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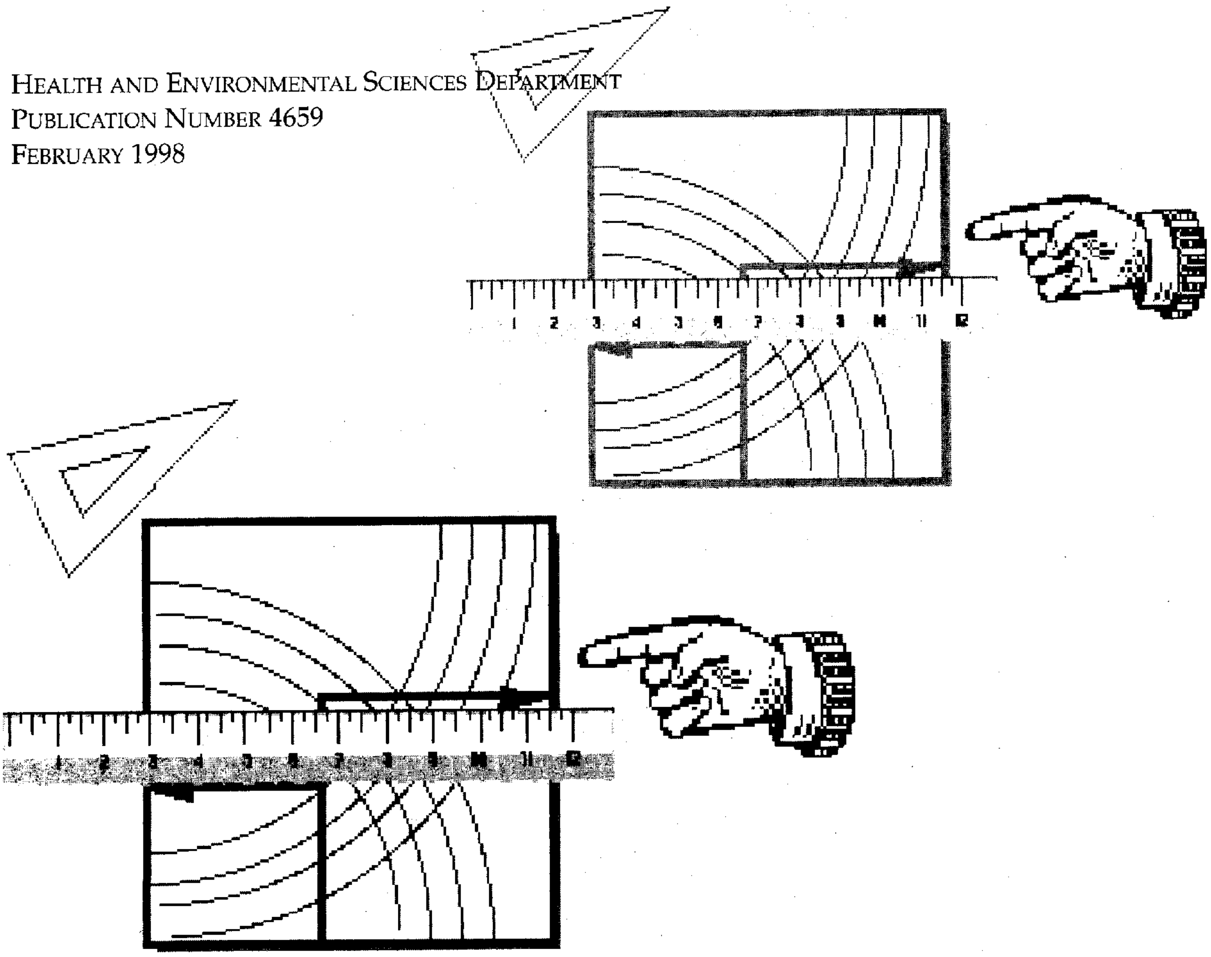
GRAPHICAL APPROACH FOR DETERMINING SITE-SPECIFIC DILUTION-ATTENUATION FACTORS (DAFs)

TECHNICAL BACKGROUND DOCUMENT

HEALTH AND ENVIRONMENTAL SCIENCES DEPARTMENT
PUBLICATION NUMBER 4659
FEBRUARY 1998



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Graphical Approach for Determining Site-Specific Dilution-Attenuation Factors (DAFs)

Technical Background Document

Health and Environmental Sciences Department

API PUBLICATION NUMBER 4659

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TABLE OF CONTENTS

TABLE OF CONTENTS (CONT.)

List of Appendices

List of Figures

List of Figures (Cont'd.)

List of Tables

EXECUTIVE SUMMARY

This document describes the technical basis for the *Graphical Approach for Determining Site-Specific Dilution-Attenuation Factors.* This is the result of a project focused on developing simplistic graphically-based approaches for deriving target soil cleanup goals for sites where groundwater is, or may be, affected by spills, leaks, or other accidental releases of liquid hydrocarbons.

This graphical approach is intended to complement methodologies used by USEPA for selecting dilution attenuation factors (DAFs). The DAF is a quantity relating leachate concentrations leaving hydrocarbon-contaminated soil zones and the resulting impact to downgradient groundwater quality. To date, many regulatory agencies have employed generic "one size fits all" DAFs that are usually conservative and disregard a site's specific characteristics. The graphical approach provides a simplistic, yet technically-defensible alternative for those desiring more site-specific values for vadose zone and submerged sources. This approach is consistent with risk-based corrective action (RBCA) approaches currently being implemented and evaluated by regulatory agencies.

The approach outlined in this report allows for varying levels of site-specificity; it can be used when one has a little, or a lot, of site-specific information. When the user has limited data, the approach will lead to smaller, thus conservative DAFs. As more characterization data become available, the same graphical approach will lead to more site-specific screening levels. Chemical specific DAFs can also be generated, however, if chemical degradation and source decay are considered negligible, then the DAF value will be the same for all chemicals at a given site. This graphical approach also provides guidance for estimating the travel time necessary for chemical migration from the source to the receptor location.

In addition to allowing for varying levels of site-specific data, this approach is unique in that the user can move away from fixed generic DAF values without having to resort to complex numerical simulations. Furthermore, the graphs visually indicate the sensitivity to various parameters, which is valuable information not easily gleaned from most numerical software simulators. Unlike the available numerical models and fixed generic values, this graphical approach is applicable to both vadose zone and submerged sources. This approach is, however, not applicable to very complex hydrogeologic settings (e.g., fractured geology), or to groundwater flows that cannot be reasonably approximated as one-dimensional (e.g., significant well pumping).

CHAPTER 1

INTRODUCTION

1.1 BACKGROUND

In the *Soil Screening Guidance* (USEPA 1996a, 1996b) the "dilution attenuation factor" (DAF) is used to relate the leachate concentration of a compound leaving a source zone to the groundwater concentration that results some distance downgradient as depicted in Figure 1-1.

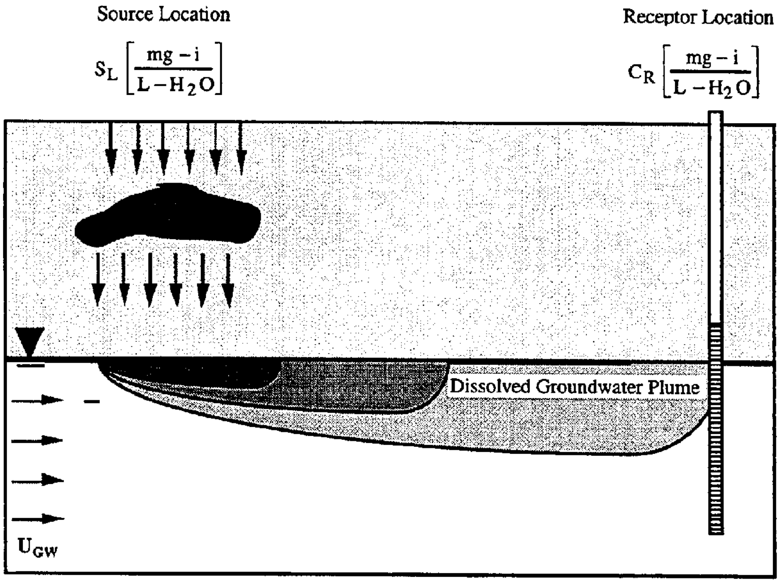


Figure 1-1. Soil-to-groundwater pathway schematic for compound "i"

The DAF plays a key role in assessing potential impact from the soil-to-groundwater pathway at sites where groundwater quality is, or may be, affected by a leak, spill, or other accidental release of hydrocarbons. In the forward calculation mode the DAF can be used to estimate potential downgradient effects of known source zone concentrations. In the reverse calculation mode the user establishes a receptor-location water quality criterion and then uses the DAF to estimate the maximum tolerable source zone leachate concentration. The following text is primarily oriented towards use of the DAF for "backward" calculations; however, the reader should note that the results of this work are equally applicable for "forward" calculations.

Conceptually, DAF-based approaches are attractive for a number of reasons, including:

a) Soil target levels derived from DAF-based approaches are often significantly less restrictive than those derived from simple equilibrium partitioning models; and

b) It is easy for regulatory agencies to adopt and implement DAF-based approaches rather than review complex fate and transport calculations at every site.

While the DAF-based approach is appealing, its development and implementation to date have been somewhat controversial. Historically, USEPA has attempted to establish generic DAF values. The USEPA Toxicity Characteristic Rule (TC Rule, 1990) first introduced a dilution factor of 20 that was based more on the specifics of the TCLP analytical protocol than on considerations of subsurface migration and transport. The 1992 draft USEPA Hazardous Waste Identification Rule (HWIR) guidance introduced DAFs of 1, 10, and 100, and these were purported to be based on results of contaminant transport modeling exercises using the EPACML model and national distributions of input parameters. These DAFs subsequently appeared in the 1993 USEPA draft Soil Screening Level Guidance. In the 1994 revision, DAF estimates were generated from a mixing-zone type mass-balance calculation.

While heavily criticized for introducing generic DAFs in the 1992 draft HWIR, USEPA can be credited with stimulating discussions regarding the efficacy of DAF-based approaches, as well as further study of the models and parameters used to generate DAFs (e.g., Chiang *et al.* 1994). For example, a single DAF cannot possibly represent the wide range of hydrologic and contaminant release settings likely to be encountered in practice. In fact, it is not difficult to imagine real settings in which the use of a generic DAF results in a target soil concentration that is either unnecessarily over-protective, or not sufficiently protective.

Thus, the development of an improved approach for establishing DAFs is needed. Ideally, any new approach would retain the simplicity of the generic DAF-based approach, but would be more appropriate for the wide range of hydrogeologic release settings and chemical properties likely to be encountered in practice.

This document describes the technical basis for the *Graphical Approach for Determining Site-Specific Dilution-Attenuation Factors.* This is the result of a project focused on developing simplistic graphically-based approaches for deriving soil screening levels for the soil-to-groundwater pathway. Ideally, this approach allows for varying levels of site-specificity. This means that the graphical approach can be used when one has a little, or a lot, of site-specific information. When the user has limited data, the approach will lead to more generic (and conservative) values which will be similar for all sites. As more characterization data become available, the same graphical approach will lead to more site-specific screening levels.

In such exercises, a balance has to be found between technical rigor and practicality in order for the system to be useful to the intended audience (regulators, consultants, project managers, etc.). Typically, as technical rigor increases, model complexity and data requirements also increase. Most state-of-the-art models require information that is not likely to be obtained during conventional site characterizations. Thus, predictive models, data requirements, and format of this graphical approach have been carefully selected and scrutinized in light of the overall project goals.

In the following chapters, the focus is on the technical basis for the graphical approach introduced in this document. Additional sections of the report discuss the use of the graphs, and the selection of parameter values, specifically:

- **Chapter 2** presents the general theoretical framework underlying the proposed graphical approach. Within this chapter, the DAF is defined mathematically for both steady and time-varying leachate sources, criteria used during model selection are discussed, and the mathematical approximations adopted in this work are presented and justified.

- **Chapter 3** focuses on the development of a graphical approach for determining DAFs for cases where the hydrocarbon-contaminated soils are in intimate contact with groundwater (submerged sources).

- **Chapter 4** focuses on the development of a graphical approach for determining DAFs for cases where the hydrocarbon-impacted soils are located entirely above the groundwater table (vadose zone sources).

- **Chapter 5** illustrates how each approach can be used with varying amounts of site-specific information.

- **Chapter 6** develops and summarizes algorithms for idealized source depletion models.

- **Chapter 7** summarizes reference materials cited in the text.

- **Appendix A** summarizes the parameters required by the graphical approach, and describes how this information is collected, or estimated based on existing databases.

- **Appendix B** provides a comparison of the full, and approximate solutions, used in developing the graphical approach.

- **Appendix C** contains a discussion on the role of vapor transport (relative to leaching) in the impacts to groundwater caused by hydrocarbon-impacted soils.

- **Appendix D** contains listings of computer codes used in this work and a brief discussion of code validation procedures.

A companion document, the *User's Guide for the Graphical Approach for Determining Site-Specific Dilution-Attenuation Factors (DAFs)*, provides a concise set of instructions for use of the graphical approach.

CHAPTER 2

GENERAL THEORETICAL FRAMEWORK

2.1 MATHEMATICAL DEFINITION OF THE DILUTION-ATTENUATION FACTOR (DAF)

For a constant-strength leachate source, USEPA defines the DAF to be:

$$\mathrm{DAF}\left[\frac{(mg_i \,/\, L_{H_2O})_{source}}{(mg_i \,/\, L_{H_2O})_{receptor}}\right]=\frac{S_L}{C_R} \qquad (2\text{-}1)$$

where:

S_L = concentration of compound "i" dissolved in leachate leaving the source zone [mg_i / L_{H2O}]

C_R = dissolved concentration of compound "i" at the receptor [mg_i / L_{H2O}]

As defined by Equation (2-1), the DAF must take on values greater than or equal to one ($DAF \geq 1$). Larger values correspond to increased attenuation through dilution, dispersion, and biodegradation.

When using the DAF to determine acceptable source zone leachate concentrations, the receptor concentration C_R is generally prescribed by regulatory guidance and is presumably developed from considerations of potential human health effects, ecological impacts, aesthetics, and other relevant criteria. It is implicit that C_R may represent a time-averaged, spatially-averaged, and/or statistically-defined quantity. For example, some C_R values may be derived based on considerations of chronic exposures over 30-y time frames (e.g., benzene groundwater quality standards), while others may be based on effects of short-term exposures (e.g., nitrate drinking water standards)

This work allows for time-varying sources. Thus the constant-strength source DAF definition given above in Equation (2-1) is extended to the following:

$$\mathrm{DAF}\left[\frac{(\mathrm{mg}_i / \mathrm{L}_{H_2O})_{\mathrm{source}}}{(\mathrm{mg}_i / \mathrm{L}_{H_2O})_{\mathrm{receptor}}}\right] = \frac{S_L^o}{\langle\langle C_R \rangle_z \rangle_{t,\max}} \tag{2-2}$$

where:

S_L^o = dissolved concentration of compound i leaving source zone at time t=0 $[\mathrm{mg}_i/\mathrm{L}_{H2O}]$

$\langle\langle C_R\rangle_z\rangle_{t,\max}$ = maximum-time-averaged and vertically-averaged centerline dissolved concentration of compound i at the receptor location $x=L_R$ $[\mathrm{mg}_i/\mathrm{L}_{H2O}]$

The reader can verify by inspection that Equation (2-2) is equivalent to Equation (2-1) for the case of a constant-strength source.

As stated above, the quantity $\langle\langle C_R\rangle_z\rangle_{t,\max}$ is often prescribed by regulatory guidance, and the user needs to identify the basis for any given value. This becomes particularly important when selecting an appropriate averaging time interval for $\langle\langle C_R\rangle_z\rangle_{t,\max}$ because water quality criteria may be based on any number of factors, including: considerations of chronic (long-term) or acute (short-term) health effects, ecological impact, aesthetic concerns, and technology limits.

2.2 GENERALIZED MATHEMATICAL APPROACH

If Equation (2-2) is used to develop DAF values, then expressions are needed to relate $\langle\langle C_R\rangle_z\rangle_{t,\max}$ to S_L^o. These relations typically originate from solutions to the General Contaminant Transport Equation, which is simply a mass balance expression accounting for accumulation, advection, dispersion, and reaction. It can be written:

$$\frac{\partial(\rho_b\ C_T)}{\partial t} = \sum_j \underline{\nabla} \bullet \phi_j\, D_j \bullet \underline{\nabla} C_j - \sum_j \phi_j\, \underline{u}_j \bullet \underline{\nabla} C_j - \sum_j \beta_j \phi_j C_j \tag{2-3}$$

In Equation (2-3):

C_T = total concentration of compound i per unit mass of soil = $\Sigma C_j\phi_j/\rho_b$ $[\mathrm{mg}_i/\mathrm{kg}_{soil}]$

C_j = concentration of contaminant i in phase j $[\mathrm{mg}_i/\mathrm{L}_{phase\text{-}j}]$

ρ_b = soil bulk density $[\mathrm{kg}_{soil}/\mathrm{L}_{soil}]$

D_j = hydrodynamic dispersion tensor for phase j $[\mathrm{m}^2/\mathrm{d}]$

$\underline{u}_j$ = interstitial (seepage) velocity vector of phase j [m/d]
t = time [d]
ϕ_j = volume fraction of phase j in the soil [$L_{phase\text{-}j}/L_{soil}$]
β_j = decay coefficient of the contaminant in phase j [d^{-1}]
$\underline{\nabla}$ = del differential vectorial operator, ($\underline{i}\,\partial/\partial x + \underline{j}\,\partial/\partial y + \underline{k}\,\partial/\partial z$) [$m^{-1}$]
x = coordinate along the axis parallel to direction of flow [m]
y = coordinate along the axis transverse to the direction of flow [m]
z = vertical coordinate perpendicular to the direction of flow [m]

In the following, C(x,y,z,t), denotes solutions to Equation (2-3). These specify the groundwater concentration (C) at any time (t) and at any point in the aquifer (x,y,z). The quantity $<<C_R>_z>_{t,max}$ appearing in the DAF definition Equation (2-2) is obtained by setting $x=L_R$ (the horizontal distance from the downgradient edge of the source to receptor), y=0 (to obtain the centerline concentration), vertically averaging over a well sampling depth H_w, and then finding the maximum time-averaged concentration for the averaging (exposure) duration T:

$$<< C_R >_z >_{t,max} = \max\left\{ \frac{1}{T}\int_{\tau}^{\tau+T} \left\{ \frac{1}{H_w}\int_{h}^{h+Hw} C(L_R,0,z,t)\,dz \right\} dt \right\} \tag{2-4}$$

where:

τ = beginning of the time-averaging period that yields the maximum time average [d]
T = averaging period duration [d]
h = elevation of top of well screen [m] (z=0 is at the ground water table)
H_w = vertical averaging depth [m]
z = vertical coordinate measured down from the ground water table [m]

2.3 MODEL SELECTION CRITERIA

Considering the goals of this work and the nature and extent of data typically available for sites of interest, the following preferred model characteristics were selected:

- all soil properties are homogeneous and constant with time;
- all flows are steady and one-dimensional;
- linear partitioning isotherms describe sorbed-dissolved phase equilibrium; and
- all reactions follow first-order kinetics.

Models describing the transport of constituents through the vadose and saturated zones are usually derived from analytical or numerical solutions to the basic three-dimensional advection-dispersion equation (Equation (2-3)). Modeling of vadose zone transport is often simplified by solving only the one or two-dimensional advection-dispersion equation.

In general, one may choose from numerical, analytical, and semi-analytical solutions. Numerical models are more versatile than analytical models and can provide solutions of complex problems involving differing boundary conditions and complex aquifer heterogeneity. The application of numerical models is typically more time-consuming than analytical models. In addition, problems may be experienced due to numerical dispersion and other inaccuracies induced by the numerical grid used in numerical solutions (Gayla, 1987). Furthermore, the application of state-of-the-art numerical models often requires data not likely to be obtained in conventional site characterizations.

Analytical models provide exact solutions to idealized scenarios that are more simplistic than those typically solved through the use of numerical models. However, the many assumptions and simplifications involving aquifer heterogeneity and boundary conditions may not be reasonable at a particular site. Analytical solutions can provide reasonable results for simulations that do not involve complex aquifer heterogeneity or boundary conditions and are attractive because they are generally less computationally demanding and can be more readily applied at sites where there is a limited amount of information available.

Given these assumptions, and since it is anticipated that this approach will be used in applications where limited site data are available, analytical and semi-analytical models are used in this work.

2.4 CONSTANT-STRENGTH AND TIME-VARYING SOURCE SOLUTIONS

Under these conditions, and for simple source geometries, it is possible to develop a number of analytical and semi-analytical solutions to Equation (2-3) for the case of constant-strength sources (e.g., Bear 1979, Yeh 1981, Hunt 1983, Javendel *et al.* 1984, Domenico 1987, Galya 1987, etc.).

In this work $C^*_{CS}(x,y,z,t)$ denotes the normalized solution for a constant-strength source (equivalent to having a source with unity leachate concentrations $S_L{}^\circ = 1$):

$$C^*_{CS}(x,y,z,t) = C(x,y,z,t) \quad \text{(for constant-strength sources with } S_L{}^\circ = 1) \tag{2-5}$$

These solutions are particularly useful as they are often analytical and can be used to derive other solutions for time-varying sources $S_L(t)$. This is accomplished through use of Duhamel's Principle (Hildebrand 1976, p 465):

$$C(x,y,z,t) = \int_0^t S_L(\omega) \frac{\partial C^*_{cs}(x,y,z,t-\omega)}{\partial t} d\omega \tag{2-6}$$

where:

$S_L(t)$ = time-varying source zone leachate concentration $[mg_i/L_{H2O}]$
ω = dummy integration variable
$C^*_{CS}(x,y,z,t)$ = normalized solution for a constant strength source [unitless]

Thus, if the constant source solution (C^*_{CS}) for a given set of boundary conditions is known, then $\langle\langle C_R \rangle_z \rangle_{t,max}$ can be calculated by inserting Equation (2-6) into Equation (2-4) and performing the necessary integrations (either analytically or numerically).

2.5 MATHEMATICAL APPROXIMATIONS

To simplify the use of Equations (2-4) and (2-6), which did not lend themselves to an obvious natural progression of graphs, an approximate solution technique was proposed, evaluated, and eventually adopted. It is based on the observation that, in the absence of significant longitudinal hydrodynamic dispersion (e.g., advection-dominated systems), one can write that the solution C(x,y,z,t) for any given source term $S_L(t)$ is given exactly by:

$$C(x,y,z,t) \approx H(t-\tau_d)\, S_L(t-\tau_d)\, C^*_{CS}(x,y,z,\infty) \tag{2-7}$$

where:

$H(t - \tau_d)$ = Heavyside step function (= 0 for $t < \tau_d$; =1 for $t \geq \tau_d$) [unitless]

$C^*_{CS}(x,y,z,\infty)$ = steady-state normalized solution for a constant-strength source [unitless]
$S_L(t - \tau_d)$ = time-varying source zone leachate concentration $[mg_i/L_{H2O}]$
τ_d = a time delay (e.g., total travel time for transport between the leachate source and the receptor location L_R) [d]

To better explain this approximation in a more graphical sense, Figure 2-2 presents the qualitative forms of the exact and approximate solutions for both constant-strength and decaying-source leachate concentrations. Figure 2-3 presents numerical results from the HPS model discussed later in Chapter 4. The exact solution, which includes longitudinal dispersion, predicts that contaminants do not arrive in a sharp front, as happens in the approximate solutions. In addition, when considering decaying sources, the peak concentration given by the approximate solution is greater than the peak concentration given by the exact solution Despite these discrepancies, the approximate solution does mimic many of the characteristics of the exact solution.

Recall also, that estimating maximum time-averaged concentrations is of greatest interest. While there may be differences between the two solutions, these may be small enough that the approximate solution reasonably estimates the time-averaged receptor location concentration given by the exact solution. In addition, considering the differences mentioned above, it may be argued that the time-averaged receptor groundwater concentration given by the approximate solution will always be greater than that given by the exact solution. In other words, the approximate solution is a conservative estimate of the exact solution results.

When C(x,y,z,t) is given by the approximation Equation (2-7), then Equation (2-4) becomes:

$$<< C_R >_z>_{t,max} \approx \left\{\frac{1}{T}\int_0^T S_L(t)dt\right\} x \left\{\frac{1}{H_w}\int_h^{h+Hw} C^*_{cs}(L_R,0,z,\infty)\,dz\right\} \qquad (2\text{-}8)$$

Approximate solution (2-8) is most accurate for scenarios in which longitudinal dispersion is minimal, or when sources decay very slowly relative to the averaging time.

Assuming that Equation (2-8) is a valid approximation, Equation (2-2) for the DAF becomes:

$$DAF = \frac{1}{\left\{\frac{1}{T}\int_0^T \frac{S_L(t)}{S_L(0)}dt\right\} x \left\{\frac{1}{H_w}\int_h^{h+Hw} C^*_{cs}(L_R,0,z,\infty)\,dz\right\}} \qquad (2\text{-}9)$$

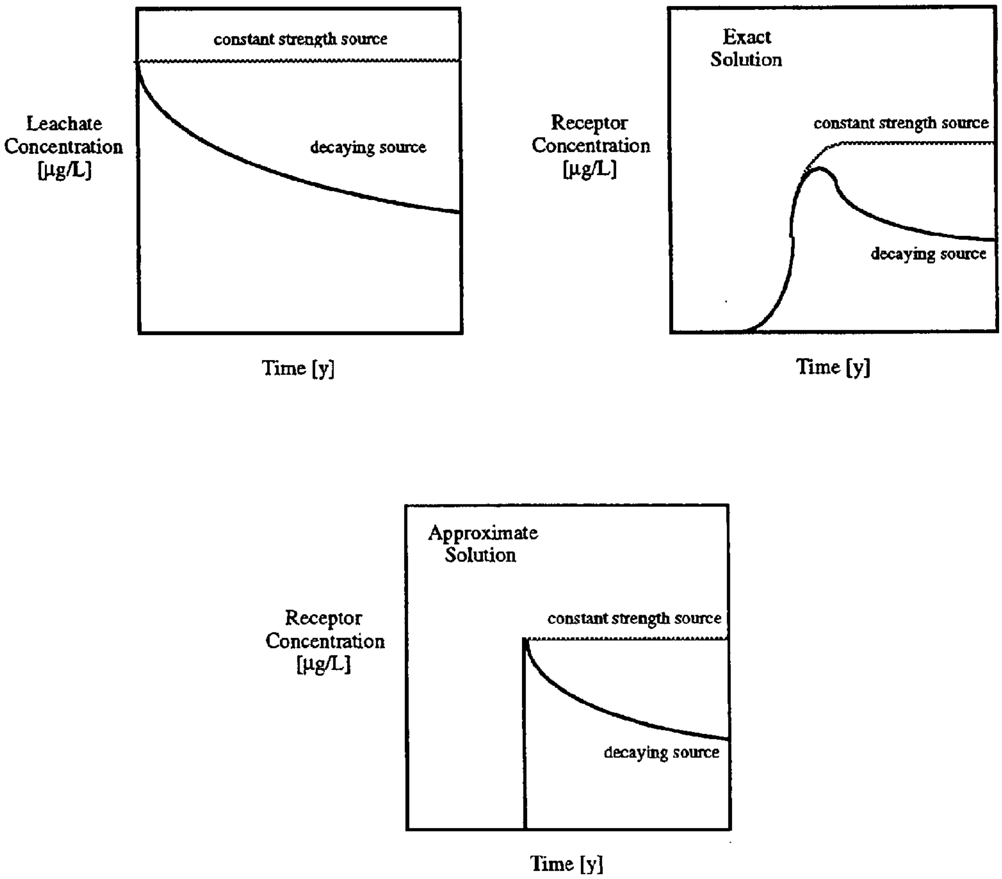


Figure 2-2. Qualitative comparison of exact and approximate solutions

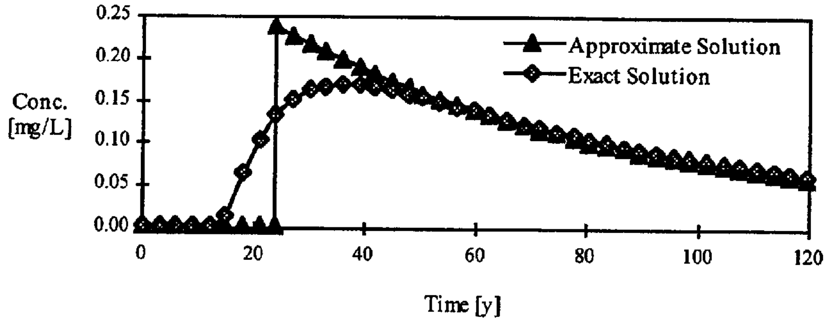


Figure 2-3. Comparison of receptor concentrations at x = 30 m (distance downgradient from center of source zone) obtained from the approximate and exact solutions for an exponentially-decaying source, using the HPS model discussed in Chapter 4

Approximation Equation (2-9) was compared with full numerical solution output from the API transport model VADSAT and from the HPS model (developed at the University of Texas at Austin during this project - see Chapter 4) for a range of groundwater velocities, source depletion rates, biodegradation rates, and receptor locations. Deviations between the approximate and exact solutions generally were less than 20 percent of the exact solution in most cases. The deviation increased as the receptor was located farther downgradient of the source zone, and the source decay rate increased. Results of this analysis are presented in Appendix B. It was decided that the level of agreement was acceptable since it was within the inherent errors of the graphical approach (i.e., within the accuracy of interpolating numerical values from the graphs) and that the approximation resulted in conservative DAF estimates.

As the agreement was acceptable, approximate Equation (2-9) was employed during this analysis, for a number of reasons, including:

- The source type (decaying, constant strength, etc.) contribution to the DAF can be calculated independent of the transport model, thereby allowing easy incorporation of multiple source types without having to redo the transport calculations.

- The time-averaged source nomographs can be generated without having to specify a specific averaging time or source decay rate.

In the following sections, specific solutions for vadose zone and groundwater zone sources are discussed, as well as the analysis of time-varying source options.

