hazard Index:		5E-08	0.00007		0E+00	0.0000		2E-09	0.000004		3E-08	0.00004		6E-08	0.00008		2E-07	0.0003		2E-10	0.000003

TABLE A-9
Risk Characterization Uncertainty Evaluation Using EPA Vapor Intrusion Screening Level Calculator – Indoor Air – On-site and Remainder Parcel Exposure Area Residential Scenario
Update to the 1999 Human Health Risk Assessment for the Frontier Fertilizer Superfund Site, Davis, California

		San	nple ID:		CH011	LS-A657A		C	CH014S-A	657A	(CH017S-A6	557A	(CH019S-A6	57A	(:H021S-A6	57A		CH027S-A	657R		CH	1028S-A657	rR
Analysis	5					1	Non-cancer			Non-cancer			Non-cancer			Non-cancer			Non-cancer				Non-cancer			Non-cancer
Method	l Analyte	CAS No.	Units	Result	Result	ELCR	HQ	Result	ELCR	HQ	Result	ELCR	HQ	Result	ELCR	HQ	Result	ELCR	HQ	Result	Result	ELCR	HQ	Result	ELCR	HQ
TO15	1,2,3-Trichloropropane	96-18-4	$\mu g/m^3$	0.054 J	0.1 =		0.01	0.18 J		0.02	0.13 J		0.01	0.13 J		0.01	0.069 J	8E-08	0.007	0.84 =	1.3 =		0.12	0.15 U		
TO15	1,2-Dibromo-3-chloropropane	96-12-8	$\mu g/m^3$	0.05 U	0.05 U			0.05 U			0.05 U			0.05 U			0.05 UJ			0.24 U	0.24 U			0.24 U		
TO15	1,2-Dibromoethane (EDB)	106-93-4	$\mu g/m^3$	0.01 U	0.01 U			0.01 U			0.01 U			0.01 U			0.01 UJ			0.19 U	0.19 U			0.19 U		
TO15	1,2-Dichloropropane	78-87-5	$\mu g/m^3$	0.05 U	0.05 U			0.05 U			0.05 U			0.05 U			0.05 UJ			9.6 =	11 =	1E-06	0.08	0.11 U		
TO15	Carbon tetrachloride	56-23-5	$\mu g/m^3$	0.08 U	0.08 U			0.08 U			0.85 =	4E-07	0.001	0.17 =	8E-08	0.0001	0.08 UJ			0.26 J	0.33 =	1E-07	0.0002	0.16 U		
	Total Ri	sk or Hazar	d Index:			0E+00	0.01		0E+00	0.02		4E-07	0.01		8E-08	0.01		8E-08	0.007			1E-06	0.2		0E+00	0.0000

(Table Continued)

		Sample II): CI	1029S-A65	7R	СНО	30S-A657	R	СНО)31S-A657F	₹	СНО)32S-A657	'R	СНО)35S-A657R			CH036S-A65	7R		CH037S-A6	57R
Analysis	;			N	lon-cance	r	1	Non-cance	r	N	lon-cance	r		Non-cance	er	N	on-cance	r		Non-cancer			Non-cancer
Method	l Analyte	CAS No. Unit	s Result	ELCR	HQ	Result	ELCR	HQ	Result	ELCR	HQ	Result	ELCR	HQ	Result	ELCR	HQ	Result	ELCR	HQ	Result	ELCR	HQ
TO15	1,2,3-Trichloropropane	96-18-4 μg/n	³ 0.41 =		0.04	0.15 U			0.15 U			0.24 J		0.02	0.45 =		0.04	1.8 =		0.2	0.15 U		
TO15	1,2-Dibromo-3-chloropropane	96-12-8 μg/n	³ 0.24 U			0.24 U			0.24 U			0.24 U			0.24 U			0.24 U			0.24 U		
TO15	1,2-Dibromoethane (EDB)	106-93-4 μg/n	³ 0.19 U			0.19 U			0.19 U			0.19 U			0.19 U			0.19 U			0.19 U		
TO15	1,2-Dichloropropane	78-87-5 μg/n	³ 0.11 U			0.11 U			0.11 U			0.11 U			0.13 J	1E-08	0.0009	0.11 U			0.11 U		
TO15	Carbon tetrachloride	56-23-5 μg/n	³ 0.16 U			0.16 U			3.3 =	1E-06	0.08	0.18 J	8E-08	0.0001	0.16 U			0.22 J	1E-07	0.0002	0.23 J	1E-07	0.0002
	Tota	l Risk or Hazard Inde	x:	0E+00	0.04		0E+00	0.0000		1E-06	0.08		8E-08	0.02		1E-08	0.04		1E-07	0.2		1E-07	0.0002

Notes:

CH011 and CH027 show two results due to collection of a duplicate.

μg/m³ = microgram(s) per cubic meter

ELCR = excess lifetime cancer risk

HQ = hazard quotient



UCL Statistics for Data Sets with Non-Detects

User Selected Options

Date/Time of Computation 3/27/2014 1:37:02 PM

From File WorkSheet.xls

Full Precision OFF
Confidence Coefficient 95%

Number of Bootstrap Operations 2000

TCP

General Statistics

Total Number of Observations	19	Number of Distinct Observations	17
Number of Detects	4	Number of Non-Detects	15
Number of Distinct Detects	4	Number of Distinct Non-Detects	13
Minimum Detect	0.11	Minimum Non-Detect	0.047
Maximum Detect	0.57	Maximum Non-Detect	5.3
Variance Detects	0.0444	Percent Non-Detects	78.95%
Mean Detects	0.26	SD Detects	0.211
Median Detects	0.18	CV Detects	0.81
Skewness Detects	1.779	Kurtosis Detects	3.23
Mean of Logged Detects	-1.557	SD of Logged Detects	0.714

Normal GOF Test on Detects Only

Shapiro Wilk GOF Test	0.799	Shapiro Wilk Test Statistic
Detected Data appear Normal at 5% Significance Level	0.748	5% Shapiro Wilk Critical Value
Lilliefors GOF Test	0.344	Lilliefors Test Statistic
Detected Data appear Normal at 5% Significance Level	0.443	5% Lilliefors Critical Value

Detected Data appear Normal at 5% Significance Level

Kaplan-Meier (KM) Statistics using Normal Critical Values and other Nonparametric UCLs

Mean	0.0971	Standard Error of Mean	0.0354
SD	0.126	95% KM (BCA) UCL	N/A
95% KM (t) UCL	0.159	95% KM (Percentile Bootstrap) UCL	N/A
95% KM (z) UCL	0.155	95% KM Bootstrap t UCL	N/A
90% KM Chebyshev UCL	0.203	95% KM Chebyshev UCL	0.252
97.5% KM Chebyshev UCL	0.318	99% KM Chebyshev UCL	0.45

Gamma GOF Tests on Detected Observations Only

A-D Test Statistic	0.407	Anderson-Darling GOF Test
5% A-D Critical Value	0.66	Detected data appear Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.296	Kolmogrov-Smirnoff GOF
5% K-S Critical Value	0.397	Detected data appear Gamma Distributed at 5% Significance Level

Detected data appear Gamma Distributed at 5% Significance Level

Gamma Statis	tics on Detec	ted Data Only
--------------	---------------	---------------

0.801	k star (bias corrected MLE)	2.538	k hat (MLE)
0.324	Theta star (bias corrected MLE)	0.102	Theta hat (MLE)
6.41	nu star (bias corrected)	20.31	nu hat (MLE)
0.29	MLE Sd (bias corrected)	0.26	MLE Mean (bias corrected)

Gamma Kaplan-Meier (KM) Statistics

22.4	nu hat (KM)	0.59	k hat (KM)
12	Adjusted Chi Square Value (22.40, β)	12.64	Approximate Chi Square Value (22.40, α)
0.181	95% Gamma Adjusted KM-UCL (use when n<50)	0.172	95% Gamma Approximate KM-UCL (use when n>=50)

Gamma ROS Statistics using Imputed Non-Detects

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

GROS may not be used when kstar of detected data is small such as < 0.1

For such situations, GROS method tends to yield inflated values of UCLs and BTVs

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

Minimum	0.01	Mean	0.0626
Maximum	0.57	Median	0.01
SD	0.136	CV	2.164
k hat (MLE)	0.528	k star (bias corrected MLE)	0.48
Theta hat (MLE)	0.119	Theta star (bias corrected MLE)	0.131
nu hat (MLE)	20.06	nu star (bias corrected)	18.23
MLE Mean (bias corrected)	0.0626	MLE Sd (bias corrected)	0.0904
		Adjusted Level of Significance (β)	0.0369
Approximate Chi Square Value (18.23, α)	9.557	Adjusted Chi Square Value (18.23, β)	9.011
95% Gamma Approximate UCL (use when n>=50)	0.119	95% Gamma Adjusted UCL (use when n<50)	N/A

Lognormal GOF Test on Detected Observations Only

Shapiro Wilk Test Statistic	0.922	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.748	Detected Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.252	Lilliefors GOF Test
5% Lilliefors Critical Value	0.443	Detected Data appear Lognormal at 5% Significance Level

Detected Data appear Lognormal at 5% Significance Level

Lognormal ROS Statistics Using Imputed Non-Detects

-4.009	Mean in Log Scale	0.063	Mean in Original Scale
1.396	SD in Log Scale	0.135	SD in Original Scale
0.12	95% Percentile Bootstrap UCL	0.117	95% t UCL (assumes normality of ROS data)
0.201	95% Bootstrap t UCL	0.152	95% BCA Bootstrap UCL
		0.139	95% H-UCL (Log ROS)

UCLs using Lognormal Distribution and KM Estimates when Detected data are Lognormally Distributed

KM Mean (logged)	-2.704	95% H-UCL (KM -Log)	0.124
KM SD (logged)	0.704	95% Critical H Value (KM-Log)	2.225

KM Standard Error of Mean (logged) 0.197

DL/2 Statistics

DL/2 Normal			DL/2 Log-Transformed		
	Mean in Original Scale	0.342	Mean in Log Scale	-2.69	
	SD in Original Scale	0.789	SD in Log Scale	1.559	
	95% t UCL (Assumes normality)	0.656	95% H-Stat UCL	0.824	

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

Nonparametric Distribution Free UCL Statistics

Detected Data appear Normal Distributed at 5% Significance Level

Suggested UCL to Use

95% KM (t) UCL 0.159 95% KM (Percentile Bootstrap) UCL N/A

Warning: One or more Recommended UCL(s) not available!

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.

Recommendations are based upon data size, data distribution, and skewness.

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

DCP

General Statistics

Total Number of Observations	19	Number of Distinct Observations	12
Number of Detects	1	Number of Non-Detects	18
Number of Distinct Detects	1	Number of Distinct Non-Detects	11

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

The data set for variable DCP was not processed!

EDB

General Statistics

Total Number of Observations	19	Number of Distinct Observations	11
Number of Detects	2	Number of Non-Detects	17
Number of Distinct Detects	2	Number of Distinct Non-Detects	11
Minimum Detect	0.028	Minimum Non-Detect	0.028
Maximum Detect	0.034	Maximum Non-Detect	5.3
Variance Detects 1	8000E-5	Percent Non-Detects	89.47%
Mean Detects	0.031	SD Detects	0.00424
Median Detects	0.031	CV Detects	0.137
Skewness Detects	N/A	Kurtosis Detects	N/A
Mean of Logged Detects	-3.478	SD of Logged Detects	0.137

Warning: Data set has only 2 Detected Values.

