Determining an Optimal Sampling Frequency for Measuring Bulk Temporal Changes in Ground-Water Quality

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Abstract

In the Data Quality Objectives (DQO) process, statistical methods are used to determine an optimal sampling and analysis plan. When the DQO decision rule for instituting remedial actions is based on a critical change in water quality, the monitoring program design must ensure that this change can be detected and measured with a specified confidence. Usually the focus is on the change at a single monitoring location and the process is limited to addressing the uncertainty inherent in the analytical methods and the variability at that location. However, new strategies that permit ranking the waste sites and prioritizing remedial activities require the means for assessing overall changes for small regions over time, where both spatial and temporal variability exist and where the uncertainty associated with these variations far exceeds measurement error. Two new methods for assessing these overall changes have been developed and are demonstrated by application to a waste disposal site in Oak Ridge, Tennessee. These methods incorporate historical data where available and allow the user to either test the statistical significance of a linear trend or of an annual change compared to a baseline year for a group of water quality wells.

Introduction

The importance of using methods that quantify the uncertainty associated with water quality data and the significance of changes in concentration is emphasized by their incorporation into the Data Quality Objectives (DQO) process (EPA, 1987a). This process is designed to ensure that sampling and analysis plans developed for environmental monitoring and remediation are sufficiently sensitive that contaminant levels and changes in contaminant concentrations can be detected at specified levels. While not explicitly addressed, the DQO process can also result in cost minimization by determining the minimum number of samples and lowest analytical level required to provide the necessary sensitivity.

In the DQO process, decision rules are developed based on the data needs, data users, and the overall problem to be addressed (EPA, 1992). These decision rules become drivers for development of the monitoring strategy by establishing the allowable uncertainty associated with conclusions drawn from the data. This uncertainty comes from two primary sources: (1) sampling and analytical uncertainty, which govern the ability to detect and quantify the level of a particular contaminant; and (2) spatial and temporal variations, which govern the ability to determine the significance of changes within a population using sample data.

The first of these sources, sampling and analytical uncertainty, is addressed by choosing approved methods and procedures that ensure accuracy at or below detection levels specified by the DQOs (e.g. EPA, 1986; 1987b). Quantifying the spatial and temporal variability is less straightforward, but must be factored in where DQO decision rules are based on net changes within an areally distributed population. Changes in site hydrologic conditions and geochemical interactions can result in temporal variations that might confound the detection of changes in actual release of contaminants from disposal areas, for example.

In order to design a monitoring program that will detect changes of the magnitude specified within the DQO process, some initial estimate of the degree of spatial and temporal variability is required. Where historical data have been obtained, these data can be used to determine statistical parameters that can then guide the initial optimization of the sampling and analysis plan. The plan can then be refined as additional data are

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Received August 1994, revised June 1995, accepted July 1995.

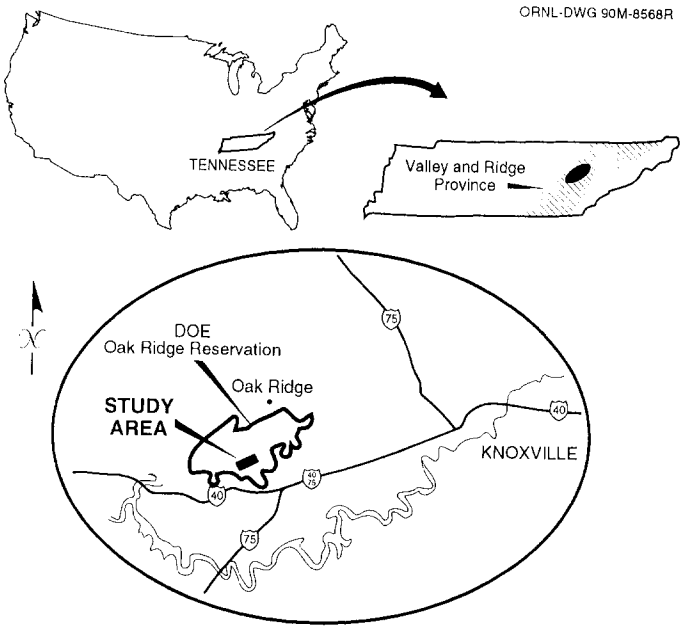

Fig. 1. The study site is located at Oak Ridge National Laboratory (ORNL) near Oak Ridge, Tennessee.

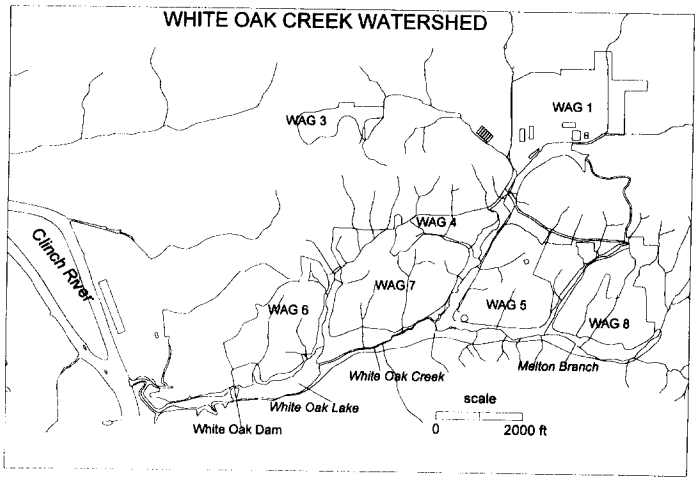

Fig. 2. Map of the White Oak Creek watershed, showing the location of WAG 6 and other WAGs relative to surface-water drainages.

obtained and the system variability is better quantified. Data sets often contain irregularly spaced data and statistical methods designed to use these data must allow for this.

