1. VISUAL ANALYSIS

Overview

Using industry standard data analysis tools (i.e., Excel), plot data (groundwater level, concentration) vs time. This allows for visual identification of trends over time. These types of plots are commonly referred to as time-series plots.

Advantages

- Easily created.
- Minimal data requirements (can be as little as two data points, although more are preferred).
- Can show different components of project (VE system turned on, VE system turned off, etc.) to aid in evaluating trends.

Disadvantages

- Data outliers can inadvertently influence “trend.”
- Does not account for variability in seasonal groundwater fluctuations.
- Trends identified can be

Example Output
MW-2
(Benzene)

![Graph showing groundwater elevation and concentration over time.](image-url)
2. LINEAR REGRESSION

Overview

A parametric statistical technique used to estimate a trend via a linear relationship between multiple data points (sample analytical results). A line with a positive slope indicates an increasing trend, whereas a negative slope is indicative of a decreasing trend. Assumptions of linear regression are as follows:

1. The difference between each concentration measurement and its predicted value from the regression equation (residuals) are approximately normal in distribution.
2. Missing data and ND’s are not part of data set.

The following conditions should be met prior to concluding a resulting trend:

1. The residuals (R) are approximately normal/reasonably symmetric in distribution.
2. A scatter plot of residuals vs concentrations yields a scatter cloud of generally uniform thickness.
3. A scatter plot of residuals vs time yields a scatter cloud of generally uniform thickness.
4. A minimum of eight measurements.
If the above conditions are met, the following can generally be applied with respect to trend interpretation:

- Where \( y = mx + b \) represents the trend line, and \( m = \text{slope} \), if \( m \) is negative, the trend (slope) is decreasing.
- Conversely, if \( m \) is positive, the trend is increasing.
- A higher \( m \) value (steeper slope) indicates a more rapid rate of degradation/contamination.
- When the above items cannot be met in an approximate sense, a non-parametric trend method should be utilized (Mann-Kendall).
- A smaller \( R^2 \) value indicates a less accurate trend line (if \( R^2 = 0 \), then the trend line would have no linear relationship). The larger the \( R^2 \) value, the less the amount of variation/deviation in the dataset from the trend line, and the more reliable the trend line is (If \( R^2 = 1 \), the dataset is defined as linear).

**Advantages**

- Least squares regression is the most commonly used regression method. Calculates a best fit line for the observed data by minimizing the sum of the squares of vertical deviations from each data point to the line.
- Can be used site-wide or for individual wells, but is best suited for individual well analysis.
- Principles can be applied to site-wide plume characteristics for site wide analysis
- Relatively simple trend analysis/data requirements.

**Disadvantages**

- Data outliers can inadvertently influence “trend.” Data input/output must be QA/QC’d prior to determining accuracy of trend (i.e., checking the residuals and/or visual).
- Extrapolation of data is not recommended in support of project decision making, yet can be useful as a general forecasting tool.
- Trends are dependent on data quality and user interpretation.
- Does not account for ND or missing data.

**Online/Free-ware availability**

Regression calculators and/or freeware are readily available online. Much of the freeware discussed in the following slides are equipped with regression analysis tools. It is also easily set up using Microsoft’s Excel program.

**Example Output**
Linear Regression (Least Squares): DECREASING
Benzene Concentration Data at One Monitoring Well Point

\[ y = -0.0404x + 1688.7 \]
\[ R^2 = 0.5007 \]
3. MANN-KENDALL (M-K)

Overview

M-K analysis is a non-parametric test for identifying trends in time-series data. In short, the analysis compares relative magnitudes of sample data (not the data values themselves). If an increasing trend exists, the sample taken first from any randomly selected pair of measurements should on average, have a lower concentration than the measurement collected at a later time.

Sources


http://www.stat.yale.edu/Courses/1997-98/101/linreg.htm
The M-K statistic (S) is given by examining all possible pairs of data points (concentrations) and scoring each pair by assigning a value (identical values = 0, earlier value > later value = -1, earlier value < later value = 1). Summing the total of the assigned values gives S. A positive S suggests an upward trend, while a negative S suggests a negative trend. The larger the value of S (+/-), the stronger the level of confidence that the trend is legitimate.

Assumptions are as follows:

1. Only relative magnitudes are required (not actual concentrations) to rank the data.
2. ND should be treated as a common value lower than any detected values.
3. At least four data points must be analyzed.

**Advantages**

- Relatively simple data requirements.
- User friendly.
- Quantifies confidence level in trends based on data.
- Enables quick identification of trends, historic and/or recent.

**Disadvantages**

- Does not account for site specific characteristics such as seepage velocity or well location.
- Analyzes only a single data point (monitoring well).
- Seasonal effects are not accounted for which can incorrectly influence trend (groundwater fluctuation through “smear zone”).
- Must address ND values…they need to be the same.

