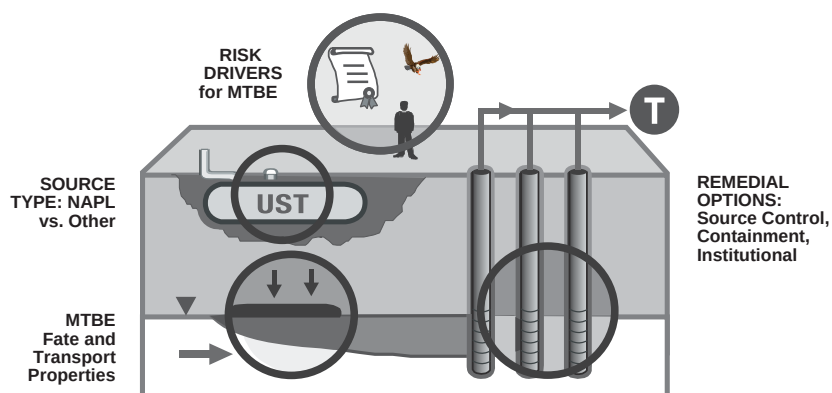


Groundwater Remediation Strategies Tool

Regulatory Analysis & Scientific Affairs Department

Publication Number 4730
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FORWARD

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ABSTRACT

This guide provides strategies for focusing remediation efforts on 1) the change in contaminant mass flux¹ in different subsurface transport compartments (e.g. the vadose zone, smear zone or a zone within an aquifer of interest) and 2) the change in remediation timeframe.

In this approach, groundwater flow and contaminant concentration data are combined to estimate the rate of contaminant mass transfer past user-selected transects across a contaminant plume. The method provides the user with a means to estimate the baseline mass flux and remediation timeframe for various transport compartments and then evaluate how different remedies reduce the mass flux and the remediation timeframe in each transport compartment.

Results from one or more transects can be used to evaluate:

- Potential water quality impacts on downgradient water supply wells.
- The natural attenuation of the contaminant mass with distance downgradient of the source.
- The relative benefits of remedies based on their anticipated reductions in mass flux from the source to the receptor.

In addition to step-by-step instructions for the strategies, several utilities are provided including:

- Worksheets for estimating baseline mass flux and remediation timeframe and evaluating potential remedies.
- Tools for calculating mass flux.
- Resources on estimating remediation lifetime and evaluating remedy flux reduction / mass removal factors.
- Tools for evaluating how long it takes for an upgradient remedial action to affect a downgradient groundwater transect zone.

¹ Strictly speaking, mass discharge

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1.0 INTRODUCTION - MASS FLUX APPROACH

Potential impacts on groundwater receptors and the need for and relative benefits of alternative remedial measures may be evaluated on the basis of the mass flux of contaminants from the source zone to the receptor. This mass-based approach to site assessment and remediation has been described by various researchers (Einarson & Mackay, 2001a,b; Gallagher et al, 1995) and identified by USEPA as a key consideration in the evaluation of natural attenuation remedies (USEPA, 1998).

Under this approach, groundwater flow and contaminant concentration data are combined to estimate the rate of contaminant mass transfer (e.g., grams per day) past selected transects through an affected groundwater plume. Strictly speaking, this is a mass discharge rate; however the term "mass flux" is typically used to describe mass discharge, and this convention will be used in this document.

Results from one or more such transects can then be used to evaluate: i) potential water quality impacts on downgradient supply wells (as determined from a mass balance analysis of the supply well pumping rate), ii) the natural attenuation of the contaminant mass with distance downgradient of the source (as defined by the reduction in mass flux between transects), and iii) the relative benefits of alternative remedies (based on their anticipated reductions in mass flux from source to receptor).

The Environmental Protection Agency's Natural Attenuation Seminar (USEPA, 1998) summarized the benefits of the mass flux approach to evaluate groundwater impacts:

"The reduction in the flux along the flowpath is the best estimate of natural attenuation of the plume as a whole."

"The flux is the best estimate of the amount of contaminant leaving the source area. This information would be needed to scale an active remedy if necessary."

"Flux estimate across the boundary to a receptor is the best estimate of loading to a receptor."

Pankow and Cherry (1996) state that:

"Therefore, the ultimate impact of plumes emanating from solvent DNAPL source zones can be evaluated in terms of the impact of relatively small annual mass fluxes to the receptor such as water-supply wells or surface waters. In some cases, the fluxes present significant risk to human health and/or the environment, and extensive remedial action is warranted. In other cases, the fluxes are insignificant, and remedial action would provide little or no actual environmental risk reduction."

In summary, the use of a mass flux approach is a powerful tool for risk management (Einarson and Mackay, 2001a), one that can be used to identify high-risk sites that require higher degrees of site investigation and corrective action. This is particularly true for MTBE, as it is attenuated less in the subsurface than other plume constituents from fuel releases at many sites.

1.1 Transport Compartments

Several researchers have identified how remediation efforts can focus on individual components of a release site. For example, Gallagher, et al. (1995) developed a "Mass-Based Corrective Action" approach where the masses in different "compartments" (soil, smear zone, and dissolved plume) were estimated and the cost per pound to remediate these masses was estimated. The concept of different transport compartments is well suited for the mass flux approach, and the conceptual remediation framework described in this document is based on evaluating the vadose zone, smear zone, and several "transect zones" in the dissolved plume.

1.2 Mass Flux and Remediation Timeframe

A logical extension of the mass flux approach is to use mass flux estimates with approximations of source masses to derive order-of-magnitude estimates of remediation timeframe. With this approach, remediation efforts can focus on the change in two key process variables:

- 1) The change in mass flux in different transport compartments;
- 2) The change in remediation timeframe.

Although estimating remediation timeframe involves considerable uncertainty, relative changes in remediation timeframe can be performed with some degree of accuracy. The conceptual remediation framework described in this document discusses methods to estimate source masses and remediation timeframes in different transport compartments.

1.3 Structure of This Document

This document expands on a mass flux framework originally proposed by Einarson and MacKay (2001a) and provides tools for evaluating mass flux at affected sites. While the framework can be used for any constituent, it was originally developed with a focus on MTBE releases from petroleum release sites.

