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ANALYSIS OF CENSORED DATA IN GROUNDWATER MONITORING WELLS AT THE SAVANNAH RIVER SITE

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ABSTRACT

It is common in environmental analyses to deal with censored data. Censored data characteristically arise through laboratory analysis of samples with contaminant concentrations less than what the analytical method is able to reliably detect. These data are called "less than detectable". Comparisons between downgradient or monitoring groundwater wells and upgradient or background wells are frequently done to determine if downgradient wells are more contaminated than background or some established maximum concentration limits (MCL's). In addition, parameter estimates are often desired. The presence of censored data complicates the statistics that can be used as estimators for individual populations or to estimate differences between two populations.

This paper describes the current process at Savannah River Site (SRS) to determine constituents of concern (COC's) for complying with groundwater monitoring and clean-up regulations. COC's are analytes found in downgradient monitoring wells in concentrations significantly greater than in background wells or significantly greater than the MCL's. Both parametric and non-parametric statistics are explored. Data plots are examined for outliers, trends, laboratory or sampling contamination, and unusually large detection limits for censored results. Wells are grouped by similar concentration levels to form a "characteristic" well, improving the estimation and decision process. Different methods are compared.

INTRODUCTION

This paper will describe the statistical analyses currently being used at SRS to develop COC lists and estimate concentration levels in the groundwater monitoring (POC) and background (BG) wells. Several parametric and non-parametric methodologies to determine a COC list are compared with the current SRS method.

For many regulatory purposes, statistical analyses of censored (less than detectable) ground water monitoring data are required to demonstrate presence or absence of statistically significant concentration levels in monitoring

wells compared with background or established maximum concentration limits (MCL's), or to determine if there is a significant health risk. One of the requirements is to develop a list of constituents of concern (COC). In addition, parameter estimates of the ground water concentration levels are often desired.

The presence of results reported at "less than detection limits" adds a complex element to the statistical analyses. The actual concentration values for these "less than detected" results are generally unavailable. In addition, the data usually contain multiple detection limits due to (1) improvement in analytical methods over time, (2) use of alternate methods with higher detection limits, (3) several laboratories analyzing the samples, or (4) matrix characteristics and sample dilution factors used by the different laboratories and analytical methods. Thus, measurements above detection are often interspersed with results reported at less than detection.

Before analyzing any of the ground water data, plots of individual results over time, by well, laboratory, and analytical method are made for each constituent with at least one result above detection limits. These plots are examined to determine if there are individual outliers, sampling, laboratory, or analytical problems. Past experience has indicated that some methods produce results with much smaller detection limits than other analytical methods. In addition, laboratory problems have been noted with a given laboratory for one or more quarters due to blank contamination, spiking of ground water samples, and significantly larger or smaller percent return than expected on the spiked quality control samples. If causes for these grouped outliers can be identified, these results are omitted from further analyses. Individual outlier results that appear not to conform to both preceding and succeeding results or that appear significantly different from replicate results either by the same laboratory or by different laboratories for the same quarter are flagged and investigated. If no cause for omitting the flagged outliers can be identified, a statistical outlier test is applied. Those results failing the outlier test at an alpha level of 0.005 are omitted from further analyses. The remaining data are again plotted to determine if there is a trend over time. The statistical analyses described in this paper

assume all outliers and results reported with large detection limits have been omitted, and there is no significant trend over time. Large detection limits are limits that when divided by two exceed all observed results over all wells.

After the data qualification process, all constituents for which there are no results above detection in any of the monitoring wells are deleted from further consideration. Typically, results are reported for around 350 constituents, but after removing those with no results above detection, about 100 constituents remain for consideration. The list of potential COC's are further pared down by elimination of indicator parameters such as pH, turbidity, total organic halogens, color, odor, specific conductance, etc. This generally reduces the number of constituents to be considered to less than 90.

DETERMINING QUARTER AVERAGES

Since contract laboratories are required to make replicate analyses and split samples are required to be sent to two or more independent laboratories for analysis, not all results are independent. Results reported from the same sample and replicate laboratory and method results within the same quarter were averaged using the following procedure.

(1) All replicate results using the same method within the same laboratory, quarter, well, and constituent are averaged for a method mean. If 50% or more of the individual replicate results are above detection, the method mean is defined as above detection.