This paper presents two methods for examining temporal changes in areally distributed ground-water quality data. The two methods provide different views of these changes and are used for somewhat different purposes depending on the sampling design and the question being addressed. The first method addresses the identification of trends over time, and the second addresses a yearly comparison to an established baseline population. The theory is first laid out then examples are given using data from a contaminated site.

Background and Site Description

Waste Area Grouping (WAG) 6 is located at the Oak Ridge National Laboratory (ORNL) in east Tennessee (Figure 1). WAG 6 has been a disposal site for radioactive, hazardous, and mixed wastes since 1969 (ORNL, 1991). In accordance with the hydrologic conceptual model for the Oak Ridge Reservation (Solomon et al., 1992), contaminated ground water and surface water from WAG 6 ultimately discharge into White Oak Lake, where they mix with contaminants released from other WAGs further upstream in the White Oak Creek watershed which drains most of Bethel and Melton Valleys (Figure 2). From there, off-site release is via White Oak Dam into the Clinch River. Currently, tritium, ^{90}Sr, and ^{137}Cs are the most significant contaminants being transported through the ground-water and surface-water systems (ORNL, 1991).

The remedial strategy for the ORNL site includes prioritizing the WAGs according to their relative contribution to the total off-site flux at White Oak Dam, thus allocating resources in a way that allows remediation of the largest contributors first (ORNL, 1993). This strategy is conceptualized as a series of funnels depicted in Figure 3. Ground water and surface water originating from each WAG or group of WAGs within a small watershed can be visualized as discharging into a funnel that empties into the White Oak Creek watershed and ultimately White Oak Lake, which functions as the overall collector. Total off-site risk is determined at White Oak Dam (WOD), the closest point at which public exposure can occur, and relative contribution to the total risk at WOD is determined by measuring contaminant contributions from the individual funnels discharging into the White Oak Creek watershed.

Currently, the relative contribution from WAG 6 is small and, therefore, a decision was made to defer remedial action at this time in order to allocate resources to WAGs with larger

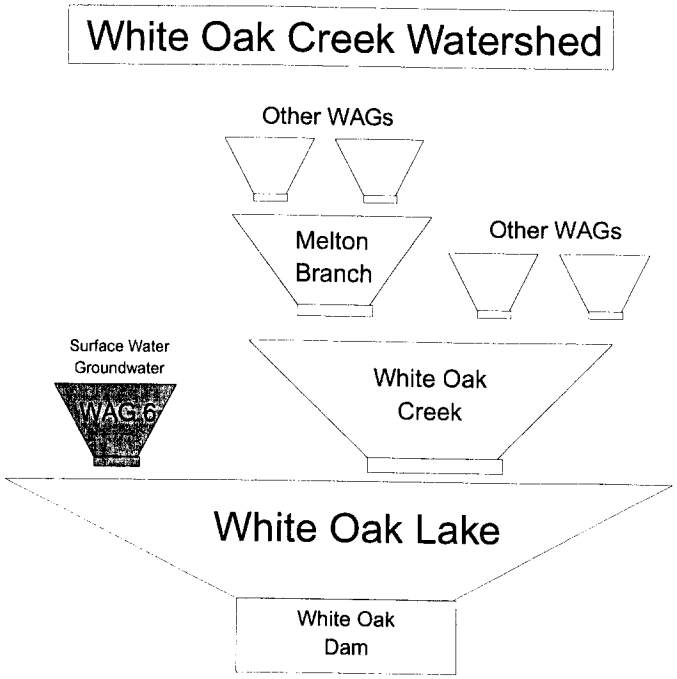

Fig. 3. Depiction of the funnel concept. Contaminants discharge from local waste disposal sites (WAGs) into surface-water drainages within the White Oak Creek watershed, where they are carried into White Oak Lake and ultimately released over White Oak Dam. Contaminants are discharged into local funnels from both surface-water and ground-water pathways.

contaminant releases. However, a monitoring strategy was required that would allow continued determination of the relative contaminant contributions to total flux at WOD over time. In addition, an early response capability was desired so that changes could be detected that would indicate that WAG 6 was approaching a magnitude of contaminant release requiring initiation of source control measures, allowing an adequate response time.

The strategy for ORNL site remediation is central to the DQO process for WAG 6 environmental monitoring because it calls for a decision rule based on summed releases from the WAG rather than on concentrations at individual monitoring locations. For example, within this strategic framework, a concentration increase at an individual well is not likely to drive contingent actions. However, a significant increase in the mean contaminant concentration within a specified group of wells could signal deterioration of existing structures that were designed to provide hydrologic isolation of the wastes. The monitoring plan for WAG 6 was developed to address activities over a five-year period, after which an evaluation will be made to determine ongoing monitoring needs (ORNL, 1993). In order for WAG 6 to be elevated to a level requiring immediate action during this time frame (i.e., relative contaminant contributions equalling the current worst contributors), it was determined that a twofold annual increase in concentration would have to occur over each of the four years following the baseline year. Thus, a twofold increase in concentration was established as the target for designing a monitoring program. While this driver was applied to both surface water and ground water as separate media, this paper addresses its application to ground water only.