This expanded mass flux framework consists of the following elements:

- Groundwater Remediation Process Flowchart (Section 2, Figure 1);
- Baseline Mass Flux and Remediation Timeframe Tool (Section 2, Worksheet 1);
- Remediation Evaluation Tool Using Mass Flux and Remediation Timeframe (Section 2, Worksheet 2);
- Mass Flux Calculation Tools (Section 3);
- Remediation Timeframe Tools (Section 4);
- Resources for Evaluating Mass Flux and Mass Reduction Factors (Section 5);
- Tools for Evaluating Changes in Groundwater Mass Flux after Remediation (Section 6 and Appendix A); and
- Method Examples (Appendix B).

1.4 Key Definitions

Action Level: Typically a concentration-based standard in either groundwater, water being extracted from a water-supply well, or a surface water quality standard.

Blending: The mixing and dilution of mass flux in either: i) a water supply well that pumps both clean water and groundwater containing a site constituent; or ii) a stream that mixes constituents in groundwater with clean surface water.

Control Point: Under a mass flux-based approach, the point where the mass flux of the constituent is to be managed. Examples include the intake of a well downgradient of a plume, or at the discharge point to a surface water body.

Flow Area: The segmented area associated with a specific concentration measurement over which an individual mass flux estimate is calculated.

Groundwater Transect Zone: The zone between two groundwater transects drawn across the dissolved constituent plume.

Mass Flux: The mass per time moving across a control area in a transport compartment in units of mass per time. This is also called the mass flowrate or the mass discharge rate. Note that some researchers refer to mass flux in units of mass per area per time. For this document, mass flux is used in a more general manner to mean mass per time crossing a transect. In this document, mass flux is represented by the symbol w .

Source Zone: The zone that includes both the affected soils in the vadose zone and the smear zone.

Transport Compartment: Either the vadose zone, smear zone, or a transect zone that has a constituent mass flux associated with it.

Variables Used in Worksheets 1 and 2: Variables used in Worksheets 1 and 2 take the form:

A_BC

Where:

- **A** indicates the parameter represented, either the **mass flux (w)**, the **timeframe (t)**, the **flux reduction factor (rw)**, or the **concentration (C)**;
- **B** indicates the chronology of the parameter, indicating its occurrence either before remediation, as a **baseline (b)**, or **after remediation (ar)**; and
- **C** indicates the transport compartment, occurring at the **vadose zone (vd)**, the **smear zone (sm)**, the **total source zone (ts)**, at one of four **groundwater transects (gw-1, gw-2, gw-3, and gw-4)**, at the **control point (cp)**, or at the **point-of-use (pou)**.

2.0 GENERAL GROUNDWATER REMEDIATION PROCESS (FLOWCHART 1)

This groundwater remediation process works by estimating the baseline mass flux and remediation timeframe for various transport compartments, and then evaluating how different remedies reduce the mass flux and remediation timeframe in each transport compartment. The effects of an upgradient remedial action (such as remediating the vadose zone) on downgradient transport compartments is also considered. The general remediation process is shown in Figure 1.

2.1 Preliminary and Detailed Site Characterization

First, a preliminary site assessment is performed. If an action level is exceeded, then a detailed site assessment is conducted. It is recommended that characterization of MTBE sites be conducted using the methods presented in "Strategies for Characterizing Subsurface Releases of Gasoline Containing MTBE" (Nichols et al., 2000) (see box below). This document provides instructions on how to use risk-based decision making in the site characterization process.

Excerpt from "Strategies for Characterizing Subsurface Releases of Gasoline Containing MTBE" (Nichols et al., 2000, www.api.org):

Risk-informed decision making is a management strategy that adds exposure and risk considerations to the traditional technical, social, and economic components of the corrective action process. The risk-informed approach presented in this bulletin uses site-specific risk factors to help determine the appropriate level of assessment at oxygenate release sites. It includes a review of the various risk factors associated with oxygenate sources, pathways, and receptors. Based on these factors, three levels of assessment are recognized. The standard level is appropriate for the greatest number of sites: it includes moderate sample spacing with some vertical characterization, as well as horizontal characterization. The limited level is appropriate at sites with fewer risk factors: it includes relatively large sample spacing with emphasis on horizontal characterization. The detailed level is warranted for sites with the most risk factors: it requires the highest level of effort for each characterization task, with relatively close sample spacing, and extensive vertical characterization of chemical concentrations and hydraulic properties.

The appropriate level of assessment is initially determined based on receptor information, since receptor data are typically

easier to obtain than source or pathway data.

Detailed information about receptors can normally be obtained from a survey of nearby wells and land uses. Receptor characterization should consider current uses and probable future uses of affected groundwater. Once receptors are characterized and an initial level of effort is established, a subsurface investigation may then be conducted to obtain detailed information about sources and pathways. The source and pathway data should be carefully reviewed as it is collected, and the level of assessment should be "upgraded" or "downgraded" accordingly. This bulletin includes a detailed overview of the tools and techniques used in the field for source and pathway characterization and subsequent monitoring at oxygenate release sites. Since traditional assessment approaches have been addressed in previous API publications, this bulletin focuses on newer technologies that allow rapid collection and field analysis of soil, soil-gas, and groundwater samples. The bulletin includes a review of the expedited site assessment process, which is particularly well suited for oxygenate assessment. It also provides a comprehensive guide to modern direct-push assessment and monitoring tools, with emphasis on their proper use at MTBE-affected sites.

