Optimal Search Strategy for the Definition of a Dense Non-Aqueous Phase Liquid (DNAPL) Source

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Introduction

DNAAPL migration through the subsurface
Overall Research Objective

To develop, test and evaluate a computer assisted analysis algorithm to help the groundwater professional identify, at least cost, the location and magnitude of a DNAPL source.
Technical Approach

• The DNAPL source location is too small to identify via borings or geophysical methods.

• The plume emanating from a DNAPL source is typically quite large and easily discovered

➤ Employ plume water-quality information to find the DNAPL source
Strategy

1. Locate possible source locations
2. Create uncertain contaminant plume consistent with these locations and known geohydrology
3. Sample wells to reduce uncertainty in contaminant plume
4. Adjust sources to be consistent with resulting more certain plume
5. Repeat 2-4 until converge to unique source location(s)
Preparatory Work

1. Gather and interpret existing field information

2. Approximate source locations and associate each with an initial weight – Choquet integral

3. Construct and run groundwater flow and transport model of the site – Monte Carlo approach

4. Generate hydraulic conductivity field – Latin hypercube sampling
5. Calculate concentration field with uncertain source locations based on their newly calculated weights.

6. Update the plume with real data from previous steps or preexisting data - **Kalman filter**

7. Select optimal sampling point – **Minimum total variance strategy** (Kalman filter– Choquet integral)

8. Optimize source strength for each potential source location using initial weights – **Simplex method**

9. Recalculate concentration field with uncertain source locations using initial weights and new strengths

10. Update new concentration field with measurement data – **Kalman filter**

11. Compare with individual plumes and obtain new weights – **α-cuts method**

Source weights stabilize? Yes → **Optimal source selected**

No → Search Algorithm
1. Gather and interpret existing field information

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Source weights stabilize? 

- yes → Optimal source selected
- no → Repeat from step 5

Examples
Initial Weighting of Potential Source Locations

Information fusion–Choquet Integral

3 identifying features of the source:
- proximity to a manufacturing facility (A)
- proximity to a waste dump (B)
- distance to the water table from the ground surface (C)

membership function capturing the meaning of “near”

membership degree (score)
## Distances and Scores

<table>
<thead>
<tr>
<th>Source no.</th>
<th>Dist. from facility (m)</th>
<th>Dist. from dump (m)</th>
<th>Dist. to water table (m)</th>
<th>Membership Scores</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>σ(A)</td>
</tr>
<tr>
<td>1</td>
<td>79</td>
<td>25</td>
<td>10.75</td>
<td>0.61</td>
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<tr>
<td>2</td>
<td>55.9</td>
<td>35.3</td>
<td>10.75</td>
<td>0.81</td>
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<tr>
<td>3</td>
<td>35.3</td>
<td>55.9</td>
<td>10.75</td>
<td>0.99</td>
</tr>
<tr>
<td>4</td>
<td>25</td>
<td>79</td>
<td>10.75</td>
<td>1</td>
</tr>
<tr>
<td>5</td>
<td>35.3</td>
<td>103</td>
<td>10.75</td>
<td>0.99</td>
</tr>
<tr>
<td>6</td>
<td>55.9</td>
<td>127.5</td>
<td>10.75</td>
<td>0.81</td>
</tr>
</tbody>
</table>
Monotone Measures

- **Monotone measures** provided by expert
- **Importance** of each individual feature and all groups of features (thereby capturing their interaction)

In our case the expert defined the 6 monotone measures as follows:

\[
\mu(A) = 0.3, \quad \mu(B) = 0.5, \quad \mu(C) = 0.2 \\
\mu(A, B) = 0.7, \quad \mu(A, C) = 0.7, \quad \mu(B, C) = 0.8 \\
\mu(A, B, C) = 1, \quad \mu(\phi) = 0
\]
All individual scores are combined and a global degree of confidence of the statement:

‘source location \(i\) belongs to the group of true source locations’

is assigned to each possible source location.

For source location 1 we have:

\[
\sigma(A) = 0.61, \quad \sigma(B) = 1, \quad \sigma(C) = 0.84 \\
\sigma_1(A) = 0.61 < \sigma_2(C) = 0.84 < \sigma_3(B) = 1
\]