**Online/Free-ware availability**

Mann-Kendall free-ware is available online. Two good options are:

1. GSI Mann-Kendall Toolkit
2. Washington State Department of Ecology (Package A)

Mann-Kendall analysis tools are also provided in the freeware packages discussed in the following slides.

**Example Output**

1. *(GSI)*
### GSI MANN-KENDALL TOOLKIT
for Constituent Trend Analysis

<table>
<thead>
<tr>
<th>Sampling Event</th>
<th>Sampling Date</th>
<th>BENZENE CONCENTRATION (µg/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2-Apr-18</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>8-Jul-19</td>
<td>0.99</td>
</tr>
<tr>
<td>3</td>
<td>25-Oct-19</td>
<td>0.99</td>
</tr>
<tr>
<td>4</td>
<td>26-Jan-11</td>
<td>0.99</td>
</tr>
<tr>
<td>5</td>
<td>18-Apr-11</td>
<td>0.50</td>
</tr>
<tr>
<td>6</td>
<td>24-Jul-11</td>
<td>0.99</td>
</tr>
<tr>
<td>7</td>
<td>18-Oct-11</td>
<td>0.99</td>
</tr>
<tr>
<td>8</td>
<td>17-Feb-12</td>
<td>0.99</td>
</tr>
<tr>
<td>9</td>
<td>7-May-12</td>
<td>0.99</td>
</tr>
<tr>
<td>10</td>
<td>17-Jul-12</td>
<td>0.99</td>
</tr>
<tr>
<td>11</td>
<td>22-Oct-12</td>
<td>0.99</td>
</tr>
<tr>
<td>12</td>
<td>23-Jan-13</td>
<td>0.99</td>
</tr>
<tr>
<td>13</td>
<td>11-Apr-13</td>
<td>0.99</td>
</tr>
<tr>
<td>14</td>
<td>10-Jul-13</td>
<td>0.99</td>
</tr>
<tr>
<td>15</td>
<td>4-Nov-13</td>
<td>0.99</td>
</tr>
<tr>
<td>16</td>
<td>23-Jan-14</td>
<td>0.99</td>
</tr>
<tr>
<td>17</td>
<td></td>
<td></td>
</tr>
<tr>
<td>18</td>
<td></td>
<td></td>
</tr>
<tr>
<td>19</td>
<td></td>
<td></td>
</tr>
<tr>
<td>20</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Coefficient of Variation</strong></td>
<td>0.00</td>
<td>0.73</td>
</tr>
<tr>
<td><strong>Mann-Kendall Statistic (S)</strong></td>
<td>0</td>
<td>-26</td>
</tr>
<tr>
<td><strong>Confidence Factor</strong></td>
<td>4.0%</td>
<td>89.0%</td>
</tr>
<tr>
<td><strong>Concentration Trend</strong></td>
<td>Stable</td>
<td>Stable</td>
</tr>
</tbody>
</table>

#### Notes:
1. At least four independent sampling events per well are required for calculating the trend. Methodology is valid for 4 to 40 samples.
2. Confidence in Trend = Confidence (in percent) that constituent concentration is increasing (S>0) or decreasing (S<0): >95% = Increasing or Decreasing; ≥ 90% = Probably Increasing or Decreasing; < 90% and S=0 = No Trend; < 90% and S<0 = No Trend; < 90% and S>0 = Stable.

#### DISCLAIMER:
The GSI Mann-Kendall Toolkit is available “as is”. Considerable care has been exercised in preparing this software product; however, no party, including without limitation GSI Environmental Inc., makes any representation or warranty regarding the accuracy, correctness, or completeness of the information contained herein, and no such party shall be liable for any direct, indirect, consequential, incidental or other damages resulting from the use of this product or the information contained herein. Information in this publication is subject to change without notice. GSI Environmental Inc. disclaims any responsibility or obligation to update the information contained herein.

GSI Environmental Inc. www.gsi-net.com
Module 1: Mann-Kendall Trend Test for Plume Stability (Non-parametric Statistical Test)

| Site Name: | ABC Corporation |
| Site Address: | Reno, NV |

Well (Sampling) Location: Well 2
Level of Confidence (Decision Criteria): 85%

Monitoring Well Information: Contaminant Concentration at a well: Quarterly sampling recommended.