CHAPTER 3

SUBMERGED (SATURATED ZONE) SOURCES

3.1 CONSTANT-STRENGTH SOURCES

Domenico (1987) published an analytical solution to Equation (2-3) for the case of solute migration from a constant-strength submerged rectangular source as depicted below in Figure 3-1.

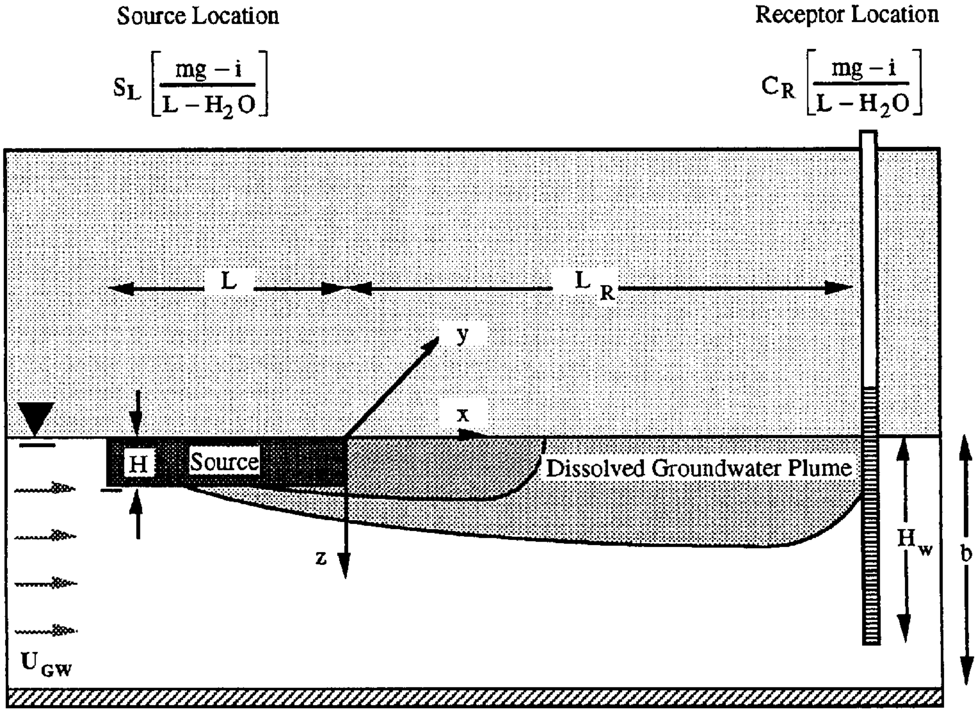


Figure 3-1. Generalized submerged source schematic

Non-retarded solute transport was assumed to occur through a homogeneous aquifer via one-dimensional advective transport, three-dimensional hydrodynamic dispersion, and first-order reaction kinetics. Domenico's original solution is:

$$
\begin{aligned}
C^{*}_{cs}(x,y,z,t) = \frac{1}{8}\exp\left\{\frac{x}{2\alpha_L}\left\{1-\sqrt{1+\frac{4\beta_s\,\alpha_L}{U_{GW}}}\right\}\right\} \\
\times\,\mathrm{erfc}\left\{\frac{x-U_{GW}t\sqrt{1+\frac{4\beta_s\,\alpha_L}{U_{GW}}}}{2\sqrt{\alpha_L U_{GW} t}}\right\} \\
\times\left\{\mathrm{erf}\left\{\frac{y+\frac{W}{2}}{2\sqrt{\alpha_T x}}\right\}-\mathrm{erf}\left\{\frac{y-\frac{W}{2}}{2\sqrt{\alpha_T x}}\right\}\right\} \\
\times\left\{\mathrm{erf}\left\{\frac{z+H}{2\sqrt{\alpha_V x}}\right\}-\mathrm{erf}\left\{\frac{z-H}{2\sqrt{\alpha_V x}}\right\}\right\}
\end{aligned}
\qquad (3\text{-}1)
$$

where:

$C^{*}_{cs}(x,y,z,t)$ = normalized transient solute concentration from a steady leachate source of concentration unity ($S_L(t)=1$), at any point in space (x,y,z) [dimensionless]

x = longitudinal distance down-gradient from the source zone measured from the down-gradient source edge [m]

y = transverse coordinate perpendicular to flow measured from the center-line of the source zone [m]

z = vertical coordinate perpendicular to flow measured down from the groundwater table [m]

α_L = the longitudinal (x-direction) dispersivity [m]

α_T = the transverse (y-direction) dispersivity [m]

α_V = the vertical (z-direction) dispersivity [m]

U_{GW} = groundwater seepage velocity [m/d]

β_s = first-order decay coefficient (reaction assumed to occur only in dissolved phase) [d^{-1}]

W = source zone width perpendicular to flow (measured in y-direction) [m]

H = thickness of source zone below the groundwater table (assumed to start at the groundwater table and extend downwards a distance H) [m]

t = time [d]

and $\mathrm{erf}(\eta)$ and $\mathrm{erfc}(\eta)$ denote the Error Function and Complementary Error Function, respectively. These are given by:

$$\mathrm{erf}(\eta)=\frac{2}{\sqrt{\pi}}\int_0^{\eta} e^{-t^2}dt \quad ; \quad \mathrm{erfc}(\eta)=1-\mathrm{erf}(\eta) \tag{3-2}$$

For the purpose of this work, the Domenico Equation (3-1) was modified to incorporate aquifers of finite thickness b [m] (through the method of images) and retarded solute transport due to sorption onto soil surfaces. Under these conditions, Domenico's original solution transforms to the following:

$$\begin{aligned}
C^*_{cs}(x,y,z,t) &= \frac{1}{8}\exp\left\{\frac{x}{2\alpha_L}\left\{1-\sqrt{1+\frac{4\beta_s\,\alpha_L}{U_{GW}}}\right\}\right\} \\
&\times \mathrm{erfc}\left\{\frac{x-U_{GW}t^*\sqrt{1+\frac{4\beta_s\,\alpha_L}{U_{GW}}}}{2\sqrt{\alpha_L U_{GW}t^*}}\right\} \\
&\times\left\{\mathrm{erf}\left\{\frac{y+\frac{W}{2}}{2\sqrt{\alpha_T x}}\right\}-\mathrm{erf}\left\{\frac{y-\frac{W}{2}}{2\sqrt{\alpha_T x}}\right\}\right\} \\
&\times\left\{\begin{aligned}
&\mathrm{erf}\left\{\frac{z+H}{2\sqrt{\alpha_V x}}\right\}-\mathrm{erf}\left\{\frac{z-H}{2\sqrt{\alpha_V x}}\right\} \\
&+\sum_{n=1}^{\infty}\left(\mathrm{erf}\left\{\frac{2nb-z+H}{2\sqrt{\alpha_V x}}\right\}-\mathrm{erf}\left\{\frac{2nb-z-H}{2\sqrt{\alpha_V x}}\right\}\right) \\
&+\sum_{n=1}^{\infty}\left(\mathrm{erf}\left\{\frac{2nb+z+H}{2\sqrt{\alpha_V x}}\right\}-\mathrm{erf}\left\{\frac{2nb+z-H}{2\sqrt{\alpha_V x}}\right\}\right)
\end{aligned}\right\}
\end{aligned} \tag{3-3}$$

where all the parameters are defined as above, except:

t^* = t/R [d]

R = saturated zone retardation factor = $1+K_d\,\rho_b/\,\phi_m$ [dimensionless]

K_d = soil-water partitioning coefficient $[(mg_i/kg_{soil})/(mg_i/L_{H2O})]$
b = finite aquifer thickness [m]

The saturated zone retardation factor R accounts for the effects of sorption on the migration of the leading edge of the plume. Rather than moving with groundwater flow, the leading edge of a dissolved chemical plume will appear to move the distance $U_{GW}\ t/R$ over the time interval t.

When evaluated at steady-state ($t^*=\infty$) and at the receptor location $x=L_R$ along the centerline (y=0), Equation (3-3) reduces to:

$$C_{cs}^*(x,y,z,t)=\exp\left\{\frac{L_R}{2\alpha_L}\left\{1-\sqrt{1+\frac{4\beta_s\,\alpha_L}{U_{GW}}}\right\}\right\}$$

$$\times\left\{\operatorname{erf}\left\{\frac{\frac{W}{2}}{2\sqrt{\alpha_T L_R}}\right\}\right\} \tag{3-4}$$

$$\times\frac{1}{2}\left\{\begin{array}{l}\operatorname{erf}\left\{\frac{z+H}{2\sqrt{\alpha_V L_R}}\right\}-\operatorname{erf}\left\{\frac{z-H}{2\sqrt{\alpha_V L_R}}\right\}\\[2ex]+\sum\limits_{n=1}^{\infty}\left(\operatorname{erf}\left\{\frac{2nb-z+H}{2\sqrt{\alpha_V L_R}}\right\}-\operatorname{erf}\left\{\frac{2nb-z-H}{2\sqrt{\alpha_V L_R}}\right\}\right)\\[2ex]+\sum\limits_{n=1}^{\infty}\left(\operatorname{erf}\left\{\frac{2nb+z+H}{2\sqrt{\alpha_V L_R}}\right\}-\operatorname{erf}\left\{\frac{2nb+z-H}{2\sqrt{\alpha_V L_R}}\right\}\right)\end{array}\right\}$$

3.2 DAF FORMULATION FOR TIME-VARYING SOURCES

As written above, Equation (3-4) is basically the product of three functions representing (from left to right) the attenuation due to: i) longitudinal dispersion and chemical reaction, ii) transverse dispersion, and iii) vertical mixing. It can be rewritten in the form:

$$C_{cs}^*(x,y,z,t)=f\left(\frac{L_R}{\alpha_L},\frac{\beta_s\,\alpha_L}{U_{GW}}\right)\times g\left(\frac{W}{\sqrt{\alpha_T L_R}}\right)\times h\left(\frac{z}{H},\frac{H}{\sqrt{\alpha_V L_R}},\frac{b}{H}\right) \tag{3-5}$$

and inserted into Equation (2-8) to obtain:

$$\mathrm{DAF} = \frac{1}{\left\{\frac{1}{T}\int_0^T \frac{S_L(t)}{S_L(0)}\,dt\right\}} \times \frac{1}{f(\frac{L_R}{\alpha_L},\frac{\beta_s\,\alpha_L}{U_{GW}}) \times g(\frac{W}{\sqrt{\alpha_T\,L_R}}) \times \left\{\frac{1}{H_w}\int_0^{Hw} h(\frac{z}{H},\frac{H}{\sqrt{\alpha_V\,L_R}},\frac{b}{H})\,dz\right\}} \qquad (3\text{-}6)$$

or:

$$\mathrm{DAF} = \frac{1}{\left\{\frac{1}{T}\int_0^T \frac{S_L(t)}{S_L(0)}\,dt\right\}} \,x\, \frac{1}{f(\frac{L_R}{\alpha_L},\frac{\beta_s\,\alpha_L}{U_{GW}})} \,x\, \frac{1}{g(\frac{W}{\sqrt{\alpha_T\,L_R}})} \,x\, \frac{1}{h^*(\frac{H_W}{b},\frac{H}{\sqrt{\alpha_V\,L_R}},\frac{H}{H_W})} \qquad (3\text{-}7)$$

This functional form suggests a very convenient arrangement for the graphical display of solutions, as the DAF depends on the product of four functions, three of which depend on two, or less, parameter groups. These three can be written:

$$\left\{\frac{1}{T}\int_0^T \frac{S_L(t)}{S_L(0)}\,dt\right\} = \frac{(1-e^{-\lambda T})}{\lambda T} \text{ (for example, for exponentially-decaying sources)} \qquad (3\text{-}8)$$

$$f(\frac{L_R}{\alpha_L},\frac{\beta_s\,\alpha_L}{U_{GW}}) = \exp\left\{\frac{(L_R/\alpha_L)}{2}\left[1-\sqrt{1+4\left(\frac{\beta_s\,\alpha_L}{U_{GW}}\right)}\right]\right\} \qquad (3\text{-}9)$$

$$g(\frac{W}{\sqrt{\alpha_T L_R}}) = \mathrm{erf}\left\{\frac{(W/\sqrt{\alpha_T L_R})}{4}\right\} \qquad (3\text{-}10)$$

and are easily presented in x-y or contour plot format. In writing Equation (3-8) an exponentially-decaying source has been assumed. Different idealized model source zones and means of estimating their decay rates are given in Chapter 6.

The fourth function, h^*, appearing in Equation (3-7) is not so easily reduced, but may be rewritten as the sum of two functions:

$$h^* = h^*_{\mathrm{inf}}(\frac{\sqrt{\alpha_V L_R}}{H},\frac{H}{H_W}) + h^*_{\mathrm{cor}}(\frac{\sqrt{\alpha_V L_R}}{b},\frac{H}{b},\frac{H}{H_W}) \qquad (3\text{-}11)$$

where:

$$h^*_{inf}\left(\frac{H}{\sqrt{\alpha_V L_R}}, \frac{H}{H_W}\right) = \frac{1}{2}\int_0^1 \left[erf\left\{\frac{Z(H_W/H)+1}{2(\sqrt{(\alpha_V L_R/H^2)}}\right\} - erf\left\{\frac{Z(H_W/H)-1}{2(\sqrt{(\alpha_V L_R/H^2)}}\right\}\right] dZ \qquad (3\text{-}12)$$

and:

$$h^*_{cor}\left(\frac{\sqrt{\alpha_V L_R}}{b}, \frac{H}{b}, \frac{H}{H_W}\right) = \frac{1}{2}\sum_{n=1}^{\infty}\int_0^1 erf\left\{\frac{2n + Z(\frac{H}{b})(\frac{H_W}{H}) + (\frac{H}{b})}{2(\frac{\sqrt{\alpha_V L_R}}{b})}\right\} dZ$$

$$-\frac{1}{2}\sum_{n=1}^{\infty}\int_0^1 erf\left\{\frac{2n + Z(\frac{H}{b})(\frac{H_W}{H}) - (\frac{H}{b})}{2(\frac{\sqrt{\alpha_V L_R}}{b})}\right\} dZ + \frac{1}{2}\sum_{n=1}^{\infty}\int_0^1 erf\left\{\frac{2n - Z(\frac{H}{b})(\frac{H_W}{H}) + (\frac{H}{b})}{2(\frac{\sqrt{\alpha_V L_R}}{b})}\right\} dZ \qquad (3\text{-}13)$$

$$-\frac{1}{2}\sum_{n=1}^{\infty}\int_0^1 erf\left\{\frac{2n - Z(\frac{H}{b})(\frac{H_W}{H}) - (\frac{H}{b})}{2(\frac{\sqrt{\alpha_V L_R}}{b})}\right\} dZ$$

Here $h^*_{inf}(H/(\alpha_V L_R)^{1/2}, (H/H_W))$ is the solution for the case of an infinite aquifer and $h^*_{cor}((\alpha_V L_R)^{1/2}/b, (H/b), (H/H_W))$ is a correction term that takes into account finite aquifer thicknesses. The former is easily plotted as a contour plot of h^*_{inf} vs. $((\alpha_V L_R)^{1/2}/H)$ and (H/H_W), while the latter is not as easily reduced, as it is a function of three parameter groups.

It is useful to examine the limits of Equations (3-12) and (3-13):

$$\lim\left(\frac{\sqrt{\alpha_V L_R}}{b} << 1\right); \quad h^*_{cor}\left(\frac{\sqrt{\alpha_V L_R}}{b}, \frac{H}{b}, \frac{H}{H_W}\right) << h^*_{inf}\left(\frac{\sqrt{\alpha_V L_R}}{H}, \frac{H}{H_W}\right) \ (i.e.\ h^* \approx h^*_{inf}) \qquad (3\text{-}14)$$

$$\lim\left(\frac{\sqrt{\alpha_V L_R}}{b} >> 1\right); \quad h^*_{cor}\left(\frac{\sqrt{\alpha_V L_R}}{b}, \frac{H}{b}, \frac{H}{H_W}\right) \rightarrow \left(\frac{H}{b}\right) \ (i.e.\ h^* \approx h^*_{cor}) \qquad (3\text{-}15)$$

$$\lim\left(\frac{H}{b} \rightarrow 1\right); \quad h^*_{inf} + h^*_{cor} \rightarrow 1 \qquad (3\text{-}16)$$

In the first limit (Equation 3-14), dispersion is not yet significant enough that the contaminant plume "sees" the aquifer bottom, and therefore the correction term (h^*_{cor}) is negligible in comparison with the infinite aquifer solution (h^*_{inf}). In the second limit (Equation 3-15), dispersion is so great that the contaminant plume has become well-mixed vertically over the aquifer thickness. In the third limit (Equation 3-16), the source and aquifer are of similar thicknesses and the contaminant begins and remains uniformly mixed across the aquifer thickness. This information can be used to quickly check that the graphs presented in the next section behave properly.

3.3 ALTERNATE WELL CONFIGURATIONS

The analysis presented above implicitly assumes a well that is constructed as shown in Figure 3-1, where the well screen extends from the upper boundary of the water table to a depth H_w below the water table. While this is the most common case encountered in practice, occasionally one will encounter situations shown in Figure 3-2, where the well is screened over some intermediate interval extending from a depth H_{w1} to a depth H_{w2}. In this case, the graphical approach can still be used with the following modification - the appropriate value of h^* to use is:

$$h^* = \frac{1}{(H_{w2} - H_{w1})}[H_{w2}\, h^*(H_{w2}) - H_{w1}\, h^*(H_{w1})] \qquad (3\text{-}17)$$

where $h^*(H_{w1})$ denotes the value of h^* calculated from the graphs for a value of $H_w = H_{w1}$.

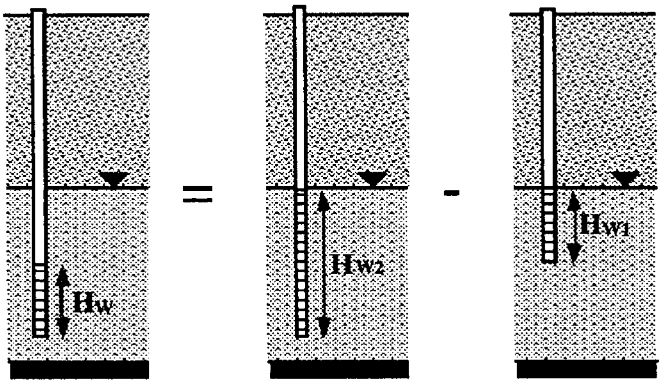


Figure 3-2. Alternate well construction configuration and graphical representation of calculation method given in Equation (3-17)

3.4 NUMERICAL METHODS

Solutions to Equations (3-8), (3-9), and (3-10) were generated with Microsoft Excel® spreadsheets. Solutions to Equations (3-12) and (3-13) were generated using the Maple V® software package distributed by Waterloo Maple Software.

3.5 SUBMERGED SOURCE DAF GRAPHS

Figures 3-3 through 3-9 present graphs of the functions f, g, h^*_{inf} and h^*_{cor}, as well as the time-averaged exponentially-decaying source term given in Equation (3-8).

Figure 3-3 presents the source decay factor for the case of an exponentially-decaying source. A discussion of idealized model source types and methods for estimating decay rates is the focus of Chapter 6. Figure 3-3 indicates that, for the case of an exponentially decaying source, the source decay factor remains essentially equal to unity until the averaging time (T) times the first-order source decay factor (λ) is greater than ≈ 1. Thus, one need not consider correcting for decaying sources unless the averaging time $T>1/\lambda$. In other words, one may treat the source as a steady source (or infinite source), as long as $T<1/\lambda$. This is also roughly equivalent to saying that one need not be concerned with correcting for decaying sources unless the averaging time T exceeds the chemical's half-life, where the half-life $t_{1/2}=\ln 2/\lambda$.

Figure 3-4 presents the dependence of the factor **f** on the parameter $(\beta_s\alpha_L/U_{GW})$. The **f** factor accounts for dissolved plume attenuation due to longitudinal dispersion and first-order chemical reactions (e.g., biodegradation). The curves presented in Figure 3-4 are presented for a range of L_R/α_L values. Based on the parameter estimation discussion given in Appendix A, a reasonable estimate for this parameter is $L_R/\alpha_L=10$. Of significance in this figure is the dependence of **f** on $(\beta_s\alpha_L/U_{GW})$. Note that for $(\beta_s\alpha_L/U_{GW})>0.1$ and $L_R/\alpha_L=10$, the factor **f** is extremely sensitive to small changes in $(\beta_s\alpha_L/U_{GW})$. Changing $(\beta_s\alpha_L/U_{GW})$ by one order of magnitude changes the value of **f** by two to three orders of magnitude. This observation has two implications:

- Chemical reaction (e.g., biodegradation), when it occurs, can be the most important attenuation mechanism (as evidenced by field observations of the differences between aromatic hydrocarbon and chlorinated solvent plumes), and

- It is critical that, if chemical reactions are to be considered when calculating a DAF, the parameter $(\beta_s\alpha_L/U_{GW})$ must be estimated as accurately as possible as the final DAF value will be strongly influenced by small variations in $(\beta_s\alpha_L/U_{GW})$. Incorrect determination of $(\beta_s\alpha_L/U_{GW})$ can lead to significant under-, or overprediction of the DAF value.

Figure 3-5 presents the dependence of the factor **g** on the parameter $(W/(\alpha_T L_R)^{1/2})$. The factor **g** accounts for attenuation of dissolved plumes due to lateral spreading caused by transverse dispersion. Given that a reasonable estimate for α_T is $\alpha_T \approx 0.03L_R$ (see Appendix A), Figure 3-5 indicates that lateral spreading contributes little to attenuation unless one is considering receptor distances at least two times greater than the source zone width (L_R>2W).

Figure 3-6 presents the dependence of the factor h^*_{inf} on the parameters $((\alpha_V L_R)^{1/2}/H)$ and (H/H_w). The factor h^*_{inf} accounts for attenuation of dissolved plumes due to vertical dispersion, as well as vertical averaging across the well screen interval. Figure 3-6 indicates that when the receptor is close to the source $((\alpha_V L_R)^{1/2}/H)<1)$, then $g \approx H/H_w$ as the reduction in concentration results from averaging concentrations across the well screen (as solutes have yet to disperse to depths not sampled by the well screen). That is why $h^*_{inf} \approx H/H_W$ (unless $H>H_W$, in which case $h^*_{inf}=1$), independent of distance from the source in this region of the graph. When the receptor location moves farther away from the source $((\alpha_V L_R)^{1/2}/H)>1)$, then vertical dispersion begins to contribute significantly to the h^*_{inf} value, and the concentration is expected to decrease with increasing distance. As h^*_{inf} is derived from the solution for an infinitely thick aquifer, it will continue to decrease as the receptor location (L_R) is moved away from the source zone.

Figures 3-7 through 3-9 present the dependence of the factor h^*_{cor} on the parameters $((\alpha_V L_R)^{1/2}/b)$ and (H/b) for (H/H_w) equal to 0.1, 1.0, and 10, respectively. Like h^*_{inf} the factor h^*_{cor} also accounts for attenuation of dissolved plumes due to vertical dispersive spreading, as well as vertical averaging across the well screen interval, but it is a correction term to account for aquifers of finite thickness. As discussed above, unbounded vertical dispersion allows h^*_{inf} to always decreases as the receptor location (L_R) is moved away from the source zone. In the case of a finite thickness aquifer, the lower boundary of the aquifer (located at a depth b) limits the vertical migration of chemicals. Thus, as one moves farther away from the source zone, solutes become uniformly mixed over the aquifer thickness, rather than continuing to decrease in concentration. Thus, the value of h $(=h^*_{inf} + h^*_{cor})$ should approach the value (H/b), independent of any other parameters. This is exactly the behavior exhibited by the contours presented in Figures 3-7 through 3-9, which show that h^*_{cor}->(H/b) as $((\alpha_V L_R)^{1/2}/b)>10$ (in this limit h^*_{inf}->0 and $h = h^*_{cor}$). Note also that Figures 3-7 through 3-9 exhibit a very weak dependence on (H/H_w), except when $(H/b) \approx 1$ and $((\alpha_V L_R)^{1/2}/b) < 1$.

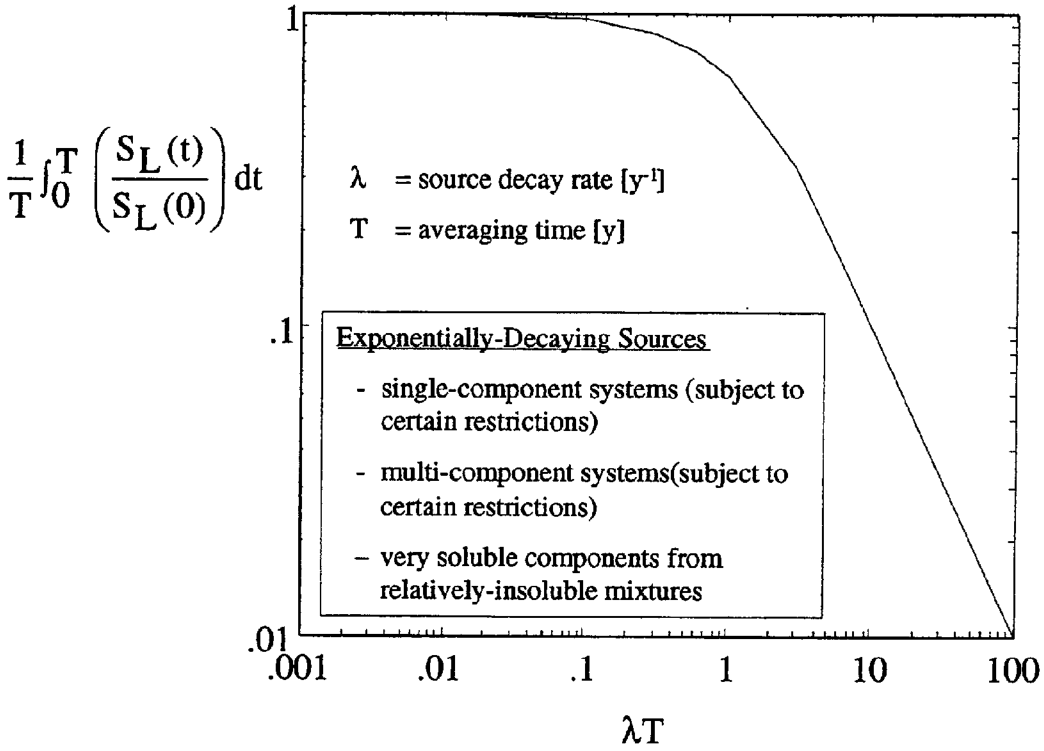
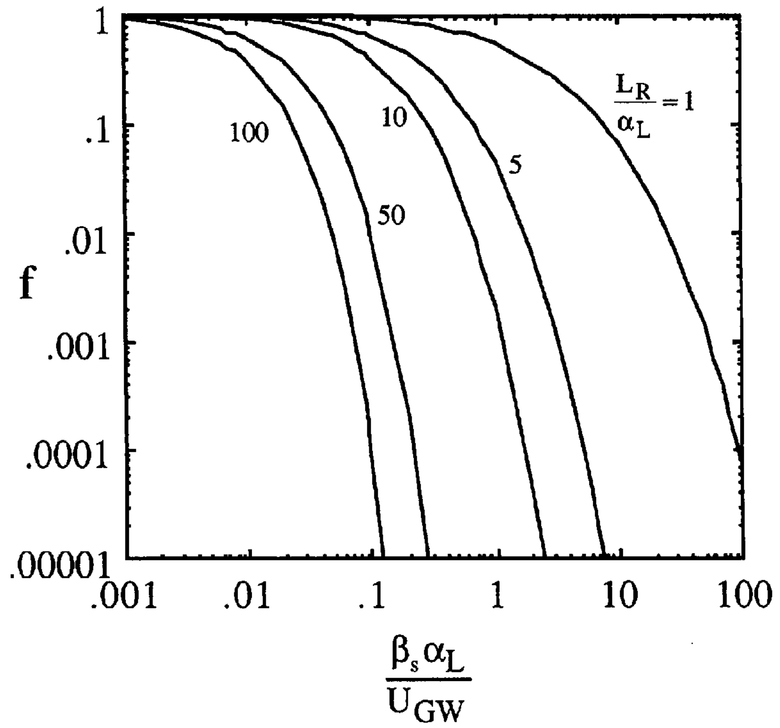


Figure 3-3. Source decay factor for exponentially-decaying sources (see Chapter 6 for calculation of decay rates and similar graphs for other idealized source decay models)



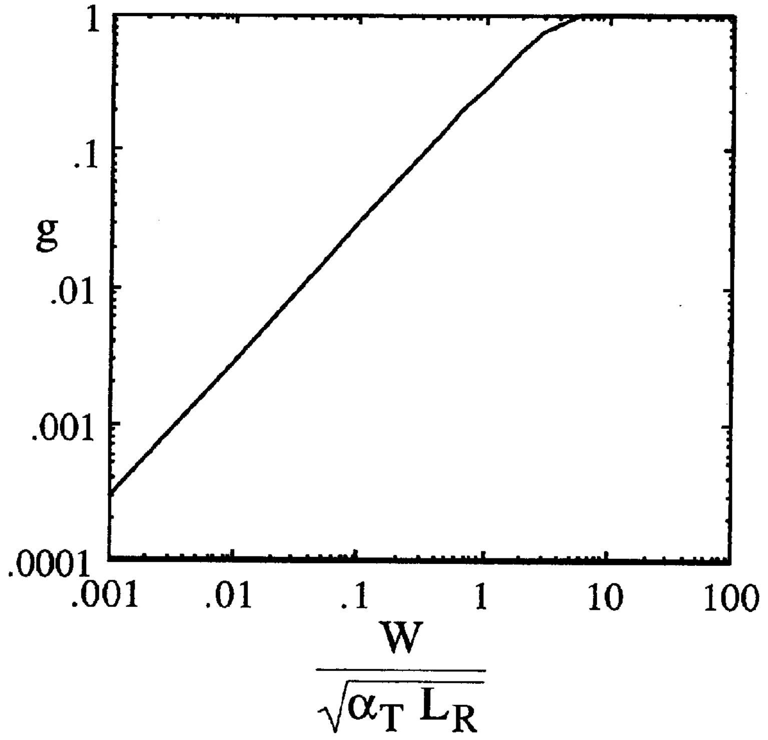
β_s = first-order biodegradation rate constant [d^{-1}]