Choquet integral calculation:

\[
h(\sigma_1, \sigma_2, \sigma_3) = \sum_{i=1}^{3} (\sigma_i - \sigma_{i-1}) \mu(\{x_i, ..., x_3\})
\]

\[
h = \sigma_1 \mu(A, C, B) + (\sigma_2 - \sigma_1) \mu(C, B) + (\sigma_3 - \sigma_2) \mu(B)
\]

\[
h = 0.61 \cdot 1 + (0.84 - 0.61)0.8 + (1 - 0.84)0.5
\]

\[
h(0.61, 0.84, 1) = 0.874
\]
Summary of Results for the Initial Weights

<table>
<thead>
<tr>
<th>Source</th>
<th>Score for facility</th>
<th>Score for waste dump</th>
<th>Score for water table</th>
<th>Global weight</th>
<th>Stand. Global weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source 1</td>
<td>0.61</td>
<td>1</td>
<td>0.84</td>
<td>0.874</td>
<td>0.96</td>
</tr>
<tr>
<td>Source 2</td>
<td>0.81</td>
<td>0.99</td>
<td>0.84</td>
<td>0.915</td>
<td>1</td>
</tr>
<tr>
<td>Source 3</td>
<td>0.99</td>
<td>0.81</td>
<td>0.84</td>
<td>0.876</td>
<td>0.96</td>
</tr>
<tr>
<td>Source 4</td>
<td>1</td>
<td>0.61</td>
<td>0.84</td>
<td>0.819</td>
<td>0.89</td>
</tr>
<tr>
<td>Source 5</td>
<td>0.99</td>
<td>0.40</td>
<td>0.84</td>
<td>0.753</td>
<td>0.82</td>
</tr>
<tr>
<td>Source 6</td>
<td>0.81</td>
<td>0.19</td>
<td>0.84</td>
<td>0.630</td>
<td>0.69</td>
</tr>
</tbody>
</table>
Latin Hypercube Sampling Strategy

- Stratified sampling
- pdf is divided into an equally probable number of non-overlapping intervals
- Samples are taken from each area
- Samples permuted such that the correlation of the field is accurately represented.

Assumptions

- Lognormal distribution of hydraulic conductivity (K)
- Statistics of K (mean, variance, covariance) assumed known

Back to flow diagram
Monte Carlo Groundwater Flow and Transport Simulation

- Employ Latin Hypercube Sampling to obtain realizations of the random hydraulic conductivity field.
- Use each realization as hydraulic conductivity input for the groundwater flow and transport model.
- Obtain the random contaminant concentration field.
- Calculate the statistics (mean and covariance matrix) of the concentration field which are going to be used as prior estimates for the Kalman filter.

Back to flow diagram
1) Update the simulated concentration field (mean and covariance matrix from Monte Carlo) using the real data at the optimal sampling locations.

2) Strategy reveals where to take a sample

The Kalman Filter obtains linear, minimum-variance, unbiased estimates for the state of a system from noisy data.
Kalman Filter Updating Equations

Update concentration at location \( i \)

\[
c^+(i) = c^-(i) + \frac{\text{Cov}^{-}(i,m)}{\text{Cov}^{-}(m,m) + \text{error}} \left[ z(m) - c^-(m) \right]
\]

- prior concentration
- estimate at location \( i \)
- measurement at location \( m \)
- Prior estimate at location \( m \)

Update covariance at location \( i, j \)

\[
\text{Cov}^+(i, j) = \text{Cov}^{-}(i, j) + \frac{\text{Cov}^{-}(i,m)\text{Cov}^{-}(m, j)}{\text{Cov}^{-}(m,m) + \text{error}}
\]

- prior covariance
- estimate at \( i, j \)

Back to flow diagram
Optimal Sampling Point Selection

Reduction in overall **uncertainty** of the field (*Kalman filter*)

**Proximity** to the source (high concentration)

**Choquet Integral**

Optimal sampling point selected

Back to flow diagram
Source Strength Optimization for Bias Correction

\[
\min \sum_{i} |c_{i} - z_{i}|
\]

s.t

\[
c_{i} = \sum_{j=1}^{k} w_{j} \frac{\partial c_{i}}{\partial m_{j}} m_{j} \quad i = 1, \ldots, n
\]

\[
m_{j} \leq m^{*} \quad j = 1, \ldots, k
\]

where:

- \(c_{i}\) : model concentration at sampling location \(i\)
- \(z_{i}\) : measured concentration at sampling location \(i\)
- \(w_{j}\) : weight associated with potential source location \(j\)
- \(m_{j}\) : source magnitude (strength) at potential source location \(j\)
- \(m^{*}\) : solubility limit for contaminant of interest
- \(n\) : total number of locations where samples have been taken
- \(k\) : total number of potential source locations

Response matrix technique

Back to flow diagram
• Plumes represented as fuzzy sets with membership functions defined as normalized concentration values.
• Several $\alpha$-cuts of the fuzzy sets are considered.