The environmental monitoring plan for WAG 6 includes a 12-18 month period of intense sampling to establish a statistical base, followed by four years of routine monitoring at reduced frequencies. Cost minimization required using subsets of the existing wells. Criteria for well selection were that all disposal areas be represented, that interior wells be selected based on historical data indicating contamination at those locations, and that perimeter wells be located either downgradient or along strike of disposal areas. Because the lithology beneath WAG 6 consists of fractured shales and carbonates, contaminants tend to migrate preferentially along discrete fracture flow paths (Solomon et al., 1992). The historical presence of contaminants, then, is an indication that a well intersects a contaminant flow path. Upgradient perimeter wells were also selected for control purposes, but do not factor into the statistical methods described in this paper. An initial sampling strategy was designed that called for quarterly sampling at all well locations during the baseline assessment, followed by quarterly sampling at downgradient perimeter wells, semiannual sampling at upgradient perimeter wells, and annual sampling at interior wells. The

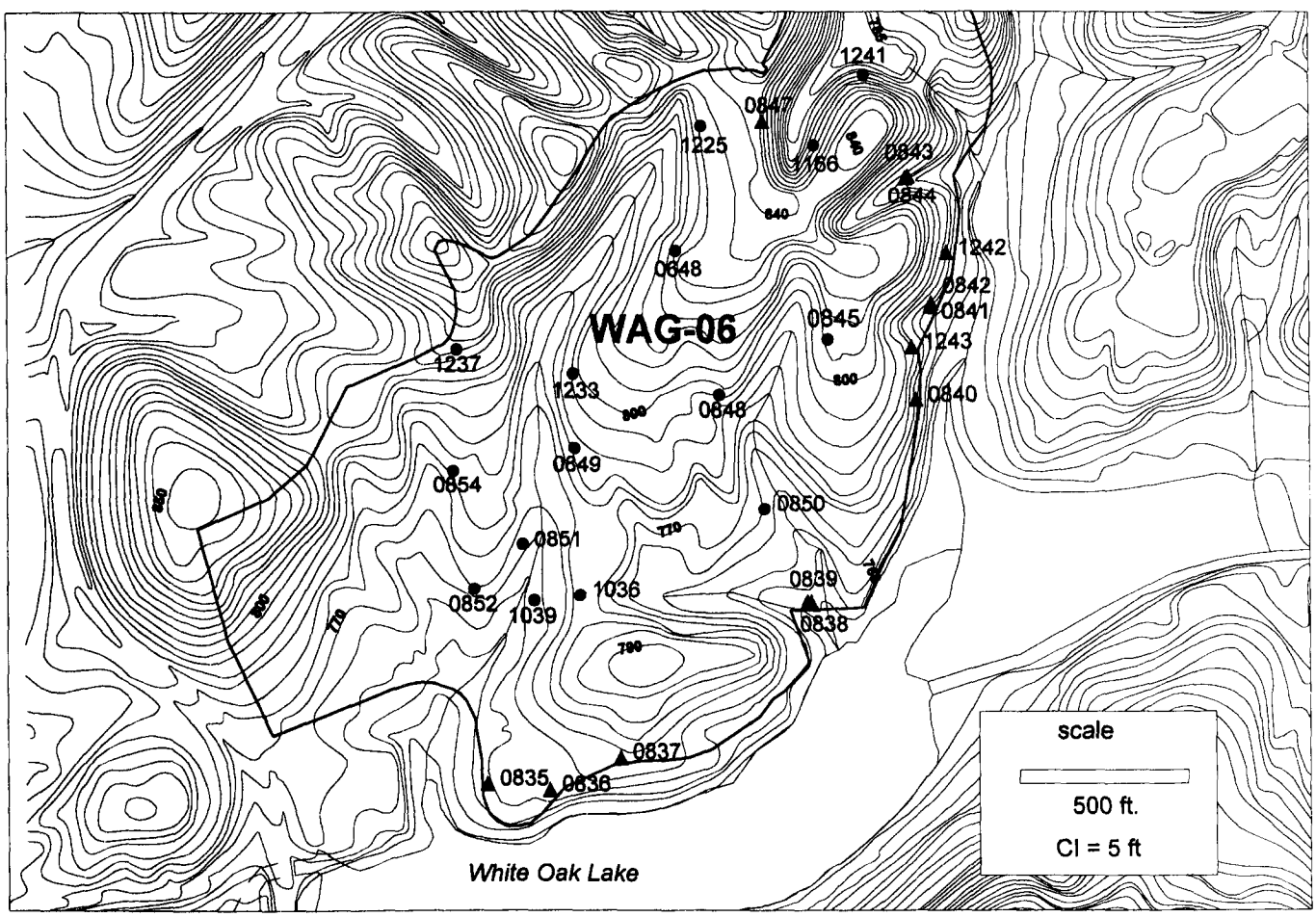

Fig. 4. Map of WAG 6 showing the distribution of water quality measurements. Circles indicate interior wells, and triangles indicate downgradient perimeter wells. These designations are for functional purposes: perimeter wells are part of the current perimeter monitoring network, and interior wells were chosen based on historical concentrations and proximity to waste disposal areas.

statistical methods described in this paper have been designed and used to test the adequacy of this sampling design for assessing changes according to the DQO decision rule.

The decision rule is applied to the monitoring strategy in the following manner. Employing the funnel concept, we are interested in a summed effect within the set of wells in the WAG interior and within the set of wells at the downgradient perimeter of the WAG. As previously stated, the two sets provide different information and therefore require different evaluations. In the WAG interior, we are interested in detecting large changes that would indicate a significant increase in the release of contaminants from the disposal units. At the perimeter we are interested in detecting trends that would indicate that contaminant release from the WAG is on the rise. Both need to be evaluated in such a manner that action can be taken before substantial contaminant releases occur. Following this rationale, the DQO driver was applied to the two populations in the following manner. Wells at the perimeter must be sampled at a frequency such that a linear trend in mean concentration leading to a factor of two increase over five years could be declared statistically significant at specified probabilities for type I and type II errors, denoted by α and β, respectively. (In this case, a type I error would occur when we say that a linear trend exists that would result in a factor of two increase when, in fact, this is not the case; and a type II error would occur when we say there does not exist a linear trend that would result in a factor of two increase when, in fact, such a linear trend did exist.) Wells within the WAG interior must be sampled at a frequency ensuring that a twofold increase for any "out year" above baseline levels when summed over the entire set of wells could be declared statistically significant at specified probabilities for type I and type II errors. In the first case we are evaluating the significance of a linear slope, and in the second case we are evaluating the significance of a change from baseline year to out year, or the "year effect." Historical tritium data have been used to establish statistical parameters for testing the initial sampling design.

