

## APPENDIX A.2: STATISTICAL TREND ANALYSIS METHODS

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This appendix details the data evaluation and remedy selection procedures employed by the Monitoring and Remediation Optimization System (MAROS) Software. The procedures outlined below were developed to assess appropriate response measures for affected groundwater plumes based on scientifically sound quantitative analyses of current and historical site groundwater conditions.

### Initial Site Investigation

Evaluation of groundwater plume conditions and appropriate response measures requires adequate site characterization, including plume delineation. Therefore, for the compliance monitoring evaluation, the minimum required site information includes:

- *Constituents of Concern (COCs):* Individual constituents must be identified along with their relevant source areas and transport mechanisms.
- *Site Hydrogeology:* Site stratigraphy and groundwater flow velocity and direction must be identified.
- *Affected Groundwater:* Plume must be completely delineated for each COC to ensure that the results of the compliance monitoring assessment are reliable and not erroneously influenced by a migrating plume.
- *Time-Series Groundwater Monitoring Data:* Historical record must be compiled for each COC and meet the minimum data requirements described below.
- *Actual and Potential Groundwater Receptors:* Well locations, groundwater-to-surface water discharge locations, underground utilities, or other points of exposure must be identified.
- *Current or Near-Term Impact?:* Any current or near-term receptor impact (defined for this evaluation as occurring in zero to two years) must be assessed. Plumes posing current or near-term impact on applicable receptors are referred for immediate evaluation of appropriate risk management measures.

### Site Conceptual Model

The EPA recommends the use of conceptual site models to integrate data and guide both investigative and remedial actions (e.g., see EPA, 1999). A conceptual site model (CSM) is a three-dimensional representation that conveys what is known or suspected about contamination sources, release mechanisms, and the transport and fate of those contaminants. The conceptual model provides the basis for assessing potential remedial technologies at the site. In the context of the MAROS software, conceptual model development prior to software use would allow the user to better utilize the information gained through the various software modules as well as provide guidance for assessing the data that would best typify historical site conditions.

It is recommended that available site characterization data should be used to develop a conceptual model for the site prior to the use of the MAROS software. The conceptual model should include a three-dimensional representation of the source area as a NAPL or region of highly contaminated ground water, of the surrounding uncontaminated area, of ground water flow properties, and of the solute transport system based on available geological, biological, geochemical, hydrological, climatological, and analytical data for the site (EPA, 1998). Data on the contaminant levels and aquifer characteristics should be obtained from wells and boreholes which will provide a clear three-dimensional picture of the hydrologic and geochemical characteristics of the site. High concentrations of dissolved contaminants can be the result of leachates, rinse waters and rupture of water conveyance lines, and are not necessarily associated with NAPLs.

This type of conceptual model differs from the more generic conceptual site models commonly used by risk assessors that qualitatively consider the location of contaminant sources, release mechanisms, transport pathways, exposure points, and receptors. However, the conceptual model of the ground water system facilitates identification of these risk-assessment elements for the exposure pathways analysis. After development, the conceptual model can be used to help determine optimal placement of additional data collection points, as necessary, to aid in the natural attenuation investigation and to develop the solute fate and transport model. Contracting and management controls must be flexible enough to allow for the potential for revisions to the conceptual model and thus the data collection effort.

Successful conceptual model development involves (EPA, 1998):

- Definition of the problem to be solved (generally the three dimensional nature, magnitude, and extent of existing and future contamination).
- Identification of the core or cores of the plume in three dimensions. The core or cores contain the highest concentration of contaminants.
- Integration and presentation of available data, including:
  - Local geologic and topographic maps,
  - Geologic data,
  - Hydraulic data,
  - Biological data,
  - Geochemical data, and
  - Contaminant concentration and distribution data.
- Determination of additional data requirements, including:
  - Vertical profiling locations, boring locations and monitoring well spacing in three dimensions,
  - A sampling and analysis plan (SAP), and
  - Other data requirements.