An $\alpha$-cut is a crisp set that contains all the elements of a fuzzy set whose membership degrees are greater or equal to the specified value of $\alpha$. 
Comparison of Plumes

- $\alpha$-cut for the updated plume (dashed line)
- $\alpha$-cut of the individual plume (solid line)
- Record common area $N_i$ (purple area)
- Weight each common area by the $\alpha$ value itself
- Sum to obtain global degree ($g$) of similarity

$$g = \sum_{i} \alpha_i N_i, \quad i = 0.1, 0.2, \ldots, 1$$

- Emphasize intersection of plumes
- Weight higher concentration values more

**Note:** The resulting weights determine how many times the particular source will be included in the Monte Carlo simulations.

Back to flow diagram
Search Algorithm Application

• **Synthetic examples (Source strength assumed known)**
  – Single source in 2-D aquifer
  – Pumping well
  – 2 sources
  – 3-D aquifer
  – Larger source targets
  – Sensitivity analysis

• **Field application (Source strength unknown)**
Synthetic Aquifer Example
Larger Source Targets

- 2-D aquifer
- 4 potential source blocks consisting of 4 nodes each
- True source belongs in block No 3 (1 out of 4 nodes)
- 60 potential sampling locations
- True source found after taking 9 samples
Simulated plume

Initial weights
Updated plume

Updated weights

Updated weights

Updated weights
Updated plume

Updated weights
Field Application

Anniston Army Depot (ANAD) location

SWMU 12 location and model domain
Site Background

SWMU 12 - Industrial waste lagoons
- abrasive dust, petroleum hydrocarbons, solvents (TCE), etc
- Used from 1960 to 1978
- emptied in 1978
- in situ chemical oxidation in 1997
Groundwater Flow and Transport Model

3 geologic layers
- Residuum
  $K = 0.028 \text{ ft/day}$
- Weathered bedrock
  $K = 0.15-850 \text{ ft/day}$
- Unweathered bedrock
  $K = 6 \text{ ft/day}$

6 numerical layers
## Groundwater Flow and Transport Model

<table>
<thead>
<tr>
<th>Well</th>
<th>PTC Layer</th>
<th>Average TCE concentration (μg/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Residuum Interval</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>02-CGW-U01</td>
<td>5</td>
<td>0.61</td>
</tr>
<tr>
<td>88EWLF-3</td>
<td>5</td>
<td>0.53</td>
</tr>
<tr>
<td>SWMU 1201</td>
<td>5</td>
<td>129,580</td>
</tr>
<tr>
<td><strong>Weathered Bedrock Interval</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>82B13</td>
<td>4</td>
<td>2.6</td>
</tr>
<tr>
<td>83B17</td>
<td>4</td>
<td>1.47</td>
</tr>
<tr>
<td>95-GOU-B01</td>
<td>4</td>
<td>0.66</td>
</tr>
<tr>
<td>88EWLF-2</td>
<td>3</td>
<td>155</td>
</tr>
<tr>
<td>02-TEW-B01</td>
<td>2</td>
<td>820</td>
</tr>
<tr>
<td>83B23</td>
<td>2</td>
<td>0.59</td>
</tr>
<tr>
<td>83B01</td>
<td>2</td>
<td>3.83</td>
</tr>
</tbody>
</table>

Not used
Boundary Conditions

- Natural boundaries are far removed from the area.
- Artificial constant head boundary conditions are used that match field data and can satisfy the horizontal flow of the aquifer.
- Vertical gradient: 0.04 ft/ft in the residuum and 0.004 ft/ft in the weathered and unweathered bedrock.
- Recharge: 3 in/year
Hydraulic Conductivity \((K_x, K_y)\) of Weathered Bedrock

Auto-calibration using 7 target water levels
Hydraulic Conductivity ($K_x, K_y$) of Weathered Bedrock
Variogram Analysis

964 mean values (that correspond to the finite element nodes) were used to create the variogram

Exponential model variogram

- Nugget = 1.06
- Sill = 14.5
- Range = 900 ft
964 mean values (that correspond to the finite element nodes) were used to create the variogram.

Variogram Analysis

- **Range = 300 ft**
- **Sill = 0.32**
- **Nugget = 0.032**
K Realizations

- The variogram and mean values were used as input to the Latin hypercube sampling strategy in order to create 300 hydraulic conductivity realizations (needed for the Monte Carlo simulation).
- These realizations capture the spatial correlation of the field as modeled with the variogram
Flow Model Results

**Colored contours:**
Monte Carlo simulation hydraulic head results.

**Black contours:**
Potentiometric map created by hydrogeologist using well water level measurements.
Potential DNAPL Source Locations

• Each block represents a potential DNAPL source location.