This is not enough to compute meaningful or reliable statistics and estimates.

Normal GOF Test on Detects Only

Not Enough Data to Perform GOF Test

Kaplan-Meier (KM) Statistics using Normal Critical Values and other Nonparametric UCLs

Mean	0.0285	Standard Error of Mean	7.3549E-4
SD	0.00172	95% KM (BCA) UCL	N/A
95% KM (t) UCL	0.0298	95% KM (Percentile Bootstrap) UCL	N/A
95% KM (z) UCL	0.0298	95% KM Bootstrap t UCL	N/A
90% KM Chebyshev UCL	0.0308	95% KM Chebyshev UCL	0.0318
97.5% KM Chebyshev UCL	0.0331	99% KM Chebyshev UCL	0.0359

Gamma GOF Tests on Detected Observations Only

Not Enough Data to Perform GOF Test

Gamma Statistics on Detected Data Only

N/A	k star (bias corrected MLE)	106.4	k hat (MLE)
N/A	Theta star (bias corrected MLE)	2.9123E-4	Theta hat (MLE)
N/A	nu star (bias corrected)	425.8	nu hat (MLE)
N/A	MLE Sd (bias corrected)	N/A	MLE Mean (bias corrected)

Gamma Kaplan-Meier (KM) Statistics

k hat (KM)	273.9	nu hat (KM)	10407
		Adjusted Level of Significance (β)	0.0369
Approximate Chi Square Value (N/A, α)	10171	Adjusted Chi Square Value (N/A, β)	10151
95% Gamma Approximate KM-UCL (use when n>=50)	0.0292	95% Gamma Adjusted KM-UCL (use when n<50)	0.0293

Lognormal GOF Test on Detected Observations Only

Not Enough Data to Perform GOF Test

Lognormal ROS Statistics Using Imputed Non-Detects

Mean in Original Scale	0.0262	Mean in Log Scale	-3.647
SD in Original Scale	0.00253	SD in Log Scale	0.092
95% t UCL (assumes normality of ROS data)	0.0272	95% Percentile Bootstrap UCL	0.0272
95% BCA Bootstrap UCL	0.0273	95% Bootstrap t UCL	0.0275
95% H-UCL (Log ROS)	N/A		

DL/2 Statistics

DI /2 Normal

DL/ 2 (10)11101		DE/ E EOS Transformed	
Mean in Original Scale	0.285	Mean in Log Scale	-3.501
SD in Original Scale	0.799	SD in Log Scale	1.578
95% t UCL (Assumes normality)	0.603	95% H-Stat UCL	0.388

DI /2 Log-Transformed

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

Nonparametric Distribution Free UCL Statistics

Data do not follow a Discernible Distribution at 5% Significance Level

Suggested UCL to Use

95% KM (t) UCL 0.0298 95% KM (% Bootstrap) UCL N/A

Warning: One or more Recommended UCL(s) not available!

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.

Recommendations are based upon data size, data distribution, and skewness.

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

UCL Statistics for Data Sets with Non-Detects

User Selected Options

Date/Time of Computation 4/15/2014 3:11:35 PM

From File WorkSheet.xls

Full Precision OFF
Confidence Coefficient 95%
Number of Bootstrap Operations 10000

1,2,3-Trichloropropane (TCP)

General Statistics

Total Number of Observations	11	Number of Distinct Observations	5
Number of Detects	3	Number of Non-Detects	8
Number of Distinct Detects	3	Number of Distinct Non-Detects	2
Minimum Detect	0.017	Minimum Non-Detect	0.00275
Maximum Detect	5.833	Maximum Non-Detect	0.005
Variance Detects	10.18	Percent Non-Detects	72.73%
Mean Detects	2.167	SD Detects	3.191
Median Detects	0.65	CV Detects	1.473
Skewness Detects	1.656	Kurtosis Detects	N/A
Mean of Logged Detects	-0.914	SD of Logged Detects	2.949

Warning: Data set has only 3 Detected Values.

This is not enough to compute meaningful or reliable statistics and estimates.

Normal GOF Test on Detects Only

Shapiro Wilk GOF Test	0.831	Shapiro Wilk Test Statistic
Detected Data appear Normal at 5% Significance Level	0.767	5% Shapiro Wilk Critical Value
Lilliefors GOF Test	0.349	Lilliefors Test Statistic
Detected Data appear Normal at 5% Significance Level	0.512	5% Lilliefors Critical Value
mal at 5% Significance Level	Detected Data appear Normal at 5% Significance Level	

Kaplan-Meier (KM) Statistics using Normal Critical Values and other Nonparametric UCLs

Mean	0.593	Standard Error of Mean	0.616
SD	1.667	95% KM (BCA) UCL	N/A
95% KM (t) UCL	1.709	95% KM (Percentile Bootstrap) UCL	N/A
95% KM (z) UCL	1.606	95% KM Bootstrap t UCL	N/A
90% KM Chebyshev UCL	2.44	95% KM Chebyshev UCL	3.277
97.5% KM Chebyshev UCL	4.438	99% KM Chebyshev UCL	6.719

Gamma GOF Tests on Detected Observations Only

Not Enough Data to Perform GOF Test

Gamma Statistics on Detected Data Only

N/A	k star (bias corrected MLE)	0.391	k hat (MLE)
N/A	Theta star (bias corrected MLE)	5.536	Theta hat (MLE)
N/A	nu star (bias corrected)	2.348	nu hat (MLE)
N/A	MLE Sd (bias corrected)	N/A	MLE Mean (bias corrected)

Gamma	Kaplan-Meier	(KM) Statistics
-------	--------------	-----	--------------

k hat (KM)	0.126	nu hat (KM)	2.782
		Adjusted Level of Significance (β)	0.0278
Approximate Chi Square Value (2.78, α)	0.311	Adjusted Chi Square Value (2.78, β)	0.218
95% Gamma Approximate KM-UCL (use when n>=50)	5.306	95% Gamma Adjusted KM-UCL (use when n<50)	7.581

Lognormal GOF Test on Detected Observations Only

8 Shapiro Wilk GOF Test	0.98	Shapiro Wilk Test Statistic
Detected Data appear Lognormal at 5% Significance Le	0.767	5% Shapiro Wilk Critical Value
32 Lilliefors GOF Test	0.232	Lilliefors Test Statistic
12 Detected Data appear Lognormal at 5% Significance Le	0.512	5% Lilliefors Critical Value

Detected Data appear Lognormal at 5% Significance Level

Lognormal ROS Statistics Using Imputed Non-Detects

Mean in Original Scale	0.591	Mean in Log Scale	-10.43
SD in Original Scale	1.75	SD in Log Scale	7.208
95% t UCL (assumes normality of ROS data)	1.547	95% Percentile Bootstrap UCL	1.594
95% BCA Bootstrap UCL	2.182	95% Bootstrap t UCL	202.2
95% H-UCL (Log ROS) 1	.515E+24		

UCLs using Lognormal Distribution and KM Estimates when Detected data are Lognormally Distributed

KM Mean (logged)	-4.537	95% H-UCL (KM -Log)	49.44
KM SD (logged)	2.55	95% Critical H Value (KM-Log)	6.43
KM Standard Error of Mean (logged)	0.942		

DL/2 Statistics

DL/2 Normal		DL/2 Log-Transformed	
Mean in Original Scale	0.592	Mean in Log Scale	-4.824
SD in Original Scale	1.749	SD in Log Scale	2.849
95% t UCL (Assumes normality)	1.548	95% H-Stat UCL	287.2

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

Nonparametric Distribution Free UCL Statistics

Detected Data appear Normal Distributed at 5% Significance Level

Suggested UCL to Use

95% KM (t) UCL 1.709 95% KM (Percentile Bootstrap) UCL N/A Warning: One or more Recommended UCL(s) not available!

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.

Recommendations are based upon data size, data distribution, and skewness.

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

1,2-Dibromoethane (EDB)

Genera	Statistics

Total Number of Observations	11	Number of Distinct Observations	4
Number of Detects	2	Number of Non-Detects	9
Number of Distinct Detects	2	Number of Distinct Non-Detects	2
Minimum Detect	1.11	Minimum Non-Detect	0.00275
Maximum Detect	6.075	Maximum Non-Detect	0.005
Variance Detects	12.33	Percent Non-Detects	81.82%
Mean Detects	3.593	SD Detects	3.511
Median Detects	3.593	CV Detects	0.977
Skewness Detects	N/A	Kurtosis Detects	N/A
Mean of Logged Detects	0.954	SD of Logged Detects	1.202

Warning: Data set has only 2 Detected Values.

This is not enough to compute meaningful or reliable statistics and estimates.

Normal GOF Test on Detects Only

Not Enough Data to Perform GOF Test

Kaplan-Meier (KM) Statistics using Normal Critical Values and other Nonparametric UCLs

0.743	Standard Error of Mean	0.655	Mean
. N/A	95% KM (BCA) UCL	1.743	SD
. N/A	95% KM (Percentile Bootstrap) UCL	2.002	95% KM (t) UCL
. N/A	95% KM Bootstrap t UCL	1.878	95% KM (z) UCL
3.895	95% KM Chebyshev UCL	2.885	90% KM Chebyshev UCL
8.05	99% KM Chebyshev UCL	5.296	97.5% KM Chebyshev UCL

Gamma GOF Tests on Detected Observations Only

Not Enough Data to Perform GOF Test

Gamma Statistics on Detected Data Only

N/A	k star (bias corrected MLE)	1.688	k hat (MLE)
N/A	Theta star (bias corrected MLE)	2.128	Theta hat (MLE)
N/A	nu star (bias corrected)	6.752	nu hat (MLE)
N/A	MLE Sd (bias corrected)	N/A	MLE Mean (bias corrected)

Gamma Kaplan-Meier (KM) Statistics

0.141	nu hat (KM)	3.111
	Adjusted Level of Significance (β)	0.0278
0.406	Adjusted Chi Square Value (3.11, β)	0.286
5.021	95% Gamma Adjusted KM-UCL (use when n<50)	7.129
	0.406	Adjusted Level of Significance (β) 0.406 Adjusted Chi Square Value (3.11, β)

Lognormal GOF Test on Detected Observations Only

Not Enough Data to Perform GOF Test

Lognormal ROS Statistics Using Imputed Non-Detects

Mean in Original Scale	0.663	Mean in Log Scale	-4.983
SD in Original Scale	1.825	SD in Log Scale	3.718
95% t UCL (assumes normality of ROS data)	1.66	95% Percentile Bootstrap UCL	1.67
95% BCA Bootstrap UCL	2.315	95% Bootstrap t UCL	70.85
95% H-UCL (Log ROS) 3	37639		

DL/2 Statistics

DL/2 Normal		DL/2 Log-Transformed	
Mean in Original Scale	0.655	Mean in Log Scale	-5
SD in Original Scale	1.828	SD in Log Scale	2.982
95% t UCL (Assumes normality)	1.654	95% H-Stat UCL	643.1

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

Nonparametric Distribution Free UCL Statistics

Data do not follow a Discernible Distribution at 5% Significance Level

Suggested UCL to Use

95% KM (BCA) UCL N/A

Warning: One or more Recommended UCL(s) not available!

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.

Recommendations are based upon data size, data distribution, and skewness.

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

1,2-Dichloroethane

General Statistics

Total Number of Observations	11	Number of Distinct Observations	2
Number of Detects	1	Number of Non-Detects	10
Number of Distinct Detects	1	Number of Distinct Non-Detects	1

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

The data set for variable 1,2-Dichloroethane was not processed!