(2) The method means from (1) within the same laboratory, quarter, well, and constituent are averaged for a laboratory mean. If 50% or more of the method means are above detection, the laboratory mean is defined as above detection.

(3) The laboratory means from (2) within quarter, well, and constituent are averaged to get a quarter mean within well and constituent. If 50% or more of the laboratory means are above detection, then the quarter mean is defined as above detection.

The resulting quarter averages are considered to be independent. Before computing the quarter averages, results reported at less than detection are replaced by half the detection limit.

DETERMINATION OF "CHARACTERISTIC" WELL

Before comparing POC with BG wells, a characteristic "worst case" well is defined for each constituent and aquifer. The well with the largest average concentration and all other wells with a similar average concentration and variability are included in the "characteristic" well. If too many wells are included, the average concentration is diluted (underestimated) and there is an increase in the variability which decreases the sensitivity or power of the POC versus BG comparison.

The following steps describe the procedure used to determine which wells are included in the "characteristic" well.

(1) If no well within the aquifer has at least 50% of the quarter means above detection, then all available wells are included in the characteristic well and steps 2 through 4 are omitted.

(2) If there are at least two wells with at least 50% of the results above detection, Levene's test for equality of variances is done. If Levene's test indicates no significant differences in variance estimates, then the variance estimates are pooled. If there are differences, then the two wells with the largest average concentrations are compared using a two sample t-test with unequal variances. If there are significant differences at an alpha level of 0.05, then only the well with the largest mean concentration is included in the characteristic well; otherwise, the two wells with the largest average concentrations are included.

(3) All wells with less than 50% above detection are grouped together and the mean concentration computed. The one "less than 50%" mean concentration is then compared with the quarter results from wells with 50% or more above detection using analysis of variance (ANOVA). If the F-test of the ratio of the between well mean square error (BMSE) to the within well mean square error (WMSE) indicates no significant difference at the 0.05 level, then all wells are included in the characteristic well.

(4) If the F-test indicates there are differences, then the Tukey-Kramer pairwise comparison test is used to determine which wells should be included in the characteristic well. The well with the largest average

concentration and all other wells that are not significantly different (based on the Tukey-Kramer test at the 0.05 level) are included in the characteristic well with one constraint. At least one well with 50% or more of the results above detection must be included in the characteristic well if one exists. That is, if the largest concentration was the mean concentration from the wells with less than 50% above detection, then from among the wells with at least 50% above detection, the one with the largest average concentration must be included even if the F-ratio from the ANOVA and the Tukey-Kramer indicated significant differences at the 0.05 level.

ESTIMATION OF AVERAGE CONCENTRATION

Mean concentrations for the POC and BG wells are based on the analyses of the characteristic wells and are only computed if at least 10% of the results are above detection. POC versus BG comparisons are also based on the comparison between the POC and BG characteristic wells and are computed only if at least one of the two wells has at least 50% of results above detection. The following steps describe the estimation process.

(1) If the characteristic well has at least 10% of the results above detection, the average of all quarter concentrations is computed.

(2) If the characteristic well has at least 50% of the results above detection, the variance and standard deviations are also computed.

(3) For the BG characteristic wells with at least 10% of the results above detection, the average is compared with the 90th percentile of all reported detection limits computed from the background wells. The larger of the 90th percentile of the detection limit and the well average is used in the POC versus BG comparison.

COMPARISON BETWEEN POC AND BG "CHARACTERISTIC" WELLS

The null hypothesis being tested is

H_0 : The POC mean concentration is not greater than BG mean concentrations in the aquifer.

The alternate hypothesis which is accepted if the null hypothesis is rejected is

H_a : The POC mean concentration is greater than the BG mean concentration in the aquifer.