Evaluating Linear Trends in Well Data: Theory

Assume that we have n observations (t_i, c_i) where $t_i = i^{th}$ observation time (sampling event), and c_i = observed average concentration from a sample of perimeter wells (possibly in log-units) of the i^{th} sampling event for $i = 1, 2, \ldots, n$. In addition, assume the mean of the response (c) at a given observation time (t) is given by the regression model $\beta_0 + \beta_1 t$. (This paper uses universal statistical notation where if β does not have a subscript it refers to a probability type II error, and if β has a subscript it refers to a coefficient in a regression model.) If the usual normality and independence assumptions are made, then the significance of β_1 will be the basis for concluding that there is a significant linear trend in the observed concentrations. In statistical terms we are testing the null hypothesis

$$H_0: \beta_1 = 0$$

against the alternative hypothesis

$$H_A: \beta_1 = \beta_1^* (> 0).$$

Under the above assumptions, the least-squares estimate of β_1, denoted by b_1, is normally distributed with mean 0 (under H_0) or β_1^* (under H_A) and variance given by

$$\mathrm{Var}(b_1) = \frac{\sigma^2}{\sum_{i=1}^{n} (t_i - \bar{t})^2} \quad (1)$$

where σ^2 is the variance of c for a given t, and $\bar{t}$ equals the mean of t from 1 to n, where the effect of sample size can be seen by the denominator. See Draper and Smith (1981) for additional discussion about regression.

If σ^2 is assumed known, the probabilities of type I and II errors for testing H_0 against H_A are given by α and β, respectively, then the value of β_1^* we would anticipate to declare as significant (at the α level of significance and a power of $1 - \beta$ for the given set of n observations) is given by

$$\beta_1^* = (z_\alpha + z_\beta)\,[\mathrm{Var}(b_1)]^{1/2} \quad (2)$$

where z_α and z_β are the $100 \times (1 - \alpha)$ and $100 \times (1 - \beta)$ percentiles, respectively, of the standard normal distribution. [See Appendix for derivation of equation (2).]

Evaluating Linear Trends in Well Data: Application

In applying the DQO decision rule to offsite contaminant release via the shallow ground-water system, we wish to be able to detect a trend in the average tritium concentration at the downgradient perimeter wells that would result in a twofold increase over five years. Thus we need to determine whether or not the initial test design of quarterly sampling over the five-year period will provide sufficient resolution to detect this change given the variability of the system. From equation (2), for a given set of statistical parameters, an estimate of the slope that would be declared significant can be determined. There is a natural slope due to radioactive decay of the sources, so in order to test a null hypothesis of zero slope, we decay-correct all data to the time of the last sampling event. Per the initial sampling design, we assume quarterly sampling at downgradient wells over a five-year period, or $n = 20$, where n is the number of sampling events in the time series for regression. If we wish to determine the value of β_1^* for probabilities of type I and type II errors both equal to 5%, then $\alpha = \beta = 0.05$ and $z_\alpha = z_\beta = 1.645$. The only other parameter required is σ^2 [equation (1)]. Here, because we are interested in the trend of the overall mean concentration, we use the error mean square from regression of the historical transformed and decay-corrected tritium concentrations on time to estimate σ^2 (i.e., the variance of the average sample event concentrations about the decay-corrected slope).

Historical tritium concentrations measured at the downgradient wells can provide a test of the assumption of initial slope of zero and an estimate of σ^2. Table 1a contains tritium data for all perimeter wells over a four-year period. The fields of this table include the well ID, observation date, tritium concentration in pCi/l, and the value of three times the counting error (3 c.e.). A measurement was considered left-censored (below detection) if the measured value was less than 3 c.e. For the sampling events (dates) with censored observations, maximum likelihood estimation methods for a censored normal distribution were used to estimate the mean concentration. Otherwise, the sample mean was used as an estimate. All data were first transformed into natural log values and subsequent calculations were made within the transformed space. Table 1b contains a summary of these calculations after log transformation for all 11 sampling events.

The statistical theory presented in the previous section is

Table 1a. Decay-Corrected Tritium Concentration Data for the Perimeter Wells

Date:	*July 1988*		*October 1988*		*January 1989*		*May 1989*		*May 1990*		*November 1990*	
Well ID	*C (pCi/l)*	*3 c.e.*	*C (pCi/l)*	*3 c.e.*	*C (pCi/l)*	*3 c.e.*	*C (pCi/l)*	*3 c.e.*	*C (pCi/l)*	*3 c.e.*	*C (pCi/l)*	*3 c.e.*
1243	NA	NA	NA	NA	NA	NA	NA	NA	794000	118500	NA	NA
835	24868	2433	32436	4054	20270	2433	26219	2433	18651	2026	21081	2433
836	3514	1621	13243	2433	<	1702	2244	1338	1649	1540	<	1500
837	NA	NA	NA	NA	<	1905	1487	1216	2433	1500	NA	NA
838	14324	2026	<	1946	11351	2433	7028	1621	24868	2433	23243	2433
839	29730	4054	8108	2433	23784	28838	26489	2433	17840	2026	23784	2433
840	21622	2433	21354	2838	11351	2433	3244	1216	4054	1621	5135	1621
841	270300	40545	243243	8109	172992	4054	216240	4054	143259	4054	129730	4054
842	648720	40545	675750	40545	567630	40545	459510	40545	183804	4054	154054	4054
843	810900	40545	919020	40545	1243380	40545	756840	40545	324360	40545	54054	40540
844	72973	4054	75684	4054	59466	3649	64872	4054	54060	4054	75676	4054
847	83793	4054	89199	4054	83793	4054	81090	36490	72981	4054	86486	4054