1,2-Dichloropropane (DCP)

General Statistics

Total Number of Observations	11	Number of Distinct Observations	4
Number of Detects	3	Number of Non-Detects	8
Number of Distinct Detects	3	Number of Distinct Non-Detects	1
Minimum Detect	0.187	Minimum Non-Detect	0.5
Maximum Detect	180	Maximum Non-Detect	0.5
Variance Detects	10234	Percent Non-Detects	72.73%
Mean Detects	63.32	SD Detects	101.2
Median Detects	9.775	CV Detects	1.598
Skewness Detects	1.715	Kurtosis Detects	N/A
Mean of Logged Detects	1.931	SD of Logged Detects	3.449

Warning: Data set has only 3 Detected Values.

This is not enough to compute meaningful or reliable statistics and estimates.

Normal GOF Test on Detects Only

Shapiro Wilk GOF Test	0.79	Shapiro Wilk Test Statistic
Detected Data appear Normal at 5% Significance Leve	0.767	5% Shapiro Wilk Critical Value
Lilliefors GOF Test	0.368	Lilliefors Test Statistic
Detected Data appear Normal at 5% Significance Leve	0.512	5% Lilliefors Critical Value

Detected Data appear Normal at 5% Significance Level

Kaplan-Meier (KM) Statistics using Normal Critical Values and other Nonparametric UCLs

19.01	Standard Error of Mean	17.41	Mean
N/A	95% KM (BCA) UCL	51.49	SD
N/A	95% KM (Percentile Bootstrap) UCL	51.87	95% KM (t) UCL
N/A	95% KM Bootstrap t UCL	48.68	95% KM (z) UCL
100.3	95% KM Chebyshev UCL	74.45	90% KM Chebyshev UCL
206.6	99% KM Chebyshev UCL	136.1	97.5% KM Chebyshev UCL

Gamma GOF Tests on Detected Observations Only

Not Enough Data to Perform GOF Test

Gamma Statistics on Detected Data Only

N/A	k star (bias corrected MLE)	0.309	k hat (MLE)
N/A	Theta star (bias corrected MLE)	204.6	Theta hat (MLE)
N/A	nu star (bias corrected)	1.857	nu hat (MLE)
N/A	MLE Sd (bias corrected)	N/A	MLE Mean (bias corrected)

Gamma Kaplan-Meier (KM) Statistics

2.514	nu hat (KM)	0.114	k hat (KM)
0.0278	Adjusted Level of Significance (β)		
0.173	Adjusted Chi Square Value (2.51, β)	0.244	Approximate Chi Square Value (2.51, α)
253.6	95% Gamma Adjusted KM-UCL (use when n<50)	179.1	95% Gamma Approximate KM-UCL (use when n>=50)

Lognormal GOF Test on Detected Observations Only

Shapiro Wilk GOF Test	0.992	Shapiro Wilk Test Statistic
Detected Data appear Lognormal at 5% Significance Leve	0.767	5% Shapiro Wilk Critical Value
Lilliefors GOF Test	0.207	Lilliefors Test Statistic
Detected Data appear Lognormal at 5% Significance Leve	0.512	5% Lilliefors Critical Value

Detected Data appear Lognormal at 5% Significance Level

Lognormal ROS Statistics Using Imputed Non-Detects

Mean in Original Scale	17.75	Mean in Log Scale	-0.961
SD in Original Scale	53.89	SD in Log Scale	3.107
95% t UCL (assumes normality of ROS data)	47.2	95% Percentile Bootstrap UCL	49.77
95% BCA Bootstrap UCL	66.92	95% Bootstrap t UCL	1027
95% H-UCL (Log ROS)	95856		

UCLs using Lognormal Distribution and KM Estimates when Detected data are Lognormally Distributed

KM Mean (logged)	-0.694	95% H-UCL (KM -Log)	248.1
KM SD (logged)	2.179	95% Critical H Value (KM-Log)	5.565
KM Standard Error of Mean (logged)	0.805		

DL/2 Statistics

DL/2 Normal	DL/2 Log-Transformed		
Mean in Original Scale	17.45	Mean in Log Scale	-0.481
SD in Original Scale	53.99	SD in Log Scale	2.186
95% t UCL (Assumes normality)	46.95	95% H-Stat UCL	320

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

Nonparametric Distribution Free UCL Statistics

Detected Data appear Normal Distributed at 5% Significance Level

Suggested UCL to Use

95% KM (t) UCL 51.87 95% KM (Percentile Bootstrap) UCL N/A

Warning: One or more Recommended UCL(s) not available!

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.

Recommendations are based upon data size, data distribution, and skewness.

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

1,3-Dichloropropane

General Statistics

Total Number of Observations	11	Number of Distinct Observations	2
Number of Detects	1	Number of Non-Detects	10
Number of Distinct Detects	1	Number of Distinct Non-Detects	1

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

The data set for variable 1,3-Dichloropropane was not processed!

Carbon Tetrachloride (CCL4)

General Statistics

Total Number of Observations	11	Number of Distinct Observations	4
Number of Detects	2	Number of Non-Detects	9
Number of Distinct Detects	2	Number of Distinct Non-Detects	2
Minimum Detect	0.2	Minimum Non-Detect	0.5
Maximum Detect	3.243	Maximum Non-Detect	2.875
Variance Detects	4.628	Percent Non-Detects	81.82%
Mean Detects	1.721	SD Detects	2.151
Median Detects	1.721	CV Detects	1.25
Skewness Detects	N/A	Kurtosis Detects	N/A
Mean of Logged Detects	-0.217	SD of Logged Detects	1.97

Warning: Data set has only 2 Detected Values.

This is not enough to compute meaningful or reliable statistics and estimates.

Normal GOF Test on Detects Only

Not Enough Data to Perform GOF Test

Kaplan-Meier (KM) Statistics using Normal Critical Values and other Nonparametric UCLs

Mean	0.477	Standard Error of Mean	0.373
SD	0.875	95% KM (BCA) UCL	N/A
95% KM (t) UCL	1.153	95% KM (Percentile Bootstrap) UCL	N/A
95% KM (z) UCL	1.09	95% KM Bootstrap t UCL	N/A
90% KM Chebyshev UCL	1.595	95% KM Chebyshev UCL	2.102
97.5% KM Chebyshev UCL	2.806	99% KM Chebyshev UCL	4.187

Gamma GOF Tests on Detected Observations Only

Not Enough Data to Perform GOF Test

Gamma Statistics on Detected Data Only

N/A	k star (bias corrected MLE)	0.783	k hat (MLE)
N/A	Theta star (bias corrected MLE)	2.197	Theta hat (MLE)
N/A	nu star (bias corrected)	3.134	nu hat (MLE)
N/A	MLE Sd (bias corrected)	N/A	MLE Mean (bias corrected)

Gamma Kaplan-Meier (KM) Statistics

k hat (KM)	0.297	nu hat (KM)	6.532
		Adjusted Level of Significance (β)	0.0278
Approximate Chi Square Value (6.53, α)	1.917	Adjusted Chi Square Value (6.53, β)	1.538
95% Gamma Approximate KM-UCL (use when n>=50)	1.624	95% Gamma Adjusted KM-UCL (use when n<50)	2.024

Lognormal GOF Test on Detected Observations Only

Not Enough Data to Perform GOF Test

Lognormal ROS Statistics Using Imputed Non-Detects

Mean in Original Scale	0.553	Mean in Log Scale	-1.392
SD in Original Scale	0.928	SD in Log Scale	1.259
95% t UCL (assumes normality of ROS data)	1.06	95% Percentile Bootstrap UCL	1.069
95% BCA Bootstrap UCL	1.315	95% Bootstrap t UCL	2.744
95% H-UCL (Log ROS)	2.228		

DL/2 Statistics

DL/2 Normal		DL/2 Log-Transformed	
Mean in Original Scale	0.625	Mean in Log Scale	-1.015
SD in Original Scale	0.939	SD in Log Scale	0.903
95% t UCL (Assumes normality)	1.139	95% H-Stat UCL	1.218

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

Nonparametric Distribution Free UCL Statistics

Data do not follow a Discernible Distribution at 5% Significance Level

Suggested UCL to Use

97.5% KM (Chebyshev) UCL 2.806

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.

Recommendations are based upon data size, data distribution, and skewness.

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

Chloroform

General Statistics

Total Number of Observations	11	Number of Distinct Observations	3
Number of Detects	1	Number of Non-Detects	10
Number of Distinct Detects	1	Number of Distinct Non-Detects	2

Warning: Only one distinct data value was detected! ProUCL (or any other software) should not be used on such a data set!

It is suggested to use alternative site specific values determined by the Project Team to estimate environmental parameters (e.g., EPC, BTV).

The data set for variable Chloroform was not processed!

Vinyl Chloride

General Statistics

Total Number of Observations	11	Number of Distinct Observations	2
Number of Detects	1	Number of Non-Detects	10
Number of Distinct Detects	1	Number of Distinct Non-Detects	1

Warning: Only one distinct data value was detected! ProUCL (or any other software) should not be used on such a data set!

It is suggested to use alternative site specific values determined by the Project Team to estimate environmental parameters (e.g., EPC, BTV).

The data set for variable Vinyl Chloride was not processed!

UCL Statistics for Data Sets with Non-Detects

User Selected Options

Date/Time of Computation 4/15/2014 3:40:58 PM

From File OnSiteData_proUCLInput.xls

Full Precision OFF
Confidence Coefficient 95%

Number of Bootstrap Operations 10000

1,2,3-Trichloropropane (TCP)

General Statistics

Total Number of Observations	32	Number of Distinct Observations	25
Number of Detects	25	Number of Non-Detects	7
Number of Distinct Detects	23	Number of Distinct Non-Detects	2
Minimum Detect	0.003	Minimum Non-Detect	0.002
Maximum Detect	26.3	Maximum Non-Detect	0.0035
Variance Detects	28.33	Percent Non-Detects	21.88%
Mean Detects	1.62	SD Detects	5.322
Median Detects	0.055	CV Detects	3.286
Skewness Detects	4.519	Kurtosis Detects	21.36
Mean of Logged Detects	-2.478	SD of Logged Detects	2.488

Normal GOF Test on Detects Only

Shapiro Wilk Test Statistic	0.337	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.918	Detected Data Not Normal at 5% Significance Level
Lilliefors Test Statistic	0.429	Lilliefors GOF Test
5% Lilliefors Critical Value	0.177	Detected Data Not Normal at 5% Significance Level

Detected Data Not Normal at 5% Significance Level

Kaplan-Meier (KM) Statistics using Normal Critical Values and other Nonparametric UCLs

0.84	Standard Error of Mean	1.266	Mean
2.869	95% KM (BCA) UCL	4.658	SD
2.804	95% KM (Percentile Bootstrap) UCL	2.691	95% KM (t) UCL
6.824	95% KM Bootstrap t UCL	2.648	95% KM (z) UCL
4.929	95% KM Chebyshev UCL	3.787	90% KM Chebyshev UCL
9.627	99% KM Chebyshev UCL	6.514	97.5% KM Chebyshev UCL

Gamma GOF Tests on Detected Observations Only

Anderson-Darling GOF Test	2.185	A-D Test Statistic
Detected Data Not Gamma Distributed at 5% Significance Level	0.88	5% A-D Critical Value
Kolmogrov-Smirnoff GOF	0.243	K-S Test Statistic
Detected Data Not Gamma Distributed at 5% Significance Level	0.192	5% K-S Critical Value