<table>
<thead>
<tr>
<th>Sampling Event</th>
<th>Date Sampled</th>
<th>Benzene</th>
<th>MTBE</th>
</tr>
</thead>
<tbody>
<tr>
<td>#1</td>
<td>2-Apr-10</td>
<td></td>
<td></td>
</tr>
<tr>
<td>#2</td>
<td>8-Jul-10</td>
<td>44</td>
<td>110</td>
</tr>
<tr>
<td>#3</td>
<td>20-Oct-10</td>
<td>73</td>
<td>80</td>
</tr>
<tr>
<td>#4</td>
<td>20-Jan-11</td>
<td>19</td>
<td>18</td>
</tr>
<tr>
<td>#5</td>
<td>18-Apr-11</td>
<td>64</td>
<td>11</td>
</tr>
<tr>
<td>#6</td>
<td>24-Jul-11</td>
<td>9.10</td>
<td>5</td>
</tr>
<tr>
<td>#7</td>
<td>18-Oct-11</td>
<td>8.90</td>
<td>5</td>
</tr>
<tr>
<td>#8</td>
<td>17-Feb-12</td>
<td>18</td>
<td>3</td>
</tr>
<tr>
<td>#9</td>
<td>7-May-12</td>
<td>51</td>
<td>3</td>
</tr>
<tr>
<td>#10</td>
<td>16-Jul-12</td>
<td>35</td>
<td>2</td>
</tr>
<tr>
<td>#11</td>
<td>22-Oct-12</td>
<td>11</td>
<td>2</td>
</tr>
<tr>
<td>#12</td>
<td>23-Jan-13</td>
<td>21</td>
<td>1</td>
</tr>
<tr>
<td>#13</td>
<td>11-Apr-13</td>
<td>20</td>
<td>2</td>
</tr>
<tr>
<td>#14</td>
<td>10-Jul-13</td>
<td>20</td>
<td>2</td>
</tr>
<tr>
<td>#15</td>
<td>4-Nov-13</td>
<td>23</td>
<td>2</td>
</tr>
<tr>
<td>#16</td>
<td>23-Jan-14</td>
<td>8.0</td>
<td>1</td>
</tr>
</tbody>
</table>

Mann-Kendall Non-parametric Statistical Test Results

<table>
<thead>
<tr>
<th>Hazardous Substance?</th>
<th>Benzene</th>
<th>MTBE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Confidence Level Calculated?</td>
<td>88.00%</td>
<td>100.00%</td>
</tr>
<tr>
<td>Plume Stability?</td>
<td>Shrinking</td>
<td>Shrinking</td>
</tr>
<tr>
<td>Coefficient of Variation?</td>
<td>n&lt;4</td>
<td>n&lt;4</td>
</tr>
<tr>
<td>Mann-Kendall Statistic &quot;S&quot; value?</td>
<td>-26</td>
<td>-86</td>
</tr>
<tr>
<td>Number of Sampling Rounds?</td>
<td>15</td>
<td>15</td>
</tr>
<tr>
<td>Average Concentration?</td>
<td>28.33</td>
<td>16.36</td>
</tr>
<tr>
<td>Standard Deviation?</td>
<td>20.61</td>
<td>32.75</td>
</tr>
<tr>
<td>Coefficient of Variation?</td>
<td>0.73</td>
<td>2.00</td>
</tr>
<tr>
<td>Blank if No Errors found</td>
<td>n&lt;4</td>
<td>n&lt;4</td>
</tr>
</tbody>
</table>
Temporal Trend: Plot of Concentration vs. Sampling Time

Hazardous substance? Benzene
Plume Stability? Shrinking

Sources


4. WASHINGTON STATE DEPARTMENT OF ECOLOGY: NATURAL ATTENUATION ANALYSIS TOOL PACKAGE FOR PETROLEUM-CONTAMINATED GROUND WATER

Overview

Comprehensive site evaluation tool based on statistical methods applied to site-specific data that accounts for historical and current data as well as hydrogeologic factors (e.g., wells, seepage velocity), and potential receptors. Analyzes individual wells, plume with respect to temporal/spatial indicators and stability. Using statistical trend analysis, helps identify temporal trends, plume characteristics (shrinking/expanding), time until target concentrations are met, influence of groundwater, evaluation of geochemical indicators, and graphical presentation of historical groundwater data. The program is divided into two packages, A and B.