α_L = longitudinal dispersivity ($\approx L_R/10$) [m]

U_{GW} = groundwater seepage velocity [m/d]

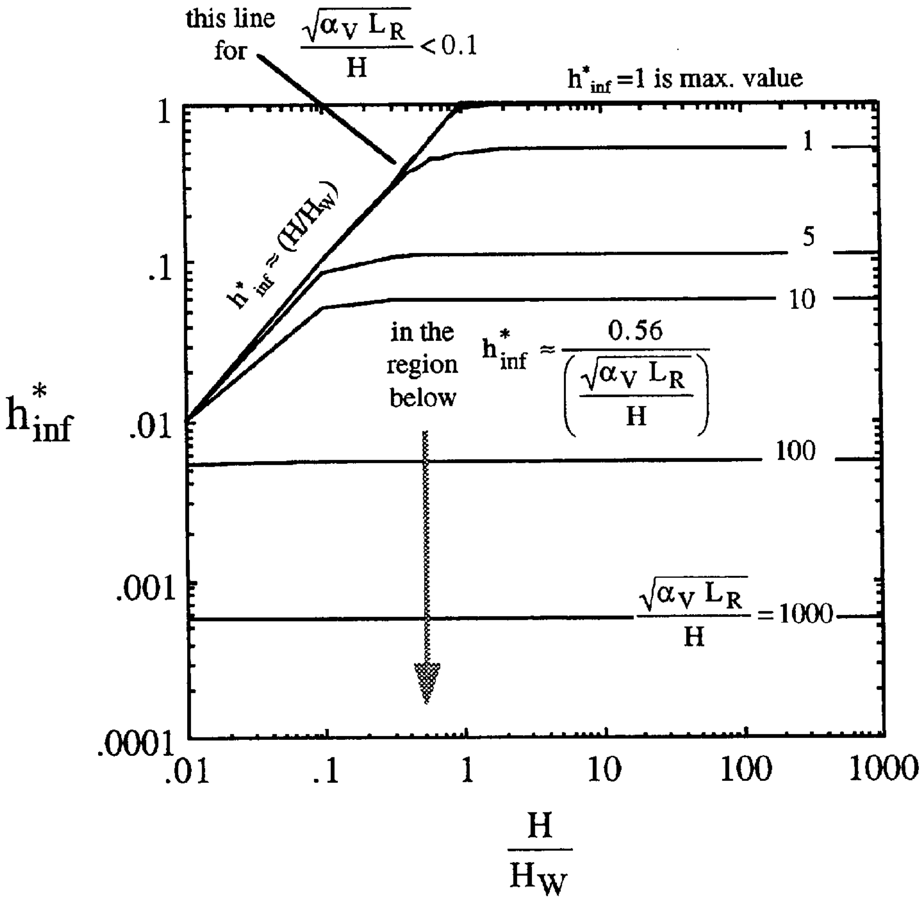
L_R = distance to receptor [m]

Figure 3-4. Longitudinal dispersion/bio-decay factor (f) for submerged sources



W = source width perpendicular to groundwater flow [m]
α_T = transverse dispersivity ($\approx 0.03\ L_R$) [m]
L_R = distance from downgradient edge of source to receptor [m]

Figure 3-5. Transverse dispersion (lateral spreading) factor (g) for submerged sources



H = vertical source thickness [m]
α_V = vertical dispersivity ($\approx 0.01\ L_R$) [m]
H_W = well screen interval thickness [m]
L_R = distance to receptor [m]
b = aquifer thickness [m]

Figure 3-6. Vertical mixing factor (h^*_{inf}) for an infinitely thick aquifer. Each line gives h^*_{inf} as a function of H/H_W for a different value of $(\alpha_V L_R)^{1/2}/H$, with accompanying simple estimation equations for interpolating for other values of $(\alpha_V L_R)^{1/2}/H$. Note that $h^* = h^*_{inf} + h^*_{cor}$ must be $\geq (H/b)$

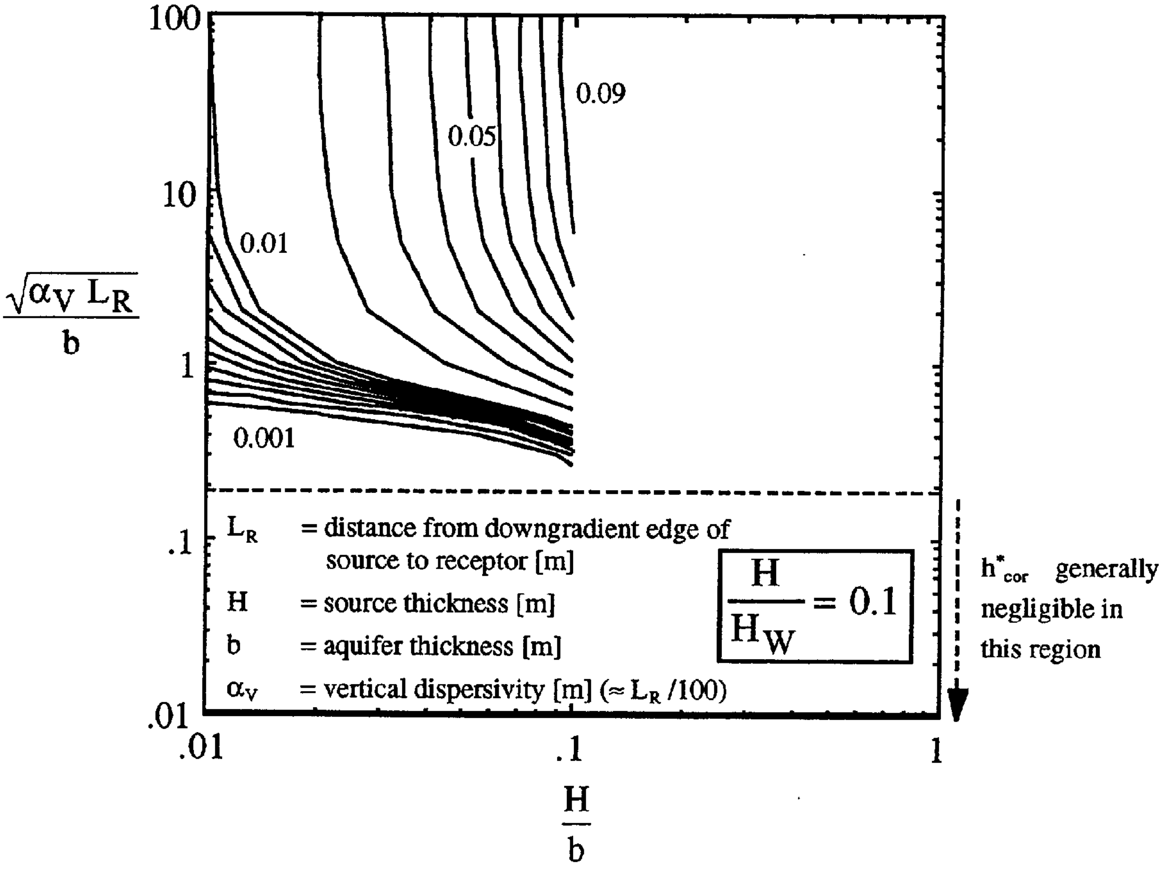


Figure 3-7. Vertical mixing correction factor (h^*_{cor}) for finite thickness aquifers, for $H/H_w=0.1$. Note that $h^* = h^*_{inf} + h^*_{cor}$ must be $\geq (H/b)$

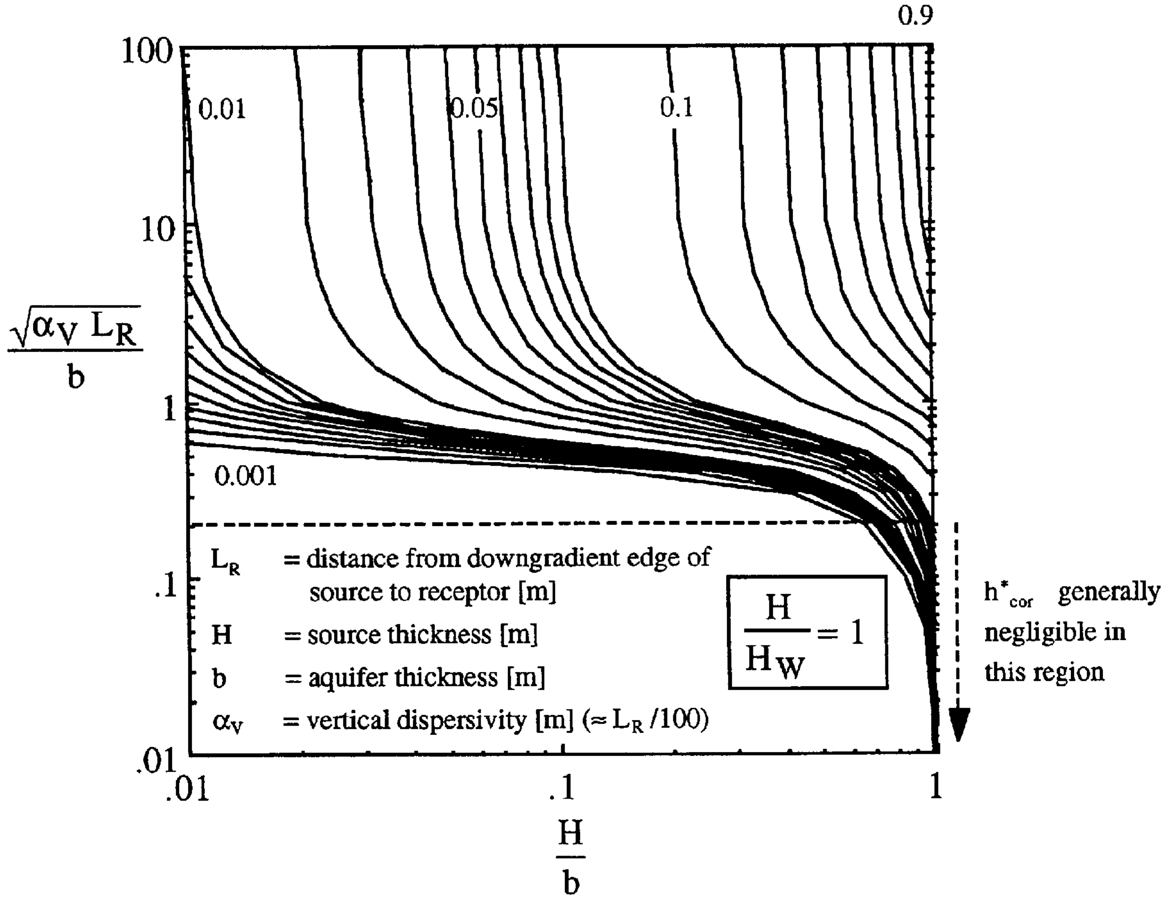


Figure 3-8. *Vertical mixing correction factor (h^*_{cor}) for finite thickness aquifers, for $H/H_w=1.0$. Note that $h^* = h^*_{inf} + h^*_{cor}$ must be $\geq (H/b)$*

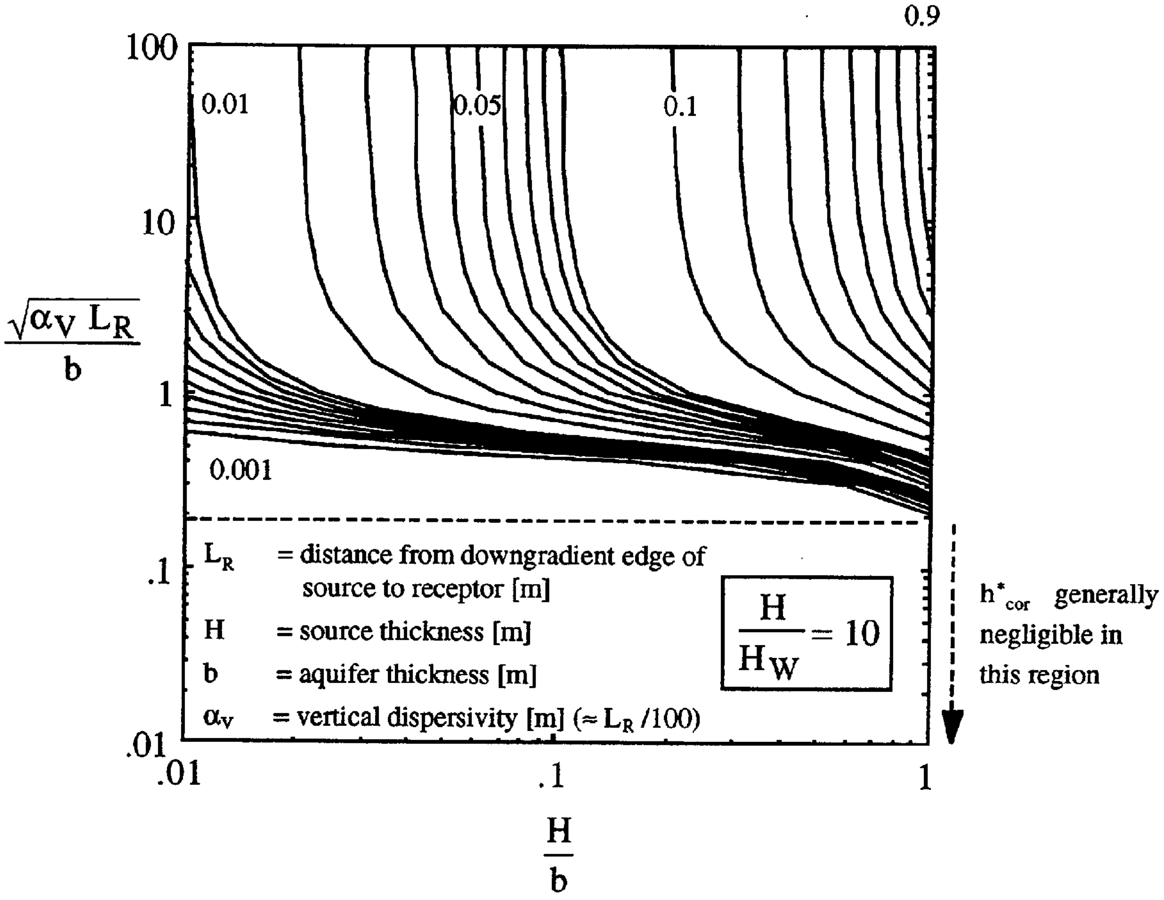


Figure 3-9. Vertical mixing correction factor (h^*_{cor}) for finite thickness aquifers, for $H/H_w=10$. Note that $h^* = h^*_{inf} + h^*_{cor}$ must be $\geq (H/b)$

CHAPTER 4

VADOSE ZONE SOURCES

4.1 INTRODUCTION

Chapter 3 focused on hydrocarbon-contaminated source soils that directly contact groundwater. That is one of the two general scenarios that might be encountered in practice. The second is the case where source zone soils are located entirely above the water table as shown below in Figure 4-1. This situation might be encountered at surface impoundments, landfills, and arid regions where the depth to groundwater is large. These vadose zone sources are the focus of this chapter.

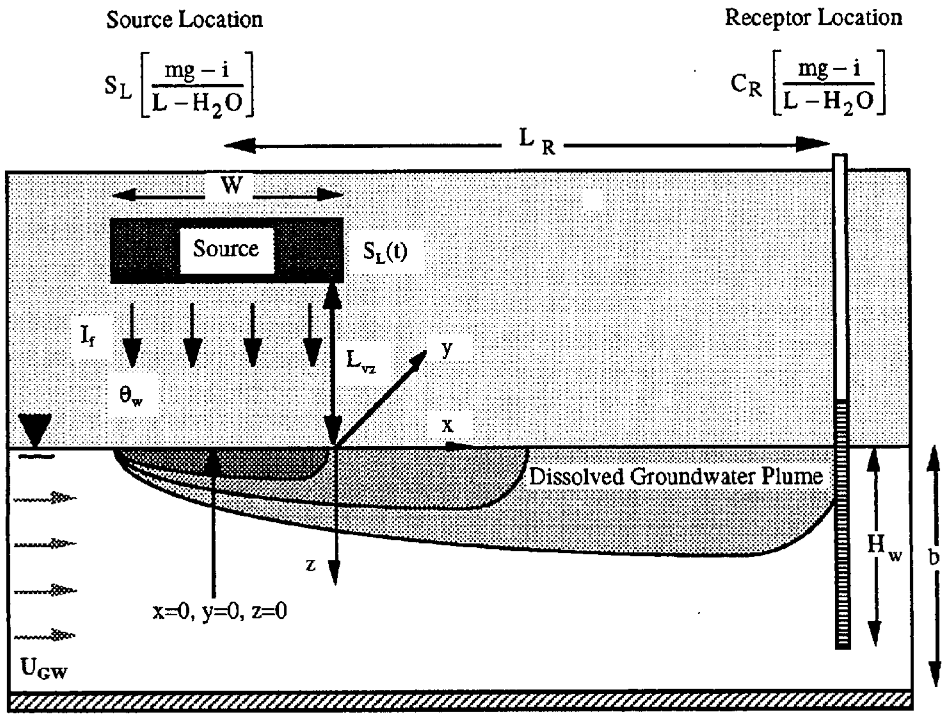


Figure 4-1. Generalized vadose zone source schematic

As in Chapter 3, the goal here is to first develop a mathematical framework for estimating dilution attenuation factors (DAFs) for vadose zone sources. Once this framework is developed, it will be used to create a more simplified graphical approach for determining DAFs.

In the case of vadose zone sources, chemical transport through both the vadose and saturated zones must be addressed. Here a compartmental model is constructed by modeling chemical transport through the vadose and saturated zones independently, and then coupling these models by requiring mass conservation across the water table boundary between the two regions.

4.2 UNSATURATED ZONE TRANSPORT MODEL

Many researchers have presented models of water flow and/or solute transport through the unsaturated zone (Nachabe *et al.*, 1995; Broadbridge and White, 1988; McWhorter and Sunada, 1990; Barry *et al.*, 1993; van Genuchten and Alves, 1982). In general, one must consider many fundamental processes (leaching, sorption, vapor migration, etc.) that contribute to chemical migration in the vadose zone. With respect to downward migration to groundwater, most have assumed that advective water flow is the most significant mechanism. This convention has been followed and only allows for downward migration via infiltrating soil moisture. Other mechanisms were considered however, and the reader will find a discussion of the estimated contribution of vapor transport to downward chemical migration in Appendix C.

The most simplistic water infiltration and solute transport models neglect transient rainfall events and seasonal changes, and simply assume constant and uniform infiltration. This infiltration rate I_f [m/d] is then set equal to the time-averaged infiltration rate (generally a yearly average). Consistent with this assumption, it is also convenient to approximate solute transport in the vadose zone as being one-dimensional, to neglect dispersion, and to approximate any chemical degradation reactions as being first-order with respect to each chemical's concentration. In this case, the solution to the General Transport Equation (2-3) for the mass flux $M_s(t)$ [mg_i /m^2-d] of chemical "i" into the aquifer is given by:

$$M_s(t) = L\,W\,I_f\,S_L(t - R_{vz}\,T_{vz})\,H(t - R_{vz}\,T_{vz})\;e^{-\beta_{vz}\,T_{vz}} \qquad (4\text{-}1)$$

where:

$M_s(t)$ = mass flux of solute "i" reaching the groundwater table at time t [mg_i /m^2-d]
L = length of source zone [m]
W = width of source zone [m]

I_f = time-averaged water infiltration rate per unit area [m/d]
$S_L(t - T_{vz} R_{vz})$ = source zone leachate concentration at time = $(t - T_{vz} R_{vz})$ [mg_i/m^3-H_2O]
$H(t - T_{vz} R_{vz})$ = Heaviside step function (=0 if $(t - T_{vz} R_{vz})<0$; =1 if $(t - T_{vz} R_{vz})>0$)
t = time [d]
T_{vz} = time for soil moisture to travel from the source zone to the water table [d]
β_{vz} = first-order chemical degradation rate constant in vadose zone[d^{-1}]
R_{vz} = vadose zone chemical-specific retardation factor [unitless]

At this point, it is useful to pause and reflect on the possible use of Equation (4-1) in the development of this graphical approach, and parameters required for its use. First, there are the parameters L and W dictated by the geometry of the source zone, which can be reasonably estimated given typical site characterization data. Second, there is the time-averaged water infiltration rate I_f, which can also be reasonably estimated if one has some knowledge of the soil types, annual precipitation and irrigation, and surface cover. The reader is referred to Appendix A for estimates of time-averaged infiltration rates for different regions of the United States. Third, Equation (4-1) requires knowledge of how the source depletes with time, which is the focus of Chapter 6. The absence of site-specific data is not too much of a hindrance here, however, as the user can always conservatively default to a constant-strength source and neglect solute degradation. Then the user need only estimate the source geometry and infiltration rate.

Of the remaining parameters, the delay time ($=T_{vz} R_{vz}$) is of little relevance when considering the maximum time-averaged aquifer impact, as discussed in §2.5. The delay time is important, however, in predicting how long it will take leachate to reach the aquifer.

This leaves the parameters β_{vz} and T_{vz} for discussion. One might treat these as a single parameter appearing in the exponential of Equation (4-1), or one could expand this grouping by inserting the following for T_{vz}:

$$T_{vz} = L_{vz}\, \phi_m / I_f \qquad (4\text{-}2)$$

where:

T_{vz} = time for soil moisture to travel from the source zone to the water table [d]
L_{vz} = vertical distance between source zone and water table [m]
ϕ_m = volumetric water content in vadose zone [m^3-water/m^3-soil]

I_f = time-averaged water infiltration rate per unit area [m/d]

Unfortunately, there are limited data available to guide the selection of the first-order degradation rate β_{vz}. Therefore, at this time, it is best to simply treat the quantity $\beta_{vz}T_{vz}$ as a single lumped fitting parameter to be determined on a site-specific basis.

In the future, however, as field methods for assessing vadose zone degradation are developed and more data are collected, it may be possible to independently determine all the quantities inherent in this lumped parameter.

For example, the volumetric soil moisture content in the vadose zone ϕ_m would have to be estimated. This could be accomplished by assuming that infiltration occurs primarily under an average unit hydraulic gradient, so that the water infiltration rate is equal to the unsaturated hydraulic conductivity at the ambient water content:

$$I_f = K_{sv}\, k_{rw} \tag{4-3}$$

where

K_{sv} = saturated hydraulic conductivity of soil in the vertical direction [m/d]
k_{rw} = relative permeability of the soil [unitless]

Studies have shown that the relative permeability, k_{rw}, is a function of the volumetric water content. Using the Brooks and Corey (1964) soil characteristic model, combined with the Burdine (1953) equations, the relative permeability function is given by:

$$k_{rw} = \left(\frac{\phi_m - \phi_{mr}}{n - \phi_{mr}} \right)^{3 + \frac{2}{\omega}} \tag{4-4}$$

where ϕ_{mr} is the irreducible water content [m^3-water/m^3-soil] and ω is the pore size distribution index as described by Brooks and Corey (1964). Using Equations (4-3) and (4-4), the vadose zone volumetric water content, ϕ_m, and infiltration rate, I_f, are then related through:

$$\phi_m = \phi_{mr} + (n - \phi_{mr})\left(\frac{I_f}{K_{sv}}\right)^{\frac{\omega}{3\omega+2}} \qquad (4\text{-}5)$$

If the reader is interested in assessing the time required for dissolved chemicals to reach the aquifer (=T_{vz} R_{vz}), T_{vz} would be calculated from Equations (4-2), (4-5) and:

$$R_{vz} = 1 + \frac{\rho_b \, f_{oc,v} \, K_{oc}}{\phi_m} \qquad (4\text{-}6)$$

which assumes that partitioning of chemicals into the gaseous phase can be neglected relative to sorption between the soil moisture and soil surfaces. Here, ρ_b [kg_{soil} /m^3] is the soil bulk density; K_{oc} [(mg_i /kg_{soil})/(mg_i /L-H_2O)] is the chemical-specific soil-organic carbon partition coefficient (see Appendix A); and f_{oc} [$kg_{organic\ carbon}$ /kg_{soil}] is the fraction of organic carbon in the soil (see Appendix A). Equation (4-6) also assumes that no immiscible-phase hydrocarbon liquids are present in soils between the source zone and the aquifer.

4.3 SATURATED ZONE TRANSPORT MODELS

There are a number of mathematical models available in the literature for describing the migration of dissolved chemical (solute) plumes. The simplest of these are the point-source plume models (Bear, 1979; Hunt, 1983; Wilson and Miller, 1978), which are useful for predicting the time development of a plume from a continuous source, or one-time point source input. In such models, infinite solute concentrations at the point source are necessary to introduce a finite chemical mass flux to the aquifer. Point-source models, therefore, are best for predicting dissolved plume behavior far from the source and are unlikely to yield reasonable predictions near the actual source location. Line-source models have also been developed (Javandel *et al.*, 1984; Ogata, 1970) and these have advantages and limitations similar to those of the point-source models.

If one is interested in predicting concentrations near the source as well as in the far-field, then a source of finite size must be considered. Vertical plane source models have been developed by researchers over the years (Domenico and Palciauskas, 1982; Ogata, 1970; Codell and Schreiber, 1972), and are often used to model contaminant sources present within the saturated zone, as in Chapter 2. Such an approach could be used for vadose zone source scenarios, but it would require the development of an additional mixing zone model to define the groundwater source zone size and concentration. This generally introduces a new unknown parameter - the mixing zone thickness, which is either arbitrarily assigned a value, or is chosen based on consideration of water table fluctuations or other site characteristics.

When considering vadose zone impacted soils, landfills, surface impoundments, or land treatment systems, the leachate percolates down through the vadose zone and enters at the aquifer through the water table. In this case, horizontal plane source models appear to be a reasonable choice.

Carslaw and Jaeger (1959) used Green's functions for the solution of the three dimensional advection-dispersion equation (Equation 2-3). Codell and Schreiber (1977) and Yeh (1981) also utilized Green's functions to develop dispersive transport models for groundwater. However, Codell and Schreiber (1977) did not consider a horizontal plane source. Gayla (1987) adapted previous work in this area, and presented a complete horizontal plane source model. It is this model that is adopted in this work.

4.4 HORIZONTAL PLANE SOURCE (HPS) MODEL

The horizontal plane source (HPS) model is a transient model derived from an analytical solution to the three-dimensional advection-dispersion equation. The source is modeled as a horizontal plane of length L [m], width W [m], and uniformly distributed strength $M_s(t)$ [mg_i /d] as shown in Figure 4-2. The groundwater seepage velocity is denoted U_{GW} [m/d] and b [m] is the aquifer thickness. The coordinate system is centered in the source area at the water table with the x-, y-, and z-coordinates oriented along the direction of groundwater flow, transverse to flow, and in the vertical direction, respectively.

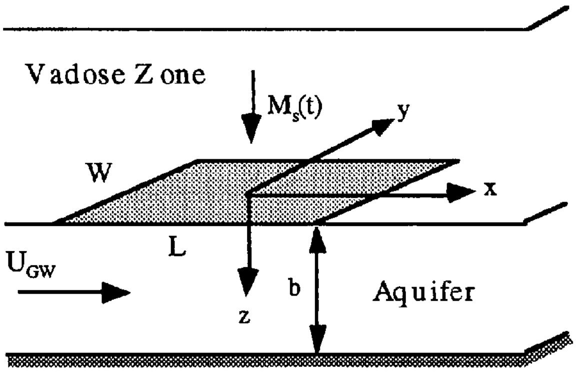


Figure 4-2. Horizontal Plane Source (HPS) Model geometry

The HPS solution developed by Galya (1987) is based on the following simplifications and assumptions:

- the aquifer is homogenous, isotropic, and initially contaminant free;
- the groundwater flow field is one-dimensional in the horizontal x-direction, and at steady-state (i.e., the groundwater velocity is constant with time and space);
- the aquifer thickness b is constant and the aquifer is infinite in horizontal extent;
- the chemical is present only in the aqueous phase or sorbed to aquifer solids; and
- chemical and/or biochemical transformations are described as a first-order process.

With these assumptions, Galya's solution can be written:

$$C(x,y,z,t) = \frac{1}{\phi_s R_s} \int_0^t M_s(\tau) X_0(x,t-\tau) Y_0(y,t-\tau) Z_0(z,t-\tau) T(t-\tau)\, d\tau \qquad (4\text{-}7)$$

where:

$$X_0(x,t) = \frac{1}{2L}[\mathrm{erf}\left(\frac{\frac{L}{2} + x - \frac{U_{GW}\, t}{R_S}}{\sqrt{4\alpha_L U_{GW}\, t / R_s}}\right) + \mathrm{erf}\left(\frac{\frac{L}{2} - x - \frac{U_{GW}\, t}{R_S}}{\sqrt{4\alpha_L U_{GW}\, t / R_s}}\right)] \qquad (4\text{-}8)$$

$$Y_0(y,t) = \frac{1}{2W}[\mathrm{erf}\left(\frac{\frac{W}{2} + y}{\sqrt{4\alpha_T U_{GW}\, t / R_s}}\right) + \mathrm{erf}\left(\frac{\frac{W}{2} - y}{\sqrt{4\alpha_T U_{GW}\, t / R_s}}\right)] \qquad (4\text{-}9)$$

$$Z_o(z,t) = \frac{1}{\sqrt{\pi \alpha_V U_{GW} t / R_s}} \sum_{n=-\infty}^{n=\infty} [\exp(\frac{-(2nb - z)^2}{4\alpha_V U_{GW} t / R_s})] \quad (4\text{-}10)$$

$$T(t) = \exp(-\beta_s t / R_s) \quad (4\text{-}11)$$

where:

C = solute concentration [mg$_i$ /L-H$_2$O]
K_d = soil-water partition coefficient [L-H$_2$O/kg-soil]
U_{GW} = groundwater seepage velocity in x-direction [m/d]
R_s = saturated zone solute retardation factor = $1 + \rho_b K_d / \phi_s$ [unitless]
t = time [d]
x = coordinate along the axis parallel to direction of flow [m]
y = coordinate along the axis transverse to direction of flow [m]
z = coordinate along the axis perpendicular to direction of flow [m]
α_L = dispersivity in the x direction (longitudinal) [m]
α_T = dispersivity in the y direction (transverse) [m]
α_V = dispersivity in the z direction (vertical) [m]
β_s = first-order saturated zone solute decay rate [d^{-1}]
ϕ_s = aquifer moisture content (assumed equal to porosity) [L-H$_2$O/L-soil]
ρ_b = soil bulk density [kg-soil/L-soil]
τ = dummy integration variable [d]

The mass loading $M_s(t)$ [mg$_i$ /d] was defined previously by Equation (4-1) in §4.2.