Date:	*February 1991*		*September 1991*		*December 1991*		*March 1992*		*May 1992*	
Well ID	*C (pCi/l)*	*3 c.e.*	*C (pCi/l)*	*3 c.e.*	*C (pCi/l)*	*3 c.e.*	*C (pCi/l)*	*3 c.e.*	*C (pCi/l)*	*3 c.e.*
1243	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
835	May-81	4054	13243	1621	NA	NA	32432	4054	NA	NA
836	2054	1459	<	1419	NA	NA	<	974	NA	NA
837	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
838	22703	2433	26216	2026	NA	NA	25405	2026	NA	NA
839	22432	2433	20811	2026	NA	NA	23243	2026	NA	NA
840	4324	1621	11081	1621	10811	1621	7027	1216	2405	1176
841	118919	4054	70270	4054	81081	4054	143243	4054	97297	4054
842	129730	4054	102703	4054	108108	4054	97297	4054	67568	4054
843	162162	40540	243243	40540	567000	81000	1080000	81000	189189	40540
844	27027	24324	78378	4054	59459	4054	64865	4054	83784	4054
847	32432	24324	72973	4054	94595	4054	97297	4054	91892	4054

Measured concentrations below three times the counting error, indicated by "<" were treated as left-censored data in the maximum likelihood estimation of the mean. Wells not included in a particular sampling event are represented by "NA."

Table 1b. Results of Maximum Likelihood Estimation for Each Sampling Event

Event	*Time (mo)*	*n*	*# Censored observations*	*Mean ln C (pCi/l)*	*Std. Dev. ln C (pCi/l)*
1	0	10	0	10.7118	1.6515
2	3	10	1	10.4819	2.0455
3	6	11	2	10.0346	2.3992
4	10	11	0	10.0801	2.0491
5	22	12	0	10.3058	1.8758
6	28	10	1	10.1354	1.5364
7	31	10	0	10.1379	1.3402
8	38	10	1	10.2632	1.5348
9	41	6	0	10.7724	0.8152
10	44	10	2	10.0576	1.6381
11	46	6	0	10.8844	1.4215

Fields are the sampling event number, time in months, number of samples per event, number of censored values, and mean and standard error in log-transformed space.

based on an assumption of sample independence. This assumption is reasonable in both spatial and temporal terms for this system. Because contaminants tend to move along discrete flow paths, concentrations at distributed locations are not as likely to impact one another. Also, as long as the sampling frequency is quarterly or less, as it is for the historical data shown, then the data are likely to be only weakly dependent if at all on previous samples (Barcelona et al., 1989).

Estimated mean concentrations ± one standard deviation about the mean are shown in Figure 5. The error bars represent the variability of values over the set of wells sampled during each event, or the between-well variance. Because we want to determine a trend in the mean, however, we are most interested in the variance of the mean over time. Correcting the data for radioactive decay causes a minor shift in the slope. Linear regression over the corrected data results in a nearly horizontal slope [$b_1 = -0.00401$ ln(pCi/l)/month] indicating that the system is currently stable at an average concentration of 10.35 ln(pCi/l). For the 11 sample event means, the error mean square from the linear regression provides an estimated value of σ^2 given by $\hat{\sigma}^2 = 0.0971$, and assuming 20 quarterly sampling periods,

$$\sum_{i=1}^{n} (t_i - \bar{t})^2 = 665. \tag{3}$$

Using the parameters described above, an estimate of the significant slope, β_1*, can be determined using

$$\hat{\mathrm{Var}}(b_1) = \frac{\hat{\sigma}^2}{\sum_{i=1}^{n} (t_i - \bar{t})^2} = \frac{0.0971}{665} = 0.000146 \tag{4}$$

and

$$\hat{\beta}_1^* = (z_\alpha + z_\beta)\,[\hat{\mathrm{Var}}(b_1)]^{1/2} = 2(1.645)\,(0.000146)^{1/2} = 0.0397. \tag{5}$$

expressed as the natural log of concentration in pCi/l per sampling period. Note that β_1 represents the rate of increase in the natural log concentration of tritium over a three-month period