Package A (Modules 1, 2, and 3) analysis tool will conduct the following:

- Non-parametric statistical tests for plume stability at each well.
  - Mann-Kendall test (previously discussed)
  - Mann-Whitney U-test

- Graphical presentation of historical ground water data.
  - Plot of temporal ground water analytical and elevation data vs. time to assess the plume status and the impact of ground water elevation fluctuation on contaminant concentrations at each well
  - Plot of spatial ground water analytical data vs. distance (for multiple wells) to assess the overall plume status

- Evaluation of geochemical indicators.
  - Estimate of expressed assimilative capacity at multiple wells
  - Simultaneous plot of concentrations of contaminant and geochemical indicators vs. distance (at multiple wells) to demonstrate biodegradation clearly

- Temporal trend (regression) analysis at each well.
  - Estimate of an average and a range of (kpoint) point decay rate (1st-order) constant for both the best-fit and a given one-tailed confidence level at each well
  - Temporal prediction at each well location under a given confidence level
  - Estimate of an average and a range (under a given confidence level) of restoration time to reach the cleanup goal at each well
  - Calculation of the correlation coefficient and confidence level (with the Pearson’s correlation coefficient) of log-linear regression analysis (for a plot of concentration vs. time at each well)
Figure A.1. Calculation Module for Natural Attenuation Analysis

Package A

Note: Modules are not linked each other.

**Description**

- **Module 1**
  - Non-Parametric Analysis for Plume Stability
    - non-parametric trend analysis
    - stability of the plume for multiple contaminants
    - well-to-well analysis
    - quarterly sampling recommended

- **Module 2**
  - Graphical and Regression Analysis for Plume Stability & Restoration Time Calculation
    - determine the stability of the plume for a contaminant; well-to-well analysis
    - quarterly sampling recommended
    - at least four sampling rounds (the most recent) over one year sampling period
    - in four or more consecutive wells

- **Module 3**
  - Historical Ground Water Data Entry
    - monitoring well information: historical contaminant concent at a well
    - monitoring well information: historical ground water elevation at a well
    - 2D location of wells with respect to plume centerline
  - Analysis of Geochemical Indicators
    - the most recent average geochemical data (Dissolved Oxygen, Nitrates, Sulphate, Manganese, Permeable Iron, Methane, Reduc Potential, Alkalinity) at up-gradient, source, and down-gradient wells
    - the most recent average contaminant concent (e.g., BTEX, or TPH) at up-gradient, source, and down-gradient wells
    - transformed 2D location of wells with respect to plume centerline

**Methodology**

- **Mann-Kendall Trend Test**
  - valid for data that exhibit random behavior
  - require at least four (the most recent) sampling rounds in four or more consecutive wells
  - one year sampling
  - plume stability test by Kendall's K statistic and Coefficient of Variation test at a user-specified confidence level

- **Mann-Whitney U Trend Test**
  - valid for data that exhibit strong seasonal behavior
  - require at least four (the most recent) consecutive sampling rounds in four or more consecutive wells
  - two years
  - plume stability test by Mann-Whitney U statistic at a user-specified confidence level

- **Graphical Presentation of Groundwater Data**
  - for individual well: statistical analysis results displayed
  - plot of conc. vs. time; conc. vs. ground water elevation
  - plot of conc. vs. plume centerline distance
  - monitoring sampling times

- **Temporal Analysis: Calculation of Restoration Time**
  - log-normal regression for conc. as a function of time
  - plume stability test by Pearson Correlation Coefficient at a user-specified confidence level
  - calculation of average and boundary restoration time at a user-specified confidence level
  - calculation of average and boundary of kstar at a well

- **Assimilative Capacity Calculation & Geochemical Indicator Plot**
  - contaminant and geochemical indicators multiple plots
  - site-specific assimilative capacity calculation at wells
Package B (Modules 4, 5, and 6) analysis tool will conduct the following calculations:

- Estimate of source mass from sampling data: for unsaturated, smear, and dissolved zones.
- Under 1-D (transformed from 2-D): steady state/continuous source assumption for only stable.
  - Plot of the concentration vs. distance
  - Estimate of an average and a range of (λ) biodegradation rate constant
  - Estimate of an average and a range of (k) bulk attenuation rate (1st-order) constant under steady state (stable plume)
  - Estimate of a percent mass removal rate by biodegradation alone
  - Temporal and spatial prediction as a function of time and well location
  - Estimate of a target source concentration in order to reach a target level at a receptor location under given restoration time
- Under 2-D; transient state (with modified Domenico model) for shrinking and stable (or any type) plumes:
  - Estimate of a biodegradation rate constant (λ) by calibration via chi-square statistics for best-fit to the normalized concentration of consecutive multiple wells by 1st-order decay model
  - Estimate of a percent mass removal rate by biodegradation alone with 1st-order decay model and instantaneous reaction model (via the calculation of mass flux)
  - Estimate of a temporal/spatial prediction at a receptor location by 1st-order decay model and instantaneous reaction model
  - Estimate of a plume stabilization time (half time to reach the steady state) at a receptor location
  - Estimate of a restoration time to reach a target level at a receptor location by 1st-order decay model and instantaneous reaction model
  - Estimate of a target source mass amount (amount of mass that should be removed from the current source zone) in order to reach a target level at a receptor location under a given restoration time by 1st-order decay model and instantaneous reaction model
  - Estimate of a contaminant mass loading rate (as a function of x-distance and time) to the adjacent surface water body by 1st-order decay model
Figure A.2. Calculation Module for Natural Attenuation Analysis
Package B