4.5 DAF FORMULATION FOR VADOSE ZONE SOURCES

Recall that in Chapter 2, the following mathematical approximation (Equation (2-9) was adopted:

$$\text{DAF} = \frac{1}{\left\{\frac{1}{T}\int_0^T \frac{S_L(t)}{S_L(0)}\,dt\right\} \text{x} \left\{\frac{1}{H_w}\int_0^{Hw} C^*_{cs}(L_R, 0, z, \infty)\,dz\right\}} \quad (4\text{-}12)$$

where:

T = averaging time [d]

$S_L(t)$ = source zone leachate strength at time t [mg_i /L-H_2O]

t = time [d]

H_w = well screen thickness [m]

$C^*_{cs}(L_R,0,z,\infty)$ = steady-state solute concentration at receptor distance L_R for constant-strength source of unit concentration [unitless]

Using Equations (4-1) and (4-7) through (4-11), one can write:

$$C^*_{cs}(x,y,z,\infty) = \frac{L\,W\,I_f\,e^{-\beta_{vz}T_{vz}}}{\phi_s R_s} \int_0^\infty X_o(x,\tau)\,Y_o(y,\tau)\,Z_o(z,\tau)\,T(\tau)\,d\tau \tag{4-13}$$

and:

$$\frac{1}{H_w}\int_0^{H_w} C^*_{cs}(L_R,0,z,\infty)\,dz =$$

$$\frac{I_f\,e^{-\beta_{vz}T_{vz}}}{H_w\,\phi_s}\int_0^{H_w}\int_0^\infty \{\frac{1}{2}[\mathrm{erf}\left(\frac{\frac{L}{2}+L_R-U_{GW}\tau}{\sqrt{4\alpha_L U_{GW}\tau}}\right)+\mathrm{erf}\left(\frac{\frac{L}{2}-L_R-U_{GW}\tau}{\sqrt{4\alpha_L U_{GW}\tau}}\right)]\bullet \tag{4-14}$$

$$[\mathrm{erf}\left(\frac{W}{\sqrt{\alpha_T U_{GW}\tau}}\right)]\bullet\ \frac{1}{\sqrt{\pi\alpha_V U_{GW}\tau}}\sum_{n=-\infty}^{n=\infty}[\exp(\frac{-(2nb-z)^2}{4\alpha_V U_{GW}\tau})]\ e^{-\beta_s\tau}\}\,d\tau\,dz$$

where L_R [m] is the distance from the center of the source zone to the receptor location. Variable transforms have been used to eliminate (t-τ) and R_s from Equations (4-7) through (4-11) when deriving Equations (4-13) and (4-14).

Equation (4-14) is dependent on L, W, I_f, ϕ_s, H_w, U_{GW}, L_R, α_L, α_T, α_V, and b. Rewriting Equation (4-14) in terms of the dimensionless variables:

$$Z = z/H_w \tag{4-15a}$$

$$\tau^* = \tau\,U_{GW}/L_R \tag{4-15b}$$

yields the following expression:

$$\frac{1}{H_w}\int_0^{H_w} C_{cs}^*(L_R, 0, z, \infty)\,dz =$$

$$\left(\frac{I_f}{U_{Gw}\,\phi_s}\right) e^{-\beta_{vz} T_{vz}} \int_0^1 \int_0^\infty \{\frac{1}{2}[\mathrm{erf}\left(\frac{\frac{1}{2}\left(\frac{L}{L_R}\right)+1-\tau^*}{\sqrt{4(\alpha_L / L_R)\tau^*}}\right) + \mathrm{erf}\left(\frac{\frac{1}{2}\left(\frac{L}{L_R}\right)-1-\tau^*}{\sqrt{4(\alpha_L / L_R)\tau^*}}\right)] \bullet \tag{4-16}$$

$$[\mathrm{erf}\left(\frac{(W / L_R)}{\sqrt{(\alpha_T / L_R)\tau^*}}\right)] \bullet$$

$$\frac{1}{\sqrt{\pi(\alpha_V / L_R)\tau^*}} \sum_{n=-\infty}^{n=\infty} [\exp(\frac{-\left(\frac{H_w}{L_R}\right)^2 (2n\left(\frac{b}{H_w}\right) - Z)^2}{4(\alpha_V / L_R)\tau^*})]\; e^{-\left(\frac{\beta_s L_R}{U_{GW}}\right)\tau^*}\}\, d\tau^*\, dZ$$

Equation (4-16) is a function of 10 dimensionless parameter groups:

$$\left(\frac{I_f}{U_{Gw}\,\phi_s}\right), (\beta_{vz} T_{vz}), \left(\frac{L}{L_R}\right), \left(\frac{\alpha_L}{L_R}\right), \left(\frac{\alpha_T}{L_R}\right), \left(\frac{\alpha_V}{L_R}\right), \left(\frac{W}{L_R}\right), \left(\frac{H_W}{L_R}\right), \left(\frac{b}{H_W}\right), \left(\frac{\beta_s L_R}{U_{GW}}\right) \tag{4-17}$$

Nine of these appear within the integrand of Equation (4-16).

In order to present a graphical solution to Equation (4-12), it is necessary to further reduce the number of parameters in Equation (4-16). To this end:

- The source length, L, and width, W, are reduced to a single length with the assumption that the source area can be approximated by a square. Then the length and width can be related to the source area, A [m^2], with $L = W = \sqrt{A}$.

- A further reduction in parameters can be achieved by relating the dispersivities, α_L, α_T, and α_V to the distance L_R between the source and receptor, as discussed below.

Characterization of aquifer dispersivities is extremely difficult and information on dispersivities is unavailable at most sites. Through a survey of available data, Gelhar, *et al.* (1992) demonstrated that longitudinal dispersivities increase as the scale of the observation increases. USEPA has used relationships between dispersivities and receptor distances when developing disposal regulations for hazardous wastes (e.g., Federal Register, 1986). Consistent with this methodology:

$$\alpha_L = \eta_L L_R \qquad (4\text{-}18a)$$

$$\alpha_T = \eta_T L_R \qquad (4\text{-}18b)$$

$$\alpha_V = \eta_V L_R \qquad (4\text{-}18c)$$

where $\eta_L = 0.1$, $\eta_T = 0.033$, and $\eta_V = 0.01$.

With these simplifications, Equation (4-16) reduces to:

$$\frac{1}{H_w}\int_0^{H_w} C^*_{cs}(L_R, 0, z, \infty)\,dz =$$

$$\left(\frac{I_f}{U_{Gw}\,\phi_s}\right) e^{-\beta_{vz} T_{vz}} \int_0^1 \int_0^\infty \{\frac{1}{2}[\mathrm{erf}\left(\frac{\frac{1}{2}\left(\frac{\sqrt{A}}{L_R}\right)+1-\tau^*}{\sqrt{4\eta_L\tau^*}}\right) + \mathrm{erf}\left(\frac{\frac{1}{2}\left(\frac{\sqrt{A}}{L_R}\right)-1-\tau^*}{\sqrt{4\eta_L\tau^*}}\right)] \bullet \qquad (4\text{-}19)$$

$$[\mathrm{erf}\left(\frac{(\sqrt{A}/L_R)}{\sqrt{\eta_T\tau^*}}\right)] \bullet \frac{1}{\sqrt{\pi\eta_V\tau^*}} \sum_{n=-\infty}^{n=\infty} [\exp(\frac{-\left(\frac{H_w}{L_R}\right)^2 (2n\left(\frac{b}{H_w}\right)-Z)^2}{4\eta_V\tau^*})]\; e^{-\left(\frac{\beta_s L_R}{U_{GW}}\right)\tau^*} \}d\tau^*\,dZ$$

which is now a function of six dimensionless parameter groups, four of which appear within the integral in Equation (4-19). To reduce the integral down to a function of three groups, the following mathematical approximation is proposed:

$$\frac{1}{H_w}\int_0^{H_w} C^*_{cs}(L_R,0,z,\infty)\,dz = <f(\frac{\sqrt{A}}{L_R},\frac{\beta_s L_R}{U_{GW}})> \bullet$$

$$\left(\frac{I_f}{U_{Gw}\,\phi_s}\right) e^{-\beta_{vz}\,T_{vz}} \int_0^1 \int_0^{\infty} \{\frac{1}{2}[\mathrm{erf}\left(\frac{\frac{1}{2}\left(\frac{\sqrt{A}}{L_R}\right)+1-\tau^*}{\sqrt{4\eta_L\,\tau^*}}\right)+\mathrm{erf}\left(\frac{\frac{1}{2}\left(\frac{\sqrt{A}}{L_R}\right)-1-\tau^*}{\sqrt{4\eta_L\,\tau^*}}\right)] \bullet \qquad (4\text{-}20)$$

$$[\mathrm{erf}\left(\frac{(\sqrt{A}/L_R)}{\sqrt{\eta_T\,\tau^*}}\right)] \bullet \frac{1}{\sqrt{\pi\,\eta_V\,\tau^*}} \sum_{n=-\infty}^{n=\infty} [\exp(\frac{-\left(\frac{H_w}{L_R}\right)^2 (2n\left(\frac{b}{H_w}\right)-Z)^2}{4\,\eta_V\,\tau^*})]\}\,d\tau^*\,dZ$$

In writing Equation (4-20), Equation (4-19) is used for the case of no solute degradation (β_s=0), and then multiplied that result by the function <f>, which is a spatial average of the function f that was introduced in Chapter 3. There, f accounted for degradation along the plume centerline, downgradient of a vertical planar source. In §4.9 the validity of this approximation will be examined.

By rearranging some of the parameter groups, Equation (4-20) can be written in the form:

$$\frac{1}{H_w}\int_0^{H_w} C^*_{cs}(L_R,0,z,\infty)\,dz = <f(\frac{\sqrt{A}}{L_R},\frac{\beta_s L_R}{U_{GW}})> \bullet \left(\frac{I_f}{U_{Gw}\,\phi_s}\right) \bullet V(\beta_{vz}\,T_{vz}) \bullet \Gamma(\frac{A}{b^2},\frac{L_R}{b},\frac{H_w}{b}) \qquad (4\text{-}21)$$

where:

$$<f> = \int_{-1/2}^{1/2} \exp[5(1-\sqrt{1+0.4(\frac{\beta_s L_R}{U_{GW}})[1-\frac{\sqrt{A}}{L_R})X]})]\,dX \quad ; \quad \frac{\sqrt{A}}{L_R}<2$$

$$(4\text{-}22a)$$

$$<f> = \frac{1}{(\frac{1}{2}+\frac{L_R}{\sqrt{A}})} \int_{-1/2}^{\frac{L_R}{\sqrt{A}}} \exp[5(1-\sqrt{1+0.4(\frac{\beta_s L_R}{U_{GW}})[1-\frac{\sqrt{A}}{L_R})X]})]\,dX \quad ; \quad \frac{\sqrt{A}}{L_R}>2$$

$$V(\beta_{vz}\,T_{vz}) = e^{-\beta_{vz}\,T_{vz}} \qquad (4\text{-}22b)$$

$$\Gamma\left(\frac{A}{b^2},\frac{L_R}{b},\frac{H_w}{b}\right)=$$

$$\int_0^1\int_0^\infty\left\{\frac{1}{2}\left[\mathrm{erf}\left(\frac{\frac{1}{2}\left(\frac{\sqrt{A}}{b}\right)\left(\frac{b}{L_R}\right)+1-\tau^*}{\sqrt{4\eta_L\tau^*}}\right)+\mathrm{erf}\left(\frac{\frac{1}{2}\left(\frac{\sqrt{A}}{b}\right)\left(\frac{b}{L_R}\right)-1-\tau^*}{\sqrt{4\eta_L\tau^*}}\right)\right]\bullet\right. \tag{4-22c}$$

$$\left.\left[\mathrm{erf}\left(\frac{\left(\frac{\sqrt{A}}{b}\right)\left(\frac{b}{L_R}\right)}{\sqrt{\eta_T\tau^*}}\right)\right]\bullet\frac{1}{\sqrt{\pi\eta_V\tau^*}}\sum_{n=-\infty}^{n=\infty}\left[\exp\left(\frac{-\left(\frac{H_w}{b}\right)^2\left(\frac{b}{L_R}\right)^2\left(2n\left(\frac{b}{H_w}\right)-Z\right)^2}{4\eta_V\tau^*}\right)\right]\right\}d\tau^*dZ$$

At this point, one final substitution is made:

$$\Gamma\left(\frac{A}{b^2},\frac{L_R}{b},\frac{H_w}{b}\right)=\Omega\left(\frac{A}{b^2},\frac{L_R}{b}\right)\bullet\sigma\left(\frac{A}{b^2},\frac{L_R}{b},\frac{H_w}{b}\right) \tag{4-23}$$

where the value of the function Ω is equal to the maximum value of Γ evaluated at any distance from the source. It is obtained by solving Γ for the case of $(H_w/b)=0$, which yields the point value of this function at the water table ($z=0$). The function σ then is a correction factor for vertically averaging across the well screen. The function σ can be viewed as a factor which represents how much the point concentration at the water table will be diluted by vertically averaging point concentrations over a well screening interval. The function Ω is easily displayed in a two-dimensional contour plot, while σ must be displayed as a sequence of graphs. At this point, Equation (4-12) can now be written as follows:

$$DAF=\frac{1}{\left\{\frac{1}{T}\int_0^T\frac{S_L(t)}{S_L(0)}dt\right\}\mathrm{x}<f>\mathrm{x}\left(\frac{I_f}{\phi_s U_{Gw}}\right)\mathrm{x}\,V\,\mathrm{x}\,\Omega\,\mathrm{x}\,\sigma} \tag{4-24}$$

4.6 ALTERNATE WELL CONFIGURATIONS

The analysis presented above implicitly assumes a well that is constructed as shown in Figure 4-1, where the well screen extends from the upper boundary of the water table to a depth H_w below the water table. While this is the most common case encountered in practice, occasionally one will encounter situations shown in Figure 4-3, where the well is screened over some intermediate interval extending from a depth H_{w1} to a depth H_{w2}. In this case, the graphical approach can still be used, with the following modification - the appropriate value of σ to use is:

$$\sigma = \frac{1}{(H_{w2} - H_{w1})}[H_{w2}\,\sigma(H_{w2}) - H_{w1}\,\sigma(H_{w1})] \tag{4-25}$$

where $\sigma(H_{w1})$ denotes the value of σ calculated from the graphs for a value of $H_w = H_{w1}$.

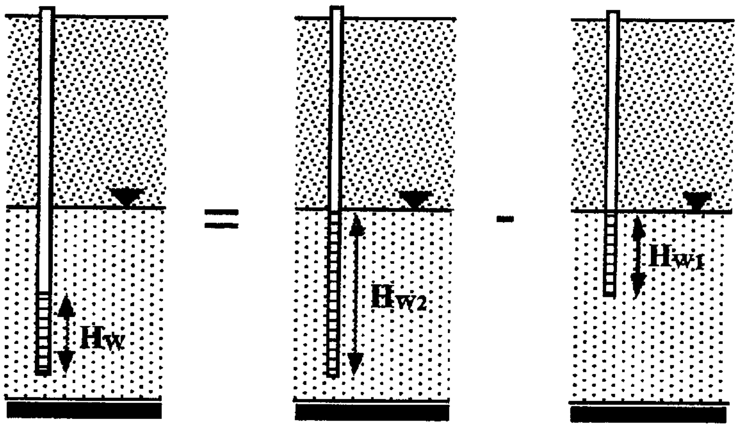


Figure 4-3. Alternate well construction configuration and graphical representation of calculation method given in Equation (4-25)

4.7 NUMERICAL METHODS

Solutions to, and graphs of, Equations (4-22a) and (4-22b) were generated with Mathematica® (Wolfram Research) and Microsoft Excel®. Solutions to Equations (4-22c) and (4-23) were generated with Fortran programs. Details of these are discussed in Appendix D.

4.8 VADOSE ZONE SOURCE DAF GRAPHS

Figures 4-4 through 4-12 present graphs of the functions defined above in Equations (4-22) and (4-23).

Figure 4-4 presents the source decay factor for the case of an exponentially-decaying source. A discussion of idealized model source types and methods for estimating decay rates is the focus of Chapter 6. Figure 4-4 indicates that, for the case of an exponentially decaying source, the source decay factor remains essentially equal to unity until the averaging time (T) times the first-order source decay factor (λ) is greater than ≈ 1. Thus, one need not consider correcting for decaying sources unless the averaging time $T > 1/\lambda$. In other words, one may treat the source as a steady source (or infinite source), as long as $T < 1/\lambda$. This is also roughly equivalent to saying that one need not be concerned with correcting for decaying sources unless the averaging time T exceeds one half-life, where the half-life $t_{1/2} = \ln 2/\lambda$. This figure is identical to the submerged source Figure 3-3 appearing in Chapter 3.

Figure 4-5 presents the vadose zone degradation function V defined by Equation (4-22b). It is a simple exponential function of the quantity ($\beta_{vz} T_{vz}$). As stated above, there are currently limited data available for guiding the selection of β_{vz}, thus at this time it may be best to treat the quantity ($\beta_{vz} T_{vz}$) as a single lumped fitting parameter to be determined on a site-specific basis.

Figure 4-6 presents the dependence of the factor <f> on the parameters ($\beta_s L_R/U_{GW}$) and (W/L_R). Here W ($=A^{1/2}$) is the source length. When (W/L_R)<2, <f> is not very sensitive to changes in (W/L_R), and the (W/L_R)<2 curves are comparable to the submerged source biodecay-factor Figure 3-4 appearing in Chapter 3, for the special case of $\alpha_L = \eta_L L_R$ and $\eta_L = 0.1$. The <f> factor accounts for dissolved plume attenuation due to first-order chemical reactions (e.g., biodegradation). Of significance in Figure 4-6 is the dependence of <f> on ($\beta_s L_R/U_{GW}$). Note that, for ($\beta_s L_R/U_{GW}$)>0.1, the factor <f> is extremely sensitive to small changes in ($\beta_s L_R/U_{GW}$), unless the receptor is located beneath the source ((W/L_R)>2). Changing ($\beta_s L_R/U_{GW}$) by one order of magnitude can change the value of <f> by two to three orders of magnitude. This observation has two implications:

- Chemical reaction (e.g. biodegradation), when it occurs, can be the most important attenuation mechanism (as evidenced by field observations of the differences between aromatic hydrocarbon and chlorinated solvent plumes); and
- It is critical that, if chemical reactions are to be considered when calculating a DAF, the parameter ($\beta_s L_R/U_{GW}$) must be estimated as accurately as possible as the final DAF value will be strongly influenced by small variations in ($\beta_s L_R/U_{GW}$). Incorrect determination of ($\beta_s L_R/U_{GW}$) can lead to under-, or over-prediction of the DAF value.

A graph of Ω appears in Figure 4-7 as a function of A/b^2 and L_R/b. The Fortran code used to generate the Ω values is included in Appendix D. The nomograph in Figure 4-7 has a predictable form; for a given receptor location, L_R, and aquifer thickness, b, the value of Ω increases as the source area, A, increases. This is expected since the mass input into the aquifer is directly related to the source area. If the values of A and b are assumed to be constant, Figure 4-7 shows that as the receptor distance, L_R, increases, receptor concentrations will decrease as expected. Finally, if A and L_R are held constant, inspection of the nomograph shows that as the aquifer thickness, b, increases, the receptor concentration will decrease. This, too, is expected since constituents will ultimately be diluted throughout a greater volume as the aquifer thickness increases.

Figures 4-8 through 4-13 include nomographs for the correction factor σ as a function of the parameters (H_w/b), (L_R/b) for a series of A/b^2 values (0.001, 0.01, 0.1, 1, 10, and 100). This correction factor represents the dilution in receptor concentration due to screening of the well into depths of the aquifer that may have constituent concentrations lower than those found at the water table. Consider a well screened over the entire aquifer depth, b. For receptor distances far from the source, or for shallow aquifers, the parameter L_R/b will be large. In either case, vertical mixing will yield uniform contaminant concentrations throughout the depth of the aquifer and the correction factor should approach a value of one. Conversely, when the parameter L_R/b is small, representing a small receptor distance or large aquifer thickness, constituents will not have penetrated the entire aquifer thickness. The correction factor should approach zero in this situation because vertical averaging of the point concentrations throughout the aquifer thickness will result in considerable dilution of the contaminant concentration found at the water table. Obviously, if one is interested only in the concentration found at the water table, then the correction factor is simply unity.

Figures 4-8 through 4-13 are consistent with this reasoning. As (H_w/b) approaches zero, the function Γ approaches Ω ($(H_w/b)=0$) corresponds to a point receptor located at the water table), and the correction factor σ approaches unity. As the well screening interval increases, the vertically averaged concentration decreases and the value of the correction factor becomes smaller and smaller, meaning that there is greater and greater correction to the value of Ω required. The correction factor nomographs also show that as the receptor distance, L_R, increases, constituents eventually become well-mixed throughout the aquifer depth and concentrations found at the water table are the same as those found at the bottom of the aquifer. For the parameter ranges considered in this research, the nomographs in Figures 4-8 through 4-13 show that aquifer concentrations essentially become vertically well-mixed when the value of L_R/b is greater than 10.

Also of significance is the apparent lack of sensitivity in σ values to changes in A/b^2, for $0.001 \le (A/b^2) \le 100$. One could practically use any of these six graphs to obtain a reasonable σ value for any given (H_w/b) and (L_R/b).

4.9 FIRST-ORDER DECAY CORRECTION FACTOR

During the development of the graphical approach for vadose zone sources, it was assumed that the exponential degradation function could be removed from the integral of Equation (4-19) and replaced by the multiplicative factor <f> appearing in Equation (4-20). The function <f> was defined in Equation (4-22a) to be:

$$<f> = \int_{-1/2}^{1/2} \exp[5(1-\sqrt{1+0.4(\frac{\beta_s L_R}{U_{GW}})[1-\frac{\sqrt{A}}{L_R})X]})] dX \quad ; \quad \frac{\sqrt{A}}{L_R} < 2$$

$$<f> = \frac{1}{(\frac{1}{2}+\frac{L_R}{\sqrt{A}})} \int_{-1/2}^{\frac{L_R}{\sqrt{A}}} \exp[5(1-\sqrt{1+0.4(\frac{\beta_s L_R}{U_{GW}})[1-\frac{\sqrt{A}}{L_R})X]})] dX \quad ; \quad \frac{\sqrt{A}}{L_R} > 2 \tag{4-22a}$$

and can be seen to depend on the parameters $(\beta_s L_R/U_{GW})$ and (W/L_R), where $W = A^{1/2}$ is the source zone length. This function is presented graphically in Figure 4-6.

This assumption was made in order to reduce the number of parameters appearing within the integral functions of Equation (4-19). While there are many possibilities, this approach was selected because:

- It is known from experience that groundwater transport solutions can be very sensitive to small changes in the parameter $(\beta_s L_R/U_{GW})$; and
- A functional dependence on the parameters $(\beta_s L_R/U_{GW})$ and (W/L_R) is suggested by the vertical planar source solution Equation (3-4).

Thus, Equation (4-22a) for <f> derives from Equation (3-9) for the function **f**. In this case, however, it is recognized that the source is distributed from $-W/2 < x < +W/2$ and that it is possible to calculate concentrations at positions beneath the source ($L_R < W/2$). To account for this, the function **f** is averaged over all x positions where the source may be introduced upstream of the receptor location. The first expression in Equation (4-22a) is appropriate for receptor positions outside the source zone ($L_R > W/2$) and the second is appropriate for receptor positions inside the source zone ($L_R < W/2$).

Approximate solution Equation (4-20) was compared with full numerical solutions of Equation (4-19) to investigate the validity of this assumption. Some of these results are presented below in Table 4-1 for a wide range of parameter values. The results suggest that Equation (4-20) provides a reasonable approximation to Equation (4-19) as long as $(\beta_s L_R/U_{GW}) < 50$. This condition should be satisfied in the majority of actual field settings, and so the approximation appears to be reasonable.

Table 4-1. Comparison of approximate and full solutions to Equation (4-19)

L_R [m]	DAF β_s=0 y^{-1}	$DAF_{Full\ Soln}$ β_s=0.365 y^{-1}	DAF_{Approx} β_s=0.365 y^{-1}	W/L_R	$\beta_s L_R/U_{GW}$
20	2.5	370	290	0.50	7.3
50	9.4	1.2×10^5	1.1×10^5	0.20	18.3
70	17	2.2×10^6	2.0×10^6	0.14	25.5
100	28	8.6×10^7	6.8×10^7	0.10	36.5
150	46	1.2×10^{10}	7.5×10^9	0.067	54.8
these values correspond to U_{GW}=1 m/y, H_W=5, I_f=0.1 m/y, W=10 m					

L_R [m]	DAF β_s=0 y^{-1}	$DAF_{Full\ Soln}$ β_s=0.0365 y^{-1}	DAF_{Approx} β_s=0.0365 y^{-1}	W/L_R	$\beta_s L_R/U_{GW}$
20	2.5	2.8	2.8	5.0	0.073
50	2.6	3.1	3.1	2.0	0.18
70	3.5	4.5	4.5	1.4	0.26
100	4.5	6.6	6.3	1.0	0.37
150	5.6	10	9.4	0.67	0.55
these values correspond to U_{GW}=10 m/y, H_W=5, I_f=0.1 m/y, W=100 m					

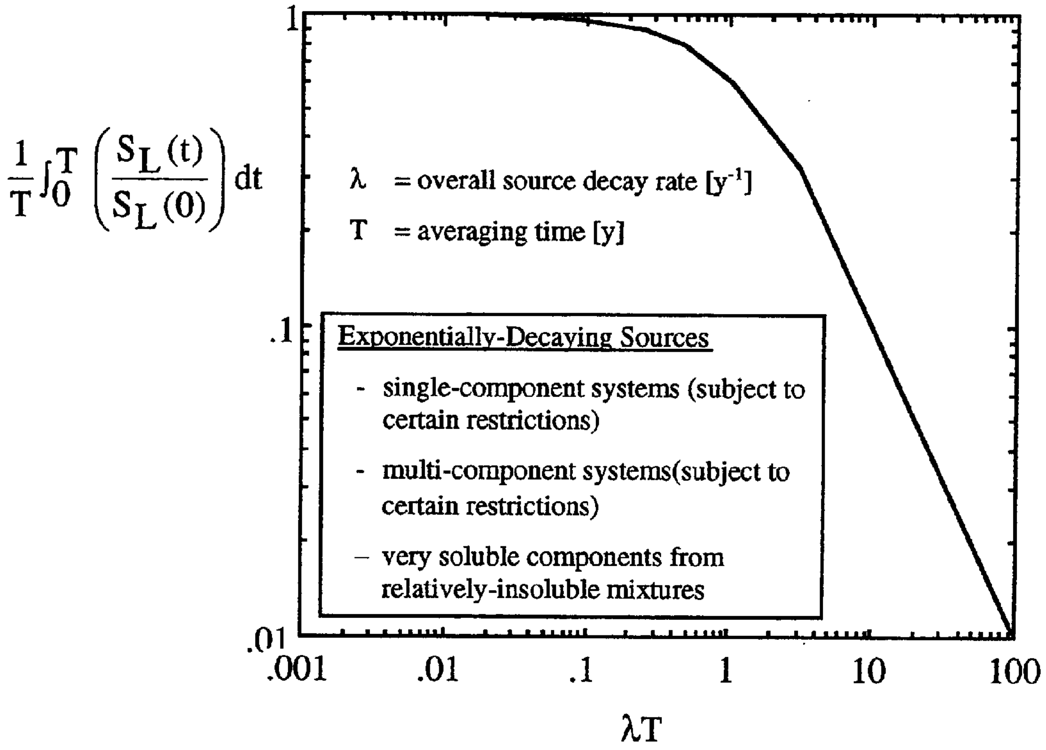


Figure 4-4. Source decay factor for exponentially-decaying sources (see Chapter 6 for calculation of decay rates and similar graphs for other idealized source decay models)