Conceptual model development prior to use of the MAROS software will allow more accurate site evaluation through quality data input (i.e. identification of source and tail wells, etc.), as well as viewing the MAROS results in light of site-specific conditions. The conceptual model will also allow the user to gain insight into the type and extent of site data that is needed to fulfill minimum data requirements in order to fully utilize the MAROS software.

## Minimum Data Requirements

Compliance Monitoring data evaluation must be based on data from a consistent set of wells over a series of periodic sampling events. Statistical validity of the constituent trend analysis requires constraints on the minimum data input. To ensure a meaningful comparison of COC concentrations over time and space, the following minimum requirements were imposed on the time-series groundwater monitoring data:

- *Number of Wells:* Evaluation should include data from at least four wells (ASTM , 1998) in which COCs have been detected. May include up to two wells which have not exhibited COCs during more recent sampling events being analyzed, but in which COCs were previously detected. As many wells should be included in the evaluation as possible, subject to the other minimum data requirements.
- *Minimum Data per Well:* Data for each well should include at least four measured concentrations over six sampling events during the time period being analyzed. For any well, data may not be missing from more than two consecutive sampling events. Guidelines given by ASTM, 1998 notes that a minimum of more than one year of quarterly monitoring data of 4 or 5 wells is needed to establish a trend.
- *Number of Sampling Events:* Evaluation should include at least six most-recent sampling events which satisfy the minimum groundwater data requirements specified above. For this evaluation, it is suggested that the user consolidate multiple sampling dates within a single quarter to consider them to be a single sampling event, with multiple measurements of the same constituent subject to a user defined consolidation (e.g. average). The sampling events do not need to be the same for each well.

**Sufficient Data:** At least four wells with four or more independent sampling events per well are available

**Insufficient Data:** Fewer than four wells or fewer than 4 independent sampling events per well are available.

Although the software will calculate trends for fewer than four wells and a minimum of 4 sampling events, the above criteria will ensure a meaningful evaluation of COC trends over time. The minimum requirements described would apply only to “well behaved” sites, for most sites more data is required to obtain an accurate representation of COC trends. Sites with significant variability in groundwater monitoring data (due to water table fluctuation, variations in groundwater flow direction, etc.) will require more data to obtain meaningful stability trends. Essentially, the plume you are evaluating should be delineated with adequate consecutive sampling data to accurately evaluate the concentration trend with time.

## Plume Stability Analysis

Confirmation of the effective performance of monitored natural attenuation as a stand-alone remedial measure requires the demonstration of *primary lines of evidence*, i.e., actual measurement of stable or shrinking plume conditions based on evaluation of historical groundwater monitoring data. For a delineated plume, a stable or shrinking condition can be identified by a stable or decreasing concentration trends over time. For this analysis, an overall plume condition was determined for each COC based on a statistical trend analysis of concentrations at each well, as described below.

## STATISTICAL TREND ANALYSIS: CONCENTRATION VS. TIME

Under optimal conditions, the natural attenuation of organic COCs at any site is expected to approximate a first-order exponential decay for compliance monitoring groundwater data. With actual site measurements, apparent concentration trends may often be obscured by data scatter arising from non-ideal hydrogeologic conditions, sampling and analysis conditions. However, even though the scatter may be of such magnitude as to yield a poor goodness of fit (typically characterized by a low correlation coefficient, e.g.,  $R^2 \ll 1$ ) for the first-order relationship, parametric and nonparametric methods can be utilized to obtain *confidence intervals* on the estimated first-order coefficient, i.e., the slope of the log-transformed data.