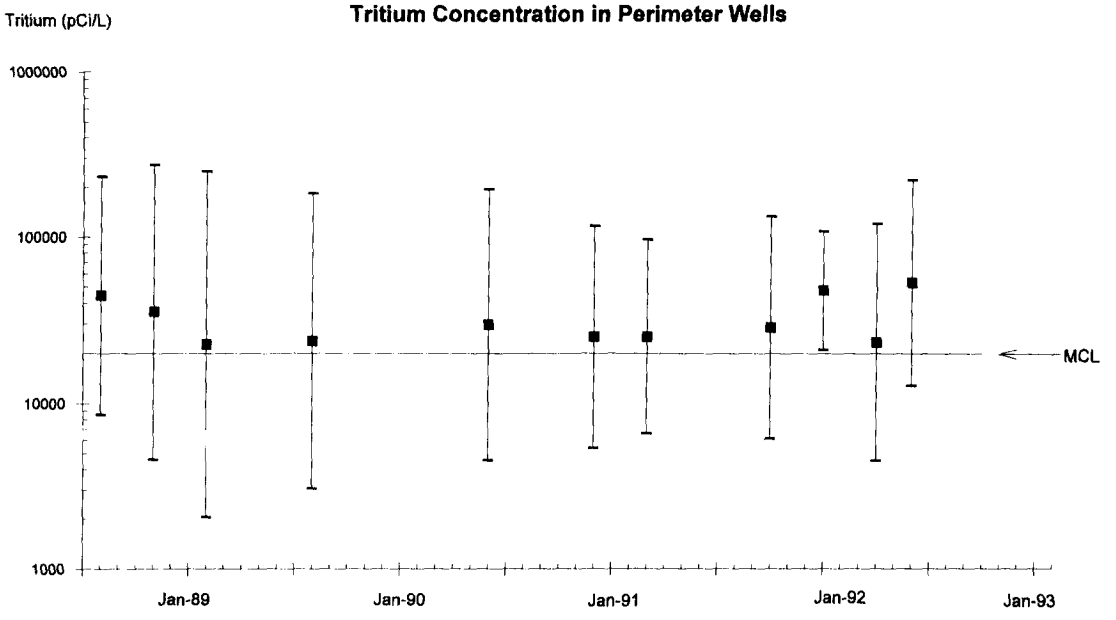

Fig. 5. Four-year trend in average decay-corrected tritium concentration in the perimeter wells. Each data point represents the mean of the sampling event and the error bars indicate ± one standard deviation about the mean. The EPA Maximum Concentration Limit (MCL) for drinking water is 20,000 pCi/l.

(quarter), and that β_1* [estimated from equation (5)] represents the value of β_1 we would declare as significantly greater than zero assuming the specified sampling design, and α and β values.

Over a five-year period, the slope calculated in equation (5) would correspond to an increase in average log concentration of 20 quarters × 0.0397 = 0.794. Starting from the current average concentration for the previous four-year period of 31,260 pCi/l, we would declare as significant a linear trend resulting in an average concentration of

$$\exp[\ln(31{,}260) + 20(0.0397)] \approx 69{,}000 \text{ pCi/l}$$

after five years, or slightly more than a factor of two increase. Thus, quarterly sampling over the five-year period will provide sufficient resolution to satisfy the DQOs.

Evaluating Shifts from Baseline in Well Data: Theory

In order to evaluate shifts from baseline in a response (e.g., tritium concentration), a group of wells will be monitored for two years. Let y_{ijk} equal the k^{th} observed response (possibly in log-units) from the j^{th} well in the i^{th} year, and assume

$$y_{ijk} = \mu + \tau_i + \gamma_j + \epsilon_{ijk} \tag{6}$$

where i = 1 (baseline year), 2 (out year); j = 1, 2, . . . , J; k = 1, 2, . . . , n_{ij}; μ is the overall mean; τ_i is the i^{th} year effect; γ_j is the j^{th} well effect; and ϵ_{ijk} is the random error component which is assumed to be normally distributed with zero mean and variance σ^2. The difference in the mean response from the baseline year (i = 1) to another specified period or "out year" (i = 2) is assumed to be

$$\delta = \tau_2 - \tau_1. \tag{7}$$

From the wells, we have independent estimates (j = 1, 2, . . . , J) of δ given by

$$\hat{\delta}_j = \overline{y_{2j}} - \overline{y_{1j}} \tag{8}$$

where

$$\overline{y_{1j}} = \sum_{k=1}^{n_{ij}} y_{ijk}/n_{ij}. \tag{9}$$

If we assume independence of the observations across years and wells, then $\hat{\delta}$ is normally distributed with

$$\text{Var}(\hat{\delta}_j) = \text{Var}(\overline{y_{1j}} - \overline{y_{2j}}) = \frac{\sigma^2}{w_j} \tag{10}$$

where

$$w_j = \left(\frac{1}{n_{1j}} + \frac{1}{n_{2j}}\right)^{-1} = n_{1j}n_{2j}/(n_{1j} + n_{2j}). \tag{11}$$

The null hypothesis of no temporal change or time effect is given by

$$H_0: \delta = 0$$

and the alternative hypothesis of an increase in the response from year 1 to year 2 is given by

$$H_A: \delta = \delta^*(> 0).$$

A weighted estimate of δ is given by

$$\hat{\delta} = \frac{\sum_{j=1}^{J} w_j\hat{\delta}_j}{\sum_{j=1}^{J} w_j} \tag{12}$$

whose variance equals

$$\text{Var}(\hat{\delta}) = \frac{\sigma^2}{\sum_{j=1}^{J} w_j}. \tag{13}$$

Under H_0, $\hat{\delta}$ has a normal distribution with zero mean and variance given by equation (13). Under H_A, $\hat{\delta}$ has a normal distribution with mean equal to δ^* and variance given by (13). If σ^2 is assumed known and the probabilities of type I and II errors are given by α and β, respectively, then the value of δ^* we would anticipate to declare as significant (at the α level of significance and a power of $1-\beta$ for the given sample) is given by

$$\delta^* = (z_\alpha + z_\beta) \frac{\sigma}{\left(\sum_{j=1}^{J} w_j \right)^{1/2}} \qquad (14)$$

where z_α amd z_β are the $100 \times (1 - \alpha)$ and $100 \times (1 - \beta)$ percentiles, respectively, of the standard normal distribution. Once the values are available for the n_{ij}'s and σ, equation (14) can be used to determine δ^* for given values of α and β.

Evaluating Shifts from Baseline in Well Data: Application

Application of the DQO decision rule to the interior wells requires detecting a twofold change in tritium concentration for any given year as compared to a baseline year. This change, referred to as the year effect (δ^*) in the previous discussion, can be estimated if the values of α and β are specified, the standard deviation (σ) of the concentrations is known, and the sample sizes n_{ij}, from which the weights w_{ij} are determined, are specified. We again obtain values for these parameters from historical data. Table 2 lists tritium concentrations for a set of interior wells sampled at varying intervals during a 50-month period. Fields listed in the table are well ID, date the sample was obtained, and tritium concentration in pCi/l. For all samples, the measured value far exceeded 3 c.e. and, therefore, there were no censored data as in the previous example.