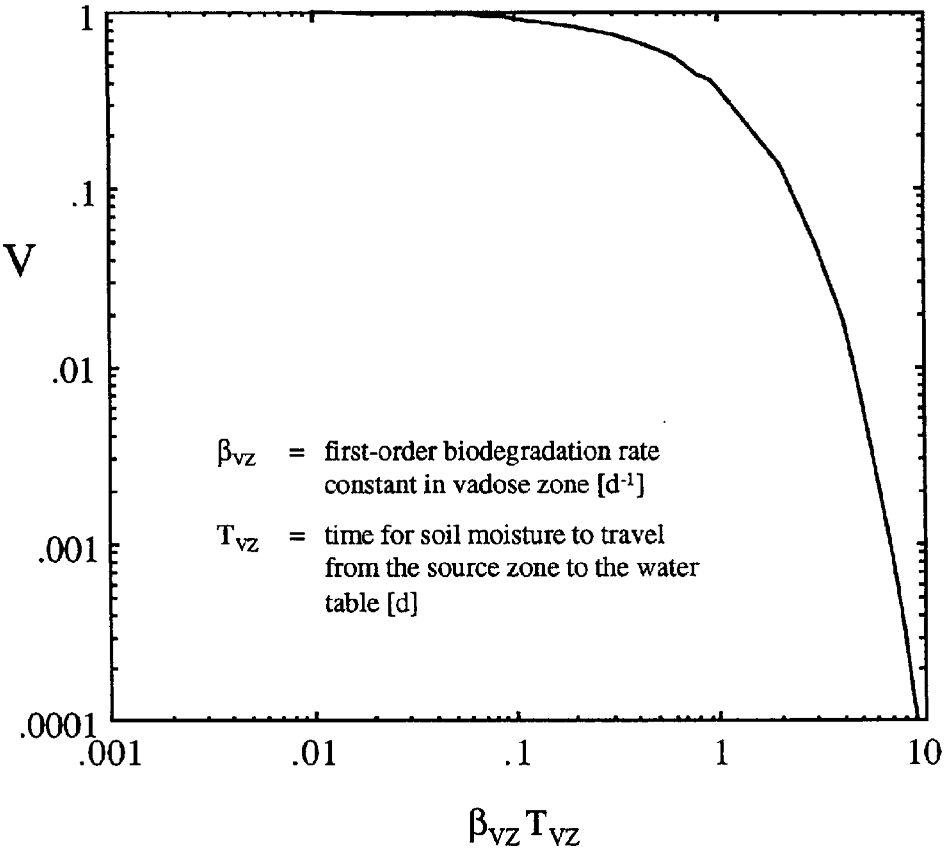


Figure 4-5. Vadose zone degradation function V

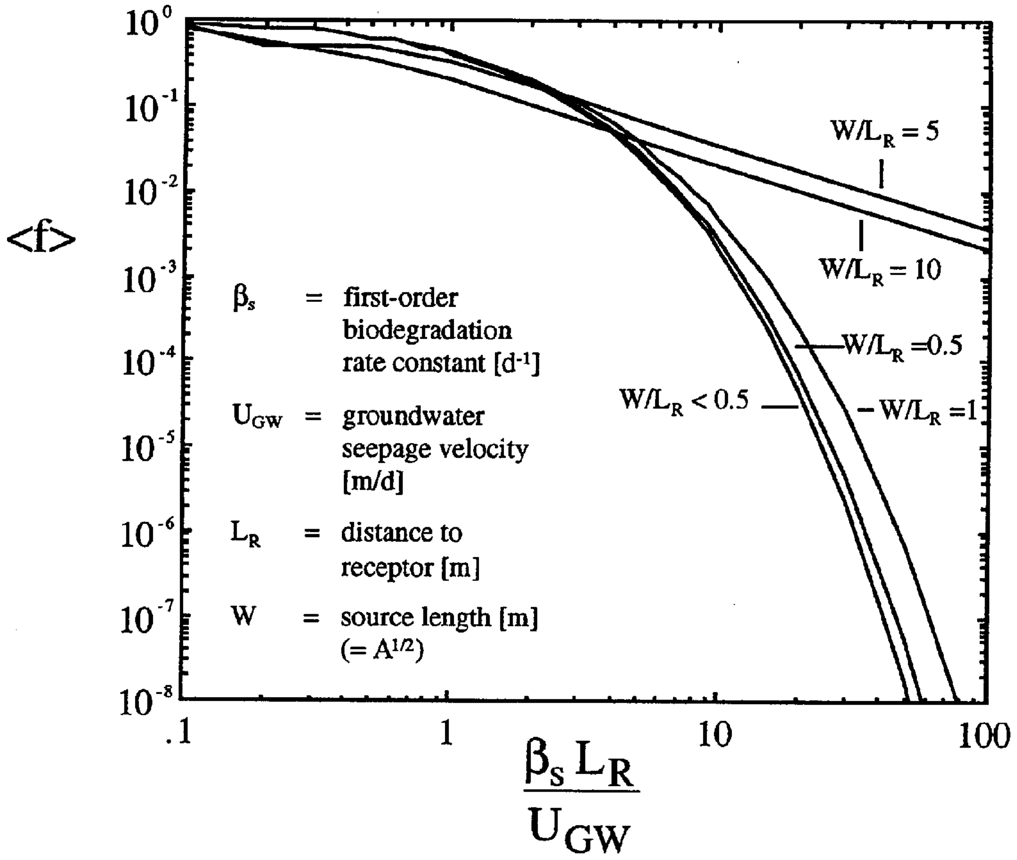


Figure 4-6. Longitudinal dispersion/bio-decay factor (f) for vadose zone sources

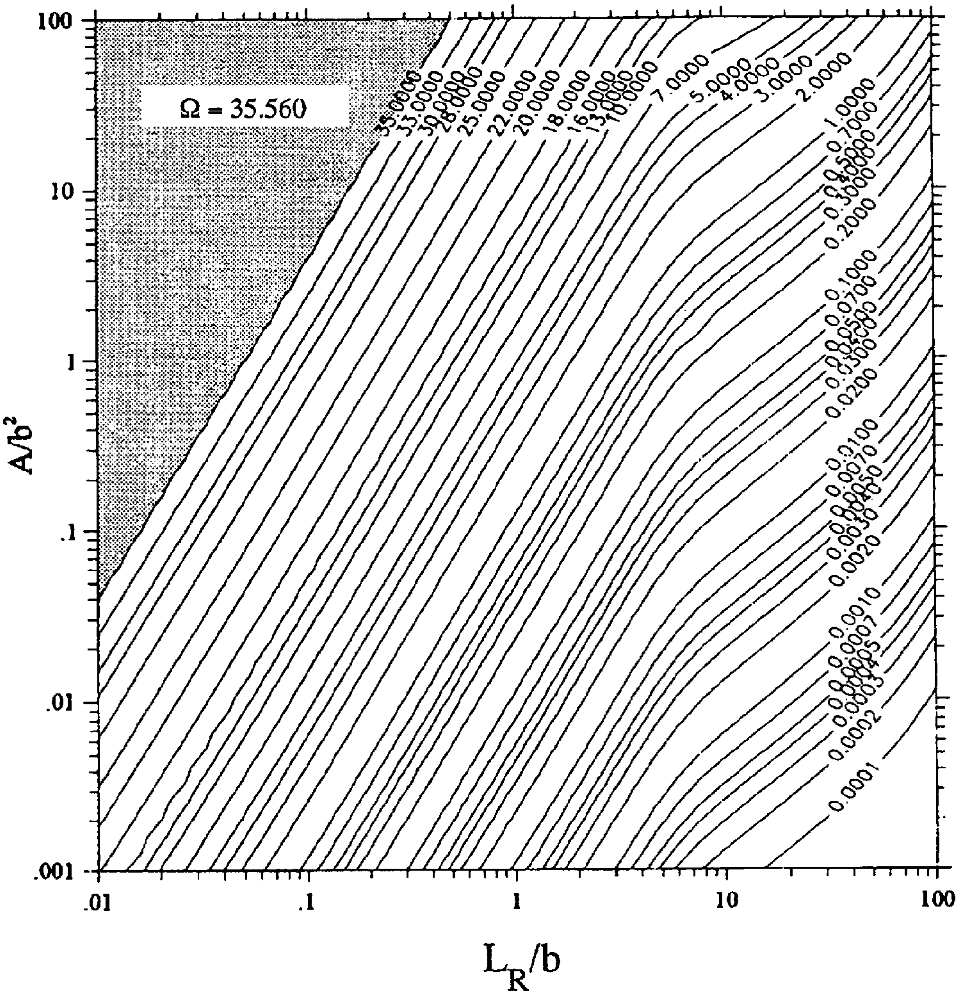


Figure 4-7. Nomograph of the function Ω

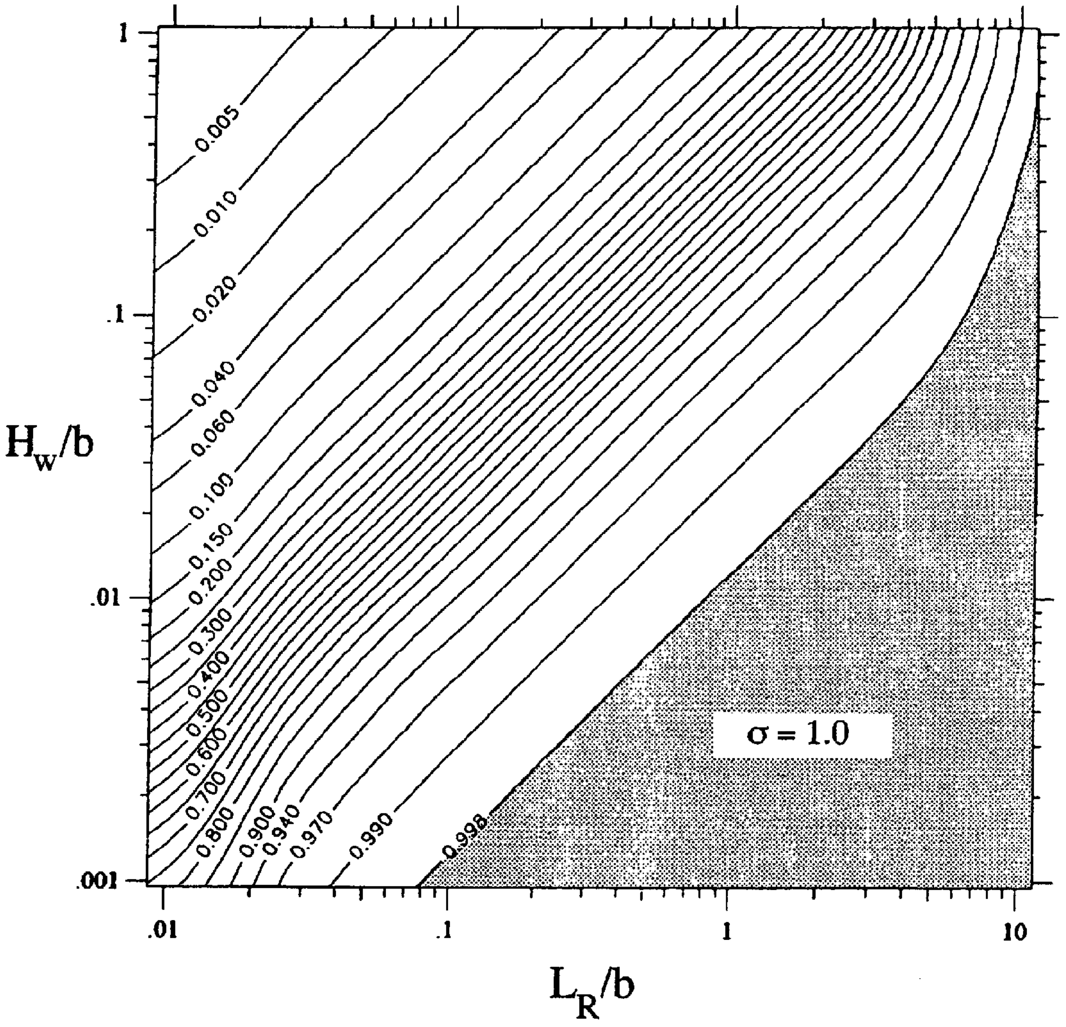


Figure 4-8. Nomograph of the function σ for $A/b^2=0.001$

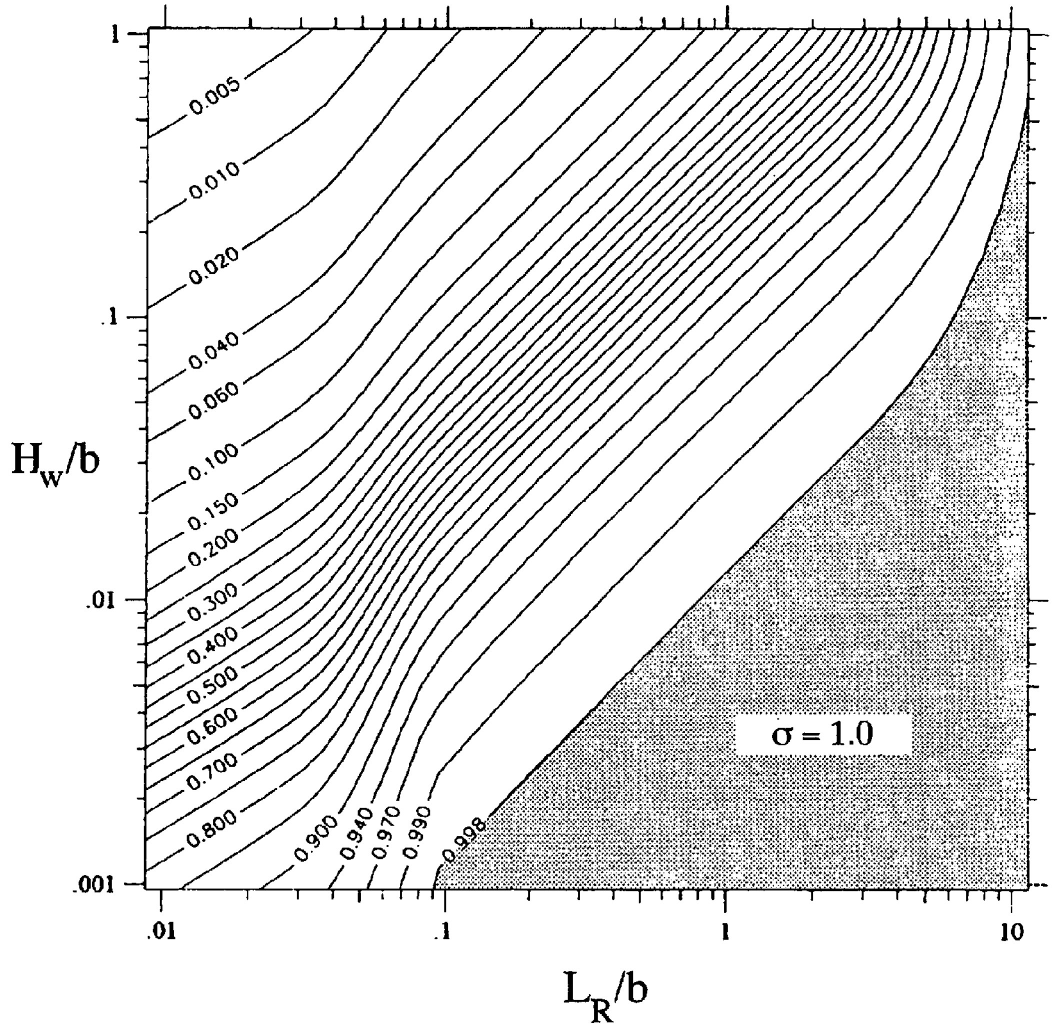


Figure 4-9. Nomograph of the function σ for $A/b^2=0.01$

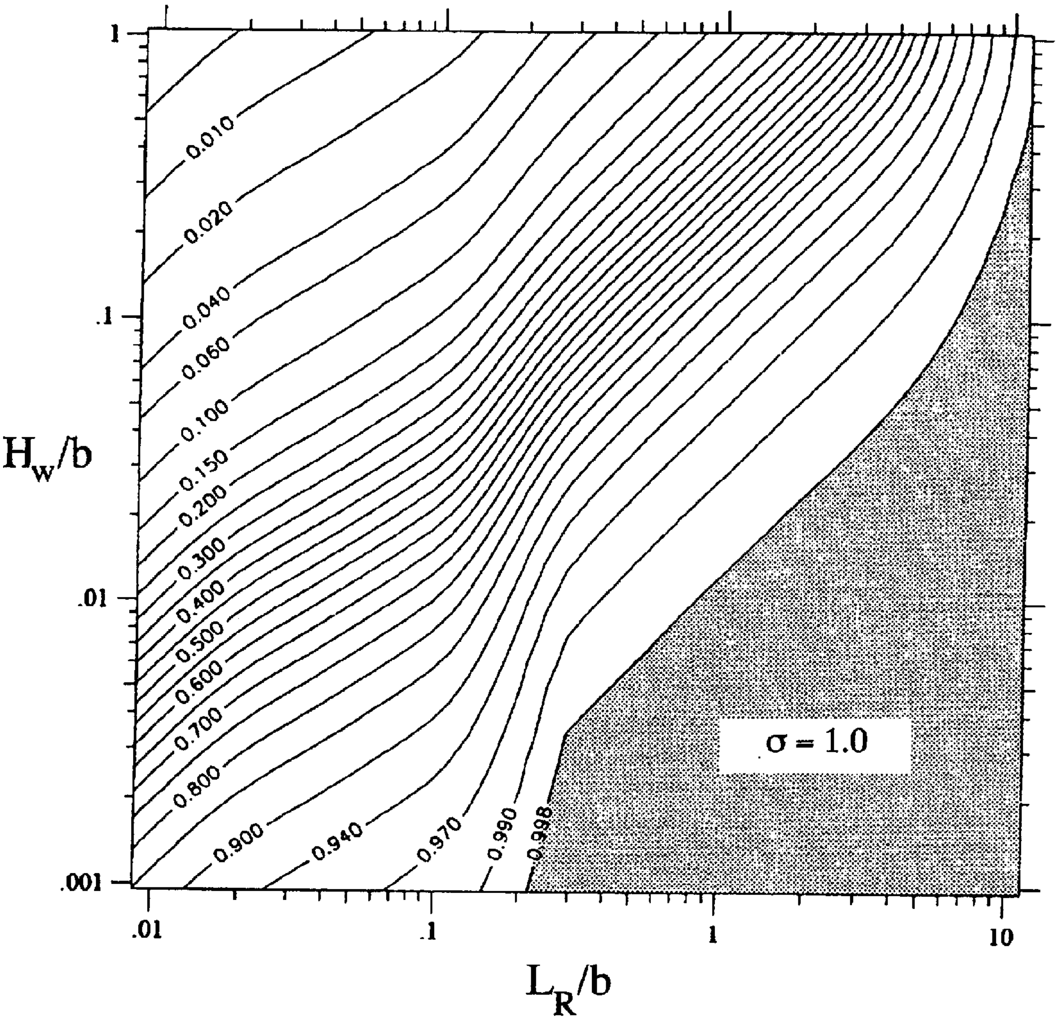


Figure 4-10. Nomograph of the function σ for $A/b^2=0.1$

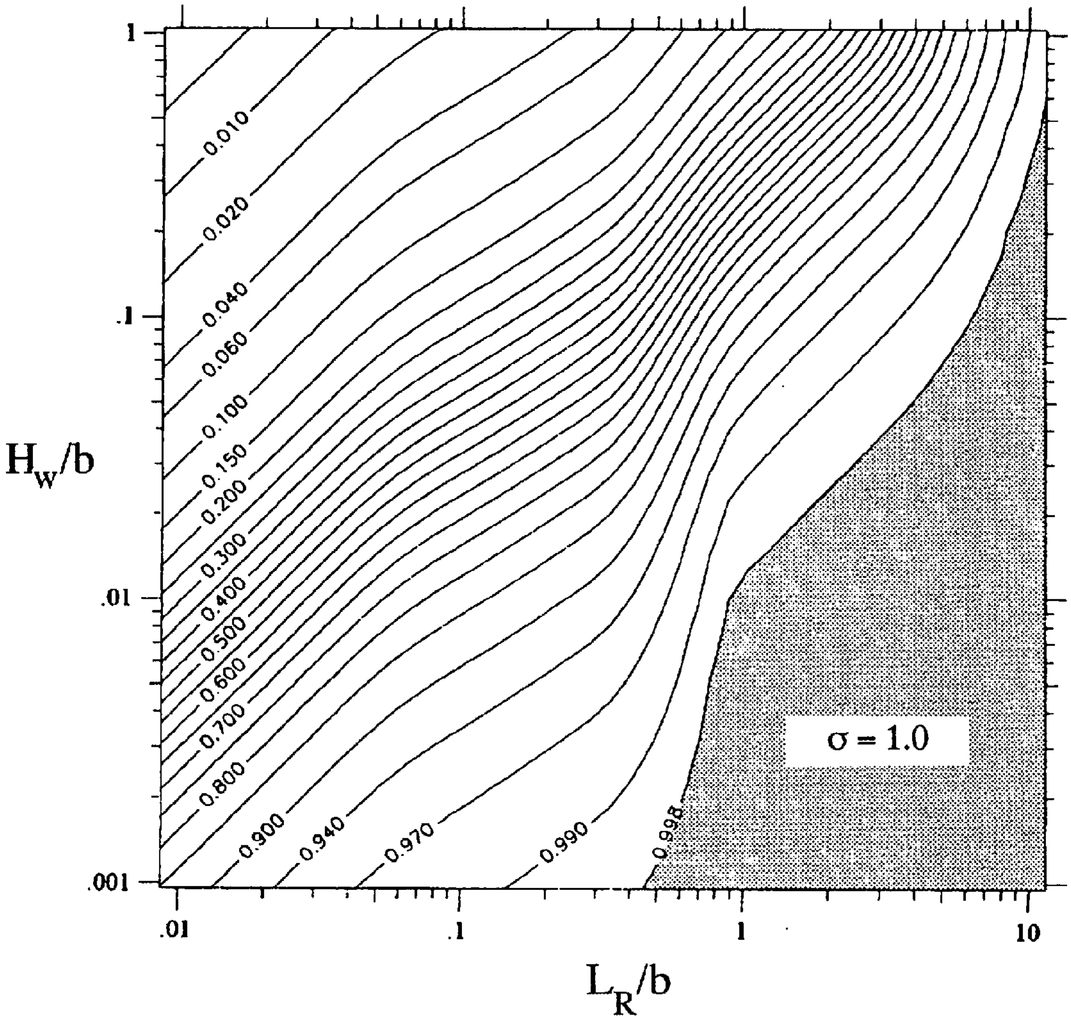


Figure 4-11. Nomograph of the function σ for A/b^2=1

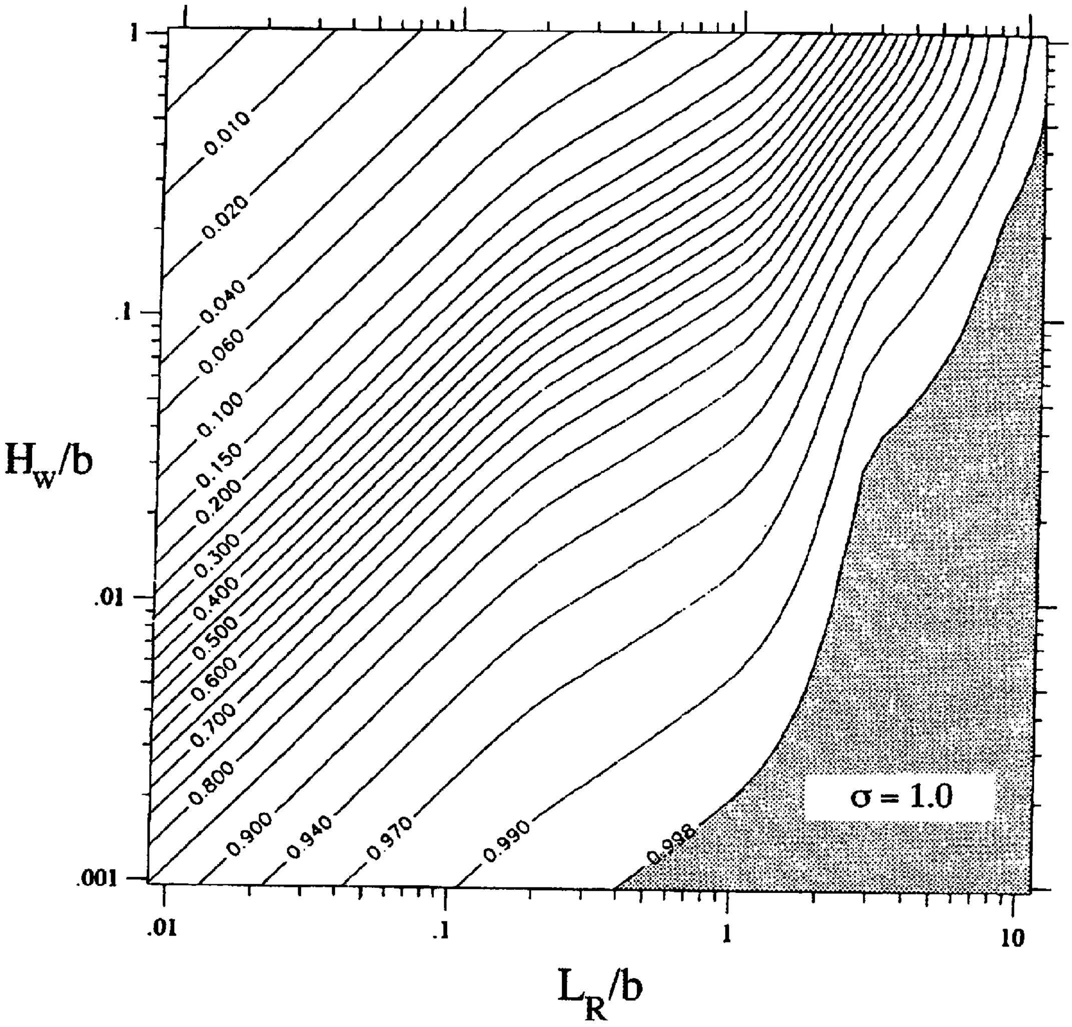


Figure 4-12. Nomograph of the function σ for $A/b^2=10$

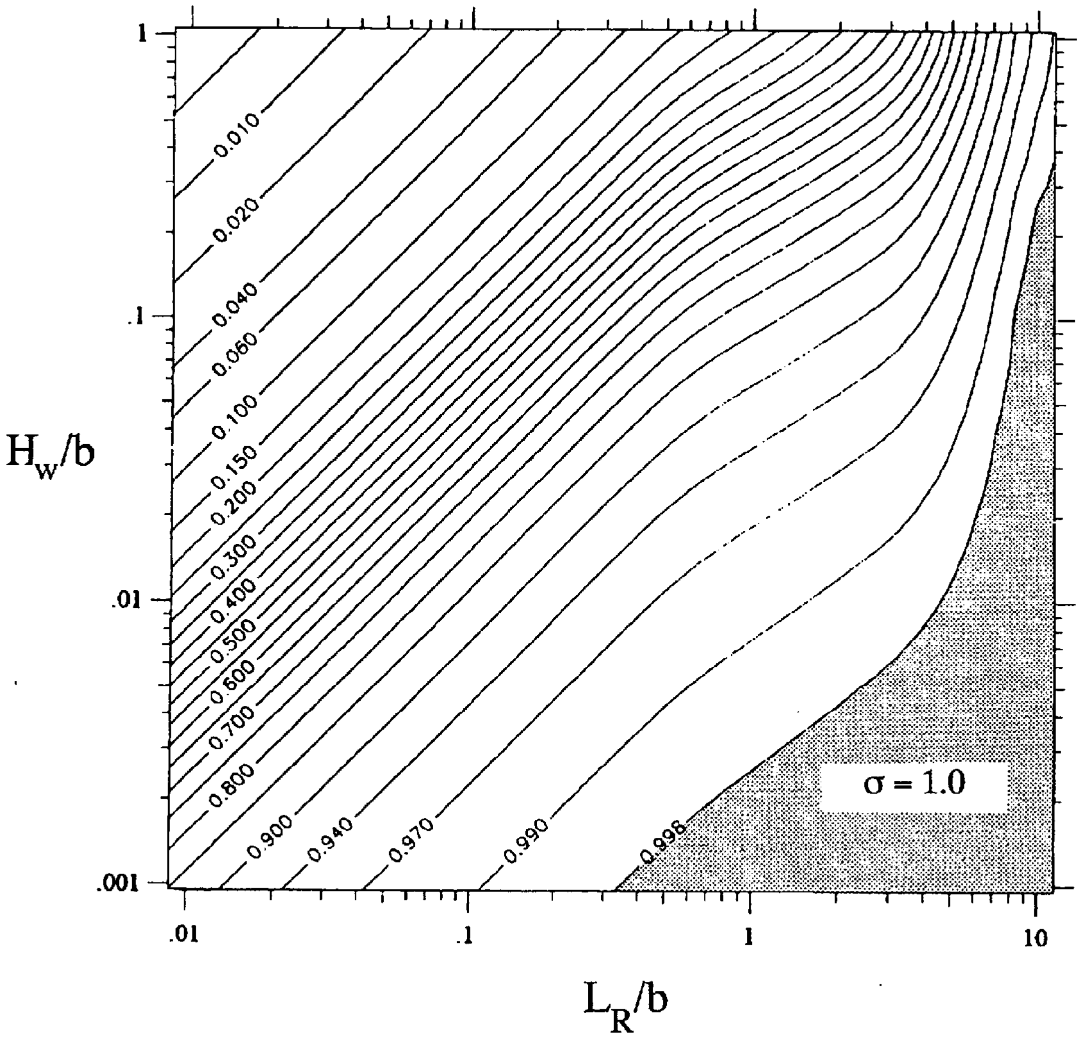


Figure 4-13. Nomograph of the function σ for $A/b^2=100$

CHAPTER 5
APPLICATION OF THE GRAPHICAL APPROACH

5.1 INTRODUCTION

In this chapter, the use of the graphical approach developed in Chapters 3 and 4 is illustrated. Hypothetical examples are presented for both vadose zone and submerged sources.

5.2 SUBMERGED SOURCE EXAMPLE

Consider the following two situations:

- A regulatory agency wishes to develop generic DAF values for underground storage tank (UST) release sites (addressed in §5.2.1); and
- The same agency and a responsible party wish to refine the DAF value for a specific site (addressed in §5.2.2).

5.2.1 GENERIC (TIER 1) DAF ESTIMATE

Equation (3-7) defines that submerged source DAF values are calculated according to the formula:

$$\mathrm{DAF} = \frac{1}{\left\{\frac{1}{T}\int_0^T \frac{S_L(t)}{S_L(0)}\,dt\right\}} \times \frac{1}{f\left(\frac{L_R}{\alpha_L}, \frac{\beta_s\,\alpha_L}{U_{GW}}\right)} \times \frac{1}{g\left(\frac{W}{\sqrt{\alpha_T\,L_R}}\right)} \times \frac{1}{h^*\left(\frac{H_W}{b}, \frac{H}{\sqrt{\alpha_V\,L_R}}, \frac{H}{H_W}\right)} \tag{5-1}$$

where:

$$h^* = h^*_{inf}\left(\frac{\sqrt{\alpha_V L_R}}{H}, \frac{H}{H_W}\right) + h^*_{cor}\left(\frac{\sqrt{\alpha_V L_R}}{b}, \frac{H}{b}, \frac{H}{H_W}\right) \tag{5-2}$$

and:

b = aquifer thickness [m]

H = thickness of source zone below the groundwater table (assumed to start at the groundwater table and extend downwards a distance H) [m]

H_W = well screen thickness (assumed to start at the groundwater table and extend downwards a distance) [m]

L_R = distance to the receptor measured from the down-gradient source edge [m]

U_{GW} = linear groundwater velocity [m/d]

W = source zone width perpendicular to flow in y-direction [m]

α_L = the longitudinal (x-direction) dispersivity [m]

α_T = the transverse (y-direction) dispersivity [m]

α_V = the vertical (z-direction) dispersivity [m]

β_s = first-order decay coefficient (reaction assumed to occur only in dissolved phase) [d^{-1}]

The functions f, g, h^*_{inf}, and h^*_{cor} are given in Figures 3-4 through 3-9.