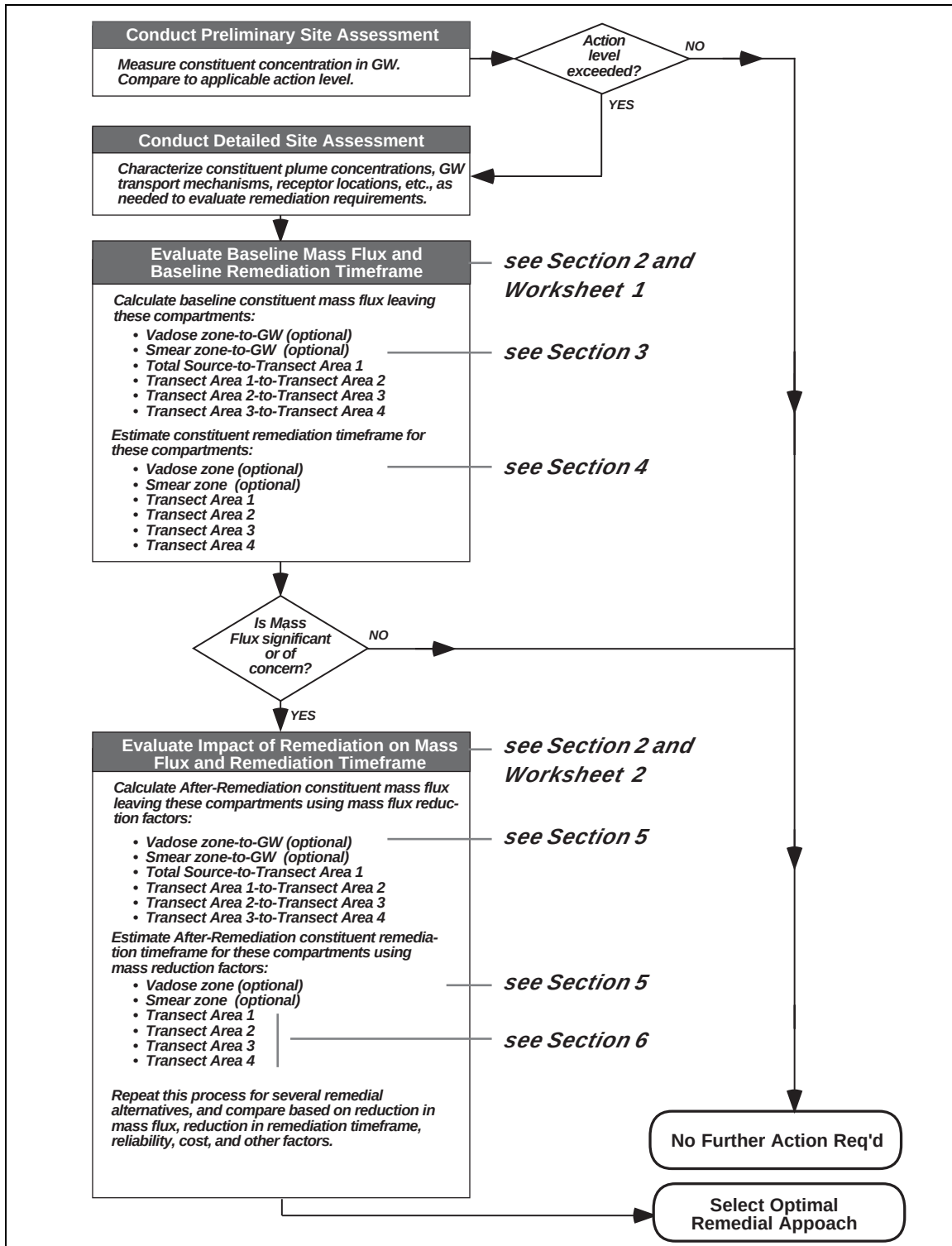


Figure 1. Groundwater Remediation Process Flowchart

2.2 Baseline Mass Flux and Remediation Timeframe Evaluation Tool (Worksheet 1)

This strategy is founded upon an analysis of constituent mass fluxes and remediation timeframes.

Baseline Mass Flux - Worksheet 1

For the baseline mass flux calculations (MFB), perform the following five steps and fill out Worksheet 1:

Step MFB-1. Calculate the Baseline Vadose Zone to Groundwater Mass Flux ($w_{b_{vd}}$) (Optional)

Using the methods and equations presented in Section 3, estimate the mass flux of the constituent leaving the vadose zone. Two main processes are typically considered: i) constituent leaving the vadose zone in recharge to water, and ii) constituent entering the groundwater via the diffusion of vapors.

Step MFB-2. Calculate the Baseline Total Source to Groundwater Mass Flux ($w_{b_{ts}}$)

Using the methods and equations presented in Section 3, estimate the mass flux of the constituent leaving the entire source zone (vadose zone plus smear zone). This is typically performed using data from the closest transect of monitoring wells located downgradient of the source zone.

Step MFB-3. Calculate the Baseline Smear Zone to Groundwater Mass Flux ($w_{b_{sm}}$) (Optional)

In most cases, the Smear Zone to Groundwater Mass Flux ($w_{b_{sm}}$) is calculated by subtracting the Baseline Vadose Zone to groundwater mass flux ($w_{b_{vd}}$) from the Baseline Total Source to Groundwater Mass Flux ($w_{b_{ts}}$), or

$$w_{b_{sm}} = w_{b_{ts}} - w_{b_{vd}}$$

Step MFB-4. Calculate the Transect Zone Mass Fluxes ($w_{b_{gw-1}}$ to $w_{b_{gw-4}}$)

Using the methods and equations presented in Section 3, estimate the mass flux of the constituent leaving the first transect zone ($w_{b_{gw-1}}$) (the portion of the constituent plume that extends from the source zone transect; i.e., the transect used to calculate the Total Source to Groundwater flux and the next downgradient transect line).

This step is repeated for each successive downgradient Transect Zone. Although Worksheet 1 only allows a maximum of 4 Transect Zones, more can be used for an individual site by tallying the results on a separate page.

Step MFB-5. Calculate the Baseline Control Point Concentration ($C_{b_{cp}}$)

Using the methods and equations presented in Section 3, determine the concentration at the control point due to blending. When an extraction well is the control point, this concentration is equal to the mass flux divided by the pumping rate of the well. When a stream is the control point, this concentration is equal to the mass flux divided by a representative low flow flowrate of the stream.