• Potential source locations are defined in both the *residuum* and *weathered bedrock* layers.

![Diagram showing potential DNAPL source locations](image)
Initial Weighting of Possible Source Locations

3 important features

- Distance from SWMU 12 borders
- Distance from high soil concentration locations
- Nearness to average TCE contour $> 10,000 \mu g/L$
Distance from SWMU 12 Borders

Membership function for "close" to SWMU 12 boundary
High Soil Concentration Locations

Membership function for "close" to high soil concentration locations

![Graph showing membership function for close to high soil concentration locations.](image)
Average TCE Contour > 10,000μg/L

Membership function for “close” to the average TCE contour > 10,000 μg/L
# Initial Weights

<table>
<thead>
<tr>
<th>distance (ft)</th>
<th>membership degree</th>
<th>distance (ft)</th>
<th>membership degree</th>
<th>membership degree</th>
<th>Global score</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>138.6</td>
<td>0.614</td>
<td>283.8</td>
<td>0.330</td>
<td>0.614</td>
</tr>
<tr>
<td>2</td>
<td>100</td>
<td>1</td>
<td>118.8</td>
<td>0.4684</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>138.6</td>
<td>0.614</td>
<td>138.6</td>
<td>0.3298</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>100</td>
<td>1</td>
<td>138.6</td>
<td>0.3298</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>0</td>
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<td>26.4</td>
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<td>1</td>
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<tr>
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</tr>
<tr>
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</tr>
<tr>
<td>8</td>
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<td>0</td>
<td>1</td>
<td>1</td>
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<td>100</td>
<td>1</td>
<td>99</td>
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<td>1</td>
</tr>
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<td>100</td>
<td>1</td>
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<td>0.0988</td>
<td>0</td>
</tr>
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<td>0.4222</td>
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<td>0.1912</td>
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<tr>
<td>13</td>
<td>138.6</td>
<td>0.614</td>
<td>330</td>
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<td>14</td>
<td>100</td>
<td>1</td>
<td>303.6</td>
<td>0</td>
<td>0</td>
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<tr>
<td>15</td>
<td>138.6</td>
<td>0.614</td>
<td>330</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
Potential Source Locations

- 3 potential source locations
- 7, 8 and 9
Search Algorithm Results

Individual source plumes with initial magnitudes (strengths)

Weathered Bedrock
Layer 3

Residuum
Layer 5
Search Algorithm Results

Weathered Bedrock - Layer 3

Residuum - Layer 5

Initial Weights

Initial Magnitudes (strength)

<table>
<thead>
<tr>
<th>Source</th>
<th>Source 1</th>
<th>Source 2</th>
<th>Source 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>W</td>
<td>50000</td>
<td>50000</td>
<td>50000</td>
</tr>
<tr>
<td>R</td>
<td>50000</td>
<td>50000</td>
<td>50000</td>
</tr>
</tbody>
</table>
Search Algorithm Results

Average TCE concentration (μg/L)

<table>
<thead>
<tr>
<th>Source</th>
<th>Weight</th>
<th>Magnitude</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source 1</td>
<td>0.0</td>
<td>3788.4</td>
</tr>
<tr>
<td>Source 2</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Source 3</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>
Search Algorithm Results

Weathered Bedrock - Layer 3

Residuum - Layer 5

Average TCE concentration (μg/L)

<table>
<thead>
<tr>
<th></th>
<th>Weathered Bedrock - Layer 3</th>
<th>Residuum - Layer 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source 1</td>
<td>3.83 W</td>
<td>820 W</td>
</tr>
<tr>
<td>Source 2</td>
<td>820 W</td>
<td></td>
</tr>
</tbody>
</table>

Weights

<table>
<thead>
<tr>
<th>Source</th>
<th>Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.0</td>
</tr>
<tr>
<td>2</td>
<td>0.0</td>
</tr>
<tr>
<td>3</td>
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Magnitudes

<table>
<thead>
<tr>
<th>Source</th>
<th>Weight (W)</th>
<th>Magnitude (W)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source 1</td>
<td>0.0</td>
<td>3598.9</td>
</tr>
<tr>
<td>Source 2</td>
<td>0.0</td>
<td>214.8</td>
</tr>
<tr>
<td>Source 3</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>
Search Algorithm Results

Average TCE concentration (μg/L)

<table>
<thead>
<tr>
<th></th>
<th>Source 1</th>
<th>Source 2</th>
<th>Source 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>W</td>
<td>0.0</td>
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<td>0.0</td>
</tr>
<tr>
<td>R</td>
<td>1100000</td>
<td>747609</td>
<td>224599</td>
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</tbody>
</table>
Search Algorithm Results