Tritium concentrations varied widely between wells, but remained relatively stable over time within each well (Figure 6). In order to avoid having the between-well variance swamp the population comparison, the standard deviation (σ) in equation (10) is determined from the pooled variance for the group of wells, a measure of the within-well variation rather than the between-well variation. For the pooled variance, a weighting scheme is used to accommodate an unequal number of samples per well. Those wells with higher numbers of samples contribute more heavily to the pooled variation.

Although the historical data listed in Table 2 span a four-year period, we treat them as a single baseline period for testing our initial sampling design of once per year for routine monitoring in the interior wells. We are interested in determining the magnitude of difference (δ^*) in tritium concentration to be detected as significant for an "out year," where we set $n_{2j} = 1$ for all j to correspond with a single sample at each well. Table 3 provides a summary of the weights and standard deviations for each well that are required for estimating δ^*. Again, all historical data are corrected to remove the effect of radioactive decay and log-transformed prior to calculations. The variance σ^2 is estimated by the pooled variance of the sample data:

$$s_p^2 = \frac{\sum_j (n_j - 1) * s_j^2}{\sum_j (n_j - 1)} \qquad (15)$$

and σ is estimated by s_p. If we wish to test with $\alpha = \beta = 0.05$, then $z_\alpha = z_\beta = 1.645$, and δ^* from (14) is estimated by:

$$\hat{\delta}^* = (z_\alpha + z_\beta) \left(\frac{\hat{\sigma}^2}{\sum_j w_j} \right)^{1/2} =$$

$$2(1.645)\left(\frac{0.376555}{11.2756} \right)^{1/2} = 0.6012 \qquad (16)$$

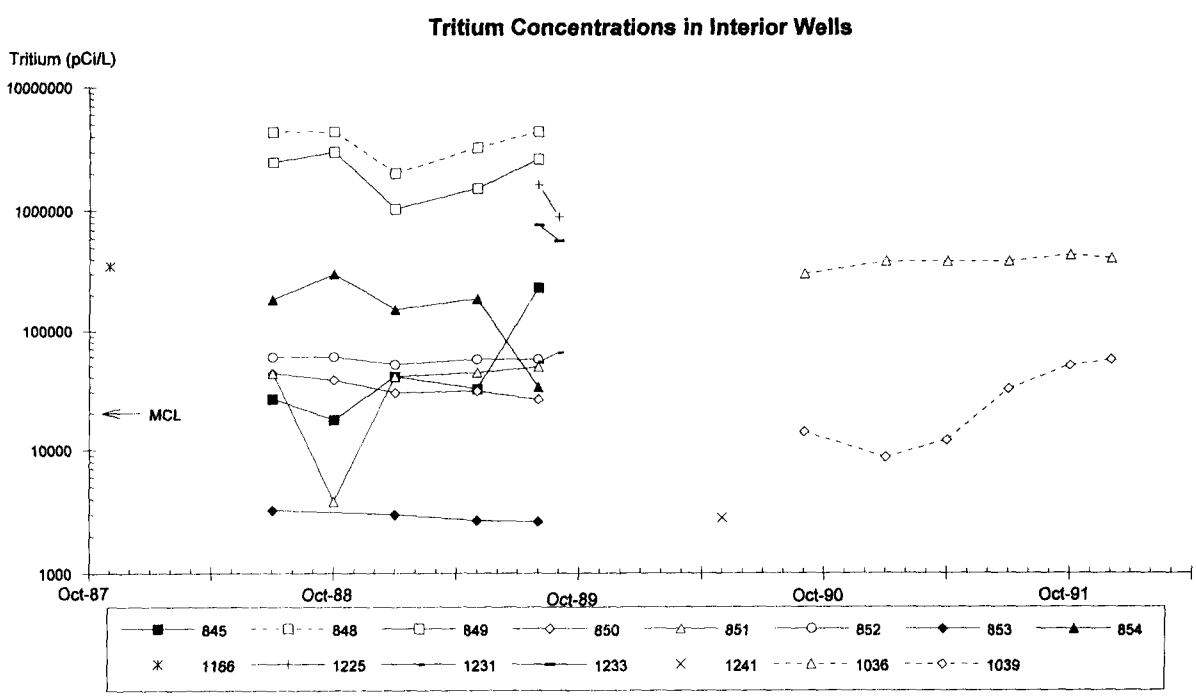

Fig. 6. Decay-corrected tritium concentrations for the interior wells used as a cumulative baseline period.

Table 2. Decay-Corrected Tritium Concentration Data for the Interior Wells

Date:	Nov-87	Jul-88	Oct-88	Jan-89	May-89	Jul-89	Sep-89	May-90	Sep-91	Jan-92	Apr-92	Jul-92	Oct-92	Dec-92
Well ID	C (pCi/l)	C (pCi/l)	C (pCi/l)	C (pCi/l)	C (pCi/l)	C (pCi/l)	C (pCi/l)	C (pCi/l)	C (pCi/l)	C (pCi/l)	C (pCi/l)	C (pCi/l)	C (pCi/l)	C (pCi/l)
1225	NA	NA	NA	NA	NA	1600000	879000	NA	NA	NA	NA	NA	NA	NA
1228	NA	NA	NA	NA	NA	10000	10900	NA	NA	NA	NA	NA	NA	NA
1229	NA	NA	NA	NA	NA	16000	16400	21200	NA	NA	NA	NA	NA	NA
1231	NA	NA	NA	NA	NA	54000	65200	NA	NA	NA	NA	NA	NA	NA
1233	NA	NA	NA	NA	NA	760000	561000	NA	NA	NA	NA	NA	NA	NA
1241	NA	NA	NA	NA	NA	NA	NA	2800	NA	NA	NA	NA	NA	NA
845	NA	26489	17569	40545	32003	NA	230000	NA	NA	NA	NA	NA	NA	NA
848	NA	4324800	4324800	2000200	3200352	NA	4300000	NA	NA	NA	NA	NA	NA	NA
849	NA	2459730	2973300	1027140	1500165	NA	2600000	NA	NA	NA	NA	NA	NA	NA
850	NA	43248	37842	27933	30603	NA	26000	NA	NA	NA	NA	NA	NA	NA
851	NA	43248	3784	400545	43904	NA	49000	NA	NA	NA	NA	NA	NA	NA
852	NA	59466	59466	51357	56906	NA	57000	NA	NA	NA	NA	NA	NA	NA
853	NA	3244	NA	2973	2660	NA	2600	NA	NA	NA	NA	NA	NA	NA
854	NA	183804	297330	151368	185020	NA	33000	NA	NA	NA	NA	NA	NA	NA
1166	351390	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
1036	NA	NA	NA	NA	NA	NA	NA	NA	300000	380000	380000	380000	430000	400000
1039	NA	NA	NA	NA	NA	NA	NA	NA	14000	8600	12000	32000	51000	57000