While this list of parameters may appear to exceed the realm of typical site assessment data, it is important to note that not all parameters are required to calculate an initial DAF estimate. For example, the regulatory agency might decide that the following conditions are fairly representative of most UST release sites:

- $W \approx 20$ m (source width)
- $H \approx 1$ m (source penetration into aquifer - for light nonaqueous phase liquids)
- $b \approx 10$ m (aquifer thickness)
- $H_W \approx 3$ m (typical well screened 3 m below, and 2 m above the water table)
- $L_R \approx 30$ m (typical distance to neighboring property boundary)

A schematic of this example is shown below in Figure 5-1.

With only this minimal data set, the graphical approach can be used to generate an initial DAF estimate, provided that the following standard estimates of dispersivities are acceptable:

$$\alpha_L = L_R/10,\ \alpha_T = L_R/30,\ \alpha_V = L_R/100 \tag{5-3}$$

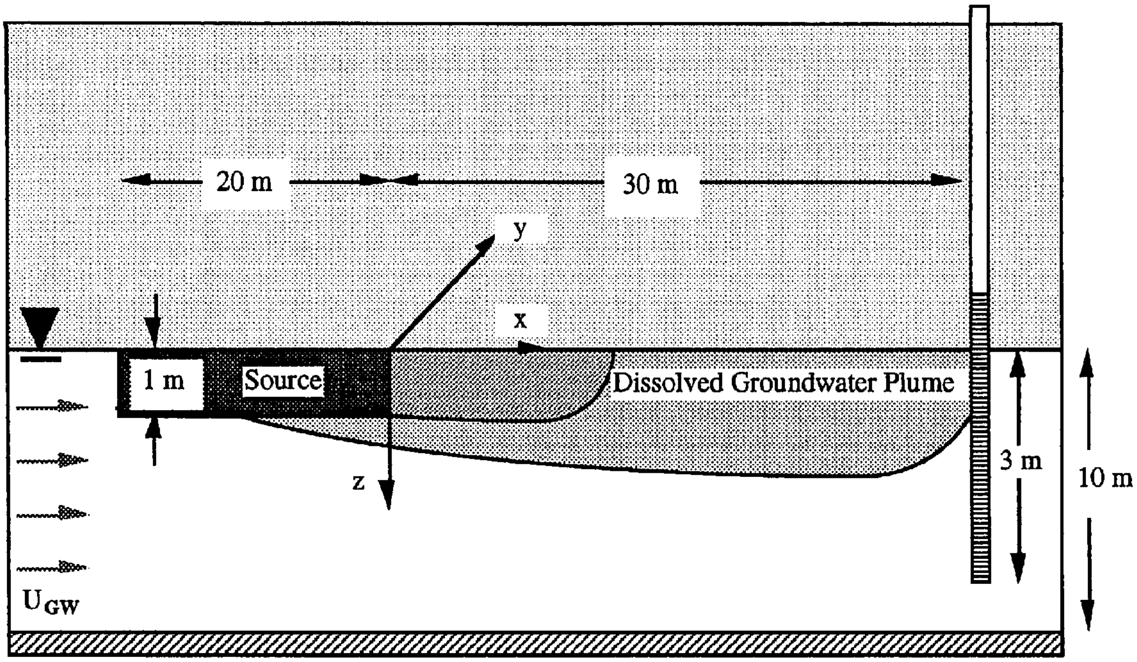


Figure 5-1. Schematic of source zone example problem (not to scale)

In making the initial DAF estimate, source decay and aerobic biodegradation are being neglected. Therefore, the only parameter groups that need to be calculated at this point are:

$$\frac{W}{\sqrt{\alpha_T L_R}} = \frac{20\text{ m}}{\sqrt{(30\text{ m}/30)(30\text{ m})}} = 3.7$$

$$\frac{\sqrt{\alpha_V L_R}}{H} = \frac{\sqrt{(30\text{ m}/100)(30\text{ m})}}{1\text{ m}} = 3.0$$

$$\frac{H}{H_W} = \frac{1\text{ m}}{3\text{ m}} = 0.3$$

$$\frac{\sqrt{\alpha_V L_R}}{b} = \frac{\sqrt{(30\text{ m}/100)(30\text{ m})}}{10\text{ m}} = 0.3$$

$$\frac{H}{b} = \frac{1\text{ m}}{10\text{ m}} = 0.1$$

Given these, the function values obtained from Figures 3-3 through 3-9 are:

$\frac{1}{T}\int_0^T \frac{S_L(t)}{S_L(0)}\,dt = 1$ (source depletion is being neglected at this point)

$f = 1$ (biodegradation is being neglected at this point)

$g \approx 0.8$

$h^*_{inf} \approx 0.18$

h^*_{cor} = negligible compared to h^*_{inf} ($h^*_{cor} << 0.18$)

and therefore the initial DAF estimate is:

$$DAF = \frac{1}{1 \times 1 \times 0.8 \times 0.18} = 7$$

Figures 5-2 through 5-4 illustrate the use of the graphs in obtaining values for g, h^*_{inf}, and h^*_{cor}.

As an indication of the magnitude of the uncertainty associated with reading values from the graphs, the actual computed values are: g=0.83, h^*_{inf} =0.17, and DAF=7.1.

At this point, the reader should note that the initial DAF estimate was generated only after specifying the geometry of the problem (source width, thickness, distance to receptor, etc.). Thus the graphical approach can be used when minimal data are available. Below, an illustration is given of how initial estimates can be refined when more site-specific information is available.

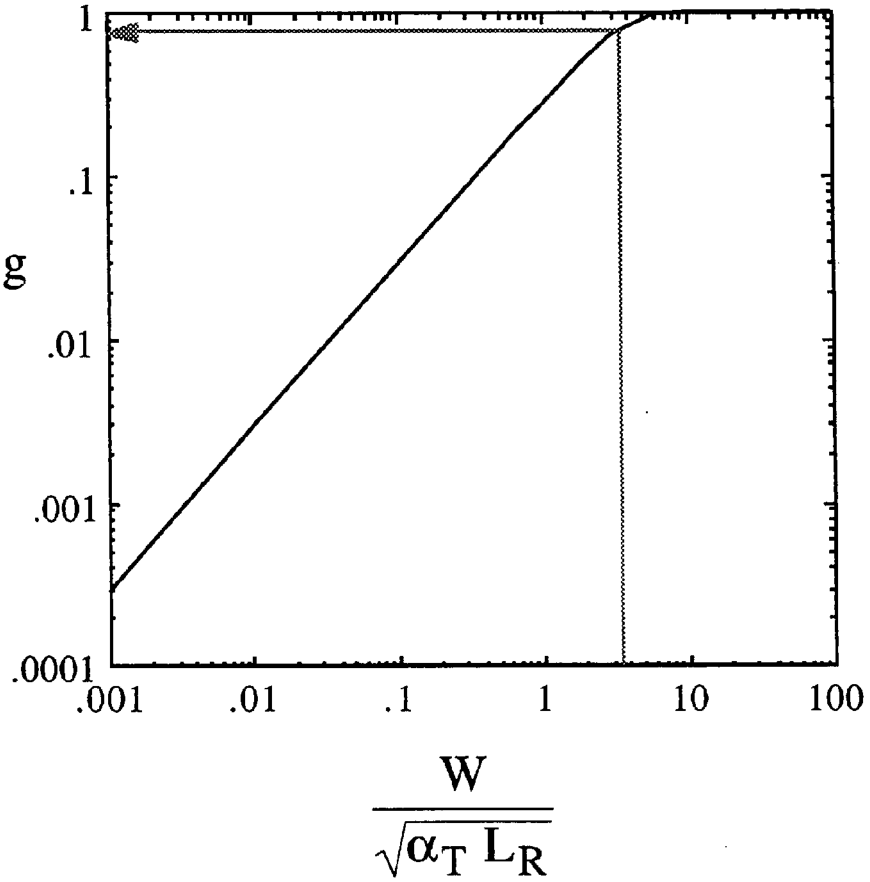


Figure 5-2. Illustration of g-value determination from the graphs for the source zone example. In this case g≈0.8.

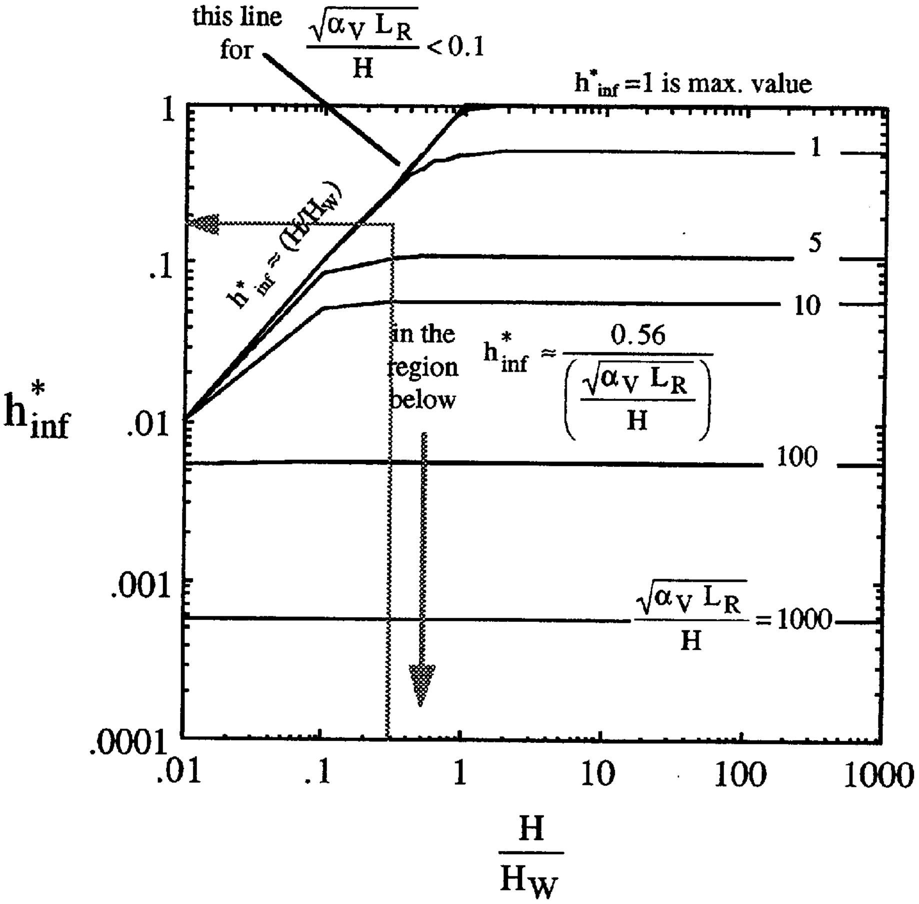


Figure 5-3. Illustration of h^*_{inf} value determination from the graphs for the source zone example. In this case $(H/H_W)=0.3$, $(\alpha_V L_R/H^2)^{1/2}=3$, and $h^*_{inf}\approx 0.18$. While a contour line for $(\alpha_V L_R/H^2)^{1/2}=3$ is not given in the figure, the estimating equation contained in the figure yields a reasonable estimate for h^*_{inf}

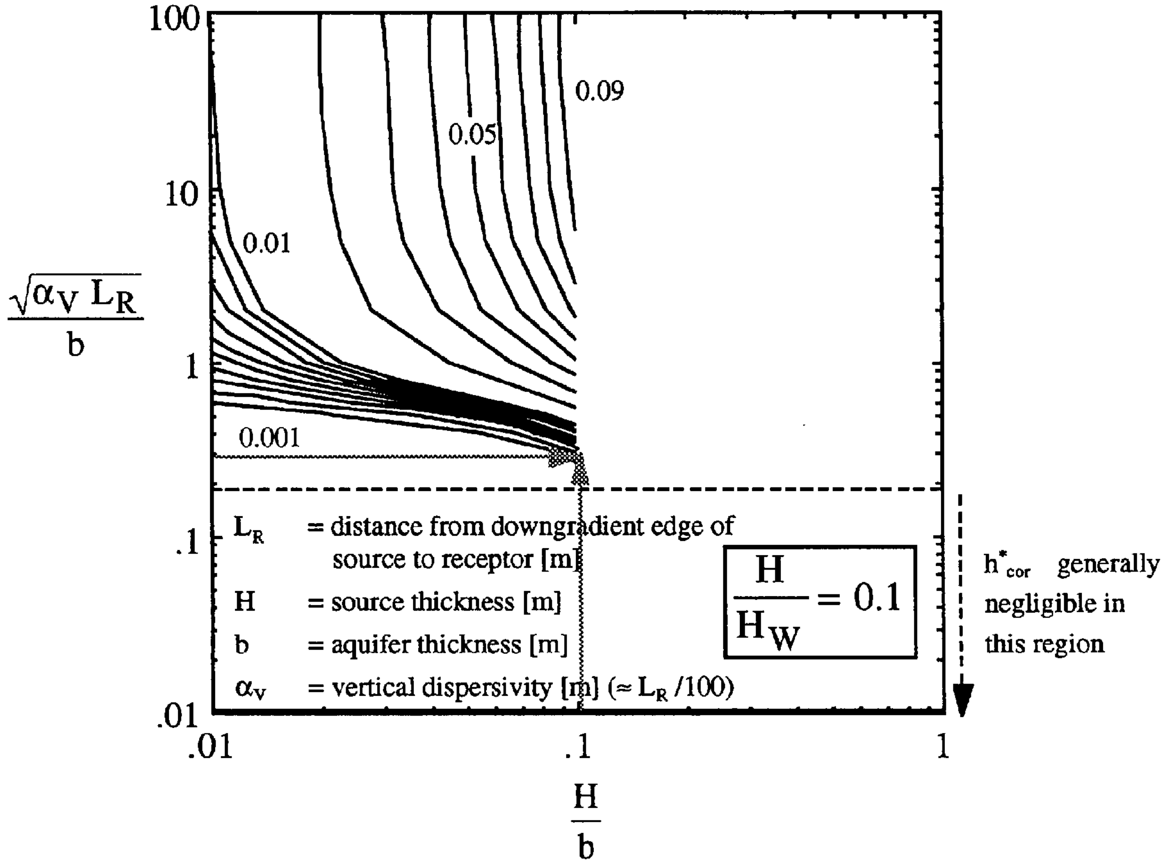


Figure 5-4. Illustration of h^*_{cor}-value determination from the graphs for the source zone example. In this case $(H/H_W)=0.3$, $(\alpha_V L_R/b^2)^{1/2}=0.3$, $H/b=0.1$, and $h^*_{cor} \approx 0.003$.

5.2.2 REFINED (TIER 2) DAF VALUES

Suppose that, for the specific site used in the previous calculations, the agency and responsible party wish to refine the generic DAF estimate. Recall that both biodegradation and source zone decay were neglected above, and both could be included when refining the DAF value. However, upon examination of Figures 3-3 and 3-4, it is apparent that accounting for biodegradation has the potential to more significantly impact the DAF estimate than accounting for a depleting source. Furthermore, focusing on biodegradation also requires the collection of fewer additional parameters (as the source decay rate depends on many other parameters).

At this particular site the groundwater velocity has been estimated to be $U_{GW} \approx 0.1$ m/d based on the water level measurements (to obtain the hydraulic gradient) and aquifer testing (to obtain the hydraulic conductivity).

Groundwater monitoring data (primarily dissolved oxygen concentrations) suggest that aerobic biodegradation is occurring at this site, although a specific rate has not been determined. The peer-reviewed literature suggests that apparent first-order degradation rates for aromatic hydrocarbons typically fall in the range 0.001 - 0.01 d^{-1}, and the agency agrees to permit the responsible party to calculate a range of refined DAF values, from which a final value will be chosen after sufficient compliance monitoring data have been collected.

In calculating the refined estimate, it has been decided that the values used above in §5.2.1 are appropriate for the site, so that the values of the functions **g** and **h*** do not change. The value of **f** (which was taken to be **f**=1 when biodegradation was neglected) is obtained by first calculating the parameter group:

$$0.03 \leq \frac{\beta_s \alpha_L}{U_{GW}} \leq 0.3$$

which leads to the following range of **f** values:

$$0.7 \leq f \leq 0.09$$

Figure 5-5 illustrates how values of **f** are obtained from the graph.

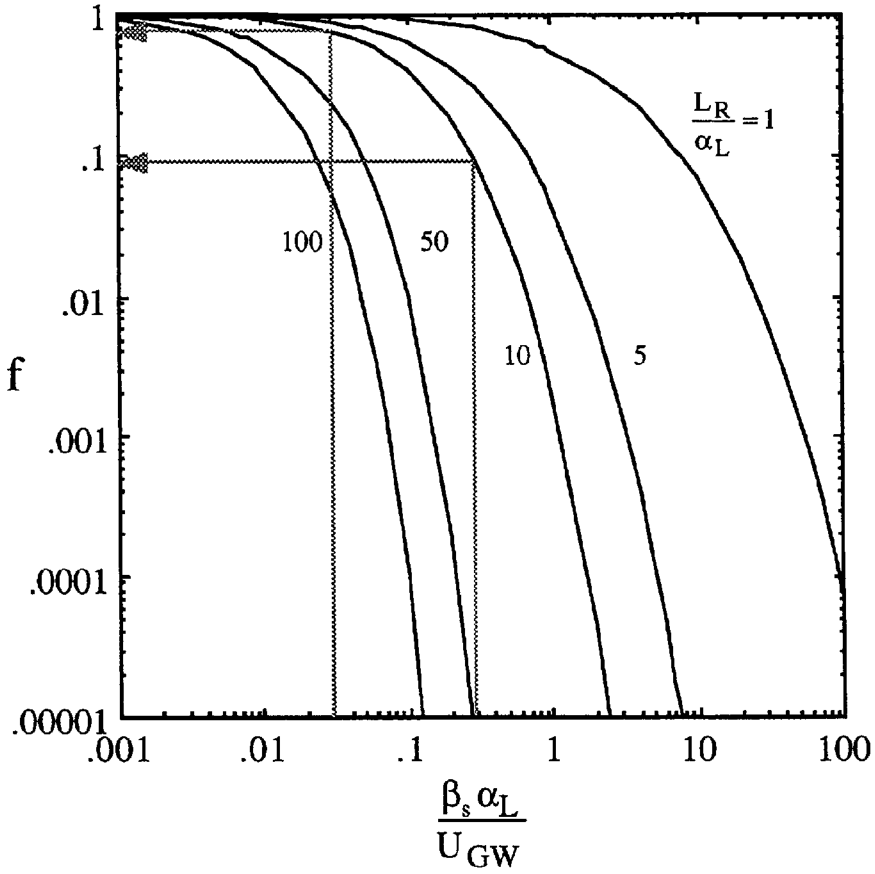


Figure 5-5. Use of the graphical approach for obtaining f values. In this case $L_R/\alpha_L=10$, $\beta_s\alpha_L/U_{GW} = 0.03$ *and* 0.3, *and* $f = 0.7$ *and* 0.09

Using Equation (5-1) this leads to the following range of refined DAF estimates:

$$\frac{1}{1 \times 0.7 \times 0.8 \times 0.18} \leq \text{DAF} \leq \frac{1}{1 \times 0.09 \times 0.8 \times 0.18}$$

or:

$$10 \leq \text{DAF} \leq 77$$

Again, as an indication of the magnitude of the uncertainty associated with reading values from the graphs, the actual computed values are: $9 \le DAF \le 70$.

These results illustrate the sensitivity of the DAF results to changes in the parameter group ($\beta_s \alpha_L / U_{GW}$). Had the distance to the receptor been larger (increasing α_L), or the groundwater velocity slower, the impact of including/neglecting biodegradation would have been even more significant.

5.3 VADOSE ZONE SOURCES

In this section the graphical approach developed in Chapter 4 is illustrated, and results are presented from an exercise in which students not familiar with this project were asked to use the graphical approach.

5.3.1 GENERIC DAF ESTIMATE (TIER 1)

Suppose that a generic DAF is to be developed for leaking UST sites where the spill does not penetrate deeply enough to reach the water table.

In this case the DAF is given by Equation (4-24):

$$DAF = \frac{1}{\left\{\frac{1}{T}\int_0^T \frac{S_L(t)}{S_L(0)}\,dt\right\} x < f > x \left(\frac{I_f}{\phi_s\, U_{Gw}}\right) x\ V\ x\ \Omega\ x\ \sigma} \tag{5-4}$$

where:

I_f = infiltration rate through vadose zone [m/d]
ϕ_s = aquifer porosity

The minimal data set required in the case of vadose zone sources is different than that for submerged sources, but is still reasonable. Suppose the agency decides that the following are representative of typical vadose zone source sites:

I_f = 0.25 m/y (infiltration rate through vadose zone)
ϕ_s = 0.43 (aquifer porosity)
U_{GW} = 10 m/y (groundwater seepage velocity)
A = 100 m^2 (source area)
H_W = 3 m (well screen thickness)
b = 10 m (aquifer thickness)
L_R = 50 m distance to receptor measured from center of source zone)

This scenario is shown schematically in Figure 5-6 below.

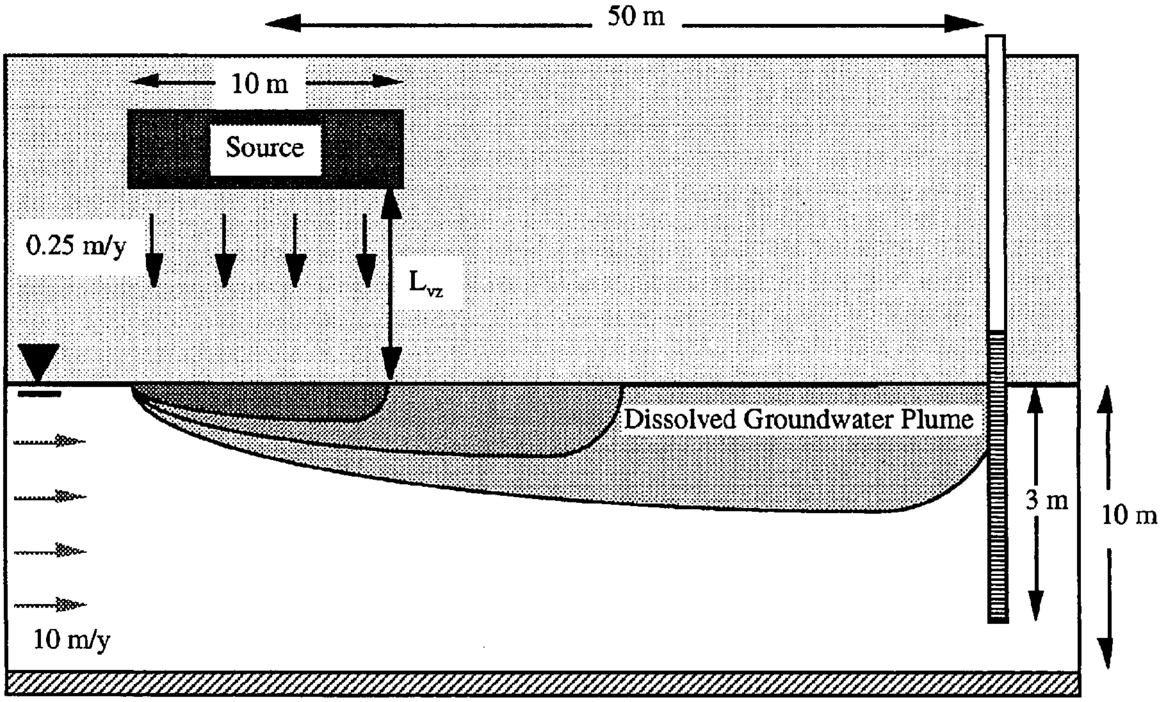


Figure 5-6. Vadose zone source example scenario.

Here again, source decay and biodegradation are neglected, so the relevant parameter groups are:

$$\frac{A}{b^2} = \frac{100\,\text{m}^2}{(10\,\text{m})^2} = 1$$

$$\frac{L_R}{b} = \frac{50\,\text{m}}{10\,\text{m}} = 5$$

$$\frac{H_W}{b} = \frac{3\,\text{m}}{10\,\text{m}} = 0.3$$

Using these and Figures 4-3 through 4-12, we can obtain:

$\frac{1}{T}\int_0^T \frac{S_L(t)}{S_L(0)}\,dt = 1$ (source depletion is being neglected at this point)

$\langle f \rangle = 1$ (biodegradation is being neglected at this point)

$V = 1$ (vadose zone biodegradation being neglected at this point)

$\Omega \approx 0.35$

$\sigma \approx 1$

and therefore the DAF estimate becomes:

$$\text{DAF} = \frac{1}{1 \times 1 \times \left(\dfrac{0.25\,\text{m}/\text{y}}{0.43 \times 10\,\text{m}/\text{y}}\right) \times 1 \times 0.35 \times 1} = 49$$

Use of the graphs is illustrated below in Figures 5-7 and 5-8.

The use of the exact HPS model (see Appendix D) for this same case results in a dilution attenuation factor of 49.1.

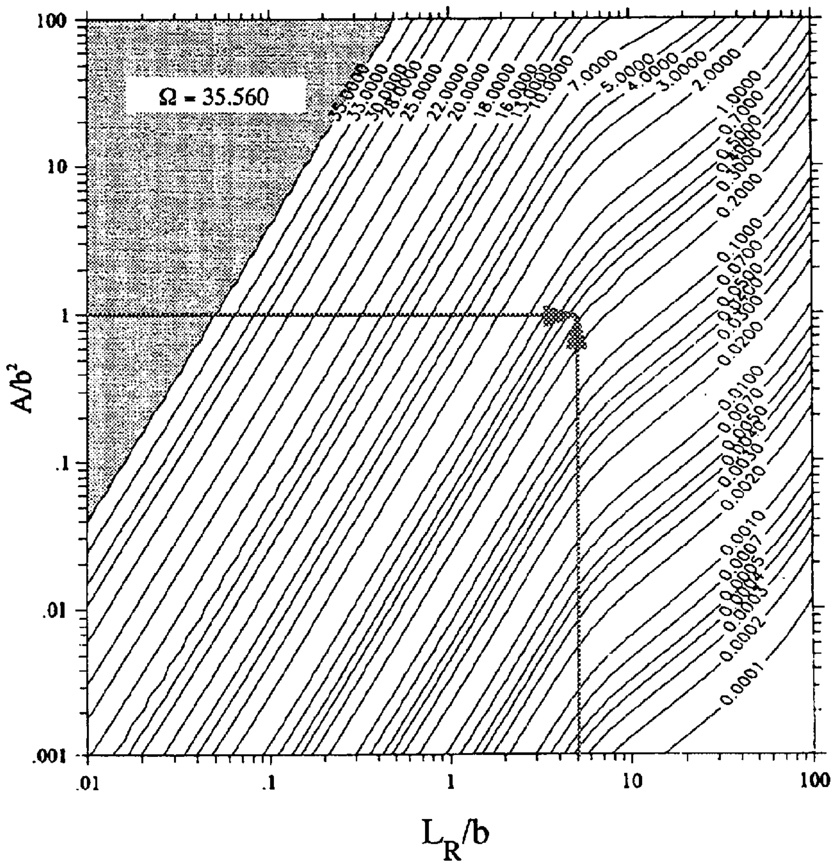


Figure 5-7. Use of the graphical approach for determining Ω. In this case $L_R/b=5$, $A/b^2=1$, and $\Omega\approx0.35$

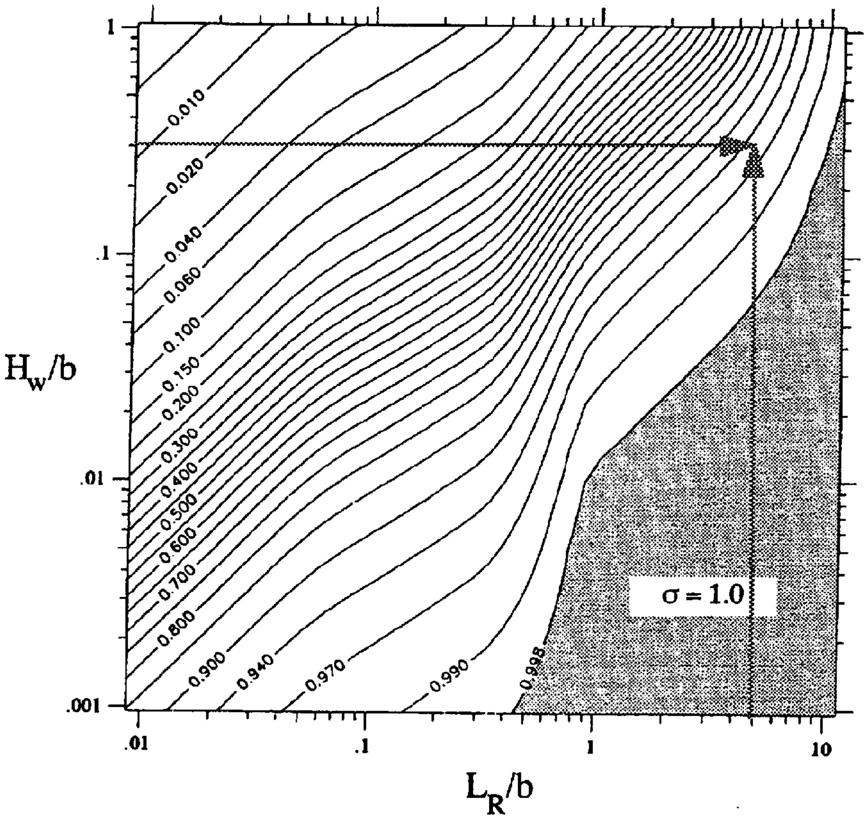


Figure 5-8. Use of the graphical approach for determining σ. In this case $L_R/b=5$, $H_w/b=0.3$, and $\sigma \approx 1$

5.3.2 ANALYSIS OF NOMOGRAPH INTERPRETATION ACCURACY

In order to determine what accuracy could be expected when using the graphical approach for vadose zone sources, a nomograph-based assignment was given to students in a graduate level groundwater hydraulics class.