Detected Data Not Gamma Distributed at 5% Significance Level

Gamma Statistics on	Detected Data Only
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0.239	k star (bias corrected MLE)	0.241	k hat (MLE)
6.778	Theta star (bias corrected MLE)	6.714	Theta hat (MLE)
11.95	nu star (bias corrected)	12.06	nu hat (MLE)
3.314	MLE Sd (bias corrected)	1.62	MLE Mean (bias corrected)

Gamma Kaplan-Meier (KM) Statistics

4.728	nu hat (KM)	0.0739	k hat (KM)
0.942	Adjusted Chi Square Value (4.73, β)	1.029	Approximate Chi Square Value (4.73, α)
6.357	95% Gamma Adjusted KM-UCL (use when n<50)	5.818	95% Gamma Approximate KM-UCL (use when n>=50)

Gamma (KM) may not be used when k hat (KM) is < 0.1

Gamma ROS Statistics using Imputed Non-Detects

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

GROS may not be used when kstar of detected data is small such as < 0.1

For such situations, GROS method tends to yield inflated values of UCLs and BTVs

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

Minimum	0.003	Mean	1.268
Maximum	26.3	Median	0.0183
SD	4.732	CV	3.732
k hat (MLE)	0.227	k star (bias corrected MLE)	0.226
Theta hat (MLE)	5.589	Theta star (bias corrected MLE)	5.6
nu hat (MLE)	14.52	nu star (bias corrected)	14.49
MLE Mean (bias corrected)	1.268	MLE Sd (bias corrected)	2.664
		Adjusted Level of Significance (β)	0.0416
Approximate Chi Square Value (14.49, α)	6.907	Adjusted Chi Square Value (14.49, β)	6.627
95% Gamma Approximate UCL (use when n>=50)	2.659	95% Gamma Adjusted UCL (use when n<50)	2.772

Lognormal GOF Test on Detected Observations Only

Shapiro Wilk GOF Test	0.934	Shapiro Wilk Test Statistic
Detected Data appear Lognormal at 5% Significance Level	0.918	5% Shapiro Wilk Critical Value
Lilliefors GOF Test	0.164	Lilliefors Test Statistic
Detected Data appear Lognormal at 5% Significance Level	0.177	5% Lilliefors Critical Value

Detected Data appear Lognormal at 5% Significance Level

Lognormal ROS Statistics Using Imputed Non-Detects

Mean in Original Scale	1.266	Mean in Log Scale	-3.749
SD in Original Scale	4.732	SD in Log Scale	3.318
95% t UCL (assumes normality of ROS data)	2.684	95% Percentile Bootstrap UCL	2.856
95% BCA Bootstrap UCL	4.074	95% Bootstrap t UCL	6.871
95% H-UCL (Log ROS)	199.4		

UCLs using Lognormal Distribution and KM Estimates when Detected data are Lognormally Distributed

KM Mean (logged)	-3.294	95% H-UCL (KM -Log)	12.48
KM SD (logged)	2.649	95% Critical H Value (KM-Log)	4.851
KM Standard Error of Mean (logged)	0.478		

DL/2 Statistics

DL/2 Normal		DL/2 Log-Transformed	
Mean in Original Scale	1.266	Mean in Log Scale	-3.43
SD in Original Scale	4.732	SD in Log Scale	2.853
95% t UCL (Assumes normality)	2.684	95% H-Stat UCL	26.95

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

Nonparametric Distribution Free UCL Statistics

Detected Data appear Lognormal Distributed at 5% Significance Level

Suggested UCL to Use

99% KM (Chebyshev) UCL 9.627

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.

Recommendations are based upon data size, data distribution, and skewness.

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

1,2-Dibromo-3-Chloropropane (DBCP)

General Statistics

Total Number of Observations	32	Number of Distinct Observations	15
Number of Detects	7	Number of Non-Detects	25
Number of Distinct Detects	7	Number of Distinct Non-Detects	8
Minimum Detect	0.006	Minimum Non-Detect	0.005
Maximum Detect	0.5	Maximum Non-Detect	14.5
Variance Detects	0.0434	Percent Non-Detects	78.13%
Mean Detects	0.17	SD Detects	0.208
Median Detects	0.053	CV Detects	1.226
Skewness Detects	1.065	Kurtosis Detects	-0.851
Mean of Logged Detects	-2.799	SD of Logged Detects	1.791

Normal GOF Test on Detects Only

Shapiro Wilk Test Statistic	0.782	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.803	Detected Data Not Normal at 5% Significance Level
Lilliefors Test Statistic	0.284	Lilliefors GOF Test
5% Lilliefors Critical Value	0.335	Detected Data appear Normal at 5% Significance Level

Detected Data appear Approximate Normal at 5% Significance Level

Kaplan-Meier (KM) Statistics using Normal Critical Values and other Nonparametric UCLs

Mean	0.044	Standard Error of Mean	0.023
SD	0.116	95% KM (BCA) UCL	0.0844
95% KM (t) UCL	0.083	95% KM (Percentile Bootstrap) UCL	0.0819
95% KM (z) UCL	0.0818	95% KM Bootstrap t UCL	0.163
90% KM Chebyshev UCL	0.113	95% KM Chebyshev UCL	0.144
7.5% KM Chebyshev UCL	0.188	99% KM Chebyshev UCL	0.273

A-D Test Statistic	0.349	Anderson-Darling GOF Test
5% A-D Critical Value	0.745	Detected data appear Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.19	Kolmogrov-Smirnoff GOF
5% K-S Critical Value	0.325	Detected data appear Gamma Distributed at 5% Significance Level

Detected data appear Gamma Distributed at 5% Significance Level

Gamma Statistics on Detected Data Only

k hat (MLE)	0.602	k star (bias corrected MLE)	0.439
Theta hat (MLE)	0.282	Theta star (bias corrected MLE)	0.387
nu hat (MLE)	8.422	nu star (bias corrected)	6.146
MLE Mean (bias corrected)	0.17	MLE Sd (bias corrected)	0.256

Gamma Kaplan-Meier (KM) Statistics

k hat (KM)	0.143	nu hat (KM)	9.173
Approximate Chi Square Value (9.17, α)	3.432	Adjusted Chi Square Value (9.17, β)	3.245
95% Gamma Approximate KM-UCL (use when n>=50)	0.118	95% Gamma Adjusted KM-UCL (use when n<50)	0.124

Gamma ROS Statistics using Imputed Non-Detects

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

GROS may not be used when kstar of detected data is small such as < 0.1

For such situations, GROS method tends to yield inflated values of UCLs and BTVs

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

Minimum	0.006	Mean	0.045
Maximum	0.5	Median	0.01
SD	0.114	CV	2.526
k hat (MLE)	0.563	k star (bias corrected MLE)	0.531
Theta hat (MLE)	0.0799	Theta star (bias corrected MLE)	0.0847
nu hat (MLE)	36.02	nu star (bias corrected)	33.98
MLE Mean (bias corrected)	0.045	MLE Sd (bias corrected)	0.0617
		Adjusted Level of Significance (β)	0.0416
Approximate Chi Square Value (33.98, α)	21.65	Adjusted Chi Square Value (33.98, β)	21.12
95% Gamma Approximate UCL (use when n>=50)	0.0706	95% Gamma Adjusted UCL (use when n<50)	0.0724

Lognormal GOF Test on Detected Observations Only

Shapiro Wilk Test Statistic	0.907	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.803	Detected Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.172	Lilliefors GOF Test
5% Lilliefors Critical Value	0.335	Detected Data appear Lognormal at 5% Significance Level

Detected Data appear Lognormal at 5% Significance Level

Lognormal ROS Statistics Using Imputed Non-Detects

-7.282	Mean in Log Scale	0.0376	Mean in Original Scale
	5		· ·
3.063	SD in Log Scale	0.116	SD in Original Scale
0.074	95% Percentile Bootstrap UCL	0.0724	95% t UCL (assumes normality of ROS data)
0.175	95% Bootstrap t UCL	0.0898	95% BCA Bootstrap UCL
		1.562	95% H-UCL (Log ROS)

UCLs using Lognormal Distribution and KM Estimates when Detected data are Lognormally Distributed

KM Mean (logged)	-4.686	95% H-UCL (KM -Log)	0.0446
KM SD (logged)	1.335	95% Critical H Value (KM-Log)	2.861
KM Standard Error of Mean (logged)	0.267		

DL/2 Statistics

DL/2 Normal		DL/2 Log-Transformed	
Mean in Original Scale	0.317	Mean in Log Scale	-4.453
SD in Original Scale	1.293	SD in Log Scale	2.243
95% t UCL (Assumes normality)	0.705	95% H-Stat UCL	0.784

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

Nonparametric Distribution Free UCL Statistics

Detected Data appear Approximate Normal Distributed at 5% Significance Level

Suggested UCL to Use

95% KM (t) UCL 0.083 95% KM (Percentile Bootstrap) UCL 0.0819

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.

Recommendations are based upon data size, data distribution, and skewness.

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

1,2-Dibromoethane (EDB)

General Statistics

Total Number of Observations	32	Number of Distinct Observations	16
Number of Detects	5	Number of Non-Detects	27
Number of Distinct Detects	5	Number of Distinct Non-Detects	12
Minimum Detect	0.00275	Minimum Non-Detect	0.002
Maximum Detect	13.27	Maximum Non-Detect	10.2
Variance Detects	34.87	Percent Non-Detects	84.38%
Mean Detects	2.703	SD Detects	5.905
Median Detects	0.081	CV Detects	2.184
Skewness Detects	2.235	Kurtosis Detects	4.998
Mean of Logged Detects	-2.539	SD of Logged Detects	3.327

Normal GOF Test on Detects Only

Shapiro Wilk Test Statistic	0.562	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.762	Detected Data Not Normal at 5% Significance Level
Lilliefors Test Statistic	0.467	Lilliefors GOF Test
5% Lilliefors Critical Value	0.396	Detected Data Not Normal at 5% Significance Level

Detected Data Not Normal at 5% Significance Level

Kaplan-Meier (KM) Statistics using Normal Critical Values and other Nonparametric UCLs

0.456	Standard Error of Mean	0.426	Mean
1.258	95% KM (BCA) UCL	2.307	SD
1.255	95% KM (Percentile Bootstrap) UCL	1.199	95% KM (t) UCL
37.17	95% KM Bootstrap t UCL	1.176	95% KM (z) UCL
2.413	95% KM Chebyshev UCL	1.793	90% KM Chebyshev UCL
4.962	99% KM Chebyshev UCL	3.273	97.5% KM Chebyshev UCL

Gamma GOF Tests on Detected Observations Only

A-D Test Statistic	0.594	Anderson-Darling GOF Test
5% A-D Critical Value	0.773	Detected data appear Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.362	Kolmogrov-Smirnoff GOF
5% K-S Critical Value	0.388	Detected data appear Gamma Distributed at 5% Significance Level

Detected data appear Gamma Distributed at 5% Significance Level

Gamma Statistics on Detected Data Only

k hat (MLE)	0.207	k star (bias corrected MLE)	0.216
Theta hat (MLE)	13.05	Theta star (bias corrected MLE)	12.5
nu hat (MLE)	2.072	nu star (bias corrected)	2.162
MLE Mean (bias corrected)	2.703	MLE Sd (bias corrected)	5.814