Table 3. Statistical Weights by Well as Determined from the Frequency of Historical Measurements

Well (j)	n1j	n2j	wj	sj
1225	2	1	0.67	0.4235
1231	2	1	0.67	0.1333
1233	2	1	0.67	0.2147
1241	1	1	0.50	—
845	5	1	0.83	0.9922
848	5	1	0.83	0.3365
849	5	1	0.83	0.4455
850	5	1	0.83	0.2033
851	5	1	0.83	1.1000
852	5	1	0.83	0.0599
853	4	1	0.80	0.1028
854	5	1	0.83	0.8386
1166	1	1	0.50	—
1036	6	1	0.86	0.1210
1039	6	1	0.86	0.8033

n1j = samples in baseline data.
n2j = samples in comparison year.
wj = weight for well j.
sj = standard deviation for well j.

The quantity $\hat{\delta}^*$ is an estimate of the difference in the mean concentration of tritium in pCi/l from the baseline year to the out year in the log-transformed space that would be declared as significant with specified variability and α and β values. This is equal to the natural log of the ratio of the untransformed mean concentrations:

$$\delta^* = \ln(\overline{C_2}) - \ln(\overline{C_1}) = \ln(\overline{C_2}/\overline{C_1}) \tag{17}$$

and

$$\overline{C_2}/\overline{C_1} = \exp(0.6012) = 1.824. \tag{18}$$

A change in average tritium concentration of slightly less than a factor of two could be detected using the historical data as a reference population. The historical data used as the baseline period for this test range from one to six samples per well, with an average of four samples per well. Thus if we assume that quarterly sampling during the actual baseline year will result in a similar estimate of the pooled variance, then annual sampling for out years will provide sufficient resolution to satisfy the DQOs.

Summary

The design and optimization of a monitoring plan within the DQO process may need to address not only the uncertainty associated with sampling and analysis, but also the larger uncertainty associated with spatial and temporal variability. While the first of these uncertainties is easily quantified, knowledge about the spatial and temporal variability of the system being studied may not be initially available. If net changes within areally distributed data are to be evaluated, then the spatial and temporal variability need to be accounted for when drawing conclusions from the data gathered. In addition, a first guess at quantifying this variability is required in order to establish nonarbitrary initial sampling frequencies.

Two methods for determining the significance of net changes in water quality data over time have been developed and presented. These temporal changes may be evaluated as either a linear trend or as a change in an out year compared to an initial or baseline year. Both methods require that the number of wells

to be sampled, the number of samples or frequency of sampling, the desired probabilities for type I and type II errors (i.e., the acceptable uncertainty), and the variance of the parameter of interest be defined as input parameters. All but the latter are user-defined. The variance is a system parameter that must be either assumed or estimated. Where historical data are present, as in the case presented here, these data can provide an initial estimate of the environmental variability that can then be used to determine an initial monitoring strategy. Where no data are present, a conservative estimate can be assumed and then later updated as data become available. In either case, iterative updating should be used to refine the monitoring strategy as the system becomes better defined.

Use of the methods described in this paper can assure that the monitoring design is sensitive enough to detect changes in contaminant concentrations that will drive remedial activities, as defined by statistical significance. In addition, the methods may result in cost savings, as they can assist in determining the minimum level of sampling required to meet specified levels of uncertainty.

Appendix: Derivation of Equation (2)

In testing the null hypothesis H_0: $\beta_1 = 0$ against the alternative hypothesis H_A: $\beta_1 = \beta_1^* (>0)$ at a given level (probability of type I error) and known σ^2, one rejects H_0 if

$$\frac{b_1}{[\mathrm{Var}(b_1)]^{1/2}} > z_\alpha \tag{19}$$

Thus

$$P[b_1 \geq z_\alpha [\mathrm{Var}(b_1)]^{1/2} \text{ given } H_0 \text{ is true}] = \alpha. \tag{20}$$

However, if the alternative hypothesis is true, the corresponding probability of a type II error β is such that

$$P[b_1 \geq \beta_1^* - z_\alpha [\mathrm{Var}(b_1)]^{1/2} \text{ given } H_A \text{ is true}] = \beta. \tag{21}$$

For the two probabilities α and β, we have

$$\beta_1^* - z_\beta [\mathrm{Var}(b_1)]^{1/2} = z_\alpha [\mathrm{Var}(b_1)]^{1/2}, \tag{22}$$

from which we obtain the result,

$$\beta_1^* = (z_\alpha + z_\beta) [\mathrm{Var}(b_1)]^{1/2}. \tag{23}$$

Acknowledgments

The authors would like to thank Regis Loffman of the Office of Environmental Compliance and Documentation, Oak Ridge National Laboratory, for providing the water quality data used in this analysis. We would also like to thank Roger Clapp and Shaw-Pin Miaou of ORNL, as well as two anonymous reviewers for their helpful comments.

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