Let

$X(\text{POC})_{ai}$	be the mean concentration for the i th constituent in aquifer-a for the POC characteristic well,
$X(\text{BG})_{ai}$	be the mean concentration for the i th constituent in aquifer-a for the BG characteristic well,
$DL90_i$	be the 90th percentile detection limit for the i th constituent computed from the BG wells over all aquifers,
$S^2(\text{POC})_{ai}$	be the estimate of variance for the i th constituent in aquifer-a if the POC characteristic well has at least 50% of the quarters above detection; otherwise, the variance is undefined,
$S^2(\text{BG})_{ai}$	be the estimate of variance for the i th constituent in aquifer-a if the BG characteristic well has at least 50% of the quarters above detection; otherwise, the variance is undefined,
$n(\text{POC})_{ai}$	be the number of quarters in the POC characteristic well for aquifer a, constituent i, and
$n(\text{BG})_{ai}$	be the number of quarters in the BG characteristic well for aquifer a, constituent i.

No comparison test is done unless $X(\text{POC})_{ai} >$ the maximum of $(DL90_i \text{ or } X(\text{BG})_{ai})$. The following procedure describes the POC and BG comparison methodology.

(1) At least 50% of the quarter means in the POC characteristic well are above detection for the constituent and aquifer, and

(a) at least 50% of the quarter means in the BG characteristic well are above detection, the BG mean is greater than $DL90_i$, and

$$X(poc)_{ai} > X(bg)_{ai} + 2.33\sqrt{S_{ai}^2(poc) / n(poc)_{ai} + S_{ai}^2(bg) / n(bg)_{ai}},$$

(b) or at least 10% and less than 50% of the quarter means in the BG characteristic well are above detection, the BG mean is greater than $DL90_i$, and

$$X(poc)_{ai} > X(bg)_{ai} + 2.33\sqrt{S_{ai}^2(poc) / n(poc)_{ai}},$$

(c) or the BG characteristic well has fewer than 10% above detection, or the BG mean is less than the 90th percentile of the detection limit, and

$$X(poc)_{ai} > DL90_i + 2.33\sqrt{S_{ai}^2(poc) / n(poc)_{ai}},$$

then the POC mean concentration is significantly greater than the BG concentration.

(2) At least 10% but less than 50% of the quarter means in the POC characteristic well are above detection, and

(a) at least 50% of the quarter means in the BG characteristic well are above detection, the BG mean is greater than $DL90_i$, and

$$X(poc)_{ai} > X(bg)_{ai} + 2.33\sqrt{S_{ai}^2(bg) / n(poc)_{ai} + S_{ai}^2(bg) / n(bg)_{ai}},$$

(b) or at least 50% of the quarter means in the BG characteristic well are above detection but the BG mean is less than $DL90_i$, and

$$X(poc)_{ai} > DL90_i + 2.33\sqrt{S_{ai}^2(bg) / n(poc)_{ai}},$$

then the POC mean concentration is significantly greater than the BG concentration.

(3) If the POC characteristic well has fewer than the 50% but at least 10% above detection, and the BG characteristic well has fewer than 50% above detection, no test comparison is done and the null hypothesis is not rejected. Both the POC and the BG means are computed.

(4) If fewer than 10% of the quarter means in the POC characteristic well are above detection, no comparison is made and the null hypothesis is not rejected.

COMPARISON WITH OTHER METHODS

Quarter results from 53 constituents were analyzed using the methodology described here. The COC list derived from the SRS analysis was compared with COC lists derived by two parametric and two non-parametric methods. The two parametric methods are Cohen's biased corrected maximum likelihood method and a regression of the normalized (Blom) ranks. Both the natural logarithm and unlogged quarter results were analyzed by the SRS and two parametric methods. The two non-parametric methods were Gehan and Wilcoxon two-sample rank sum. The chosen constituents had at least 50% of the results above detection in the POC wells and at least 9 quarter results in both the BG and POC characteristic wells.

The presence of multiple censoring limits complicates the comparisons for the parametric methods. A censoring limit (CL) equal to twice the largest quarter average less than detection was defined for each of the 53 constituents. All quarter results less than or equal to the CL were considered to be "less than" regardless of whether it was originally less than detection or was based on a reported result. The CL generally equaled the previously defined 90th percentile background detection limit.

Cohen's method is based on maximum likelihood estimates which are obtained by determining values for μ and σ that maximize Eq. (1).

$$\ln[L(\mu, \sigma)] = -[(n - k) / 2] \ln(2\pi\sigma^2) - \left[\sum_{i=k+1}^n (x_i - \mu)^2 / (2\sigma^2) \right] + k \ln \Phi(x < CL), \quad (1)$$

where CL is the censoring limit, k is the number of results less than or equal to CL, n is the total number of quarters, and $F(CL)$ is the cumulative normal distribution at $x=CL$.