Gamma Kaplan-Meier (KM) Statistics

2.181	nu hat (KM)	0.0341	k hat (KM)
0.16	Adjusted Chi Square Value (2.18, β)	0.178	Approximate Chi Square Value (2.18, α)
5.789	95% Gamma Adjusted KM-UCL (use when n<50)	5.219	95% Gamma Approximate KM-UCL (use when n>=50)

Gamma (KM) may not be used when k hat (KM) is < 0.1

Gamma ROS Statistics using Imputed Non-Detects

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

GROS may not be used when kstar of detected data is small such as < 0.1

For such situations, GROS method tends to yield inflated values of UCLs and BTVs

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

Minimum	0.00275	Mean	0.431
Maximum	13.27	Median	0.01
SD	2.342	CV	5.437
k hat (MLE)	0.212	k star (bias corrected MLE)	0.213
Theta hat (MLE)	2.033	Theta star (bias corrected MLE)	2.023
nu hat (MLE)	13.57	nu star (bias corrected)	13.63
MLE Mean (bias corrected)	0.431	MLE Sd (bias corrected)	0.934
		Adjusted Level of Significance (β)	0.0416
Approximate Chi Square Value (13.63, α)	6.317	Adjusted Chi Square Value (13.63, β)	6.051
95% Gamma Approximate UCL (use when n>=50)	0.929	95% Gamma Adjusted UCL (use when n<50)	0.97

Lognormal GOF Test on Detected Observations Only

Shapiro Wilk GOF Test	0.928	Shapiro Wilk Test Statistic
Detected Data appear Lognormal at 5% Significance Level	0.762	5% Shapiro Wilk Critical Value
Lilliefors GOF Test	0.216	Lilliefors Test Statistic
Detected Data appear Lognormal at 5% Significance Level	0.396	5% Lilliefors Critical Value

Detected Data appear Lognormal at 5% Significance Level

Lognormal ROS Statistics Using Imputed Non-Detects

Mean in Original Scale	0.422	Mean in Log Scale	-12.17
SD in Original Scale	2.344	SD in Log Scale	5.439
95% t UCL (assumes normality of ROS data)	1.125	95% Percentile Bootstrap UCL	1.249
95% BCA Bootstrap UCL	2.073	95% Bootstrap t UCL	69.19
95% H-UCL (Log ROS) 1	43538		

UCLs using Lognormal Distribution and KM Estimates when Detected data are Lognormally Distributed

KM Mean (logged)	-5.561	95% H-UCL (KM -Log)	0.0652
KM SD (logged)	1.824	95% Critical H Value (KM-Log)	3.563
KM Standard Error of Mean (logged)	0.376		

DL/2 Statistics

	,		
DL/2 Normal		DL/2 Log-Transformed	
Mean in Original Scale	0.627	Mean in Log Scale	-4.827
SD in Original Scale	2.476	SD in Log Scale	2.813
95% t UCL (Assumes normality)	1.369	95% H-Stat UCL	5.561

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

Nonparametric Distribution Free UCL Statistics

Detected Data appear Gamma Distributed at 5% Significance Level

Suggested UCL to Use

95% KM (t) UCL	1.199	95% GROS Adjusted Gamma UCL	0.97
95% Adjusted Gamma KM-UCL	5.789		

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.

Recommendations are based upon data size, data distribution, and skewness.

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

1,2-Dichloroethane

General Statistics

Total Number of Observations	32	Number of Distinct Observations	10
Number of Detects	9	Number of Non-Detects	23
Number of Distinct Detects	9	Number of Distinct Non-Detects	2
Minimum Detect	0.07	Minimum Non-Detect	0.438
Maximum Detect	2.133	Maximum Non-Detect	0.5
Variance Detects	0.516	Percent Non-Detects	71.88%
Mean Detects	0.634	SD Detects	0.719
Median Detects	0.24	CV Detects	1.133
Skewness Detects	1.405	Kurtosis Detects	1.168
Mean of Logged Detects	-1.078	SD of Logged Detects	1.22

Normal GOF Test on Detects Only

Shapiro Wilk Test Statistic	0.804	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.829	Detected Data Not Normal at 5% Significance Level
Lilliefors Test Statistic	0.264	Lilliefors GOF Test
5% Lilliefors Critical Value	0.295	Detected Data appear Normal at 5% Significance Level

Detected Data appear Approximate Normal at 5% Significance Level

Kaplan-Meier (KM) Statistics using Normal Critical Values and other Nonparametric UCLs

Mean	0.286	Standard Error of Mean	0.0834
SD	0.424	95% KM (BCA) UCL	0.445
95% KM (t) UCL	0.428	95% KM (Percentile Bootstrap) UCL	0.431
95% KM (z) UCL	0.423	95% KM Bootstrap t UCL	0.539
90% KM Chebyshev UCL	0.536	95% KM Chebyshev UCL	0.65
97.5% KM Chebyshev UCL	0.807	99% KM Chebyshev UCL	1.116

Gamma GOF Tests on Detected Observations Only

A-D Test Statistic	0.387	Anderson-Darling GOF Test
5% A-D Critical Value	0.746	Detected data appear Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.226	Kolmogrov-Smirnoff GOF
5% K-S Critical Value	0.288	Detected data appear Gamma Distributed at 5% Significance Level

Detected data appear Gamma Distributed at 5% Significance Level

Gamma Statistics on Detected Data Only

0.697	k star (bias corrected MLE)	0.935	k hat (MLE)
0.909	Theta star (bias corrected MLE)	0.678	Theta hat (MLE)
12.55	nu star (bias corrected)	16.83	nu hat (MLE)
0.759	MLE Sd (bias corrected)	0.634	MLE Mean (bias corrected)

Gamma Kaplan-Meier (KM) Statistics

29.16	nu hat (KM)	0.456	k hat (KM)
17.36	Adjusted Chi Square Value (29.16, β)	17.83	Approximate Chi Square Value (29.16, α)
0.481	95% Gamma Adjusted KM-UCL (use when n<50)	0.468	95% Gamma Approximate KM-UCL (use when n>=50)

Gamma ROS Statistics using Imputed Non-Detects

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

GROS may not be used when kstar of detected data is small such as < 0.1

For such situations, GROS method tends to yield inflated values of UCLs and BTVs

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

Minimum	0.01	Mean	0.305
Maximum	2.133	Median	0.123
SD	0.458	CV	1.505
k hat (MLE)	0.554	k star (bias corrected MLE)	0.523
Theta hat (MLE)	0.55	Theta star (bias corrected MLE)	0.582
nu hat (MLE)	35.46	nu star (bias corrected)	33.47
MLE Mean (bias corrected)	0.305	MLE Sd (bias corrected)	0.421
		Adjusted Level of Significance (β)	0.0416
Approximate Chi Square Value (33.47, α)	21.24	Adjusted Chi Square Value (33.47, β)	20.72
95% Gamma Approximate UCL (use when n>=50)	0.48	95% Gamma Adjusted UCL (use when n<50)	0.492

Lognormal GOF Test on Detected Observations Only

Shapiro Wilk Test Statistic	0.941	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.829	Detected Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.168	Lilliefors GOF Test
5% Lilliefors Critical Value	0.295	Detected Data appear Lognormal at 5% Significance Level

Detected Data appear Lognormal at 5% Significance Level

Lognormal ROS Statistics Using Imputed Non-Detects

Mean in Original Scale	0.31	Mean in Log Scale	-1.737
SD in Original Scale	0.435	SD in Log Scale	1.026
95% t UCL (assumes normality of ROS data)	0.44	95% Percentile Bootstrap UCL	0.446
95% BCA Bootstrap UCL	0.496	95% Bootstrap t UCL	0.579
95% H-UCL (Log ROS)	0.47		

UCLs using Lognormal Distribution and KM Estimates when Detected data are Lognormally Distributed

KM Mean (logged)	-1.744	95% H-UCL (KM -Log)	0.349
KM SD (logged)	0.839	95% Critical H Value (KM-Log)	2.25
(M Standard Error of Mean (logged)	0.237		

DL/2 Statistics

DL/2 Normal	DL/2 Log-Transformed			
Mean in Original Scale	0.357	Mean in Log Scale	-1.304	
SD in Original Scale	0.405	SD in Log Scale	0.637	
95% t UCL (Assumes normality)	0.478	95% H-Stat UCL	0.42	

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

Nonparametric Distribution Free UCL Statistics

Detected Data appear Approximate Normal Distributed at 5% Significance Level

Suggested UCL to Use

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.

Recommendations are based upon data size, data distribution, and skewness.

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

1,2-Dichloropropane (DCP)

General Statistics

24	Number of Distinct Observations	32	Total Number of Observations
10	Number of Non-Detects	22	Number of Detects
2	Number of Distinct Non-Detects	22	Number of Distinct Detects
0.5	Minimum Non-Detect	0.1	Minimum Detect
29.73	Maximum Non-Detect	1065	Maximum Detect
31.25%	Percent Non-Detects	50964	Variance Detects
225.8	SD Detects	64.69	Mean Detects
3.49	CV Detects	0.965	Median Detects
20.97	Kurtosis Detects	4.539	Skewness Detects
2.513	SD of Logged Detects	1.081	Mean of Logged Detects

Normal GOF Test on Detects Only

0.306	Shapiro Wilk GOF Test
0.911	Detected Data Not Normal at 5% Significance Level
0.397	Lilliefors GOF Test
0.189	Detected Data Not Normal at 5% Significance Level
	0.911 0.397

Detected Data Not Normal at 5% Significance Level

Kaplan-Meier (KM) Statistics using Normal Critical Values and other Nonparametric UCLs

Mean	44.65	Standard Error of Mean	33.52
SD	185.3	95% KM (BCA) UCL	112
95% KM (t) UCL	101.5	95% KM (Percentile Bootstrap) UCL	109.2
95% KM (z) UCL	99.8	95% KM Bootstrap t UCL	450.5
90% KM Chebyshev UCL	145.2	95% KM Chebyshev UCL	190.8
97.5% KM Chebyshev UCL	254	99% KM Chebyshev UCL	378.2

Gamma GOF Tests on Detected Observations Only

Anderson-Darling GOF Test	2.187	A-D Test Statistic
Detected Data Not Gamma Distributed at 5% Significance Level	0.881	5% A-D Critical Value
Kolmogrov-Smirnoff GOF	0.242	K-S Test Statistic
Detected Data Not Gamma Distributed at 5% Significance Level	0.204	5% K-S Critical Value

Detected Data Not Gamma Distributed at 5% Significance Level

Gamma Statistics on Detected Data Only

0.231	k star (bias corrected MLE)	0.233	k hat (MLE)
279.8	Theta star (bias corrected MLE)	278.1	Theta hat (MLE)
10.17	nu star (bias corrected)	10.24	nu hat (MLE)
134.5	MLE Sd (bias corrected)	64.69	MLE Mean (bias corrected)

Gamma Kaplan-Meier (KM) Statistics

3.717	nu hat (KM)	0.0581	k hat (KM)
0.553	Adjusted Chi Square Value (3.72, β)	0.613	Approximate Chi Square Value (3.72, α)
300.2	95% Gamma Adjusted KM-UCL (use when n<50)	270.6	95% Gamma Approximate KM-UCL (use when n>=50)