Description

Estimation of Contaminant Mass at a Source Zone
- to be used as an input for Module 6
- types of data needed: measured contaminant concentration at source area elements, dissolved, particulate, total dissolved solids, and total solids

1-D Steady-State Mode:
- continuous source & steady-state mode
- Boltzmann’s equation used
- data needed: hydrology (Q, R, α, R)
- the most recent and representative contaminant concentrations, in line or across the source zone
- contiguous sections (2-D) of wells with respect to plane centerline

Module 5

Inputs
- run data entry worksheet for a contaminant source
- calibration of A for 1st order decay
- calculation of A for 1st order decay
- density flow rate (for Modules 6 only)

Calculation of Rate Constant Temporal/Spatial Prediction
- log-linear regression of half-life vs. distance
- calculation of rate constant vs. distance
- calculation of distance from source to point of interest
- calculation of target source mass to reach the target level at a given restoration time and location of receptor

Module 6

2-D Transient State Mode:
- modified Darcian flow method used: three models used: 1st order decay, instantaneous reaction models with decaying source data
- dissolved concentrations, dissolved solids, and dissolved solids
- dissolved solids, dissolved solids, and dissolved solids
- dissolved solids, dissolved solids, and dissolved solids
- dissolved solids, dissolved solids, and dissolved solids
- dissolved solids, dissolved solids, and dissolved solids

Inputs
- run data entry worksheet for a contaminant source
- calibration of A for 1st order decay
- calculation of A for 1st order decay
- density flow rate (for Modules 6 only)

Methodology

Source Zone Analysis
- simple Thoreau Polygon Network used for the discrimination of the source zone
- determination of soil source mass in a source zone
- calculation of mass distribution pattern

Comparison: Field Data vs. Predicted
- plot of conc. (measured and the predicted) vs. distance
- plot of normalized conc. (measured and the predicted) vs. distance

Calculation Mass Removal Rate by Biodegradation
- mass removal rate by biodegradation
- calculation of mass flux rate along the plane of distance
- calculation of mass flux rate along the plane of distance

Calculation of Target Source Mass and Restoration Time
- calculation of target source mass from a receptor location and time (multiple locations and multiple times)
- calculation of restoration time to reach the target level (time, location, and multiple times)
- calculation of target level restoration time

Surface Water Mass Loading Rate
- calculation of mass loading rate from surface water from ground water source at a given distance and time period
- calculation of mass loading rate from surface water from ground water source at a given distance and time period

Note: Modules 5 and 6 are the same input worksheet.
Advantages

- User friendly
- Quantifies confidence level in trends based on data
- Enables quick identification of trends, historic and/or recent
- Comprehensive site analysis
- Incorporates hydrogeologic site data and potential receptors in analysis
- Geochemical/Biodegradation assessment/modeling capability
- 2-D Modeling capability

Disadvantages

- Complex data requirements (depending on module)
- Time intensive (depending on module)
- Does not use real world coordinates in 2-D modeling components
- Does not provide site optimization recommendations

Online/Freeware availability

Free-ware is available online:

http://www.ecy.wa.gov/programs/tcp/policies/pol_main.html

Example Output
1. Input data used for this module

<table>
<thead>
<tr>
<th>Hazardous Substance:</th>
<th>Benzene</th>
</tr>
</thead>
<tbody>
<tr>
<td>Seepage Velocity (Average), ( V_{s\text{avg}} ), ft/yr</td>
<td>1.138</td>
</tr>
<tr>
<td>Longitudinal Dispersion, ( \alpha_x ), ft</td>
<td>13.45</td>
</tr>
<tr>
<td>Retardation Factor, ( R )</td>
<td>2.05</td>
</tr>
<tr>
<td>Current Continuous Source Concentration, ( C_{\text{avg}} ), ug/L</td>
<td>6500</td>
</tr>
</tbody>
</table>

2. Enter Decision Criteria

Level of Confidence (Decision Criteria used) \( 85\% \)


**Log-linear Regression Results:**

- Average Slope \( \beta \): \( 1.65E-02 \)
- Lower Boundary Slope \( (@ 85\% \text{ C.L.}) \): \( 1.06E-02 \)
- Intercept \( \alpha \): \( 8248.0 \)
- Coefficient of Determination, \( r^2 \): 0.789
- Correlation Coefficient, \( r \): -0.888
- Number of Data Point, \( n \): 8
- t-statistics: 5.35
- Level of significance calculated for the slope: 99.9%