The estimates of μ and σ^2 are given by

$$\hat{\mu} = \bar{x}_{n-k} - \hat{\sigma} \left(\frac{k}{n-k} \right) \frac{\varphi(e)}{\Phi(e)}, \text{ and} \quad (2)$$

$$\hat{\sigma}^2 = [S_{n-k}^2 + (\bar{x}_{n-k} - \hat{\mu})^2] / [1 + \varepsilon \left(\frac{k}{n-k} \right) \frac{\varphi(\varepsilon)}{\Phi(\varepsilon)}], \quad (3)$$

$$\text{where } \bar{x}_{n-k} = \sum_{i=n-k}^n x_i / (n-k), \quad (4)$$

$$S_{n-k}^2 = \frac{\sum_{i=k+1}^n (x_i - \bar{x}_{n-k})^2}{(n-k)}, \quad (5)$$

$\varphi(\varepsilon)$ is the normal probability density function,

$$\text{and } \varepsilon = \frac{(DL - \hat{\mu})}{\hat{\sigma}}. \quad (6)$$

Cohen (1959, 1961) describes a procedure to minimize the bias of the above estimates.

(1) Compute the proportion less than CL, $h = k / n$. (7)

(2) Compute the mean and variance of the (n-k) measurements above the CL by

$$\bar{x}_a = \frac{1}{(n-k)} \sum_{i=k+1}^n y_i \text{ and} \quad (8)$$

$$s_a^2 = \frac{1}{(n-k)} \sum_{i=k+1}^n (x_i - \bar{x}_a)^2. \quad (9)$$

$$(3) \text{ Compute } \hat{\gamma} = \frac{s_a^2}{(\bar{x}_a - CL)^2}. \quad (10)$$

(4) Obtain an estimate of the parameter λ from Table A15 in Gilbert (1987) using linear interpolation if necessary and estimate the mean and variance by

$$\hat{\mu} = \bar{x}_a - \hat{\lambda}(\bar{x}_a - CL), \text{ and} \quad (11)$$

$$\hat{\sigma}_x^2 = s_a^2 + \hat{\lambda}(\bar{x}_a - CL)^2. \quad (12)$$

The regression method computes the Blom ranks for the quarter means using SAS[®] PROC RANK (ref. 11) and then fits a linear regression

with the original data as the dependent variable and the Blom ranks as the independent variable. The quarter results are ranked separately within the POC and BG characteristic well from smallest to largest. Tied values are given averaged ranks. Normal scores (Blom ranks) are computed from the ranks by

$$y_i = F^{-1}[(r_i - 3/8)/(n + 1/4)]. \quad (13)$$

The results above the CL are regressed on the Blom ranks as defined in eq. (13).

$$x_i = \hat{a} + \hat{b}y_i, \quad (14)$$

where $\hat{a}$ estimates the mean and $\hat{b}$ estimates the standard deviation.

The BG mean concentration was set equal to the larger of the 90th percentile detection limit or the estimated mean before making the POC-BG comparison. Both Cohen's and the Blom rank regression estimates of mean concentration can be negative. When this occurred, the estimate was replaced by the 90th percentile detection limit. Cohen's method has another disadvantage in that the estimate of $\hat{\gamma}$ occasionally exceeds 1 and biased corrected estimates cannot be computed by the above method. This occurred for 13 of the 53 constituents using the unlogged data and once using the logged data.

The Wilcoxon two sample rank test was done after replacing the less than detection results with half the detection limit. Gehan does not require replacement of the less than detected results with any assumed value. If the data are censored with only one detection limit, the Wilcoxon Rank Sum Test is equivalent to the Gehan method, which is discussed in Millard and Deveral (1988). The Gehan statistic is defined as follows: Let m_B and m_S denote the number of quarterly means in the BG and POC characteristic wells. Let $N = m_B + m_S$. Let $t_1 < t_2 < \dots < t_k$ denote the ordered distinct uncensored observations for the combined BG and POC characteristic wells for a given constituent and aquifer. For $i = 1, \dots, k$, let d_{Bj} denote the number of quarter means from the BG well that are equal to t_j , and d_{Sj} is similarly defined for the POC well. Set $d_j = d_{Bj} + d_{Sj}$. If there are no tied uncensored measurements, then d_j will always be equal to 1.