Gamma (KM) may not be used when k hat (KM) is < 0.1

Gamma ROS Statistics using Imputed Non-Detects

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

GROS may not be used when kstar of detected data is small such as < 0.1

For such situations, GROS method tends to yield inflated values of UCLs and BTVs

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

Minimum	0.01	Mean	44.48
Maximum	1065	Median	0.448
SD	188.3	CV	4.233
k hat (MLE)	0.168	k star (bias corrected MLE)	0.173
Theta hat (MLE)	264.3	Theta star (bias corrected MLE)	256.6
nu hat (MLE)	10.77	nu star (bias corrected)	11.09
MLE Mean (bias corrected)	44.48	MLE Sd (bias corrected)	106.8
		Adjusted Level of Significance (β)	0.0416
Approximate Chi Square Value (11.09, α)	4.636	Adjusted Chi Square Value (11.09, β)	4.413
95% Gamma Approximate UCL (use when n>=50)	106.4	95% Gamma Adjusted UCL (use when n<50)	111.8

Lognormal GOF Test on Detected Observations Only

Shapiro Wilk Test Statistic	0.913	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.911	Detected Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.198	Lilliefors GOF Test
5% Lilliefors Critical Value	0.189	Detected Data Not Lognormal at 5% Significance Level

Detected Data appear Approximate Lognormal at 5% Significance Level

Lognormal ROS Statistics Using Imputed Non-Detects

Mean in Original Scale	44.62	Mean in Log Scale	0.335
SD in Original Scale	188.2	SD in Log Scale	2.461
95% t UCL (assumes normality of ROS data)	101	95% Percentile Bootstrap UCL	109.4
95% BCA Bootstrap UCL	150.2	95% Bootstrap t UCL	444.3
95% H-UCL (Log ROS)	216		

UCLs using Lognormal Distribution and KM Estimates when Detected data are Lognormally Distributed

KM Mean (logged)	0.39	95% H-UCL (KM -Log)	129.7
KM SD (logged)	2.315	95% Critical H Value (KM-Log)	4.32

KM Standard Error of Mean (logged) 0.428

DL/2 Statistics

DL/2 Normal		DL/2 Log-Transformed	
Mean in Original Scale	45.01	Mean in Log Scale	0.438
SD in Original Scale	188.2	SD in Log Scale	2.388
95% t UCL (Assumes normality)	101.4	95% H-Stat UCL	179.6

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

Nonparametric Distribution Free UCL Statistics

Detected Data appear Approximate Lognormal Distributed at 5% Significance Level

Suggested UCL to Use

99% KM (Chebyshev) UCL 378.2

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.

Recommendations are based upon data size, data distribution, and skewness.

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

1,3-Dichloropropane

General Statistics

Total Number of Observations	32	Number of Distinct Observations	6
Number of Detects	6	Number of Non-Detects	26
Number of Distinct Detects	6	Number of Distinct Non-Detects	1
Minimum Detect	0.06	Minimum Non-Detect	0.5
Maximum Detect	1.537	Maximum Non-Detect	0.5
Variance Detects	0.319	Percent Non-Detects	81.25%
Mean Detects	0.454	SD Detects	0.565
Median Detects	0.272	CV Detects	1.244
Skewness Detects	1.847	Kurtosis Detects	3.595
Mean of Logged Detects	-1.453	SD of Logged Detects	1.287

Normal GOF Test on Detects Only

Shapiro Wilk Test Statistic	0.755	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.788	Detected Data Not Normal at 5% Significance Level
Lilliefors Test Statistic	0.301	Lilliefors GOF Test
5% Lilliefors Critical Value	0.362	Detected Data appear Normal at 5% Significance Level

Detected Data appear Approximate Normal at 5% Significance Level

Kaplan-Meier (KM) Statistics using Normal Critical Values and other Nonparametric UCLs

Mean	0.225	Standard Error of Mean	0.0951
SD	0.288	95% KM (BCA) UCL	0.436
95% KM (t) UCL	0.386	95% KM (Percentile Bootstrap) UCL	0.412
95% KM (z) UCL	0.381	95% KM Bootstrap t UCL	0.942
90% KM Chebyshev UCL	0.51	95% KM Chebyshev UCL	0.639
97.5% KM Chebyshev UCL	0.819	99% KM Chebyshev UCL	1.171

A-D Test Statistic	0.455	Anderson-Darling GOF Test
5% A-D Critical Value	0.718	Detected data appear Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.286	Kolmogrov-Smirnoff GOF
5% K-S Critical Value	0.342	Detected data appear Gamma Distributed at 5% Significance Level

Detected data appear Gamma Distributed at 5% Significance Level

Gamma Statistics on Detected Data Only

k hat (MLE)	0.883	k star (bias corrected MLE)	0.553
Theta hat (MLE)	0.514	Theta star (bias corrected MLE)	0.822
nu hat (MLE)	10.6	nu star (bias corrected)	6.633
MLE Mean (bias corrected)	0.454	MLE Sd (bias corrected)	0.611

Gamma Kaplan-Meier (KM) Statistics

k hat (KM)	0.609	nu hat (KM)	38.97
Approximate Chi Square Value (38.97, α)	25.67	Adjusted Chi Square Value (38.97, β)	25.1
95% Gamma Approximate KM-UCL (use when n>=50)	0.341	95% Gamma Adjusted KM-UCL (use when n<50)	0.349

Gamma ROS Statistics using Imputed Non-Detects

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

GROS may not be used when kstar of detected data is small such as < 0.1

For such situations, GROS method tends to yield inflated values of UCLs and BTVs

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

Minimum	0.01	Mean	0.232
Maximum	1.537	Median	0.115
SD	0.305	CV	1.314
k hat (MLE)	0.692	k star (bias corrected MLE)	0.648
Theta hat (MLE)	0.336	Theta star (bias corrected MLE)	0.358
nu hat (MLE)	44.3	nu star (bias corrected)	41.48
MLE Mean (bias corrected)	0.232	MLE Sd (bias corrected)	0.289
		Adjusted Level of Significance (β)	0.0416
Approximate Chi Square Value (41.48, α)	27.72	Adjusted Chi Square Value (41.48, β)	27.11
95% Gamma Approximate UCL (use when n>=50)	0.348	95% Gamma Adjusted UCL (use when n<50)	0.355

Lognormal GOF Test on Detected Observations Only

Shapiro Wilk Test Statistic	0.896	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.788	Detected Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.261	Lilliefors GOF Test
5% Lilliefors Critical Value	0.362	Detected Data appear Lognormal at 5% Significance Level

Detected Data appear Lognormal at 5% Significance Level

Lognormal ROS Statistics Using Imputed Non-Detects

Mean in Original Scale	0.214	Mean in Log Scale	-2.039
SD in Original Scale	0.28	SD in Log Scale	0.979
95% t UCL (assumes normality of ROS data)	0.298	95% Percentile Bootstrap UCL	0.301
95% BCA Bootstrap UCL	0.339	95% Bootstrap t UCL	0.372
95% H-UCL (Log ROS)	0.321		

UCLs using Lognormal Distribution and KM Estimates when Detected data are Lognormally Distributed

KM Mean (logged)	-1.989	95% H-UCL (KM -Log)	0.3
KM SD (logged)	0.903	95% Critical H Value (KM-Log)	2.321
KM Standard Error of Mean (logged)	0.41		

DL/2 Statistics

DL/2 Normal		DL/2 Log-Transformed	
Mean in Original Scale	0.288	Mean in Log Scale	-1.399
SD in Original Scale	0.241	SD in Log Scale	0.517
95% t UCL (Assumes normality)	0.36	95% H-Stat UCL	0.338

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

Nonparametric Distribution Free UCL Statistics

Detected Data appear Approximate Normal Distributed at 5% Significance Level

Suggested UCL to Use

95% KM (t) UCL 0.386 95% KM (Percentile Bootstrap) UCL 0.412

 $Note: Suggestions\ regarding\ the\ selection\ of\ a\ 95\%\ UCL\ are\ provided\ to\ help\ the\ user\ to\ select\ the\ most\ appropriate\ 95\%\ UCL.$

Recommendations are based upon data size, data distribution, and skewness.

These recommendations are based upon the results of the simulation studies summarized in Singh, Maichle, and Lee (2006).

However, simulations results will not cover all Real World data sets; for additional insight the user may want to consult a statistician.

Benzene

General Statistics

Total Number of Observations	32	Number of Distinct Observations	14
Number of Detects	12	Number of Non-Detects	20
Number of Distinct Detects	12	Number of Distinct Non-Detects	3
Minimum Detect	0.083	Minimum Non-Detect	0.5
Maximum Detect	93	Maximum Non-Detect	14.5
Variance Detects	863.8	Percent Non-Detects	62.5%
Mean Detects	16.53	SD Detects	29.39
Median Detects	1.7	CV Detects	1.778
Skewness Detects	2.01	Kurtosis Detects	3.659
Mean of Logged Detects	0.587	SD of Logged Detects	2.531

Normal GOF Test on Detects Only

Shapiro Wilk Test Statistic	0.647	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.859	Detected Data Not Normal at 5% Significance Level
Lilliefors Test Statistic	0.357	Lilliefors GOF Test
5% Lilliefors Critical Value	0.256	Detected Data Not Normal at 5% Significance Level

Detected Data Not Normal at 5% Significance Level

Kaplan-Meier (KM) Statistics using Normal Critical Values and other Nonparametric UCLs

3.503	Standard Error of Mean	6.301	Mean
12.7	95% KM (BCA) UCL	18.97	SD
12.3	95% KM (Percentile Bootstrap) UCL	12.24	95% KM (t) UCL
20.93	95% KM Bootstrap t UCL	12.06	95% KM (z) UCL
21.57	95% KM Chebyshev UCL	16.81	90% KM Chebyshev UCL
41.16	99% KM Chebyshev UCL	28.18	97.5% KM Chebyshev UCL

Gamma GOF	Tests on Detected	Observations Only
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Anderson-Darling GOF Test	0.707	A-D Test Statistic
Detected data appear Gamma Distributed at 5% Significance Leve	0.822	5% A-D Critical Value
Kolmogrov-Smirnoff GOF	0.271	K-S Test Statistic
Detected Data Not Gamma Distributed at 5% Significance Level	0.265	5% K-S Critical Value

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

Gamma Statistics on Detected Data Only

k hat (MLE)	0.309	k star (bias corrected MLE)	0.288
Theta hat (MLE)	53.43	Theta star (bias corrected MLE)	57.48
nu hat (MLE)	7.424	nu star (bias corrected)	6.901
MLE Mean (bias corrected)	16.53	MLE Sd (bias corrected)	30.82

Gamma Kaplan-Meier (KM) Statistics

k hat (KM)	0.11	nu hat (KM)	7.061
Approximate Chi Square Value (7.06, α)	2.204	Adjusted Chi Square Value (7.06, β)	2.062
95% Gamma Approximate KM-UCL (use when n>=50)	20.18	95% Gamma Adjusted KM-UCL (use when n<50)	21.58

Gamma ROS Statistics using Imputed Non-Detects

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

GROS may not be used when kstar of detected data is small such as < 0.1

For such situations, GROS method tends to yield inflated values of UCLs and BTVs

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

Minimum	0.01	Mean	6.217
Maximum	93	Median	0.01
SD	19.3	CV	3.104
k hat (MLE)	0.172	k star (bias corrected MLE)	0.177
Theta hat (MLE)	36.08	Theta star (bias corrected MLE)	35.12
nu hat (MLE)	11.03	nu star (bias corrected)	11.33
MLE Mean (bias corrected)	6.217	MLE Sd (bias corrected)	14.78
		Adjusted Level of Significance (β)	0.0416
Approximate Chi Square Value (11.33, α)	4.788	Adjusted Chi Square Value (11.33, β)	4.561
95% Gamma Approximate UCL (use when n>=50)	14.71	95% Gamma Adjusted UCL (use when n<50)	15.44