Baseline Natural Attenuation Timeframe - Worksheet 1

For the baseline remediation timeframe calculations (RTB), perform the following four steps and fill out Worksheet 1:

Step RTB-1. Estimate the Vadose Zone Natural Attenuation Timeframe ($t_{b_{vd}}$) (Optional)

Using the methods and equations presented in Section 4, estimate how long the constituent source will persist if no active remediation is performed.

Step RTB-2. Estimate the Smear Zone Natural Attenuation Timeframe ($t_{b_{sm}}$) (Optional)

Using the methods and equations presented in Section 4, estimate how long the constituent in the smear zone will persist if no active remediation is performed.

Step RTB-3. Estimate the Total Source Zone Natural Attenuation Timeframe ($t_{b_{ts}}$) (Optional)

Use the maximum value for $t_{b_{vd}}$ and $t_{b_{sm}}$.

Step RTB-4. Calculate the Transect Zone Natural Attenuation Timeframe ($t_{b_{gw-1}}$ through $t_{b_{gw-4}}$)

Estimate the travel time from the source to the transect (divide distance from source to transect by seepage velocity and retardation factor) and add this number to the total source natural attenuation timeframe ($t_{b_{ts}}$) estimated in Step RTB-3. This will provide an order-of-magnitude approximation for how long natural attenuation alone could remediate the transect zones.

2.3 Remedy Evaluation Tool Using Mass Flux and Remediation Timeframe (Worksheet 2)

The remedy evaluation tool provides a framework for evaluating how a remedial action will reduce the mass flux at the control point, and how the remediation timeframe will be affected. A different Remedy Evaluation Tool (Worksheet 2) should be completed for every remedial alternative being considered. Successful remedial alternatives (i.e., ones that meet the required reduction in mass flux and remediation timeframe) should be compared against each other based on cost, reliability, and other factors to select the best remedial approach.

After-Remediation Mass Flux - Worksheet 2

For the after-remediation mass flux calculations (MFAR), perform the following five steps and fill out Worksheet 2:

Step MFAR-1. Calculate the After-Remediation Vadose Zone to Groundwater Mass Flux (w_{arvd}) (Optional)

Using the resources referenced in Section 5, estimate the Flux Reduction Factor for the Vadose Zone (rw_{vd}) that the proposed remedial alternative will achieve. For example, if soil vapor extraction (SVE) is being considered in a coarse sand, then a 90% reduction in the vadose zone MTBE mass flux could be expected (so that $rw_{vd} = 0.1$). However, if the remedial alternative is pump-and-treat, then the Flux Reduction Factor for the Vadose Zone would be 1.0 (no change). Flux reduction factors should reflect what can be achieved in a reasonable timeframe, such as 1-5 years.

Step MFAR-2. Calculate the After-Remediation Smear Zone to Groundwater Mass Flux ($w_{ar_{sm}}$) (Optional)

Using the resources referenced in Section 5, estimate the Flux Reduction Factor for the Smear Zone (rw_{sm}) that the proposed remedial alternative will achieve. For example, if LNAPL skimming is being considered, then a significant reduction in the smear zone mass flux would be used (such as $rw_{sm} = 0.50$ if the hydrogeologic conditions are appropriate for LNAPL skimming). However, if the remedial alternative is pump-and-treat in a low permeability water-bearing unit, then little reduction might be anticipated (such as $rw_{sm} = 0.90$). Flux reduction factors should reflect what can be achieved in a reasonable timeframe, such as 1-5 years.

Step MFAR-3. Calculate the After-Remediation Flux Reduction Factor for the Total Source Zone to Groundwater Mass Compartment (rw_{ts})

Add the after-remediation flux for the vadose zone (w_{arvd}) and the after-remediation flux for the smear zone ($w_{ar_{sm}}$) to get the after remediation flux for the total source-to-gw compartment ($w_{ar_{ts}}$). Then divide $w_{ar_{ts}}$ by the baseline total source-to-gw flux ($w_{b_{ts}}$) to get the total source-to-gw flux reduction factor (rw_{ts}). This flux reduction factor should reflect what can be achieved by remediation in a reasonable timeframe, such as 1-5 years.

Step MFAR-4. Calculate the After-Remediation Transect Zone Mass Fluxes ($w_{ar_{gw-1}}$ to $w_{ar_{gw-4}}$)

Using the resources referenced in Section 5, estimate the Flux Reduction Factor for the Transect Zones (rw_{gw-1} to rw_{gw-4}) that the proposed remedial alternative will achieve. Note that the flux reduction factors are cumulative; in other words upstream flux reduction factors are reflected in downgradient flux reduction factors by multiplying them together. The goal is to get the ultimate reduction in flux.

Step MFAR-5. Calculate the Baseline Control Point Concentration ($C_{ar_{cp}}$)

Using the resources referenced in Section 5, determine the Control Point Flux Reduction Factor (rw_{pou}) from any point-of-use remediation technology. Multiply this factor (if present) with all other Mass Flux reduction factors ($w_{ar_{ts}}$ and $w_{ar_{gw-1}}$ to $w_{ar_{gw-4}}$) to get the after-remediation mass flux to the well, and then divide by the control point flowrate to get the after-remediation control point concentration.

After-Remediation Remediation Timeframe - Worksheet 2

To evaluate the after-remediation remediation timeframe (RTAR) that the remedial technology is likely to achieve, perform the four following steps:

Step RTAR-1. Calculate the After-Remediation Vadose Zone Remediation Timeframe ($t_{ar_{vd}}$) (Optional)

Using the resources referenced in Section 5, estimate how long the source will persist if active remediation is performed.

Step RTAR-2. Calculate the After-Remediation Smear Zone Remediation Timeframe ($t_{ar_{sm}}$) (Optional)

Using the resources referenced in Section 5, estimate how long the smear zone will persist if active remediation is performed.

Step RTAR-3. Select Mass Flux Curve in Appendix A That Best Represents Source (Optional)

Using the results from Steps RTAR-1 and RTAR-2, choose either a decaying source or a step-function source that best represents the mass flux from the source during and after remediation. Refer to Section 6 and Appendix A for more information on how to make this selection.