Nonparametric tests such as the Mann-Kendall test for trend are suitable for analyzing data that do not follow a normal distribution. Nonparametric methods focus on the location of the probability distribution of the sampled population, rather than specific parameters of the population. The outcome of the test is not determined by the overall magnitude of the data points, but depends on the ranking of individual data points. Assumptions on the distribution of the data are not necessary for nonparametric tests. The Mann-Kendall test for trend is a nonparametric test which has no distributional assumptions and irregularly spaced measurement periods are permitted. The advantage gained by this approach involves the cases where outliers in the data would produce biased estimates of the least squares estimated slope. Parametric tests such as first-order regression analysis make assumptions on the normality of the data distribution, allowing results to be affected by outliers in the data in some cases. However, the advantage of parametric methods involve more accurate trend assessments result from data where there is a normal distribution of the residuals. Therefore, when the data is normally distributed the nonparametric method, the Mann-Kendall test, is not as efficient. Both tests are utilized in the MAROS software.

## Primary Line of Evidence 1: Mann-Kendall Analysis

### GENERAL

The Mann-Kendall test is a non-parametric statistical procedure that is well suited for analyzing trends in data over time (Gilbert, 1987). The Mann-Kendall test can be viewed as a nonparametric test for zero slope of the first-order regression of time-ordered concentration data versus time. The AFCEE MAROS Tool includes this test to assist in the analysis of groundwater plume stability. The Mann-Kendall test does not require any assumptions as to the statistical distribution of the data (e.g. normal, lognormal, etc.) and can be used with data sets which include irregular sampling intervals and missing data. The Mann-Kendall test is designed for analyzing a single groundwater constituent, multiple constituents are analyzed separately.

For this evaluation, a decision matrix was used to determine the "Concentration Trend" category for each well, as presented on Table 2.

### MANN-KENDALL STATISTIC (S)

The Mann-Kendall statistic (S) measures the trend in the data. Positive values indicate an increase in constituent concentrations over time, whereas negative values indicate a decrease in constituent concentrations over time. The strength of the trend is proportional to the magnitude of the Mann-Kendall Statistic (i.e., large magnitudes indicate a strong trend).

Data for performing the Mann-Kendall Analysis should be in time sequential order. The first step is to determine the sign of the difference between consecutive sample results.  $Sgn(x_i - x_{i-1})$  is an

indicator function that results in the values 1, 0, or -1 according to the sign of  $x_j - x_k$  where  $j > k$ , the function is calculated as follows

$$\begin{aligned} \text{sgn}(x_j - x_k) &= 1 && \text{if } x_j - x_k > 0 \\ \text{sgn}(x_j - x_k) &= 0 && \text{if } x_j - x_k = 0 \\ \text{sgn}(x_j - x_k) &= -1 && \text{if } x_j - x_k < 0 \end{aligned}$$

The Mann-Kendall statistic (S) is defined as the sum of the number of positive differences minus the number of negative differences or

$$S = \sum_{k=1}^{n-1} \sum_{j=k+1}^n \text{sgn}(x_j - x_k).$$

The *confidence in the trend* for the Mann-Kendall statistic is calculated using a Kendall probability table (e.g. Hollander, M. and Wolfe, D.A., 1973, incorporated into the software as 'tblMK\_Probabilities'). By assessing the S result along with the number of samples, n, the Kendall table provides the probability of rejecting the null hypothesis ( $H_0 = \text{no trend}$ ) for a given level of significance. MAROS calculates a 'confidence level' percentage by subtracting the probability (p) from 1 (Confidence = 1-p %). Confidence of 90% represents a significance level of  $\alpha = 0.1$ , and 95% confidence corresponds to  $\alpha = 0.05$ . The resulting confidence in the trend is applied in the Mann Kendall trend analysis as outlined in Table A.2.1. The Mann-Kendall test used in MAROS is limited to 40 sample events.

#### **AVERAGE**

The arithmetic mean of a sample of n values of a variable is the average of all the sample values written as

$$\bar{x} = \frac{\sum_{i=1}^n x_i}{n}$$

#### **STANDARD DEVIATION**

The standard deviation is the square root of the average of the square of the deviations from the sample mean written as

$$s = \sqrt{\frac{\sum_{i=1}^n (x_i - \bar{x})^2}{n - 1}}.$$

The standard deviation is a measure of how the value fluctuates about the arithmetic mean of the data.