<table>
<thead>
<tr>
<th>Average TCE concentration (μg/L)</th>
<th>Weathered Bedrock - Layer 3</th>
<th>Residuum - Layer 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>820 W</td>
<td><img src="Weathered_Bedrock.png" alt="Graph" /></td>
<td><img src="Residuum.png" alt="Graph" /></td>
</tr>
<tr>
<td>3.83 W</td>
<td></td>
<td></td>
</tr>
<tr>
<td>155 W</td>
<td></td>
<td></td>
</tr>
<tr>
<td>129,580 R</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Weights

![Bar Graph](Weights.png)

Magnitudes

<table>
<thead>
<tr>
<th>Source 1</th>
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<tr>
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<td>1100000</td>
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Search Algorithm Results

Average TCE concentration (μg/L)

<table>
<thead>
<tr>
<th></th>
<th>820 W</th>
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<th>129,580 R</th>
<th>2.6 W</th>
</tr>
</thead>
</table>

Weathered Bedrock - Layer 3

Residuum - Layer 5

Weights

Magnitudes

<table>
<thead>
<tr>
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<td>0.0</td>
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</table>
Search Algorithm Results

### Average TCE concentration (μg/L)

<table>
<thead>
<tr>
<th>Source</th>
<th>Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weathered Bedrock - Layer 3</td>
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</tr>
<tr>
<td>Residuum - Layer 5</td>
<td>2.6 W</td>
</tr>
<tr>
<td></td>
<td>0.53 R</td>
</tr>
</tbody>
</table>

### Weathered Bedrock - Layer 3

#### Weights

<table>
<thead>
<tr>
<th>Source</th>
<th>Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source 1</td>
<td>0.0</td>
</tr>
<tr>
<td>Source 2</td>
<td>0.0</td>
</tr>
<tr>
<td>Source 3</td>
<td>0.0</td>
</tr>
</tbody>
</table>

### Residuum - Layer 5

#### Magnitudes

<table>
<thead>
<tr>
<th>Source</th>
<th>Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source 1</td>
<td>1100000</td>
</tr>
<tr>
<td>Source 2</td>
<td>1100000</td>
</tr>
<tr>
<td>Source 3</td>
<td>0.0</td>
</tr>
</tbody>
</table>
Search Algorithm Results

**Average TCE concentration (μg/L)**
- 820 W
- 3.83 W
- 155 W
- 129,580 R
- 2.6 W
- 0.53 R
- 0.66 W

**Weights**

**Magnitudes**

<table>
<thead>
<tr>
<th></th>
<th>Source 1</th>
<th>Source 2</th>
<th>Source 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>W</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>R</td>
<td>0.0</td>
<td>1100000</td>
<td>1100000</td>
</tr>
</tbody>
</table>
Search Algorithm Results

Average TCE concentration (μg/L)

<table>
<thead>
<tr>
<th>Source</th>
<th>Magnitude</th>
</tr>
</thead>
<tbody>
<tr>
<td>W</td>
<td>0.0</td>
</tr>
<tr>
<td>R</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Weathered Bedrock - Layer 3

Residuum - Layer 5

Weights

Magnitudes

<table>
<thead>
<tr>
<th>Source</th>
<th>Source 2</th>
<th>Source 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>W</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>R</td>
<td>0.0</td>
<td>1100000</td>
</tr>
</tbody>
</table>
Search Algorithm Results

Average TCE concentration (μg/L)

- Weathered Bedrock - Layer 3:
  - Source 1: 129,580 R
  - Source 2: 243100
  - Source 3: 162100

- Residuum - Layer 5:
  - Source 1: 1100000
  - Source 2: 1100000

Weights and Magnitudes:

<table>
<thead>
<tr>
<th>Source</th>
<th>W</th>
<th>R</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>2</td>
<td>0.0</td>
<td>1100000</td>
</tr>
<tr>
<td>3</td>
<td>0.0</td>
<td>1100000</td>
</tr>
</tbody>
</table>
True Source Location

- **Best estimate of true source location**: Entire SWMU 12 area (blocks 5, 8, 11) *(partially confirmed by algorithm – actual source area larger than identified, block 8)*

- Suspecting potential movement to the east of SWMU 12 *(confirmed by algorithm, block 9)*

- **Best estimate of DNAPL depth**: Residuum interval *(confirmed by algorithm)*

- Suspecting potential movement to the weathered bedrock interval *(not confirmed by algorithm)*
Conclusions

• Algorithm successful when tested using synthetic examples that represent various situations that can be encountered in the field.
• Field application results acceptable. Depth of DNAPL source confirmed, areal extend may have been underestimated…or may not have been.
The End