Step RTAR-4. Estimate the Transect Zone Remediation Timeframes ($t_{ar_{gw-1}}$ to $t_{ar_{gw-4}}$)

Using the curve selected in Step RTAR-3, estimate how long it will take to remediate each transect zone.

When Worksheet 2 is completed, review the following information:

1. The after-remediation concentration at the control point ($C_{ar_{cp}}$) (See Step MFAR-5);
2. How long it will take to remediate each compartment (Steps RTAR-1 through RTAR-4).

Based on these factors, determine if a particular remediation alternative provides acceptable performance. If so, evaluate cost, implementability, and other factors to determine if the remediation alternative should be applied at the site.

3.0 TOOLS FOR CALCULATING MASS FLUX

The following pages contain sheets summarizing the major methods that can be used to calculate mass fluxes. These tools are provided:

- Section 3.1:** Groundwater Mass Flux Calculation - Transect Method
- Section 3.2:** Groundwater Mass Flux Calculation - Solute Transport Model Method
- Section 3.3:** Groundwater Mass Flux Calculation - Extraction Well Method
- Section 3.4:** Control Point Concentration Calculation
- Section 3.5:** Vadose Zone to Groundwater Mass Flux Calculation

3.1 Groundwater Mass Flux Calculation - Transect Method

Transect Method – Summary

FLUX TERM	GROUNDWATER MASS FLUX – TRANSECT METHOD	
Equation	$w = \sum_{i=1}^{i=n} C_i q_i A_i CF$ w = total mass flux from source zone (g/day) (also called mass discharge)	
Input Data	C_i = concentration of constituent at individual measurement point in transect (mg/L) q_i = specific discharge (also called Darcy velocity) through flow area associated with an individual measurement i (cm/sec). q_i can be calculated using: $q_i = K \cdot i \quad \text{where}$ K = hydraulic conductivity (cm/sec) i = hydraulic gradient (cm/cm) A_i = area associated with an individual measurement (ft²) CF = conversion factor = 80.3 (ft/cm)/(sec/day)(L/ft³)(g/mg)	
Typical Input Values	C_i = 0.001 mg/L to 10,000 mg/L (for MTBE) K (Clays) = $<1 \times 10^{-6}$ cm/s K (Silts) = 1×10^{-6} to 1×10^{-3} cm/sec K (Silty sands) = 1×10^{-5} to 1×10^{-3} cm/sec K (Clean sands) = 1×10^{-3} to 1 cm/sec K (Gravel) = > 1 cm/sec i = 0.0001 to 0.01 ft/ft A_i = 100 to 100,000 ft²	

How to Calculate / Example

Estimation of mass flux across one or more transects through an affected groundwater plume involves the following principal steps:

- 1. Characterize Plume Concentrations:** For each selected plume transect, sufficient groundwater sampling points must be available to define i) the full width and thickness of the plume and ii) the distribution of contaminant concentrations within the plume. Either single-level or multilevel groundwater monitoring points may be used for this purpose. Multilevel monitoring points can provide a more detailed three-dimensional characterization of contaminant concentrations in groundwater. However, single-level groundwater monitoring networks, while less accurate than multi-level networks, can still provide sufficient accuracy to support a mass flux analysis at many sites.

(NOTE: an alternative method is to use the concentrations from contour lines as measurement points. The locations where the transect intersects contour lines from plume maps can be used to construct flow areas for the mass flux calculations).

2. **Characterize Groundwater Flow:** To characterize the specific discharge (q) across each plume transect, representative measurements are required for both the hydraulic flow gradient (i) and the hydraulic conductivity (K) of the flow system (where $q = K \times i$). The groundwater flow direction and hydraulic gradient for each segment of a transect line can be determined from a potentiometric surface contour map based on static water level measurements of available sampling points. Representative measurements of the hydraulic conductivity of the groundwater-bearing unit should be obtained at one or more locations, using appropriate slug test or pumping test methods.
3. **Select Plume Transects:** To characterize mass flux, transects should be located at points where sufficient data are available to define affected groundwater concentrations and specific discharge, as defined in Steps 1 and 2 above. For two-dimensional data (i.e., from single-screen monitoring wells), the transect will represent a line extending across the full width of the plume, perpendicular to the direction of groundwater flow (see Figures 2 and 3). For uniform flow fields, this transect will be a straight line, but, for converging or diverging flowlines, the transect will be curvilinear in shape. For three-dimensional data (i.e., from multilevel monitoring wells), the transect line will represent a vertical plane through the groundwater plume, positioned perpendicular to groundwater flow (see Figures 4 and 5).

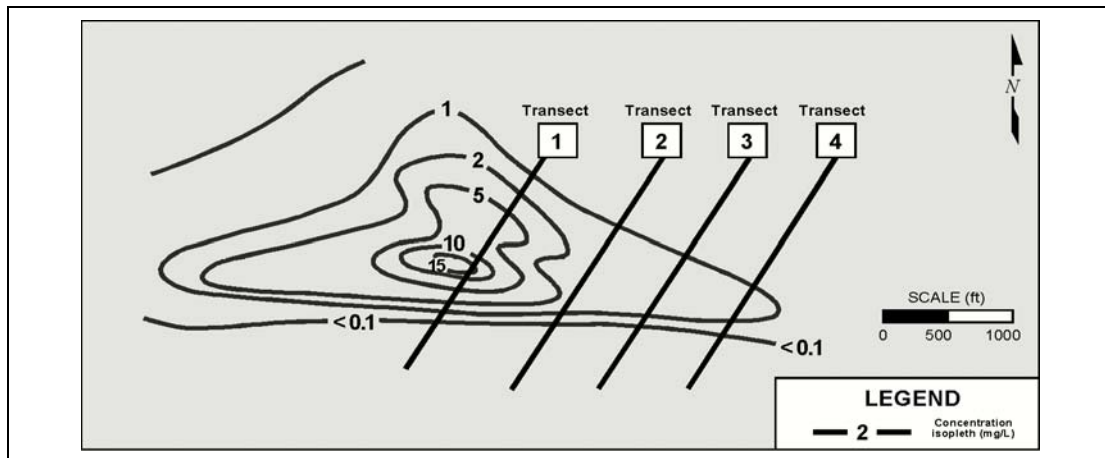


Figure 2. Example Transects through 2-D Plume Contour Map, Dover AFB, Delaware (Adapted from: Einarson, 2001)