**COEFFICIENT OF VARIATION (COV)**

The Coefficient of Variation (COV) is a statistical measure of how the individual data points vary about the mean value. The coefficient of variation, defined as the standard deviation divided by the average or

$$C.O.V. = \frac{s}{\bar{x}}$$

Values less than or near 1.00 indicate that the data form a relatively close group about the mean value. Values larger than 1.00 indicate that the data show a greater degree of scatter about the mean.

**RESULTS AND INTERPRETATION OF RESULTS: MANN-KENDALL ANALYSIS**

The Constituent Trend Analysis results are presented in the *Mann-Kendall Analysis* Screen (accessed from the *Plume Analysis Menu*). The software uses the input data to calculate the Coefficient of Variation (COV) and the Mann-Kendall statistic (S) for each well with at least four sampling events (see Figure A.2.1). A "Concentration Trend" and "Confidence in Trend" are reported for each well with at least four sampling events. If there is insufficient data for the well trend analysis, N/A (Not Applicable) will be displayed in the "Concentration Trend" column.

Statistical Analysis Results. Last column is the result for the trend.

Well	S/T	COV	MK (S)	Confidence in Trend	Concentration Trend
MW-8	S	0.985	-11	70.50%	S
MW-7	S	0.249	-7	62.60%	S
MW-14	S	1.606	-50	99.90%	D
MW-13	S	1.106	-53	99.80%	D
MW-12	S	1.591	-68	100.00%	D
MW-1	S	1.701	-15	98.50%	D
MW-6	T	0.000	0	47.80%	S
MW-5	T	0.851	-31	99.80%	D

Note: Increasing (I); Probably Increasing (PI); Stable (S); Probably Decreasing (PD); Decreasing (D); No Trend (NT); Not Applicable (N/A); Source/Tail (S/T); COV (Coefficient of Variation); MK(S) Mann-Kendall Statistic

FIGURE A.2.1 MANN-KENDALL ANALYSIS RESULTS

- The Coefficient of Variation (COV) is a statistical measure of how the individual data points vary about the mean value. Values less than or near 1.00 indicate that the data form a relatively close group about the mean value. Values larger than 1.00 indicate that the data show a greater degree of scatter about the mean.
- The Mann-Kendall statistic (MK (S)) measures the trend in the data. Positive values indicate an increase in constituent concentrations over time, whereas negative values indicate a decrease in constituent concentrations over time. The strength of the trend is proportional to the magnitude of the Mann-Kendall Statistic (i.e., large magnitudes indicate a strong trend).

- The “Confidence in Trend” (1-*p*) is the statistical probability that the constituent concentration is increasing ( $S > 0$ ) or decreasing ( $S < 0$ ). The null hypothesis (no trend) is rejected for confidence above 90%.
- The “Concentration Trend” for each well is determined according to the following rules, where COV is the coefficient of variation:

TABLE A.2.1 MAROS MANN-KENDALL ANALYSIS DECISION MATRIX

Mann-Kendall Statistic	Confidence in Trend	Concentration Trend
$S > 0$	> 95%	Increasing
$S > 0$	90 - 95%	Probably Increasing
$S > 0$	< 90%	No Trend
$S \leq 0$	< 90% and $COV \geq 1$	No Trend
$S \leq 0$	< 90% and $COV < 1$	Stable
$S < 0$	90 - 95%	Probably Decreasing
$S < 0$	95%	Decreasing

The MAROS Mann-Kendall Analysis Decision Matrix was developed in-house by Groundwater Services Inc. Strongly Increasing or Decreasing trends indicate a higher level of statistical significance. The confidence can be used as a qualitative measure of the statistical strength of the trend when evaluating the overall stability of the plume. The user can choose not to apply one of the two statistical plume analysis decision matrices. Choose “Not Used” in the Trend Result weighting screen. If the user would like to use another decision matrix to determine stability of the plume, they would need to do this outside the software.