**Rates Calculated:**

<table>
<thead>
<tr>
<th></th>
<th>unit</th>
<th>@ Avg Slope</th>
<th>@ Lower Boundary Slope (@85% C.L.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bulk Attenuation Rate Constant, ( K )</td>
<td>yr(^{-1})</td>
<td>1.88</td>
<td>1.21</td>
</tr>
<tr>
<td>Half Life of ( K )</td>
<td>yr</td>
<td>0.37</td>
<td>0.57</td>
</tr>
<tr>
<td>Biodegradation Rate Constant, ( \Lambda )</td>
<td>yr(^{-1})</td>
<td>1.12</td>
<td>0.67</td>
</tr>
<tr>
<td>Half Life of ( \Lambda )</td>
<td>yr</td>
<td>0.62</td>
<td>1.63</td>
</tr>
<tr>
<td>Ratio of ( K/\Lambda )</td>
<td>%</td>
<td>59%</td>
<td>56%</td>
</tr>
</tbody>
</table>

4. 1-D Temporal/Spatial Prediction with Bear Equation (1979); Transient Plug flow model with a longitudinal dispersion

<table>
<thead>
<tr>
<th>Temporal/Spatial Prediction</th>
<th>Predicted Concentration, ( C_{\text{avg}} ), ug/L</th>
<th>Calculation of Target Source Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Location of a Receptor</td>
<td></td>
<td>Calculate Target Source concentration</td>
</tr>
<tr>
<td>x-direction, ft</td>
<td>200</td>
<td></td>
</tr>
<tr>
<td>y-direction, ft</td>
<td>15</td>
<td>202.8</td>
</tr>
<tr>
<td>Simulation Time, yr</td>
<td>14</td>
<td>694.2</td>
</tr>
</tbody>
</table>

Prediction as a function of simulation time at a receptor’s location given above

Prediction as a function of x-distance at a simulation time given above (\( @ y=0 \))
### Module 6: Calculation of Mass Removal Rate by Biodegradation

#### Site Name: Dummy XYZ site

#### Site Address: 1234, Olympia, WA 98501

#### Hazardous Substance: Benzene

<table>
<thead>
<tr>
<th>Transverse Distance, y-direction (ft)</th>
<th>Ground water Concentrations in Plume (ng/L at z=0)</th>
<th>Distance from Source, x-direction (ft)</th>
<th>Choose a Model below to Display:</th>
</tr>
</thead>
<tbody>
<tr>
<td>108.0</td>
<td>56.3</td>
<td>39.6</td>
<td>No Degradation Model</td>
</tr>
<tr>
<td>55.0</td>
<td>4669.0</td>
<td>1611.7</td>
<td>1st Order Decay Model</td>
</tr>
<tr>
<td>0.0</td>
<td>3723.5</td>
<td>1503.6</td>
<td>Instantaneous Reaction Model</td>
</tr>
<tr>
<td>-50.0</td>
<td>4669.0</td>
<td>1016.7</td>
<td></td>
</tr>
<tr>
<td>-100.0</td>
<td>56.3</td>
<td>39.6</td>
<td></td>
</tr>
</tbody>
</table>

**FLUX (mg/day)**

| Mass 1.90E-4 | 7.95E-4 | 3.46E-3 | 1.79E-3 | 8.71E-3 | 4.99E-2 | 2.96E-2 | 9.39E-1 | 4.63E-1 | 3.31E-1 | 1.14E-1 |

**Target Ground-water Conc. mg/L** 5.0

**Modelled Area Length (L), ft** 550.0

**Modelled Area Width (W), ft** 200.0

*Displayed Model is 1st-order Decay.

#### Plume and Source Masses (Order-of-Magnitude Accuracy)

- **Plume Mass if No Biodegradation:** 98.2 Ag
  - Actual Plume Mass: 5.3 Ag
  - Change in Electron Acceptor/Byp product Mass, kg:
    - Oxygen: na
    - Nitrate: na
    - Fumaric acid: na
    - Sulfate: na
    - Methane: na
    - Manganese: na

- Contaminant Mass in Source (t=0 years): 296.0 Ag
- Contaminant Mass in Source Now (t=12 years): 103.8 Ag
- Current Volume of Groundwater in Plume: 10.4 ac-ft³
- Flowrate of Water Through Source Zone: 1.960 ac-ft³

---

**Note:**

- All concentrations are in nanograms per liter (ng/L).
- The model assumes a 1st-order decay for biodegradation.
- The mass calculations are approximate and for demonstration purposes.