Lognormal GOF Test on Detected Observations Only

Shapiro Wilk Test Statistic	0.914	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.859	Detected Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.156	Lilliefors GOF Test
5% Lilliefors Critical Value	0.256	Detected Data appear Lognormal at 5% Significance Level

Detected Data appear Lognormal at 5% Significance Level

Lognormal ROS Statistics Using Imputed Non-Detects

-1.176	Mean in Log Scale	6.362	Mean in Original Scale
2.411	SD in Log Scale	19.25	SD in Original Scale
12.38	95% Percentile Bootstrap UCL	12.13	95% t UCL (assumes normality of ROS data)
21.17	95% Bootstrap t UCL	14.99	95% BCA Bootstrap UCL
		39.06	95% H-UCL (Log ROS)

UCLs using Lognormal Distribution and KM Estimates when Detected data are Lognormally Distributed

KM Mean (logged)	-1.076	95% H-UCL (KM -Log)	10.05
KM SD (logged)	2.002	95% Critical H Value (KM-Log)	3.835
KM Standard Error of Mean (logged)	0.396		

DL/2 Statistics

DL/2 Normal		DL/2 Log-Transformed	
Mean in Original Scale	6.591	Mean in Log Scale	-0.504
SD in Original Scale	19.21	SD in Log Scale	1.84
95% t UCL (Assumes normality)	12.35	95% H-Stat UCL	10.76

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

Nonparametric Distribution Free UCL Statistics

Detected Data appear Approximate Gamma Distributed at 5% Significance Level

Suggested UCL to Use

95% KM (t) UCL	12.24	95% GROS Adjusted Gamma UCL	15.44
95% Adjusted Gamma KM-UCL	21.58		

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.

Recommendations are based upon data size, data distribution, and skewness.

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

Carbon Tetrachloride (CCL4)

General Statistics

14	Number of Distinct Observations	32	Total Number of Observations
20	Number of Non-Detects	12	Number of Detects
2	Number of Distinct Non-Detects	12	Number of Distinct Detects
0.5	Minimum Non-Detect	0.11	Minimum Detect
1.625	Maximum Non-Detect	13.4	Maximum Detect
62.5%	Percent Non-Detects	24.04	Variance Detects
4.903	SD Detects	3.94	Mean Detects
1.244	CV Detects	1.22	Median Detects
-0.184	Kurtosis Detects	1.073	Skewness Detects
1.971	SD of Logged Detects	0.0762	Mean of Logged Detects

Normal GOF Test on Detects Only

Shapiro Wilk Test Statistic	0.789	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.859	Detected Data Not Normal at 5% Significance Level
Lilliefors Test Statistic	0.263	Lilliefors GOF Test
5% Lilliefors Critical Value	0.256	Detected Data Not Normal at 5% Significance Level

Detected Data Not Normal at 5% Significance Level

Kaplan-Meier (KM) Statistics using Normal Critical Values and other Nonparametric UCLs

0.63	Standard Error of Mean	1.568	Mean
2.657	95% KM (BCA) UCL	3.412	SD
2.636	95% KM (Percentile Bootstrap) UCL	2.637	95% KM (t) UCL
3.355	95% KM Bootstrap t UCL	2.605	95% KM (z) UCL
4.315	95% KM Chebyshev UCL	3.459	90% KM Chebyshev UCL
7.838	99% KM Chebyshev UCL	5.503	97.5% KM Chebyshev UCL

Gamma (GOF 1	Tests on	Detected	Observations Only
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Anderson-Darling GOF Test	0.702	A-D Test Statistic
Detected data appear Gamma Distributed at 5% Significance Level	0.787	5% A-D Critical Value
Kolmogrov-Smirnoff GOF	0.228	K-S Test Statistic
Detected data appear Gamma Distributed at 5% Significance Level	0.259	5% K-S Critical Value

Detected data appear Gamma Distributed at 5% Significance Level

Gamma Statistics on Detected Data Only

.E) 0.424	k star (bias corrected MLE)	0.492	k hat (MLE)
E) 9.285	Theta star (bias corrected MLE)	8.013	Theta hat (MLE)
d) 10.18	nu star (bias corrected)	11.8	nu hat (MLE)
d) 6.049	MLE Sd (bias corrected)	3.94	MLE Mean (bias corrected)

Gamma Kaplan-Meier (KM) Statistics

k hat (KM)	0.211	nu hat (KM)	13.52
Approximate Chi Square Value (13.52, α)	6.244	Adjusted Chi Square Value (13.52, β)	5.98
95% Gamma Approximate KM-UCL (use when n>=50)	3.396	95% Gamma Adjusted KM-UCL (use when n<50)	3.546

Gamma ROS Statistics using Imputed Non-Detects

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

GROS may not be used when kstar of detected data is small such as < 0.1

For such situations, GROS method tends to yield inflated values of UCLs and BTVs

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

Minimum	0.01	Mean	1.692
Maximum	13.4	Median	0.123
SD	3.454	CV	2.041
k hat (MLE)	0.275	k star (bias corrected MLE)	0.27
Theta hat (MLE)	6.161	Theta star (bias corrected MLE)	6.273
nu hat (MLE)	17.58	nu star (bias corrected)	17.26
MLE Mean (bias corrected)	1.692	MLE Sd (bias corrected)	3.258
		Adjusted Level of Significance (β)	0.0416
Approximate Chi Square Value (17.26, α)	8.86	Adjusted Chi Square Value (17.26, β)	8.537
95% Gamma Approximate UCL (use when n>=50)	3.297	95% Gamma Adjusted UCL (use when n<50)	3.421

Lognormal GOF Test on Detected Observations Only

Shapiro Wilk Test Statistic	0.85	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.859	Detected Data Not Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.211	Lilliefors GOF Test
5% Lilliefors Critical Value	0.256	Detected Data appear Lognormal at 5% Significance Level

Detected Data appear Approximate Lognormal at 5% Significance Level

Lognormal ROS Statistics Using Imputed Non-Detects

Mean in Original Scale	1.667	Mean in Log Scale	-1.105
SD in Original Scale	3.434	SD in Log Scale	1.806
95% t UCL (assumes normality of ROS data)	2.696	95% Percentile Bootstrap UCL	2.724
95% BCA Bootstrap UCL	3.018	95% Bootstrap t UCL	3.438
95% H-UCL (Log ROS)	5.327		

UCLs using Lognormal Distribution and KM Estimates when Detected data are Lognormally Distributed

KM Mean (logged)	-1.2	95% H-UCL (KM -Log)	2.317
KM SD (logged)	1.534	95% Critical H Value (KM-Log)	3.138
KM Standard Error of Mean (logged)	0.294		

DL/2 Statistics

DL/2 Normal		DL/2 Log-Transformed	
Mean in Original Scale	1.651	Mean in Log Scale	-0.801
SD in Original Scale	3.433	SD in Log Scale	1.378
95% t UCL (Assumes normality)	2.68	95% H-Stat UCL	2.389

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

Nonparametric Distribution Free UCL Statistics

Detected Data appear Gamma Distributed at 5% Significance Level

Suggested UCL to Use

95% KM (t) UCL 2.637 95% GROS Adjusted Gamma UCL 3.421 95% Adjusted Gamma KM-UCL 3.546

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.

Recommendations are based upon data size, data distribution, and skewness.

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

Chloroform

General Statistics

Total Number of Observations	32	Number of Distinct Observations	18
Number of Detects	15	Number of Non-Detects	17
Number of Distinct Detects	15	Number of Distinct Non-Detects	3
Minimum Detect	0.089	Minimum Non-Detect	0.415
Maximum Detect	24	Maximum Non-Detect	0.5
Variance Detects	36.66	Percent Non-Detects	53.13%
Mean Detects	2.231	SD Detects	6.055
Median Detects	0.61	CV Detects	2.714
Skewness Detects	3.802	Kurtosis Detects	14.6
Mean of Logged Detects	-0.591	SD of Logged Detects	1.448

Normal GOF Test on Detects Only

Shapiro Wilk Test Statistic	0.369	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.881	Detected Data Not Normal at 5% Significance Level
Lilliefors Test Statistic	0.43	Lilliefors GOF Test
5% Lilliefors Critical Value	0.229	Detected Data Not Normal at 5% Significance Level

Detected Data Not Normal at 5% Significance Level

Kaplan-Meier (KM) Statistics using Normal Critical Values and other Nonparametric UCLs

0.757	Standard Error of Mean	1.142	Mean
2.671	95% KM (BCA) UCL	4.134	SD
2.601	95% KM (Percentile Bootstrap) UCL	2.425	95% KM (t) UCL
10.9	95% KM Bootstrap t UCL	2.387	95% KM (z) UCL
4.44	95% KM Chebyshev UCL	3.412	90% KM Chebyshev UCL
8.67	99% KM Chebyshev UCL	5.867	97.5% KM Chebyshev UCL

Gamma GOF Tests on Detected Observations Only

Anderson-Darling GOF Test	1.641	A-D Test Statistic
Detected Data Not Gamma Distributed at 5% Significance Level	0.801	5% A-D Critical Value
Kolmogrov-Smirnoff GOF	0.263	K-S Test Statistic
Detected Data Not Gamma Distributed at 5% Significance Level	0.235	5% K-S Critical Value

Detected Data Not Gamma Distributed at 5% Significance Level

Gamma Statistics on Detected Data Only

0.414	k star (bias corrected MLE)	0.462	k hat (MLE)
5.391	Theta star (bias corrected MLE)	4.832	Theta hat (MLE)
12.41	nu star (bias corrected)	13.85	nu hat (MLE)
3.468	MLE Sd (bias corrected)	2.231	MLE Mean (bias corrected)

Gamma Kaplan-Meier (KM) Statistics

4.887	nu hat (KM)	0.0764	k hat (KM)
1.009	Adjusted Chi Square Value (4.89, β)	1.1	Approximate Chi Square Value (4.89, α)
5.531	95% Gamma Adjusted KM-UCL (use when n<50)	5.073	95% Gamma Approximate KM-UCL (use when n>=50)

Gamma (KM) may not be used when k hat (KM) is < 0.1

Gamma ROS Statistics using Imputed Non-Detects

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

GROS may not be used when kstar of detected data is small such as < 0.1

For such situations, GROS method tends to yield inflated values of UCLs and BTVs

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

1.08	Mean	0.01	Minimum
0.105	Median	24	Maximum
3.904	CV	4.217	SD
0.268	k star (bias corrected MLE)	0.272	k hat (MLE)
4.035	Theta star (bias corrected MLE)	3.965	Theta hat (MLE)
17.13	nu star (bias corrected)	17.43	nu hat (MLE)
2.088	MLE Sd (bias corrected)	1.08	MLE Mean (bias corrected)
0.0416	Adjusted Level of Significance (β)		
8.445	Adjusted Chi Square Value (17.13, β)	8.766	Approximate Chi Square Value (17.13, α)
2.191	95% Gamma Adjusted UCL (use when n<50)	2.111	95% Gamma Approximate UCL (use when n>=50)

Lognormal GOF Test on Detected Observations Only

Shapiro Wilk GOF Test	0.912	Shapiro Wilk Test Statistic
Detected Data appear Lognormal at 5% Significance Leve	0.881	5% Shapiro Wilk Critical Value
Lilliefors GOF Test	0.135	Lilliefors Test Statistic
Detected Data appear Lognormal at 5% Significance Leve	0.229	5% Lilliefors Critical Value

Detected Data appear Lognormal at 5% Significance Level

Lognormal ROS Statistics Using Imputed Non-Detects

Mean in Original Scale	1.164	Mean in Log Scale	-1.227
SD in Original Scale	4.196	SD in Log Scale	1.298
95% t UCL (assumes normality of ROS data)	2.422	95% Percentile Bootstrap UCL	2.615
95% BCA Bootstrap UCL	3.45	95% Bootstrap t UCL	11.13
95% H-UCL (Log ROS)	1.312		

UCLs using Lognormal Distribution and KM Estimates when Detected data are Lognormally Distributed

KM Mean (logged)	-1.22	95% H-UCL (KM -Log)	1.001
KM SD (logged)	1.16	95% Critical H Value (KM-Log)	2.629
1. 15	0.222		

KM Standard Error of Mean (logged) 0.233

DL/2 Statistics

DL/2 Normal		DL/2 Log-Transformed			
Mean in Original Scale	1.176	Mean in Log Scale	-1.023		
SD in Original Scale	4.192	SD in Log Scale	1.058		
95% t UCL (Assumes normality)	2.433	95% H-Stat UCL	1.011		

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

Nonparametric Distribution Free UCL Statistics

Detected Data appear Lognormal Distributed at 5% Significance Level

Suggested UCL to Use

95% KM (BCA) UCL 2.671

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.