## Statistical Plume Analysis 2: Linear Regression Analysis

### GENERAL

Linear Regression is a parametric statistical procedure that is typically used for analyzing trends in data over time. However, with the usual approach of interpreting the log slope of the regression line, concentration trends may often be obscured by data scatter arising from non-ideal hydrogeologic conditions, sampling and analysis conditions, etc. Even though the scatter may be of such magnitude as to yield a poor goodness of fit (typically characterized by a low correlation coefficient, e.g.,  $R^2 \ll 1$ ) for the first-order relationship, *confidence intervals* can nonetheless be constructed on the estimated first-order coefficient, i.e., the slope of the log-transformed data. Using this type of analysis, a higher degree of scatter simply corresponds to a wider confidence interval about the average log-slope. Assuming the *sign* (i.e., positive or negative) of the estimated log-slope is correct, a level of confidence that the slope is not zero can be easily determined. Thus, despite a poor goodness of fit, the overall *trend* in the data may still be ascertained, where low levels of confidence correspond to “Stable” or “No Trend” conditions (depending on the degree of scatter) and higher levels of confidence indicate the stronger likelihood of a trend. The coefficient of variation, defined as the standard deviation divided by the average, is used as a secondary measure of scatter to distinguish between “Stable” or “No Trend” conditions for negative slopes. The Linear Regression Analysis is designed for analyzing

a single groundwater constituent, multiple constituents are analyzed separately. The MAROS software includes this test to assist in the analysis of groundwater plume stability.

For this evaluation, a decision matrix was used to determine the “Concentration Trend” category for each well, as presented on Table A.2.2.

**LINEAR REGRESSION**

The objective of linear regression analysis is to find the trend in the data through the estimation of the log slope as well as placing confidence limits on the log slope of the trend. Regression begins with the specification of a model to be fitted. A linear relationship is one expressed by a linear equation. The Linear Regression analysis in MAROS is performed on Ln (COC Concentration) versus Time. The regression model assumes that for a fixed value of x (sample date) the expected value of y (log COC concentration) is some function. For a particular value,  $x_i$  or sample date the predicted value for y (log COC concentration) is given by

$$\hat{y}_i = a + bx_i .$$

The fit of the predicted values to the observed values ( $x_i, y_i$ ) are summarized by the difference between the observed value  $y_i$  and the predicted value  $\hat{y}_i$  (the residual value.) A reasonable fit to the line is found by making the residual values as small as possible. The method of least squares is used to obtain estimates of the model parameters (a, b) that minimize the sum of the squared residuals,  $S^2$  or the measure of the distance between the estimate and the values we want to predict (the y’s).

$$S^2 = \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

The values for the intercept (a) and the slope (b) of the line that minimize the sum of the squared residuals ( $S^2$ ), are given by

$$b = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} \quad \text{and} \quad a = \bar{y} - b\bar{x}$$

where  $\bar{x}$  and  $\bar{y}$  are the mean x and y (log COC concentration) values in the dataset.

In order to test the confidence on the regression trend, there is a need to place confidence limits on the slope of the regression line. In this stage of the trend analysis, it is assumed that for each x value, the y-distribution is normal. A t-test may be used to test that the true slope is different from zero. This t-test is preferentially used on data that is not serially correlated or seasonally cyclic or skewed.

The variance of  $y_i$  ( $\sigma^2$ ) is estimated by the quantity  $S^2_{y..x}$  where this quantity is defined as

$$S^2_{y|x} = \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n - 2}$$

where n is the number of samples.