---

**Plot All Data**

**Plot Data > Target**
Module 5: Calculation of Rate Constants: Temporal/Spatial Prediction

1. Input data used for this module

<table>
<thead>
<tr>
<th>Hazardous Substance:</th>
<th>Benzene</th>
</tr>
</thead>
<tbody>
<tr>
<td>Seepage Velocity (Average), $V_{avg}$, ft/yr</td>
<td>113.8</td>
</tr>
<tr>
<td>Longitudinal Dispersivity, $\alpha_x$, ft</td>
<td>13.45</td>
</tr>
<tr>
<td>Retardation Factor, $R$</td>
<td>2.05</td>
</tr>
<tr>
<td>Current Continuous Source Concentration, ug/L</td>
<td>6500</td>
</tr>
</tbody>
</table>


**Log-linear Regression Results:**

- Average Slope: $1.65 \times 10^{-2}$
- Lower Boundary Slope (@85% C.L.): $1.06 \times 10^{-2}$
- Intercept: 8248.0
- Coefficient of Determination, $r^2$: 0.789
- Correlation Coefficient, $r$: 0.888
- Number of Data Point, $n$: 5
- t-statistics: 5.35
- Level of significance calculated for the slope: 95.0%

**Rates Calculated:**

- Bulk Attenuation Rate Constant, $k$: $1.88 \times 10^{-2}$, $1.21 \times 10^{-2}$
- Half Life of $k$: $0.57 \times 10^{-2}$
- Biodegradation Rate Constant, $k$: $1.12 \times 10^{-2}$, $0.67 \times 10^{-2}$
- Half Life of $k$: $1.63 \times 10^{-2}$
- Ratio of $k$: $0.59 \times 10^{-2}$, $0.56 \times 10^{-2}$

4. 1-D Temporal/Spatial Prediction with Bear Equation (1979): Transient Plug flow model with a longitudinal dispersion

<table>
<thead>
<tr>
<th>Location of a Receptor</th>
<th>Predicted Concentration, ug/L</th>
<th>Calculation of Target Source Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>x-direction, ft</td>
<td>@ Avg Slope</td>
<td>@ Lower Boundary Slope (85% C.L.)</td>
</tr>
<tr>
<td>y-direction, ft</td>
<td>200</td>
<td>15</td>
</tr>
<tr>
<td>Simulation Time, yr</td>
<td>14</td>
<td>202.8, 694.2</td>
</tr>
</tbody>
</table>

**Prediction as a function of simulation time at a receptor's location given above**

**Prediction as a function of x-distance at a simulation time given above (@ y=0)**
Module 6: Calculation of Target Source Mass and Restoration

1. Input data used for this Module

<table>
<thead>
<tr>
<th>Hazardous Substance</th>
<th>Release, kg</th>
</tr>
</thead>
<tbody>
<tr>
<td>Current Source Mass</td>
<td>100</td>
</tr>
<tr>
<td>Source Release time, yr</td>
<td>3</td>
</tr>
<tr>
<td>Seepage Velocity, V_s, D/yr</td>
<td>113.91</td>
</tr>
<tr>
<td>Longitudinal Dispersion, ( \alpha_x ), ft</td>
<td>13.45</td>
</tr>
<tr>
<td>Transverse Dispersion, ( \alpha_y ), ft</td>
<td>1.35</td>
</tr>
<tr>
<td>Retardation Factor, R</td>
<td>2.054</td>
</tr>
<tr>
<td>Biodegradation Rate Constant, ( \lambda ), yr(^{-1} )</td>
<td>0.027</td>
</tr>
</tbody>
</table>

2. Enter Decision Criteria

| Simulation Start time, yr | 0.001 |
| Simulation End time, yr  | 30    |
| Target Level at receptors, mg/L | 100   |

3. Temporal Prediction at a Receptor (at z=0)

<table>
<thead>
<tr>
<th>Location of Receptor</th>
<th>Type of Model Used</th>
<th>Half Time to reach the steady-state, yr</th>
<th>Predicted Concentration, mg/L</th>
<th>Time to reach the Target level without source removal, yr</th>
<th>Target Source information to reach target level (100 mg/L) and at Simulation End Time (50 yr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Receptor 1</td>
<td>x-direction, ft 50</td>
<td>No degradation</td>
<td>1.2</td>
<td>1925.2</td>
<td>42.0</td>
</tr>
<tr>
<td></td>
<td>y-direction, ft 30</td>
<td>1st Order Decay</td>
<td>1.0</td>
<td>1169.4</td>
<td>37.5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Instant Reaction</td>
<td>NA</td>
<td>0.0</td>
<td>NA</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Target mass: 79.5, Removal needed: 20.5</td>
</tr>
<tr>
<td>Receptor 2</td>
<td>x-direction, ft 20</td>
<td>No degradation</td>
<td>3.9</td>
<td>2440.2</td>
<td>44.2</td>
</tr>
<tr>
<td></td>
<td>y-direction, ft 20</td>
<td>1st Order Decay</td>
<td>3.1</td>
<td>333.1</td>
<td>26.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Instant Reaction</td>
<td>NA</td>
<td>0.0</td>
<td>NA</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Target mass: 65.0, Removal needed: 35.0</td>
</tr>
</tbody>
</table>