Dilution attenuation factors were to be determined using an infiltration rate, I_f=0.2 m/y and a Darcy velocity $\phi_s U_{GW}$=5.0 m/y for the following conditions:

Case 1:
Source area, A = 100 m^2; aquifer thickness, b = 10 m; source decay rate, λ = 0.015/y; averaging period, T = 1 y; and

Receptor 1: distance = 10 m, well screen length = 4.0 m
Receptor 2: distance = 80 m, well screen length = 2.5 m
Receptor 3: distance = 150 m, well screen length = 1.5 m

Case 2:
Source area, A = 1400 m^2; aquifer thickness, b = 20 m; source decay rate, λ = 0.025/y; averaging period, T = 30 y; and

Receptor 1: distance = 25 m, well screen length = 3.0 m
Receptor 2: distance = 65 m, well screen length = 10.0 m
Receptor 3: distance = 130 m, well screen length = 1.25 m

Case 3:
Source area, A = 125 m^2; aquifer thickness, b = 15 m; source decay rate, λ = 0.010/y; averaging period, T = 3 y; and

Receptor 1: distance = 12 m, well screen length = 5.0 m
Receptor 2: distance = 60 m, well screen length = 5.0 m
Receptor 3: distance = 140 m, well screen length = 0.1 m

Student responses are tabulated and compared with the true values in Table 5-1.

As seen in Table 5-1, the DAFs predicted by the students generally were very close to the actual DAF value. A few students read the numbers from the nomographs correctly, and then simply made a computation error that resulted in an incorrect DAF. In cases where the students made computational errors, the errors are not corrected here. Generally, the error in the DAFs computed by the students is low when the outliers in the responses are thrown out. If the outliers are neglected, the error in the DAF estimates is usually less than ten percent.

Being only a homework assignment, some students were rather careless in their estimations, and in cases where the dilution attenuation factor derived from the nomographs is meant to be applied to an actual site, it can be expected that users will be more accurate in their attention to detail when using the nomographs. However, these responses show that the nomographs are rather easy to use and, when used correctly and accurately, the dilution attenuation factors derived from the graphical approach are reproducible and consistent.

Table 5-1. Student responses to the dilution attenuation factor homework problems.

	DAF Answers Given by Students For Each Case								
Student	**1.1**	**1.2**	**1.3**	**2.1**	**2.2**	**2.3**	**3.1**	**3.2**	**3.3**
1	10.4	144.0	258.0	5.4	22.3	44.6	14.6	98.1	329.0
2	10.4	128.2	221.8	212.1	558.0	1339.3	41.5	289.7	919.1
3	10.6	139.2	263.2	4.7	18.8	44.6	6.2	89.6	316.2
4	11.3	128.0	213.0	4.5	16.2	39.7	13.2	96.6	306.0
5	8.6	137.2	271.7	4.9	19.4	42.0	10.7	58.5	154.8
6	5.0	134.3	1275.5	4.9	19.2	42.0	12.8	92.4	283.4
7	11.8	141.1	295.5	4.6	16.7	34.7	19.8	136.1	446.4
8	7.3	132.0	263.0	4.8	17.9	44.6	13.9	94.3	292.0
9	8.4	132.0	1320.0	4.4	19.6	48.9	126.0	148.0	278.0
10	11.1	131.0	260.0	4.9	17.9	42.0	13.4	97.4	299.0
11	12.9	102.2	170.0	4.2	17.8	48.3	16.4	114.4	30.9
12	8.2	140.0	280.0	6.0	20.0	42.0	14.0	140.0	290.0
13	11.5	140.0	263.0	4.8	19.2	42.0	15.0	112.3	33.4
14	11.3	1.5	255.0	4.3	17.8	35.7	143.0	91.4	286.0
15	14.6	128.8	255.1	4.1	5.2	43.4	13.9	94.3	526.3
16	11.7	132.2	263.2	4.7	19.4	59.5	14.6	94.3	328.9
17	10.1	129.5	214.8	4.1	16.7	39.2	124.0	97.2	283.5
Actual Answer:	**10.9**	**125.2**	**223.6**	**4.9**	**20.2**	**45.0**	**13.2**	**90.6**	**295.1**

CHAPTER 6

IDEALIZED SOURCE DEPLETION MODELS

6.1 INTRODUCTION

As a result of leaching, volatilization, biodegradation, and other natural processes, source zone soil and leachate concentrations will slowly decline with time. The theoretical framework outlined in Chapter 2 of this document allows for time-varying sources, and Equation (2-2) defines the dilution attenuation factor (DAF) to be:

$$\mathrm{DAF}\left[\frac{(mg_i\ /\ L_{H_2O})_{source}}{(mg_i\ /\ L_{H_2O})_{receptor}}\right]=\frac{S_L^o}{<<C_R>_z>_{t,max}} \qquad (6\text{-}1)$$

where:

S_L^o = dissolved concentration of compound i leaving source zone at time t=0 $[mg_i/L_{H2O}]$

$<<C_R>_z>_{t,max}$ = maximum-time-averaged and vertically-averaged centerline dissolved concentration at the receptor location $x=L_R$ $[mg_i/L_{H2O}]$

It was also shown that Equation (6-1) can be reduced to the following (Equation (2-9)):

$$\mathrm{DAF}=\frac{1}{\left\{\frac{1}{T}\int_0^T \frac{S_L(t)}{S_L(0)}\,dt\right\} \times \left\{\frac{1}{H_w}\int_0^{H_w} C_{cs}^*(L_R,0,z,\infty)\,dz\right\}} \qquad (6\text{-}2)$$

where:

$S_L(t)$ = time-varying source zone leachate concentration of chemical i $[mg_i/L_{H2O}]$

T = averaging time (often the exposure duration upon which the receptor location tolerance criterion is based) [d]

H_w = well screen interval (screen interval is assumed to extend from the water table downwards) [m]

L_R = distance downgradient to receptor [m]

$C^*_{CS}(L_R,0,z,\infty)$ = steady-state normalized concentration distribution along the dissolved plume centerline for a steady source of unit strength [dimensionless]

For the case of constant strength sources:

$$\frac{1}{T}\int_0^T \frac{S_L(t)}{S_L(0)}\,dt = 1 \qquad (6\text{-}3)$$

and the user need only know $C^*_{CS}(L_R,0,z,\infty)$ to be able to calculate a DAF value. Otherwise, the user must have knowledge of how the source zone leachate concentration $S_L(t)$ changes with time.

There is one additional reason why a user may require knowledge of what is occurring in the source zone. Often, once a DAF is calculated and then used to determine an initial source zone leachate concentration $S_L(t{=}0){=}S^o_L$ [mg_i/L_{H2O}], the user may also wish to estimate a total soil concentration C^o_T [mg_i/kg_{soil}] that corresponds to S^o_L (i.e. a soil screening level):

$$S^o_L \xrightarrow{?} C^o_T \qquad (6\text{-}4)$$

Thus, in this chapter the modeling of the source zone is focused towards two objectives:

- calculating the expression:

  $$\frac{1}{T}\int_0^T \frac{S_L(t)}{S_L(0)}\,dt \qquad (6\text{-}5)$$

  which is required to complete the DAF estimation, and

- finding relationships between S^o_L [mg_i/L_{H2O}] and a soil screening level C^o_T [mg_i/kg_{soil}].

In the following, a few idealized time-varying source zone models are presented, the relationships (6-4) and (6-5) are developed, and guidance for selecting among the different models is presented. Table 6-1 summarizes the nomenclature used in the following sections, while Table 6-2 summarizes the idealized time-varying source zone models discussed below.

Table 6-1. Nomenclature used in Chapter 6.

Quantity	Definition
C_V	vapor phase concentration of chemical "i" in the soil matrix [mg_i/L_{air}]
C_S	concentration of chemical "i" sorbed to soil particle surfaces [mg_i/kg_{soil}]
$C_{T,mix}$	total soil concentration of a multi-component mixture [$mg_{mixture}/kg_{soil}$]
C_T	total soil concentration (all phases) of chemical "i" [mg_i/kg_{soil}]
C_T^{o}	total soil concentration (all phases) of chemical "i" at time t=0 [mg_i/kg_{soil}]
C_I	immiscible (free-phase) concentration of "i" in the source zone [mg_i/kg_{soil}]
$<<C_R>_z>_{t,max}$	time-averaged solute concentration at the receptor location [mg_i/L_{H2O}]
H	source zone thickness [m]
D^{eff}	effective gas phase diffusion coefficient in soil matrix [m^2/y] (chemical specific)
DAF	dilution attenuation factor [dimensionless] (chemical specific)
f_{oc}	fraction of organic carbon in soil matrix [kg_{carbon}/kg_{soil}]
I	water flux through the source zone [m^3/m^2-d]
K_H	Henrys law coefficient [(mg_i/L_{air})/(mg_i/L_{H2O})] (chemical specific)
K_d	soil/water partition coefficient [(mg_i/kg_{soil})/(mg_i/L_{H2O})] (chemical specific)
K_{oc}	organic carbon partition coefficient [(mg_i/kg_{soil})/(mg_i/L_{H2O})] (chemical specific)
L	length of the source zone parallel to groundwater flow direction [m]
L_C	depth of soil cover overlaying the source zone [m]
L_d	diffusion path length for volatile source zone losses = $L_c + 1/2\ H$ [m]
M_L	mass of compound in the source zone soil pore water [mg_i] (chemical specific)
M_V	mass of compound in the source zone vapor space [mg_i] (chemical specific)
M_S	mass of compound sorbed onto source zone soil particles [mg_i] (chemical specific)
M_W	molecular weight of a single component in a mixture [g/$moles_i$] (chemical specific)
$M_{W,avg}$	average molecular weight of the mixture [$g_{mixture}/moles_{mixt}$] (mixture specific)
n	total soil porosity [L_{voids}/L_{soil}]
P^V	pure phase vapor pressure of compound [atm] (chemical specific)
R	Universal Gas Constant [0.0821 L-atm/mole-K]

Table 6-1. Nomenclature used in Chapter 6 (cont.).

Quantity		Definition
S	-	pure phase aqueous solubility of chemical "i" [mg_i/L_{H2O}] (chemical specific)
S_{avg}	-	average aqueous solubility of a multi-component mixture [$mg_{mixture}/L_{H2O}$] (mixture specific)
S_L	-	source zone leachate concentration of chemical "i" [mg_i/L_{H2O}]
S_L^o	-	source zone leachate concentration of chemical "i" at time t=0 [mg_i/L_{H2O}]
t	-	time [d]
t_o	-	time period for depletion of immiscible (free-phase) chemical [d] (chemical specific)
T	-	averaging time (for time period $T_2 < t < T_1$)[d]
T_S	-	temperature in the source zone [K]
U_{GW}	-	groundwater seepage velocity [m/d]
W	-	width of source zone perpendicular to groundwater flow direction [m]
X_i	-	mole fraction of constituent i in a mixture [$moles_i/moles_{mixture}$] (chemical specific)
β_{source}	-	first-order biodegradation constant for source zone dissolved phase[d^{-1}] (chemical specific)
ϕ_m	-	moisture content [L_{H2O}/L_{soil}]
ϕ_A	-	air-filled porosity [L_{air}/L_{soil}]
γ	-	dissolved phase overall partitioning coefficient [L_{H2O}/kg_{soil}] (chemical specific)
λ	-	overall first-order source-zone leachate strength decay coefficient [d^{-1}] (chemical specific)
ρ_b	-	soil bulk density [kg_{soil}/L_{soil}]
ρ_s	-	density of soil particles [kg_{soil}/L_{soil}]

Table 6-2. Summary of Algorithms for the Idealized Source Models Described in Chapter 6.

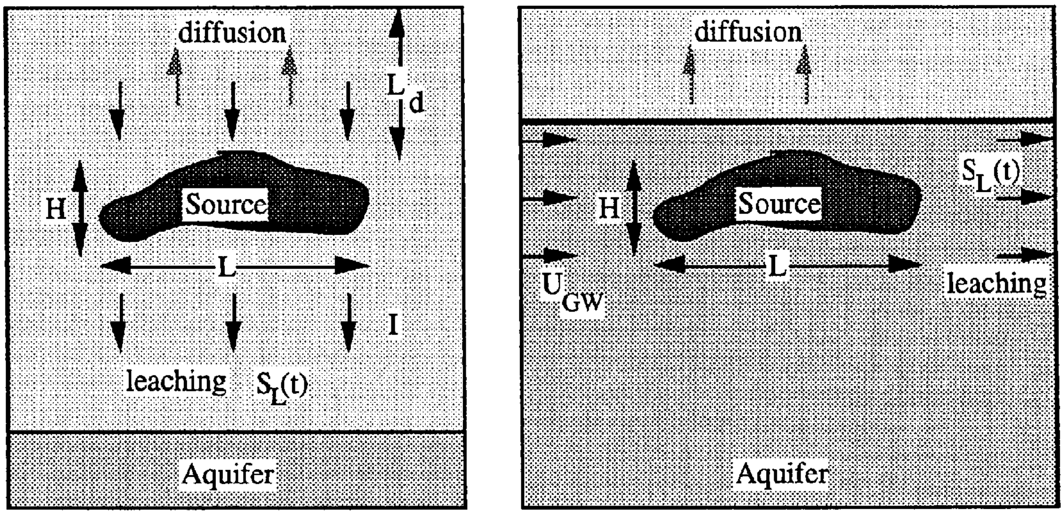
Source Type	Source Zone Leachate $S_L(t)$	Decay Constant λ	Soil Screening Level C^{o}_{T}	Restrictions
CONSTANT STRENGTH SOURCES				
A) no immiscible phase present, single or multiple compounds	$S_L(t) = S^o_L$ $\frac{1}{T}\int_0^T \frac{S_L(t)}{S_L(0)}\,dt = 1$	$\lambda = 0$	$C^o_T = S^o_L\left(\frac{\phi_m}{\rho_b} + \frac{\phi_A K_H}{\rho_b} + K_d\right)$	$\sum_{i=1}^{i=n}\left(\frac{S^o_L}{S}\right)_i < 1$ *(sum over all compounds present)*
B) immiscible phase, single or multiple components	$S_L(t) = S^o_L = X_i S$ $\frac{1}{T}\int_0^T \frac{S_L(t)}{S_L(0)}\,dt = 1$	$\lambda = 0$	mixtures: $C^o_T = \frac{M_W}{M_{W,avg}}\left(\frac{S^o_L}{S}\right) C_{T,mix}$ for single components: $C^o_T \geq S\left(\frac{\phi_m}{\rho_b} + \frac{\phi_A K_H}{\rho_b} + K_d\right)$	for mixtures: $\sum_{i=1}^{i=n}\left(\frac{S^o_L}{S}\right)_i = 1$ *(sum over all compounds present)* single components: $S^o_L = S$
Exponentially-Decaying Sources				
A) no immiscible phase, single or multiple compounds	$S_L(t) = S^o_L\, e^{-\lambda t}$ $\frac{1}{T}\int_0^T \frac{S_L(t)}{S_L(0)}\,dt = \frac{(1 - e^{-\lambda T})}{\lambda T}$	$\lambda = \frac{\left(\frac{I}{H} + \frac{K_H D^{eff}}{H L_d} + \beta_{source}\,\phi_m\right)}{\phi_m + \phi_A K_H + \rho_b K_d}$ the equation above is specific for vadose zone sources; for submerged sources replace (I/H) with ($U_{GW}\phi_m/L$).	$C^o_T = S^o_L\left(\frac{\phi_m}{\rho_b} + \frac{\phi_A K_H}{\rho_b} + K_d\right)$	$\sum_{i=1}^{i=n}\left(\frac{S^o_L}{S}\right)_i < 1$ *(sum over all compounds present)*

Table 6-2. Summary of Algorithms for the Idealized Source Models Described in Chapter 6.

Source Type	Source Zone Leachate $S_L(t)$	Decay Constant λ	Soil Screening Level C^o_T	Restrictions
EXPONENTIALLY-DECAYING SOURCES				
B) immiscible phase, leaching of relatively soluble compounds from an insoluble mixture	$S_L(t) = S^o_L e^{-\lambda t}$ $\frac{1}{T}\int_0^T \frac{S_L(t)}{S_L(0)} dt = \frac{(1-e^{-\lambda T})}{\lambda T}$ $S^o_L = X_i S$	$\lambda = (\frac{I}{H} + \frac{K_H D^{eff}}{H L_d} + \beta_{source} \phi_m) \times \left(\frac{S}{\rho_b C_{T,mix}}\right)\left(\frac{M_{w,avg}}{M_w}\right)$ the equation above is specific for vadose zone sources; for submerged sources replace (I/H) with ($U_{GW}\phi_m/L$).	$C^o_T = \frac{M_W}{M_{W,avg}}\left(\frac{S^o_L}{S}\right) C_{T,mix}$	$\sum_{i=1}^{i=n}\left(\frac{S^o_L}{S}\right)_i = 1$ *(sum over all compounds present)* and $S >> S_{avg}$
DELAYED EXPONENTIALLY-DECAYING SOURCES				
A) Single Component	$S_L(t) = S \; ; \; t \le t_o$ $S_L(t) = S^o_L e^{-\lambda(t-t_o)};$ $t_o \le t$ $\frac{1}{T}\int_0^T \frac{S_L(t)}{S_L(0)} dt = \left(\frac{t_o}{T}\right) + \frac{(1-e^{-\lambda(T-t_o)})}{\lambda T}$	$\lambda = \frac{(\frac{I}{H} + \frac{K_H D^{eff}}{H L_d} + \beta_{source} \phi_m)}{\phi_m + \phi_A K_H + \rho_b K_d}$ the equation above is specific for vadose zone sources; for submerged sources replace (I/H) with ($U_{GW}\phi_m/L$).	$C^o_T = S[\lambda t_o + \gamma]/\rho_b$ where: $\gamma = (\frac{\phi_m}{\rho_b} + \frac{\phi_A K_H}{\rho_b} + K_d)$	single component only, $T > t_o$
GENERAL CASE				
General Case	$S_L(t) = f(t)$	no general form	to be determined numerically	none

6.2 GENERAL APPROACH - CONCEPTUAL MODEL

In general, sources may be located above or within the groundwater zone as shown in Figure 6-1. In either case, water passes through the source zone and some degree of leaching, volatilization, and chemical degradation may occur. In the following, general mass loss rate and chemical equilibrium partitioning expressions are developed. These equations form the theoretical basis for the analysis of simplistic limiting cases discussed in subsequent sections.



vadose zone source scenario

submerged source zone scenario

Figure 6-1. Conceptual source zone scenarios

6.2.1 MATHEMATICAL FRAMEWORK - SOURCE ZONE MASS BALANCE

The following approach is applicable to both vadose-zone and submerged source zones, although the equations will be derived in the context of vadose zone sources.

Allowing for mass loss due to leaching, volatilization, and biodegradation, vadose zone source zone mass loss rates can be approximated with the following:

$$\frac{d}{dt}(\rho_b C_T L W H) = -I L W S_L - \frac{D^{eff}}{L_d} C_V L W - \beta_{source} \phi_m S_L L W H \qquad (6\text{-}6)$$

where:

ρ_b = soil bulk density $[kg_{soil}/L_{soil}]$
C_T = total concentration of contaminant in soil (all phases) $[mg_i/kg_{soil}]$
S_L = source zone pore water (leachate) concentration $[mg_i/L_{H2O}]$
C_V = vapor phase concentration in soil matrix $[mg_i/L_{air}]$
I = water infiltration rate [m/d]
L = length of the source zone parallel to groundwater flow direction [m]
W = source zone width perpendicular to groundwater flow direction [m]
H = source zone thickness (vertical dimension) [m]
D^{eff} = effective porous medium gas phase diffusion coefficient $[m^2/d]$
L_d = diffusion path length [m]
β_{source} = first-order biodegradation coefficient for source zone solute $[d^{-1}]$
ϕ_m = moisture content $[L_{H2O}/L_{soil}]$

The first term in Equation (6-6) accounts for mass loss due to leaching, the second term is an estimate of volatilization losses, and the third term approximates biodegradation as a first-order reaction. In the case of submerged sources, the volatilization loss term will typically be negligible in comparison to leaching losses, and the term ($ILWS_L$) should be replaced with ($U_{GW}\phi_m HWS_L$).

Equation (6-6) can be rearranged:

$$\frac{d}{dt}(\rho_b C_T) = -\left(\frac{I}{H} + \beta_{source}\,\phi_m\right)S_L - \frac{D^{eff}}{H\,L_d}C_V \quad \text{(for vadose zone sources)} \tag{6-7a}$$

$$\frac{d}{dt}(\rho_b C_T) = -\left(\frac{U_{GW}\,\phi_m}{L} + \beta_{source}\,\phi_m\right)S_L - \frac{D^{eff}}{H\,L_d}C_V \quad \text{(for submerged sources)} \tag{6-7b}$$

6.2.2 MATHEMATICAL APPROACH - CHEMICAL PARTITIONING

Relationships among C_T, C_V, and S_L are required to solve Equation (6-7). In general, for multi-component mixtures over a wide range of compositions and concentrations, there are no analytical closed-form equations relating these quantities (Rixey, 1996). However, there are limiting forms which may be used, provided that restrictions for their use are not violated. Two of these are examined below.

Equilibrium Partitioning - Single or Multi-Component Systems - Immiscible Phase not Present

An immiscible phase will not be present in the soil matrix when the following condition is satisfied:

$$\sum_{i=1}^{i=n} \left(\frac{S^o_L}{S} \right)_i < 1 \qquad (6\text{-}8)$$

where:

S^o_L = initial source zone leachate concentration of chemical "i" at time t=0 [mg_i / L_{H2O}]
S = pure component solubility of chemical "i" [mg_i / L_{H2O}]

In this case, the total mass of a chemical "i" is distributed among the pore water, soil air, and soil particle surfaces in the soil matrix. A mathematical description of this mass distribution can be written:

$$M_{T,i} = M_{L,i} + M_{V,i} + M_{S,i} \qquad (6\text{-}9)$$

where:

$M_{L,i}$ = the mass of chemical "i" in the soil pore water [mg_i]
$M_{V,i}$ = the mass of chemical "i" in the vapor phase [mg_i]
$M_{S,i}$ = the mass of chemical "i" sorbed onto soil particles [mg_i]

Equation (6-9) can also be written in terms of chemical concentrations in the three phases:

$$\rho_b C_T = \phi_m S_L + \phi_A C_V + \rho_b C_S \qquad (6\text{-}10)$$

where:

C_T = total soil concentration of chemical "i" in the soil matrix $[mg_i / kg_{soil}]$
S_L = source zone pore water (leachate) concentration of chemical "i" $[mg_i / L_{H2O}]$
C_V = vapor phase concentration of chemical "i" in soil matrix $[mg_i / L_{air}]$
C_S = sorbed concentration of chemical "i" in soil matrix $[mg_i / kg_{soil}]$
ρ_b = soil bulk density $[kg_{soil}/L_{soil}]$
ϕ_m = volumetric soil moisture content $[L_{H2O}/L_{soil}]$
ϕ_A = air-filled soil porosity $[L_{void}/L_{soil}]$

It is common to relate concentrations in each phase through linear partitioning expressions:

$$C_V = K_H S_L \tag{6-11}$$

$$C_S = K_d S_L \tag{6-12}$$

where:

K_H = Henrys law coefficient for chemical "i" $[(mg_i / L_{air})/(mg_i / L_{H2O})]$
K_d = Linear soil/water partition coefficient for chemical "i" $[(mg_i / kg_{soil})/(mg_i / L_{H2O})]$

Note that both K_H and K_d are chemical specific properties. After substituting Equations (6-11) and (6-12) into Equation (6-10) and rearranging, the total soil concentration of a given compound, C_T, may be expressed only in terms of the pore water concentration, and chemical and soil parameters:

$$C_T(t) = \gamma S_L(t) \tag{6-13}$$

where:

$$\gamma = \left(\frac{\phi_m}{\rho_b} + \frac{\phi_a K_H}{\rho_b} + K_d\right) \tag{6-14}$$

The term γ [L_{H2O}/kg_{soil}] can be viewed as an overall dissolved phase partitioning coefficient for chemical "i", and is typically considered to be constant with time for a given compound and soil matrix.

Based on Equation (6-13), the restriction given in Equation (6-8) can be rewritten as:

$$\sum_{i=1}^{i=n}\left(\frac{S_L^o}{S}\right)_i < 1 \quad \text{or} \quad \sum_{i=1}^{i=n}\left(\frac{C_T^o/\gamma}{S}\right)_i \leq 1 \qquad (6\text{-}15)$$

Equilibrium Partitioning - Single or Multi-Component Systems - Immiscible Phase Present

An immiscible phase will be present in the soil matrix when the following condition is satisfied:

$$\sum_{i=1}^{i=n}\left(\frac{S_L^o}{S}\right)_i = 1 \quad \text{or} \quad \sum_{i=1}^{i=n}\left(\frac{C_T^o/\gamma}{S}\right)_i \geq 1 \qquad (6\text{-}16)$$

where:

S^o_L = initial source zone leachate concentration of chemical "i" at time t=0 [mg_i/L_{H2O}]
S = pure component solubility of chemical "i" [mg_i/L_{H2O}]
C^o_T = initial source zone soil concentration of chemical "i" at (t=0) [mg_i/kg_{soil}]
γ = overall soil partition coefficient for chemical "i" as defined in Equation (6-14) [L_{H2O}/kg_{soil}]

In this case, the total mass of chemical "i" is distributed among four phases in the soil matrix: pore water, soil vapor, sorbed onto soil particle surfaces, and an immiscible phase.

Equations (6-11) and (6-12) are still used to relate concentrations of chemical "i" in the vapor, sorbed, and dissolved phases; however, an additional equation is required to describe partitioning from the immiscible phase. Here the ideal solution assumption is invoked; thus, it is assumed that the leachate concentration of chemical "i", S_L [mg_i/L_{H2O}], is proportional to its mole fraction in the immiscible phase, X_i [$moles_i$/total moles], and the pure compound solubility S [mg_i/L_{H2O}]:

$$S_L = S X_i \qquad (6\text{-}17)$$

where:

$$X_i = \left(\frac{C_T}{C_{T,mix}}\right)\left(\frac{M_{W,avg}}{M_W}\right) \qquad (6\text{-}18)$$

and:

$C_{T,mix}$ = total concentration of mixture (sum of all compounds) in the soil matrix $[mg_{mixture}/kg_{soil}]$
C_T = total concentration of chemical "i" in the soil matrix $[mg_i /kg_{soil}]$
M_W = molecular weight of chemical "i" $[g_i /mole_i]$
$M_{W,avg}$ = mixture average molecular weight $[g_{mixture} /mole_{mixture}]$

In writing Equation (6-18), it has been assumed that the immiscible phase contains the majority of the total contaminant mass.

Assuming that the immiscible free-phase behaves as an ideal solution (i.e., obeys Raoult's law), the soil vapor concentration C_v $[mg_i /L_{vapor}]$ of any chemical "i" is given by:

$$C_V = X_i\left(\frac{P^V M_W}{R\,T_S}\right) = K_H\,S_L \qquad (6\text{-}19)$$

where:

P^V = pure phase vapor pressure of chemical "i" [atm]
R = Universal Gas Constant [= 0.0821 L-atm/mole-K]
T_S = temperature in the soil matrix [K]
K_H = Henrys law coefficient for chemical "i" $[(mg_i /L_{air})/(mg_i /L_{H2O})]$

6.3 CONSTANT-STRENGTH (INFINITE) SOURCES

Though most source zones contain a finite mass of contaminant which necessarily decreases over time due to natural processes, constant-strength source models are often employed for a number of reasons, including:

- The user does not have to estimate a source zone depletion rate, which often requires additional data that may not be available; or

- The source zone decay rate may be so slow that small changes in the source strength occur during the period of interest.

In any case, it is recognized that the use of constant-strength source zone models typically result in conservative estimates of actual impacts to groundwater. Here "conservative" implies that the predicted leachate concentration always equals or exceeds the actual leachate concentration at any given time.

Figure 6-2 displays how the leachate concentration depends on time for a constant-strength source.

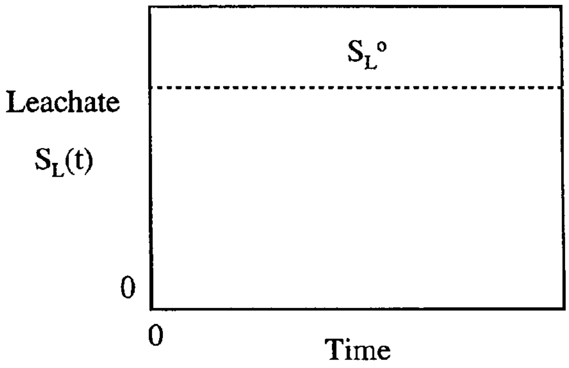


Figure 6-2. *Dependence of source zone leachate concentration S_L [mg_i/L_{H2O}] on time for a constant-strength source*

In this case, independent of the equilibrium partitioning behavior in the source zone, we can write:

$$S_L(t) = S_L^o \tag{6-20}$$

and

$$\frac{1}{T}\int_0^T \frac{S_L(t)}{S_L(0)}\,dt = 1 \qquad (6\text{-}21)$$

Equation (6-21) is the expression that would be used in DAF Equation (6-2) for a constant-strength source.