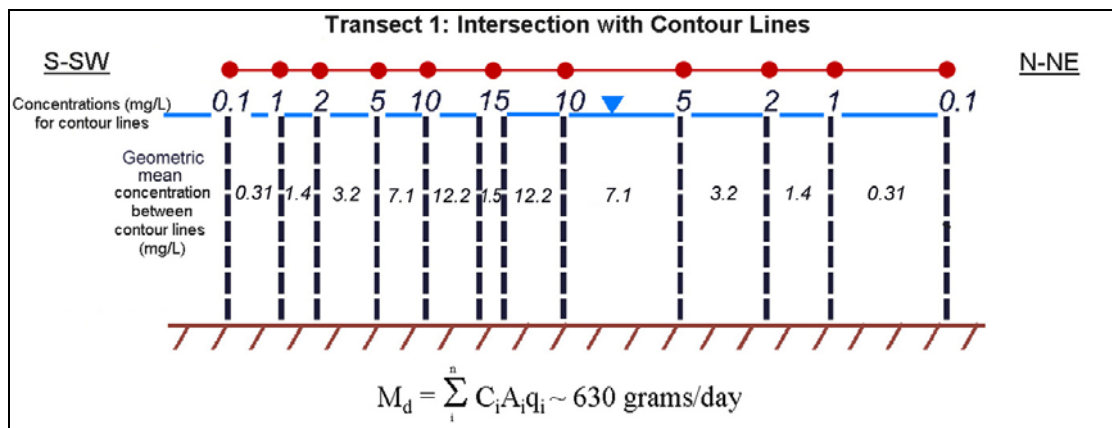


Figure 3. Concentration Profile for 2-D Transect No. 1 Based on Concentration Contours Shown in Figure 2 (Adapted from: Einarson, 2001)

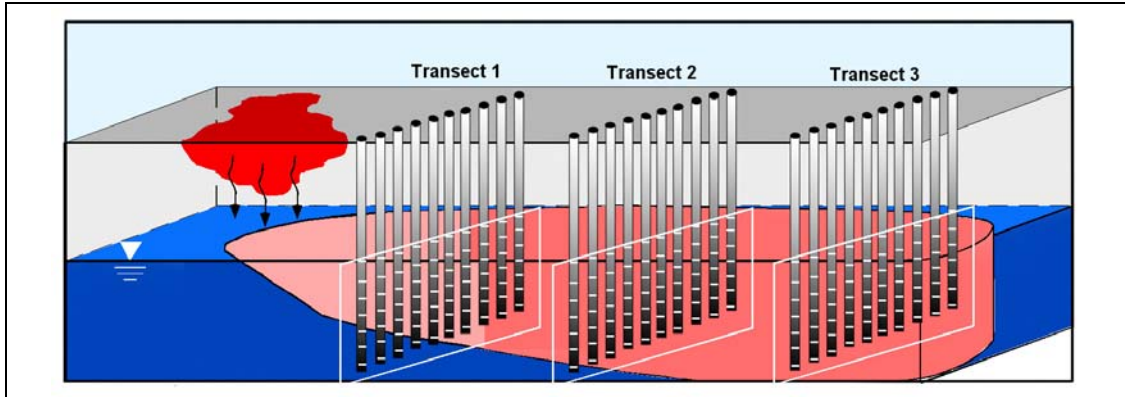


Figure 4. Example Transects through 3-D Plume Delineation

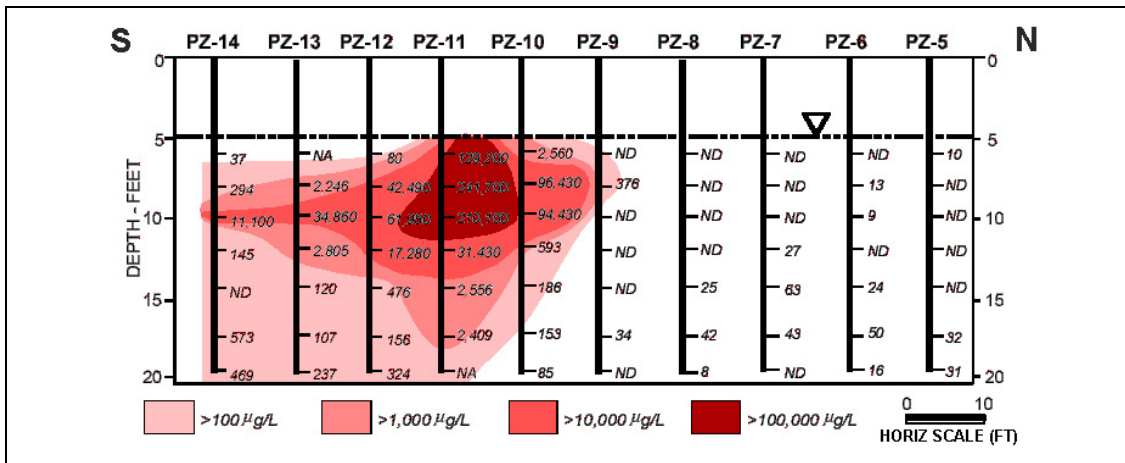


Figure 5. MTBE Concentration Profile for 3-D Transect No. 1 Shown in Figure 4
(Adapted from: Einarson, 2001)

4. **Subdivide Transects Into Subareas:** Each transect should be divided into subareas. Typically, each subarea represents a different concentration value. Two methods are commonly applied. For Method 1, subareas are divided to represent the area between concentration isopleths on a contour map of the plume. The concentration is assumed to be the geometric mean of the two contour values. For Method 2, sufficient monitoring points are located directly on the transect to construct transect subareas. The dividing line between subareas is typically halfway between the measurement points. In some cases, a combination of Method 1 and Method 2 can be applied. For three-dimensional transects, the transect plume should be subdivided into polygons bounded by contour data (Method 1) or centered on available measuring points (Method 2) (See Figures 4 and 5 for an example of Method 2).
5. **Calculate Cumulative Mass Flux Across Transect:** The total contaminant mass flux across the transect is calculated as follows:

$$w = \sum_{i=1}^{i=n} C_i q_i A_i CF$$

where:

- w = total mass flux from source zone (g/day) (also called mass discharge)
- C_i = concentration of constituent at flow area in transect (mg/L)
- q_i = specific discharge (also called Darcy velocity) through flow area associated with an individual constituent measurement i (cm/sec). q_i can be calculated using:

$$q_i = K \cdot i \quad \text{where:}$$

- K = hydraulic conductivity (cm/sec)
 i = hydraulic gradient (cm/cm)
 A_i = Flow area associated with an individual constituent measurement (ft²)
 CF = conversion factor = 80.3 (ft/cm)/(sec/day)(L/ft³)(g/mg)

For the two dimensional example, mass flux is calculated as:

	C_i (mg/L)	q_i (cm/sec)	Width of Transect (ft)	Thickness of Transect (ft)	A_i (ft ²)	w_i (g/day)
1	0.31	5.00E-05	8	15	120	0.15
2	1.4	5.00E-05	5	15	75	0.42
3	3.2	5.00E-05	10	15	150	1.93
4	7.1	5.00E-05	8	15	120	3.42
5	12.2	5.00E-05	9	15	135	6.61
6	15	5.00E-05	4	15	60	3.61
7	12.2	5.00E-05	9	15	135	6.61
8	7.1	5.00E-05	19	15	285	8.12
9	3.3	5.00E-05	14	15	210	2.70
10	1.4	5.00E-05	10	15	150	0.84
11	0.31	5.00E-05	19	15	285	0.35
TOTAL						34.8

Table 1. Mass Flux Calculation for 2-D Transect No. 1 (see Figure 3)
 (assumes $K = 0.1$ cm/sec, $i = 0.005$ ft/ft). (Adapted from: Einarson, 2001)

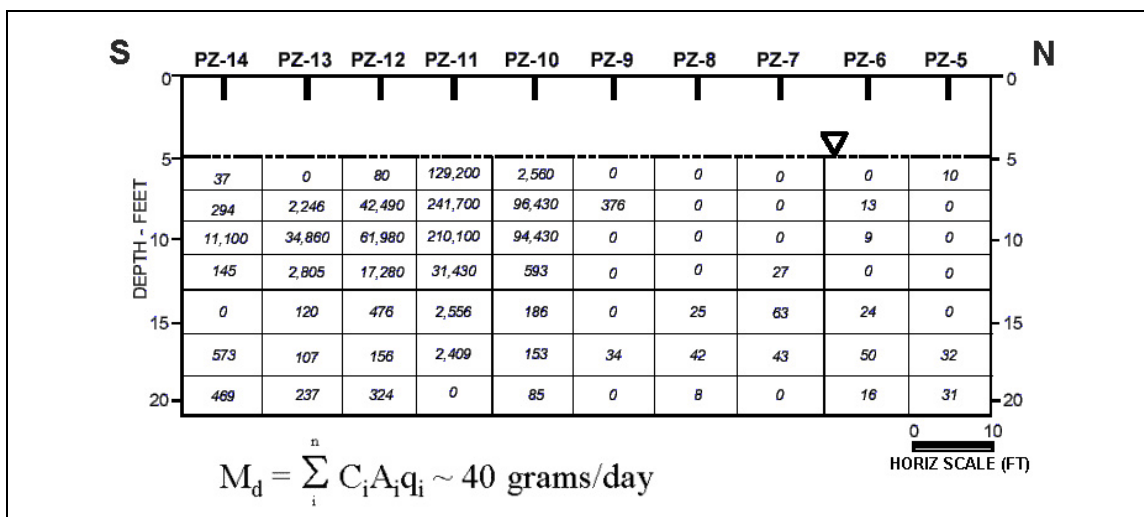


Figure 6. MTBE Concentration and Area for Each Polygon of Transect
 (see Figures 4 and 5)(Adapted from: Einarson, 2001)

3.2 Groundwater Mass Flux Calculation - Solute Transport Model Method

A solute transport model can be used to estimate mass flux in groundwater. In some models, mass flux is presented directly on the output screens (e.g., BIOSCREEN, BIOCHLOR). Other models (e.g., numerical models) can provide either flow or concentrations, or both, but supplemental calculations are required to calculate a flux.

Models containing mass flux terms directly are listed below:

BIOSCREEN: An easy-to-use spreadsheet-based analytical model originally designed to be used for BTEX plumes. It can be adapted for MTBE by using the first-order decay method to simulate biodegradation or by using a first order rate constant of zero if biodegradation of MTBE is not occurring at a particular site. Mass flux is estimated from a 5x11 array of concentration values provided by the model. BIOSCREEN is a 2-D model (Newell et al, 1996).

BIOCHLOR: An easy-to-use spreadsheet-based analytical model originally designed to be used for chlorinated solvent plumes. As with BIOSCREEN, it can be adapted for MTBE by using the first-order decay method to simulate biodegradation or by using a first order rate constant of zero if biodegradation of MTBE is not occurring at a particular site. BIOCHLOR allows computation of two different degradation zones, where different first-order rate constants can be entered. Mass flux is estimated from a 5x11 array of concentration values provided by the model. BIOCHLOR is a 2-D model (Aziz et al, 2000).

3.3 Groundwater Mass Flux Calculation - Extraction Well Method

An extraction well downgradient of a source zone is pumped at a rate to capture the water flowing through the source zone. After waiting for the flow field to stabilize, the mass discharge from the well(s) is measured, which is equal to the mass flux leaving the source zone.