Location of Receptor #1 is 50 ft direction & 100 y direction, Location of Receptor #2 is 200 ft direction & 200 y direction

4. Temporal Spatial Prediction along Plume Centerline (at y & z = 0) with 1st-order Decay Model

Modelled Overall Plume Centerline Distance to evaluate, ft: 400
Modelled Overall Simulation Time to evaluate, year: 12

Temporal Prediction as a function of Time at Receptor Locations

Temporal and Spatial Prediction along Plume Centerline

<table>
<thead>
<tr>
<th>Distance along plume centerline x-direction (at y=0, z=0), ft</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
</tr>
<tr>
<td>100</td>
</tr>
<tr>
<td>200</td>
</tr>
<tr>
<td>300</td>
</tr>
<tr>
<td>400</td>
</tr>
<tr>
<td>500</td>
</tr>
</tbody>
</table>

Provisional Draft, June, 2014
5. MONITORING AND REMEDIATION OPTIMIZATION SYSTEM (MAROS)

Overview

Developed by GSI for the Air Force Center for Environmental Excellence (AFCEE), in accordance with the AFCEE Long Term Monitoring Optimization Guide.

Comprehensive site evaluation tool based on statistical methods applied to site-specific data that accounts for historical and current data as well as hydrogeologic factors (e.g., wells, seepage velocity), and potential receptors. Analyzes individual wells, plume with respect to spatial indicators and stability, and site optimization. Using database trend analysis, helps identify constituents of concern (CoC), significance of temporal trends, redundancy of data points (monitoring wells), adequate sampling frequency, and data gaps.

MAROS will conduct the following calculations:

- **Summary Statistics for Individual Wells**
  - Calculates the detection frequency, date range of data, maximum concentration, range of concentrations, and date of maximum result for up to 5 COCs for all wells
  - Summary Statistics using Kaplan-Meier Method: Mean, median standard deviation and percentiles for individual well data are calculated using the Kaplan-Meier method to account for datasets with a higher percentage of non-detect (ND) data
  - Outliers for Individual Wells: uses Dixon’s method to identify high or low outliers in a dataset
  - Data Distribution: MAROS Uses the Shapiro-Wilk method to identify individual well datasets that do not have Normal or Log-normal data distributions

- **Trend Analysis for Individual Wells**
  - Mann Kendall
  - Linear Regression

- **Data Sufficiency for Individual Wells**
  - Cleanup Status: Sequential T-Test and Student’s T-Test are used to determine if concentrations are statistically below the cleanup goal
  - Power Analysis: Estimates how many more samples may be required to demonstrate location is statistically below the cleanup level
  - Prioritizes well importance using a qualitative method based on individual well statistics and well monitoring objectives

- **Moment Analysis**
- Uses the full dataset to estimate moments and the Mann-Kendall trends of each metric.
- Total dissolved mass in the plume
- Center of mass: Coordinates of the center of mass
- Spread of mass about the center of the plume

- Evaluation of aggregate concentration trends for source area, tail and User-defined well groups

- Spatial/Temporal Optimization
  - Provides several qualitative and quantitative metrics for identifying redundant monitoring locations and for identifying areas of high uncertainty that may require more monitoring locations
  - Provides several qualitative and quantitative metrics for assessing appropriate sampling frequency for well networks
Advantages

- Comprehensive site analysis
- Incorporates hydrogeologic site data and potential receptors in analysis
- Recommendations for sampling optimization (potential for cost reduction)
- Recommendations for potential well locations (data gaps)
- EPA accepted data analysis tool for project decision support
- Uses real world coordinates in 2-D modeling components

Disadvantages

- Complex data requirements
- Time intensive
- Does not analyze geochemical/biodegradation components (work-around required)

Online/Freeware availability


Example Output
Mann Kendall Plot

Select a well and chemical below to graph. The concentration trend result in the box below reflects the chemical and well chosen to be graphed.

Select: 
- Well: MW-11
- Chemical: BENZENE

Graph Type
- Log
- Linear

MK (S):
8.5

Confidence in Trend:
99.3%

COV:
0.51

MK Concentration Trend: I

Note: Increasing (I); Probably Increasing (PI); Stable (S); Probably Decreasing (PD); Decreasing (D); No Trend (NT); Not Applicable (N/A) - due to insufficient data.
Sources