The estimation of the standard deviation or standard error of the slope (s.e.b.) is defined as

$$s.e.b. = \sqrt{\frac{S_{y|x}^2}{\sum_{i=1}^n (x_i - \bar{x}_i)^2}}$$

To test significance of the slope calculated, the following t-test result can be used to find the confidence interval for the slope.

$$t = \frac{b}{s.e.b.}$$

The t result along with the degrees of freedom (n-2) are used to find the confidence in the trend by utilizing a t-distribution table found in most statistical textbooks (e.g. Fisher, L.D. and van Belle, G., 1993). The resulting confidence in the trend is utilized in the linear regression trend analysis as outlined in Table A.2.2.

**RESULTS AND INTERPRETATION OF RESULTS: LINEAR REGRESSION ANALYSIS**

The Constituent Trend Analysis Results are presented in the Linear Regression Analysis Screen (accessed from the Mann-Kendall Analysis screen). The software uses the input data to calculate the Coefficient of Variation (COV) and the first-order coefficient (Ln Slope) for each well with at least four sampling events. A "Concentration Trend" and "Confidence in Trend" are reported for each well with at least four sampling events. If there is insufficient data for the well trend analysis, N/A (Not Applicable) will be displayed in the "Concentration Trend" column (Figure A.2.2)

Statistical Analysis Results. Last column is the result for the trend.

Well	S/T	Average	Ln Slope	COV	Confidence in Trend	Concentration Trend
MW-8	S	6.8E-04	-9.5E-05	9.8E-01	82.2%	S
MW-7	S	5.4E-04	-3.1E-05	2.5E-01	78.1%	S
MW-14	S	9.5E-03	-1.0E-03	1.6E+00	99.6%	D
MW-13	S	1.7E-02	-1.5E-03	1.1E+00	100.0%	D
MW-12	S	3.6E-02	-1.7E-03	1.6E+00	100.0%	D
MW-1	S	3.6E-01	-1.4E-03	1.7E+00	99.6%	D
MW-6	T	5.0E-04	0.0E+00	0.0E+00	100.0%	S

Note: Increasing (I); Probably Increasing (PI); Stable (S); Probably Decreasing (PD); Decreasing (D); No Trend (NT); Not Applicable (N/A); Source/Tail (S/T); COV (Coefficient of Variation)

FIGURE A.2.2 LINEAR REGRESSION ANALYSIS RESULTS

- The Coefficient of Variation (COV) is a statistical measure of how the individual data points vary about the mean value. Values less than or near 1.00 indicate that the data form a relatively close group about the mean value. Values larger than 1.00 indicate that the data show a greater degree of scatter about the mean.
- The Log Slope (Ln Slope) measures the trend in the data. Positive values indicate an increase in constituent concentrations over time, whereas negative values indicate a decrease in constituent concentrations over time.
- The “Confidence in Trend” is the statistical probability that the constituent concentration is increasing (ln slope>0) or decreasing (ln slope<0).
- The “Concentration Trend” for each well is determined according to the following rules, where COV is the coefficient of variation:

TABLE A.2.2 MAROS LINEAR REGRESSION ANALYSIS DECISION MATRIX

Confidence in Trend	Ln Slope	
	Positive	Negative
<90%	No Trend	COV < 1 Stable COV > 1 No Trend
90% - 95%	Probably Increasing	Probably Decreasing
> 95%	Increasing	Decreasing

COV = Coefficient of Variation

The MAROS Linear Regression Analysis Decision Matrix was developed in-house by Groundwater Services Inc. The user can choose not to apply one of the two statistical plume analysis decision matrices. Choose “Not Used” in the Trend Results weighting screen. If the user would like to use another decision matrix to determine stability of the plume, they would need to do this outside the software.

## Further Considerations

The results of a constituent concentration trend analysis form just one component of a plume stability analysis. Additional considerations in determining the over-all plume stability include:

- Multiple constituent concentration trend analyses;
- Time-frame over which the trend is evaluated;
- Adequate delineation of the plume;
- Status of the COC as a parent or daughter product;
- Proximity of monitoring wells with stable or decreasing constituent trends to the downgradient edge of the plume.

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