Recommendations are based upon data size, data distribution, and skewness.

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

cis-1,3-Dichloropropene

General Statistics

Total Number of Observations	32	Number of Distinct Observations	5
Number of Detects	3	Number of Non-Detects	29
Number of Distinct Detects	3	Number of Distinct Non-Detects	3
Minimum Detect	0.22	Minimum Non-Detect	0.5
Maximum Detect	0.5	Maximum Non-Detect	14.5
Variance Detects	0.0229	Percent Non-Detects	90.63%
Mean Detects	0.327	SD Detects	0.151
Median Detects	0.26	CV Detects	0.464
Skewness Detects	1.597	Kurtosis Detects	N/A
Mean of Logged Detects	-1.185	SD of Logged Detects	0.434

Warning: Data set has only 3 Detected Values.

This is not enough to compute meaningful or reliable statistics and estimates.

Normal GOF Test on Detects Only

Shapiro Wilk Test Statistic	0.855	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.767	Detected Data appear Normal at 5% Significance Level
Lilliefors Test Statistic	0.337	Lilliefors GOF Test
5% Lilliefors Critical Value	0.512	Detected Data appear Normal at 5% Significance Level

Detected Data appear Normal at 5% Significance Level

Kaplan-Meier (KM) Statistics using Normal Critical Values and other Nonparametric

Mean	0.249	Standard Error of Mean	0.0197
SD	0.0506	95% KM (BCA) UCL	N/A
95% KM (t) UCL	0.282	95% KM (Percentile Bootstrap) UCL	N/A
95% KM (z) UCL	0.281	95% KM Bootstrap t UCL	N/A
90% KM Chebyshev UCL	0.308	95% KM Chebyshev UCL	0.335
97.5% KM Chebyshev UCL	0.372	99% KM Chebyshev UCL	0.445

Gamma GOF Tests on Detected Observations Only

Not Enough Data to Perform GOF Test

Gamma Statistics on Detected Data Only

N/A	k star (bias corrected MLE)	7.742	k hat (MLE)
N/A	Theta star (bias corrected MLE)	0.0422	Theta hat (MLE)
N/A	nu star (bias corrected)	46.45	nu hat (MLE)
N/A	MLE Sd (bias corrected)	N/A	MLE Mean (bias corrected)

Gamma Kaplan-Meier (KM) Statistics

1543	nu hat (KM)	24.11	k hat (KM)
0.0416	Adjusted Level of Significance (β)		
1448	Adjusted Chi Square Value (N/A, β)	1453	Approximate Chi Square Value (N/A, α)
0.265	95% Gamma Adjusted KM-UCL (use when n<50)	0.264	95% Gamma Approximate KM-UCL (use when n>=50)

Lognormal GOF Test on Detected Observations Only

Shapiro Wilk GOF Test	0.895	Shapiro Wilk Test Statistic
Detected Data appear Lognormal at 5% Significance Leve	0.767	5% Shapiro Wilk Critical Value
Lilliefors GOF Test	0.312	Lilliefors Test Statistic
Detected Data appear Lognormal at 5% Significance Leve	0.512	5% Lilliefors Critical Value

Detected Data appear Lognormal at 5% Significance Level

Lognormal ROS Statistics Using Imputed Non-Detects

Mean in Original Scale	0.256	Mean in Log Scale	-1.403
SD in Original Scale	0.0772	SD in Log Scale	0.288
95% t UCL (assumes normality of ROS data)	0.279	95% Percentile Bootstrap UCL	0.279
95% BCA Bootstrap UCL	0.281	95% Bootstrap t UCL	0.283
95% H-UCL (Log ROS)	0.281		

UCLs using Lognormal Distribution and KM Estimates when Detected data are Lognormally Distributed

KM Mean (logged)	-1.406	95% H-UCL (KM -Log)	0.26
KM SD (logged)	0.156	95% Critical H Value (KM-Log)	1.724
VM Standard Error of Moan (logged)	0.0750		

KM Standard Error of Mean (logged) 0.0759

DL/2 Statistics

DL/2 Normal		DL/2 Log-Transformed	
Mean in Original Scale	0.494	Mean in Log Scale	-1.225
SD in Original Scale	1.238	SD in Log Scale	0.632
95% t UCL (Assumes normality)	0.864	95% H-Stat UCL	0.452

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

Nonparametric Distribution Free UCL Statistics

Detected Data appear Normal Distributed at 5% Significance Level

Suggested UCL to Use

95% KM (t) UCL 0.282 95% KM (Percentile Bootstrap) UCL N/A

Warning: One or more Recommended UCL(s) not available!

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.

Recommendations are based upon data size, data distribution, and skewness.

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

Vinyl Chloride

General Statistics

Total Number of Observations	32	Number of Distinct Observations	8
Number of Detects	6	Number of Non-Detects	26
Number of Distinct Detects	5	Number of Distinct Non-Detects	3
Minimum Detect	0.098	Minimum Non-Detect	0.5
Maximum Detect	0.25	Maximum Non-Detect	14.5
Variance Detects	0.00548	Percent Non-Detects	81.25%
Mean Detects	0.15	SD Detects	0.074
Median Detects	0.105	CV Detects	0.495
Skewness Detects	0.963	Kurtosis Detects	-1.829
Mean of Logged Detects	-1.991	SD of Logged Detects	0.455

Normal GOF Test on Detects Only

Shapiro Wilk Test Statistic 0.694	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value 0.788	Detected Data Not Normal at 5% Significance Level
Lilliefors Test Statistic 0.371	Lilliefors GOF Test
5% Lilliefors Critical Value 0.362	Detected Data Not Normal at 5% Significance Level

Detected Data Not Normal at 5% Significance Level

Kaplan-Meier (KM) Statistics using Normal Critical Values and other Nonparametric UCLs

Mean	0.15	Standard Error of Mean	0.0302
SD	0.0676	95% KM (BCA) UCL	0.2
95% KM (t) UCL	0.201	95% KM (Percentile Bootstrap) UCL	0.2
95% KM (z) UCL	0.199	95% KM Bootstrap t UCL	0.802
90% KM Chebyshev UCL	0.24	95% KM Chebyshev UCL	0.281
97.5% KM Chebyshev UCL	0.338	99% KM Chebyshev UCL	0.45

Gamma GOF Tests on Detected Observations Only

A-D Test Statistic	1.012	Anderson-Darling GOF Test
5% A-D Critical Value	0.698	Detected Data Not Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.375	Kolmogrov-Smirnoff GOF
5% K-S Critical Value	0.333	Detected Data Not Gamma Distributed at 5% Significance Level

Detected Data Not Gamma Distributed at 5% Significance Level

Gamma Statistics on Detected Data Only

2.906	k star (bias corrected MLE)	5.59	k hat (MLE)
0.0515	Theta star (bias corrected MLE)	0.0268	Theta hat (MLE)
34.88	nu star (bias corrected)	67.09	nu hat (MLE)
0.0878	MLE Sd (bias corrected)	0.15	MLE Mean (bias corrected)

313.9	nu hat (KM)	4.905	k hat (KM)
271.8	Adjusted Chi Square Value (313.89, β)	273.8	Approximate Chi Square Value (313.89, α)
0.173	95% Gamma Adjusted KM-UCL (use when n<50)	0.172	95% Gamma Approximate KM-UCL (use when n>=50)

Gamma ROS Statistics using Imputed Non-Detects

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

GROS may not be used when kstar of detected data is small such as < 0.1

For such situations, GROS method tends to yield inflated values of UCLs and BTVs

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

Minimum	0.0321	Mean	0.152
Maximum	0.329	Median	0.142
SD	0.0727	CV	0.479
k hat (MLE)	4.234	k star (bias corrected MLE)	3.858
Theta hat (MLE)	0.0359	Theta star (bias corrected MLE)	0.0394
nu hat (MLE)	271	nu star (bias corrected)	246.9
MLE Mean (bias corrected)	0.152	MLE Sd (bias corrected)	0.0773
		Adjusted Level of Significance (β)	0.0416
Approximate Chi Square Value (246.88, α)	211.5	Adjusted Chi Square Value (246.88, β)	209.8
95% Gamma Approximate UCL (use when n>=50)	0.177	95% Gamma Adjusted UCL (use when n<50)	0.179

Lognormal GOF Test on Detected Observations Only

Shapiro Wilk Test Statistic	0.709	Shapiro Wilk GOF Test
5% Shapiro Wilk Critical Value	0.788	Detected Data Not Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.349	Lilliefors GOF Test
5% Lilliefors Critical Value	0.362	Detected Data appear Lognormal at 5% Significance Level

Detected Data appear Approximate Lognormal at 5% Significance Level

Lognormal ROS Statistics Using Imputed Non-Detects

Mean in Original Scale	0.15	Mean in Log Scale	-1.991
SD in Original Scale	0.0671	SD in Log Scale	0.435
95% t UCL (assumes normality of ROS data)	0.17	95% Percentile Bootstrap UCL	0.169
95% BCA Bootstrap UCL	0.171	95% Bootstrap t UCL	0.172
95% H-UCL (Log ROS)	0.174		

UCLs using Lognormal Distribution and KM Estimates when Detected data are Lognormally Distributed

KM Mean (logged)	-1.991	95% H-UCL (KM -Log)	0.171
KM SD (logged)	0.415	95% Critical H Value (KM-Log)	1.87
KM Standard Error of Mean (logged)	0.186		

DL/2 Statistics

DL/2 Normal		DL/2 Log-Transformed	
Mean in Original Scale	0.468	Mean in Log Scale	-1.358
SD in Original Scale	1.243	SD in Log Scale	0.717
95% t UCL (Assumes normality)	0.84	95% H-Stat UCL	0.437

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

Nonparametric Distribution Free UCL Statistics

Detected Data appear Approximate Lognormal Distributed at 5% Significance Level

Suggested UCL to Use

95% KM (t) UCL 0.201

95% KM (% Bootstrap) UCL

0.2

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.

Recommendations are based upon data size, data distribution, and skewness.

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