For averages less than detection, let e_{bj} = the number of quarter means from the BG well with censoring levels that fall into the interval $(t_{j-1}, t_j]$ where $t_0 = -\infty$; e_{sj} is similarly defined for the POC well. Let n_{Lbj} be the number of quarter results from the BG comparison well known to be less than or equal to t_j ; n_{Lsj} is similarly defined for the POC well. Define $e_j = e_{bj} + e_{sj}$ and $n_{Lj} = n_{Lbj} + n_{Lsj}$. For the two-sample case, the score statistic can be written as

$$v = \sum_{i=1}^k (d_{sicj} + e_{sj}C_j), \quad (15)$$

where $c_j = n_{Lj} - (k - i + 1)$ and $C_j = -(k - i + 1)$. If the quarter means in the POC characteristic well are larger than those in the BG characteristic well, the statistic will be large. If ties occur among the uncensored data, then, as for the case of singly censored data, the average scores should be assigned to the tied measurements.

If the censoring mechanism is the same for the POC and BG wells, the permutation variance for the v score is given by

$$\text{Var}_p = [m_b m_s / (N(N-1))] \sum_{i=1}^k (d_{icj}^2 + e_{icj}^2). \quad (16)$$

The standardized Gehan statistic is $z = v / \sqrt{\text{Var}_p}$ with p values computed from the standard normal distribution.

RESULTS

A total of 27 different COC's were identified by at least one of the six parametric method combinations (SRS, Blom regression, and Cohen's ML with both logged and unlogged data). These are broken down by method combinations in Tables 1 and 2. All 25 COC's based on the SRS-unlogged method were also identified by at least one other parametric method combination. All but one of the SRS-logged COC's (23) were identified by at least one other parametric method. The Gehan method identified 37 COC's and the Wilcoxon method identified 31. Gehan identified all 27 of the parametric COC's and Wilcoxon identified 26 out of the 27.

Estimates of the BG mean concentration exceeded the POC estimated mean concentration for two of the Gehan COC's. Gehan was the only method declaring these two constituents as COC's. The SRS method without the constraint of comparing to the larger of the BG mean or the 90th percentile detection limit, would have identified 4 additional COC's which were identified by both Gehan and Wilcoxon.

Table 1: Number of COC's Identified by Each Method

Status of Data	SRS	Blom Rank Reg.	Cohen's ML	Gehan	Wilcoxon 2-sample
Unlogged	25	22	19*	37	31
Logged	24	23	24**		
Common to both logged & unlogged					
	22	20	18		

*13 constituents could not be tested.

**1 constituent could not be tested.

Table 2: Breakdown of COC's by Multiple Method Combinations

Method Combination	Number of COC's
All 6 parametric methods	18
All except Cohen's-unlogged (could not be tested)	2
SRS & Cohen's unlogged (tested)	19
SRS & Regression-unlogged	22
Regression & Cohen's-unlogged (tested)	19
All three parametric methods-logged	22
SRS & Regression-logged	22
SRS & Cohen's-logged	23
SRS-logged and Gehan, 0 unlogged	1
Gehan & at least one parametric method	27
Wilcoxon & at least one parametric method	26
Gehan & Wilcoxon	31
Only Gehan	4

CONCLUSIONS

The advantages of the SRS method is that it is easy to implement using current statistical computing packages, it yields COC's that have practical (above 90th percentile detection limit) as well as statistical significance, and always yields estimates of mean concentration equal to

or greater than the 90th percentile detection limit. Negative estimates of mean concentration can occur with both Cohen's and Blom rank regression methods. In addition, the POC-BG comparison cannot always be done with Cohen's method. Log transformation before analyzing the data is recommended when using Cohen's method if many of the constituents cannot be tested. The two non-parametric tests, Gehan and Wilcoxon, can include as COC's constituents that may have no practical difference. Gehan identified 2 COC's for which the BG mean concentration exceeded the POC mean concentration.

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