3.4 Control Point Concentration Calculation

Control Point Concentration – Summary

FLUX TERM	CONTROL POINT CONCENTRATION
Equation	$C_{b_{cp}} = \frac{w_{gw-n}}{Q_{cp}}$
Input Data	$C_{b_{cp}}$ = concentration of constituent at the control point, such as a water-supply well or stream after blending (mg/L) w_{gw-n} = The mass flux at the farthest downgradient transect (the closest transect to the control point) (g/day) Q_{cp} = The total flowrate at the control point, such as the pumping rate of a water supply well, or the flowrate in a stream after blending with groundwater containing constituent (L/day)
Typical Input Values	w_{gw-n} = 0.1 to 1000 g/day Q_{cp} = 500 to 500,000 L/day
Comments	This is the calculation where mass flux is used to estimate the concentration of the constituent in water at the control point (such as a water supply well or stream) after blending with groundwater containing the constituent (Einarson and Mackay, 2001a).

How to Calculate

The mass flux at a particular transect is divided by the flowrate from a pumping well at the control point. This yields a maximum concentration at the control point.

Example

Problem: Determine the control point concentration of MTBE for a transect with 100 g/day MTBE. A 100,000 L/day water supply well is located at the edge of the plume.

Solution: $C_{bcp} = (100 \text{ g/day}) / (100,000 \text{ L/day}) * (1000 \text{ mg/g}) = 1 \text{ mg/L}$

3.5 Vadose Zone to Groundwater Mass Flux Calculation**Vadose Zone to Groundwater Mass Flux Summary**

FLUX TERM	VADOSE ZONE TO GROUNDWATER MASS FLUX
Equation	$w_{bvd} = \frac{C_T}{(\theta_{ws} / \rho_b) + k_d + H(\theta_{as} / \rho_b)} \left(\frac{L_1}{L_2} \right) (I_f) (A) (CF)$ where $k_d = k_{oc} f_{oc}$ and $I_f = 0.0018 P^2 \text{ for sandy soils (empirical relationship; results are in cm/yr)}$ $I_f = 0.0009 P^2 \text{ for silty soils (empirical relationship; results are in cm/yr)}$ $I_f = 0.00018 P^2 \text{ for clay soils (empirical relationship; results are in cm/yr)}$
Input Data	w_{bvd} = mass flux from vadose zone (mg/yr) C_T = bulk contaminant concentration on soil mass for all phases (mg/kg) θ_{ws} = volumetric water content of surface soils ($\text{cm}^3 \text{ H}_2\text{O}/\text{cm}^3 \text{ soil}$) ρ_b = soil bulk density (g soil/$\text{cm}^3 \text{ soil}$) k_d = soil-water distribution (partition) coefficient ($\text{cm}^3 \text{ H}_2\text{O}/\text{g soil}$) H = Henry's law constant for contaminant ($\text{cm}^3 \text{ H}_2\text{O}/\text{cm}^3 \text{ air}$) θ_{as} = volumetric air content of vadose zone soils ($\text{cm}^3 \text{ air}/\text{cm}^3 \text{ soil}$) k_{oc} = organic carbon partition coefficient for contaminant ($\text{cm}^3 \text{ H}_2\text{O}/\text{g C}$) f_{oc} = fraction of organic carbon (g C/g soil) L_1 = thickness of contaminated soil zone (cm) L_2 = distance from top of contaminated soil zone to top of water-bearing unit (cm) I_f = Net infiltration (cm/yr) A = area of contaminated soil zone (cm^2) P = mean annual precipitation (cm/yr) CF = conversion factor 2.74×10^{-9} (l-g-yr / cm^3 - mg - day)
Typical Input Values	C_T = 0.010 – 10,000 mg/kg (for MTBE) θ_{ws} = 0.08 to 0.38 $\text{cm}^3 \text{ H}_2\text{O}/\text{cm}^3 \text{ soil}$ ρ_b = 1.7 g soil/$\text{cm}^3 \text{ soil}$ k_d = 0.072 $\text{cm}^3 \text{ H}_2\text{O}/\text{g soil}$ H = 0.024 $\text{cm}^3 \text{ H}_2\text{O}/\text{cm}^3 \text{ air}$ (for MTBE) θ_{as} = 0.02 to 0.33 $\text{cm}^3 \text{ air}/\text{cm}^3 \text{ soil}$ k_{oc} = $10^{1.08} \text{ cm}^3 \text{ H}_2\text{O}/\text{g C}$ (for MTBE) f_{oc} = 0.006 g C/g soil L_1 = 60 to 305 cm L_2 = 60 to 305 cm A = 152 to 7620 cm^2 P = 6 to 160 cm/yr

How To Calculate

The mass flux from the vadose zone to the saturated zone can be estimated using an estimated infiltration rate, the concentration of the constituent in vadose zone soils, and partitioning equations.

Example

Problem: A site has an average MTBE concentration in vadose zone soils of 220 mg/kg. The site receives 100 cm of annual precipitation. The estimated soil properties are: soil bulk density of 1.7 g soil/cm³ soil, volumetric water content = 0.08 cm³ H₂O/cm³ soil, and volumetric air content = 0.33 cm³ air/cm³ soil. The contaminated soils are clean, well-graded sands. The top 61 cm of the soil is affected and is underlain by 60 cm of clean unsaturated soils before reaching the water table. The measured f_{oc} of the soil is 0.006, and the log K_{oc} value for MTBE is 1.08. The Henry's law constant for MTBE is 0.024 cm³ H₂O/cm³ air. The source zone is 1981 cm long in the direction parallel to groundwater flow and 183 cm long in the direction perpendicular to groundwater flow.

Solution: First estimate the annual infiltration in the vadose zone. For sandy soils:
 $I_f = 0.0018(100)^2 = 18 \text{ cm/yr}$

Next, estimate the area of the contaminated soil zone:
 $A = (1981)(183) = 362,523 \text{ cm}^2$

Then estimate the vadose zone to groundwater mass flux:

$$w - b_{vd} = \left(\frac{220}{(0.08 / 1.7) + 0.006(10^{1.08}) + 0.024(0.33 / 1.7)} \right) \left(\frac{61}{61 + 60} \right) (18)(362,523)(2.74 \times 10^{-9})$$

Vadose zone mass flux = 16.0 g/day