Assuming that the user had calculated a DAF, and a resulting initial source leachate concentration S^o_L [mg_i/L_{H2O}], Equations (6-13) and (6-14), or Equations (6-17) and (6-18) would be used to estimate a soil screening level C^o_T [mg_i/kg_{soil}]:

(single or multi-component systems without immiscible phase present)

$$C^o_T = S^o_L\left(\frac{\phi_m}{\rho_b} + \frac{\phi_a K_H}{\rho_b} + K_d\right) \textit{ provided that } \sum_{i=1}^{i=n}\left(\frac{S^o_L}{S}\right)_i < 1 \qquad (6\text{-}22)$$

or

(single or multi-component systems with immiscible phase present)

$$C^o_T = \frac{M_W}{M_{W,avg}}\left(\frac{S^o_L}{S}\right)C_{T,mix} \quad \textit{provided that } \sum_{i=1}^{i=n}\left(\frac{S^o_L}{S}\right)_i = 1 \qquad (6\text{-}23)$$

Note that use of Equation (6-23) requires an estimate of the total soil concentration of all compounds present $C_{T,mix}$ [mg_i/kg_{soil}] ($C_{T,mix} = \Sigma C^o_T$).

It is also important that the user verify that the restrictions given in Equations (6-22) and (6-23) are satisfied.

6.4 EXPONENTIALLY-DECAYING SOURCES

The source zone leachate concentration dependence on time, $S_L(t)$ [mg_i/L_{H2O}], for an exponentially-decaying source is given by:

$$S_L(t) = S^o_L\, e^{-\lambda t} \qquad (6\text{-}24)$$

and

$$\frac{1}{T}\int_0^T \frac{S_L(t)}{S_L(0)}\,dt = \frac{(1-e^{-\lambda T})}{\lambda T} \tag{6-25}$$

where:

λ = overall first-order decay rate of source zone leachate strength [d^{-1}]
T = averaging time [d]

This functional dependence is shown in Figures 6-3 and 6-4 below.

The challenge now is to determine the overall first-order leachate source-strength decay constant λ [d^{-1}]. This is derived from mass balance Equation (6-7) and equilibrium partitioning relations Equations (6-11) and (6-12), or (6-17), (6-18), and (6-19).

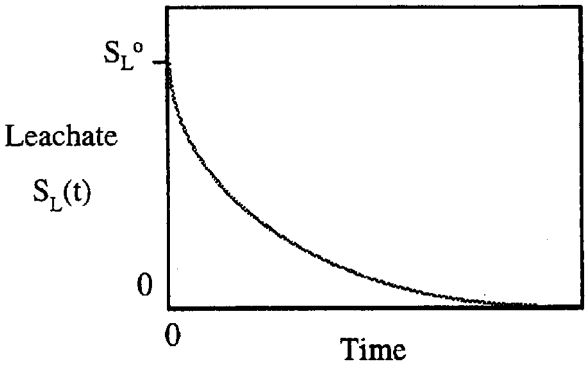


Figure 6-3. Dependence of source zone leachate concentration S_L [mg_i/L_{H2O}] on time for an exponentially-decaying source

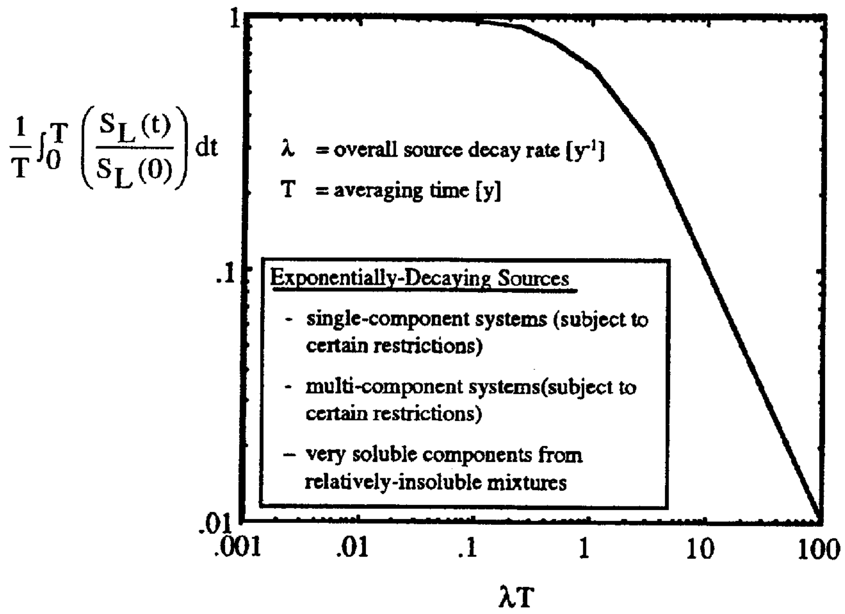


Figure 6-4. *Dependence of time-averaged and normalized source zone leachate concentration (Equation 6-25) on averaging time for an exponentially-decaying source*

First-Order Source Decay Rate: Single, or Multi-Component Mixtures without Immiscible Phase Present

Equation (6-8) dictates the condition under which an immiscible phase is not present in the soil matrix. In this case, the total mass of a chemical "i" is distributed among the pore water, soil air, and soil particle surfaces in the soil matrix. Partitioning Equations (6-11) and (6-12) apply, and when combined with Equation (6-7) yield:

$$\frac{d}{dt}(S_L) = -\left\{\frac{[(\frac{I}{H} + \beta_{source}\,\phi_m) + \frac{D^{eff}}{H\,L_d}\,K_H]}{[\phi_m + \phi_A\,K_H + \rho_b K_d]}\right\} S_L \quad \text{(vadose zone sources)} \qquad (6\text{-}26a)$$

$$\frac{d}{dt}(S_L) = -\left\{\frac{[(\frac{U_{GW}\,\phi_m}{L} + \beta_{source}\,\phi_m) + \frac{D^{eff}}{H\,L_d}\,K_H]}{[\phi_m + \phi_A\,K_H + \rho_b K_d]}\right\} S_L \quad \text{(submerged sources)} \qquad (6\text{-}26b)$$

which predicts a first-order decay in leachate strength with time, with a decay constant λ given by:

$$\lambda = \frac{\left(\frac{I}{H} + \frac{K_H D^{eff}}{H L_d} + \beta_{source}\,\phi_m\right)}{\phi_m + \phi_A K_H + \rho_b K_d} \quad \textit{immiscible phase not present (vadose zone sources)} \qquad (6\text{-}27a)$$

$$\lambda = \frac{\left(\frac{U_{GW}\,\phi_m}{L} + \frac{K_H D^{eff}}{H L_d} + \beta_{source}\,\phi_m\right)}{\phi_m + \phi_A K_H + \rho_b K_d} \quad \textit{immiscible phase not present (submerged sources)} \qquad (6\text{-}27b)$$

Here:

K_H = Henrys law coefficient for chemical "i" $[(mg_i/L_{air})/(mg_i/L_{H2O})]$
K_d = soil/water partition coefficient for chemical "i" $[(mg_i/kg_{soil})/(mg_i/L_{H2O})]$
ϕ_m = volumetric soil moisture content $[L_{H2O}/L_{soil}]$
ϕ_A = air-filled soil porosity $[L_{void}/L_{soil}]$
ρ_b = soil bulk density $[kg_{soil}/L_{soil}]$
I = water infiltration rate [m/d]
H = source zone thickness (vertical dimension) [m]
D^{eff} = effective porous medium diffusion coefficient for chemical "i" $[m^2/d]$
L_d = diffusion path length [m]
U_{GW} = groundwater seepage velocity [m/d]
β_{source} = first-order biodegradation coefficient for dissolved chemical "i" $[d^{-1}]$
L = length of source parallel to groundwater flow direction [m]

For these same conditions, the relationship between the initial source zone leachate concentration, S^o_L $[mg_i/L_{H2O}]$, and initial soil concentration, C^o_T $[mg_i/kg_{soil}]$, of any compound is given by:

$$C^o_T = S^o_L\left(\frac{\phi_m}{\rho_b} + \frac{\phi_A K_H}{\rho_b} + K_d\right) \quad \textit{provided that} \quad \sum_{i=1}^{i=n}\left(\frac{S^o_L}{S}\right)_i < 1 \qquad (6\text{-}28)$$

First-Order Source Decay Rate: Single or Multi-Component Mixtures with Immiscible Phase Always Present

Equation (6-16) dictates the conditions under which an immiscible phase is present in the soil matrix. In this case, the total mass of a compound "i" is distributed among the pore water, soil air, soil particle surfaces, and immiscible phase in the soil matrix. Partitioning Equations (6-17), (6-18), and (6-19) apply, and when combined with Equation (6-7) yield:

$$\frac{d}{dt}(C_T) \;=\; -\,[(\frac{I}{H}+\beta_{source}\,\phi_m\,)+\frac{D^{eff}}{H\,L_d}\,K_H]\left(\frac{S}{\rho_b\,C_{T,mix}}\right)\left(\frac{M_{w,avg}}{M_w}\right)C_T \text{ (vadose zone sources)} \quad (6\text{-}29a)$$

$$\frac{d}{dt}(C_T)=-\,[(\frac{U_{GW}\,\phi_m}{L}+\beta_{source}\,\phi_m\,)+\frac{D^{eff}}{H\,L_d}\,K_H]\left(\frac{S}{\rho_b\,C_{T,mix}}\right)\left(\frac{M_{w,avg}}{M_w}\right)C_T \text{ (submerged sources)} \quad (6\text{-}29b)$$

Thus:

$$\lambda=[(\frac{I}{H}+\beta_{source}\,\phi_m\,)+\frac{D^{eff}}{H\,L_d}\,K_H]\left(\frac{S}{\rho_b\,C_{T,mix}}\right)\left(\frac{M_{w,avg}}{M_w}\right) \textit{ immiscible phase present} \text{ (vadose sources)}$$

(6-30a)

$$\lambda=[(\frac{U_{GW}\,\phi_m}{L}+\beta_{source}\,\phi_m\,)+\frac{D^{eff}\,K_H}{H\,L_d}]\left(\frac{S}{\rho_b\,C_{T,mix}}\right)\left(\frac{M_{w,avg}}{M_w}\right) \textit{immiscible phase present} \text{ (submerged sources)}$$

(6-30b)

where:

K_H = Henry's law coefficient for chemical "i" $[(mg_i\,/L_{air})/(mg_i\,/L_{H2O})]$
ϕ_m = volumetric soil moisture content $[L_{H2O}/L_{soil}]$
ρ_b = soil bulk density $[kg_{soil}/L_{soil}]$
I = water infiltration rate [m/d]
H = source zone thickness (vertical dimension) [m]
D^{eff} = effective porous medium diffusion coefficient for chemical "i" $[m^2/d]$
L_d = diffusion path length [m]
β_{source} = first-order biodegradation coefficient for dissolved chemical "i" $[d^{-1}]$
S = pure component solubility of chemical "i" $[mg_i\,/L_{H2O}]$

$C_{T,mix}$ = total concentration of mixture (sum of all compounds) in the soil matrix [$mg_{mixture}/kg_{soil}$]
C_T = total concentration of chemical "i" in the soil matrix [mg_i/kg_{soil}]
M_W = molecular weight of chemical "i" [$g_i/mole_i$]
$M_{W,avg}$ = mixture average molecular weight [$g_{mixture}/mole_{mixture}$]

For these same conditions, the relationship between the initial source zone leachate concentration, S^o_L [mg_i/L_{H2O}], and initial soil concentration, C^o_T [mg_i/kg_{soil}], of any compound is given by:

$$C^o_T = \frac{M_W}{M_{W,avg}}\left(\frac{S^o_L}{S}\right)C_{T,mix} \quad \textit{provided that} \quad \sum_{i=1}^{i=n}\left(\frac{S^o_L}{S}\right)_i = 1 \qquad (6\text{-}31)$$

Delayed Exponentially Decaying Sources - Single Component Systems Only

Here, the source zone contains a single compound with initial concentration C^o_T [mg_i/kg_{soil}] that is large enough to ensure that:

$$C^o_T > S\left[\frac{\phi_m}{\rho_b} + \frac{\phi_A K_H}{\rho_b} + K_d\right] \qquad (6\text{-}32)$$

where:

K_H = Henrys law coefficient of chemical "i" [$(mg_i/L_{air})/(mg_i/L_{H2O})$]
K_d = Linear soil/water partition coefficient for chemical "i" [$(mg_i/kg_{soil})/(mg_i/L_{H2O})$]
ϕ_m = volumetric soil moisture content [L_{H2O}/L_{soil}]
ϕ_A = air-filled soil porosity [L_{void}/L_{soil}]
ρ_b = soil bulk density [kg_{soil}/L_{soil}]
S = pure component aqueous solubility of chemical "i" [mg_i/L_{H2O}]
L = length of source parallel to groundwater flow direction [m]

Then, as the source decays:

$$S_L(t) = S \qquad \text{for} \qquad C_T(t) > S\left[\frac{\phi_m}{\rho_b} + \frac{\phi_A\, K_H}{\rho_b} + K_d\right] \tag{6-33}$$

and:

$$S_L(t) = \frac{C_T(t)}{\left[\dfrac{\phi_m}{\rho_b} + \dfrac{\phi_A\, K_H}{\rho_b} + K_d\right]} \qquad \text{for} \qquad C_T(t) \le S\left[\frac{\phi_m}{\rho_b} + \frac{\phi_A\, K_H}{\rho_b} + K_d\right] \tag{6-34}$$

Inserting Equations (6-33) and (6-34) into Equation (6-7) yields the following expression for $S_L(t)$:

$$S_L(t) = S \qquad \text{for} \qquad t < t_o \tag{6-35}$$

and:

$$S_L(t) = S\, e^{-\lambda\,(t - t_o)} \qquad \text{for}\ t \ge t_o \tag{6-36}$$

where:

$$\lambda = \left\{ \frac{\left(\dfrac{I}{H} + \dfrac{K_H\, D^{eff}}{H\, L_d} + \beta_{source}\, \theta_m\right)}{\phi_m + \phi_A\, K_H + \rho_b K_d} \right\} \ \text{(vadose zone sources)} \tag{6-37a}$$

$$\lambda = \left\{ \frac{\left(\dfrac{U_{GW}\, \phi_m}{L} + \dfrac{K_H\, D^{eff}}{H\, L_d} + \beta_{source}\, \theta_m\right)}{\phi_m + \phi_A\, K_H + \rho_b K_d} \right\} \ \text{(submerged sources)} \tag{6-37b}$$

and:

$$t_o = \frac{\left\{\rho_b C_T^o - S\left[\phi_m + \phi_A\, K_H + \rho_b K_d\right]\right\}}{\left[\left(\dfrac{I}{H} + \beta_{source}\, \phi_m\right) + \dfrac{K_H\, D^{eff}}{H\, L_d}\right] S} \ \text{(for vadose zone sources)} \tag{6-38a}$$

$$t_o = \frac{\left\{\rho_b C_T^o - S\left[\phi_m + \phi_A\, K_H + \rho_b K_d\right]\right\}}{\left[\left(\dfrac{U_{GW}\, \phi_m}{L} + \beta_{source}\, \phi_m\right) + \dfrac{K_H\, D^{eff}}{H\, L_d}\right] S} \ \text{(for submerged sources)} \tag{6-38b}$$

In Equations (6-37) and (6-38):

K_H = Henry's law coefficient for chemical "i" $[(mg_i/L_{air})/(mg_i/L_{H2O})]$
K_d = soil/water partition coefficient for chemical "i" $[(mg_i/kg_{soil})/(mg_i/L_{H2O})]$
ϕ_m = volumetric soil moisture content $[L_{H2O}/L_{soil}]$
ϕ_A = air-filled soil porosity $[L_{void}/L_{soil}]$
ρ_b = soil bulk density $[kg_{soil}/L_{soil}]$
I = water infiltration rate [m/d]
H = source zone thickness (vertical dimension) [m]
D^{eff} = effective porous medium diffusion coefficient for chemical "i" $[m^2/d]$
L_d = diffusion path length [m]
U_{GW} = groundwater seepage velocity [m/d]
β_{source} = first-order biodegradation coefficient for dissolved chemical "i" $[d^{-1}]$

For these conditions:

$$\frac{1}{T}\int_0^T \frac{S_L(t)}{S_L(0)}\,dt = \left(\frac{t_o}{T}\right) + \frac{(1 - e^{-\lambda(T - t_o)})}{\lambda T} \qquad (6\text{-}39)$$

This functional dependence is shown in Figures 6-5 and 6-6 below.

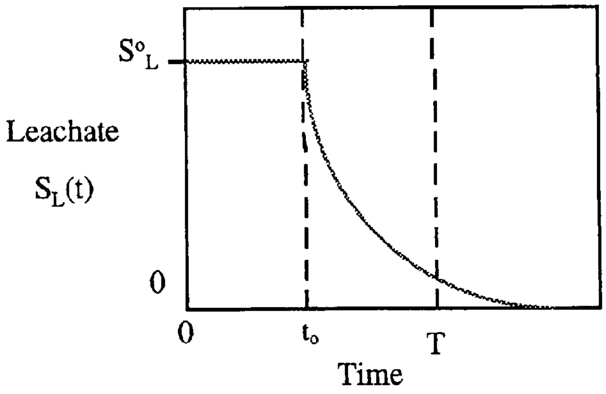


Figure 6-5. Dependence of source zone leachate concentration S_L $[mg_i/L_{H2O}]$ on time for a time-delayed exponentially-decaying source

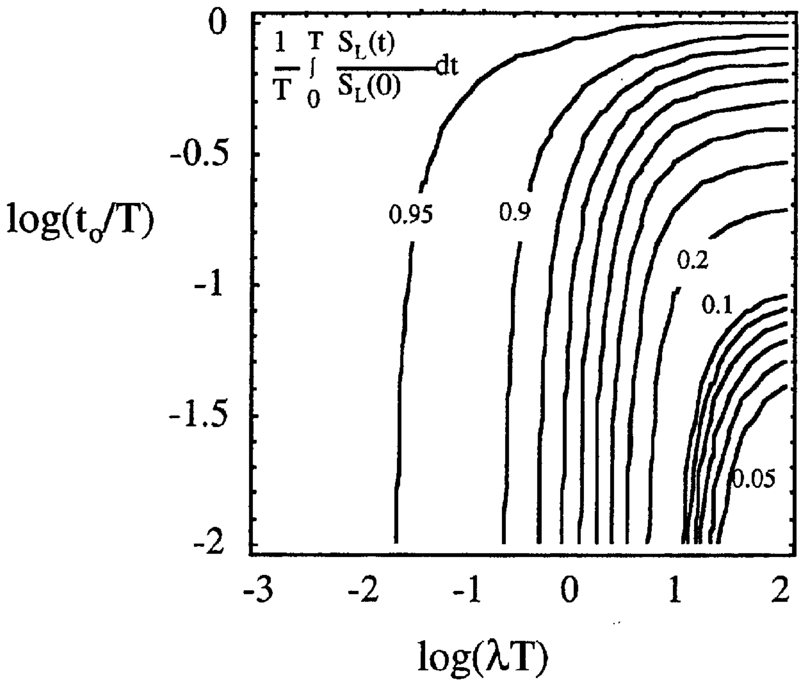


Figure 6-6. ***Dependence of time-averaged and normalized source zone leachate concentration (Equation 6-39) on averaging time for a time-delayed exponentially-decaying source***

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APPENDIX A

DATA/PARAMETER SELECTION GUIDE

INTRODUCTION

Determination of site-specific dilution attenuation factors (DAFs) with the graphical technique described in this document may require as many as 25 individual parameter values. These are listed in Table A-1, along with "typical" ranges of values obtained from various published references. In addition, for each parameter, an indication of the DAF determination process sensitivity is given. The qualitative sensitivity indication for each parameter gives the user an indication of how changes, or uncertainty, in the parameter will affect the calculated DAF. The following pages, qualitative scale was used to rank the parameters listed in Table A-1:

high = potential to cause much greater than an order of magnitude change in the DAF
moderate = potential to cause up to an order of magnitude change in the DAF
low = potential to cause much less than an order of magnitude change in the DAF

As will be seen, not all of these parameters are required to generate a DAF estimate for a given site.

In the following pages each parameter is discussed briefly, and guidance is given for selecting reasonable parameter values.

Residual Water Filled Soil Porosity

The residual water content may be determined empirically on a mass basis by comparing the mass of an undisturbed sample to its dried mass. In the absence of empirical data, the residual water content may be estimated from soil type (Carsel and Parrish 1988). A soil data base compiled by Carsel *et al.* (1988) was used to obtain bulk density and clay content for the 12 Soil Conservation Service (SCS) textural classifications, which include: clay, clay loam, loam, loamy sand, silt, silt loam, silty clay, silty clay loam, sand, sandy clay, sandy clay loam, and sandy loam. Residual water content was then estimated from bulk density on a volume basis (Rawls and Brakensiek 1985), values for SCS soil textures are listed in Table A-2.

Table A-1. Parameter values, DAF sensitivity indicator, and ranges of reasonable values

Parameter	Range	Sensitivity	Reference
SOURCE ZONE PARAMETERS - ONLY REQUIRED FOR CALCULATING SOIL TARGET LEVELS FROM DAFs			
ϕ_m - residual water content [L_{H2O}/L_{soil}]	0.034- 0.1	low	Carsel 1988
ϕ_A - air-filled porosity [L_{void}/L_{soil}]	0.28 - 0.42	low	Carsel 1988
K_{OC} - organic carbon partition coefficient [$(mg/kg_{soil})/(mg/L_{H2O})$]	83- 1.8×10^5	high	Montgomery 1991
f_{oc} - fraction of organic carbon in soil [kg/kg]	0 - 0.063	moderate	Carsel 1988
ρ_b - soil bulk density [kg_{soil}/L_{H2O}]	1.4 - 1.7	low	Carsel 1988
K_H - "dimensionless" Henrys Law constant for compound i [$(mg/L_{air})/(mg/L_{H2O})$]	10^{-7} -3.5	low	Mackay 1981
S - aqueous solubility of compound i [mg/L]	10^{-3} - 10^5	high	Verschueren 1983
SOURCE ZONE PARAMETERS - ONLY REQUIRED WHEN CONSIDERING TIME-VARYING SOURCE STRENGTHS			
I_f - water infiltration rate through source zone [m/y]	0.00007 -1	high	Help Model
*β - first-order biodegradation rate constant [d^{-1}]	0.0006 - 0.01*	high	Chiang 1989, Buscheck 1992
L - length of source zone [m]	3 - 30	moderate	Experience
W - width of source zone [m]	3 - 30	moderate	Experience
H - thickness of source zone [m]	3 - 30	moderate	Experience
D^{eff} - effective vapor-phase diffusion coefficient for compound i [m^2/d]	0.39 - 0.82	low	Marrero 1973
L_C - depth below ground surface to the top of the source zone [m]	1 - 10	low	Experience
L_d - mean diffusion path length = L_c + 0.5 H [m]	1 - 10	low	Experience
$C_{T,mix}$ - total soil concentration of a mixture (sum of all components) [mg_{mix}/kg_{soil}] ♦	10^2 - 10^5	high	Experience
M_w - molecular weight of component i [g/mole] ♦	16 - 400	high	Verschueren 1983
$M_{w,avg}$ - average mixture molecular weight [$g_{mix}/moles_{mix}$] ♦	60 - 300	low	Experience
K_H - Henrys law coefficient for compound i [$(mg/L_{air})/(mg/L_{H2O})$]	10^{-7} - 3.5	low	Mackay 1981
S - pure phase aqueous solubility of contaminant i [mg/L_{H2O}] ♦	10^{-3} - 10^5	high	Verschueren 1983

Table A-1. Parameter values, DAF sensitivity indicator, and ranges of reasonable values (cont.)

Parameter	Range	Sensitivity	Reference
VADOSE ZONE PARAMETERS - ONLY REQUIRED FOR VADOSE-ZONE SOURCES			
I_f - water infiltration rate through vadose zone [m/y]	0.00007 -1	high	Help Model
L_{vz} - distance from the bottom of the source zone to the aquifer [m]	0 - 100	high	Empirical
ϕ_m - water-filled porosity [L_{H2O}/kg_{soil}]	0.034- 0.1	low	Carsel 1988
β_{vz} - first order biodegradation rate constant [d^{-1}]*	0.0006 - 0.01*	high	Chiang 1989, Buscheck 1992
SATURATED ZONE PARAMETERS			
U_{GW} - linear groundwater velocity [m/d]	0.005 - 0.5	high - when including biodegradation; moderate otherwise	Newell 1990
ρ_b - soil bulk density [kg_{soil}/L_{H2O}]	1.32 - 1.87	low	Carsel 1988
K_{OC} - organic carbon partition coefficient [(mg/kg_{soil})/(mg/L_{H2O})]	83- 1.8x10^5	low	Montgomery 1991
f_{oc} - fraction of organic carbon in soil [kg/kg]	0 - 0.063	low	Carsel 1988
β_s - first order biodegradation rate constant [d^{-1}]*	0.0006 - 0.01*	high	Chiang 1989, Buscheck 1992
α_L - longitudinal dispersivity [m]	0.015 - 20	moderate	Gelhar 1992
α_T - transverse dispersivity [m]	0.03 - 0.1	moderate	Gelhar 1992
α_V - vertical dispersivity [m]	0.0006 - 0.15	moderate	Gelhar 1992
b - aquifer thickness [m]	5 - 560	low	EPA 1993
H_w - well screen sampling interval thickness [m]	1.5 - 4.5	high	Experience
L_R - distance from source zone to the receptor [m]	0 - 150	high	Experience

* based on reported first-order decay rates from saturated-zone transport studies. Values may not be appropriate for other uses (e.g., vadose zone, or source zone biodegradation rates)

♦ necessary only for finite sources with immiscible phase present

Air Filled Soil Porosity

Air filled soil porosity may be calculated from the total porosity and the residual water content by:

$$\phi_A = n - \phi_m$$

where:

ϕ_A = air filled soil porosity$[L_{air}/L_{soil}]$
ϕ_m = residual water content $[L_{water}/L_{soil}]$
n = total soil porosity $[L_{void}/L_{soil}]$

The total soil porosity may be determined empirically, or estimated from soil type (Rawls and Brakensiek 1985). Table A-2 lists values for SCS soil textures.

Soil Bulk Density

Soil bulk density determined on a dry weight basis is defined as the mass of soil per unit volume. This value may be determined experimentally, or may be calculated by the following relationship:

$$\rho_b = \rho_s (1-n)$$

where:

ρ_b = dry soil bulk density $[kg_{soil}/L_{soil}]$
ρ_s = soil particle density $[kg_{soil}/L_{soil}]$
n = total soil porosity $[L_{void}/L_{soil}]$

The soil particle density does not vary widely. A value of 2.65 [kg/L] was used for determination of the range of values presented in Table A-1.

Table A-2. Mean soil porosity and residual water contents for SCS soil types (Carsel and Parrish 1988)

Soil Type	Soil Porosity (n) L_{void}/L_{soil}		Residual Water Content L_{H2O}/L_{soil}	
	Mean	Std. Dev.	Mean	Std. Dev.
Clay	0.38	0.09	0.068	0.034
Clay loam	0.41	0.09	0.095	0.010
Loam	0.43	0.10	0.078	0.013
Loamy sand	0.41	0.09	0.057	0.015
Silt	0.46	0.11	0.034	0.010
Silt Loam	0.45	0.08	0.067	0.015
Silty Clay	0.36	0.07	0.070	0.023
Silty clay loam	0.43	0.07	0.089	0.009
Sand	0.43	0.06	0.045	0.010
Sandy clay	0.38	0.05	0.100	0.013
Sandy clay loam	0.39	0.07	0.100	0.006
Sandy loam	0.41	0.09	0.065	0.017

Organic Carbon Partitioning Coefficient

The organic carbon partitioning coefficient K_{oc} [(mg/kg$_{carbon}$)/(mg/L$_{H2O}$)] is a chemical specific property, measuring the extent to which an organic compound partitions itself between the solid and solution phases of a saturated or unsaturated soil. K_{oc} is defined as the ratio of the mass of chemical adsorbed per unit weight of organic carbon in the soil to the equilibrium concentration of the chemical in solution:

$$K_{oc} = \frac{(mg_i / kg_{carbon})}{(mg_i / L_{H2O})}$$

Values of K_{oc} (in the above units) may range from 10 to 1,000,000 (Lyman 1982). Known methods for estimating K_{oc} values are approximate at best, thus measured values should be used if available. Table A-7 located at the end of this appendix contains K_{oc} values for selected chemicals.

Fractional Organic Carbon Content

The fractional organic carbon content of a given soil may be estimated from the percent organic matter by the following empirical relationship (Enfield 1982):

$$f_{oc} = \frac{\%OM}{174}$$

where:

f_{oc} = fractional organic carbon content
%OM = percent organic matter
174 = conversion factor

Organic carbon content generally decreases exponentially with depth (Brady 1990), due to decreases in the presence of plant matter. This implies that aquifers generally will have a low organic carbon content compared to shallow vadose zone soils. Table A-3 summarizes measured organic carbon contents of 24 aquifer sediments (API 1994).

Chemical Properties

The chemical properties of selected organic compounds, including: molecular weight, Henry's law coefficient, diffusion coefficient, and aqueous solubility are listed in Table A-7 at the end of this appendix. These values were compiled from the following sources: Montgomery and Wilkom (1990), Verschueren (1983), Mackay (1981), and Marrero and Mason (1973).

Total Mixture Soil Concentration

This parameter is required only if the source contains an immiscible mixture. The total soil concentration ($C_{T,mix}$) is the sum of the masses of all components per unit mass of soil. In this work, it is often assumed that immiscible mixtures are comprised mostly of insoluble compounds, the compounds of most interest are much more soluble than other compounds in the mixture, and they comprise only a small fraction of the total (e.g., benzene in gasoline). Thus, the total mixture concentration is assumed to remain relatively constant as the soluble compounds are leached.

Average Mixture Molecular Weight

This parameter is required only if a finite immiscible mixture source is being considered. It is a function of the mole fractions (X_i) and molecular weights (Mw_i) of all compounds in the mixture, and can change over time.

$$Mw_{ave} = \sum_{n=1}^{k} x_i \, Mw_n$$

In this work, it is assumed that immiscible mixtures are comprised mostly of insoluble compounds, and the soluble compounds of most interest comprise only a small fraction of the total. Thus, the total concentration is assumed to remain relatively constant as the soluble compounds are leached, and the average molecular weight is treated as a constant.

Reasonable carbon number ranges and average molecular weights for petroleum fuel products are (based on data given in Bruce and Schmidt 1994):

gasoline	C_4 - C_{12} (average molecular weight ≈90 g/mole)
kerosene	C_8 - C_{16} (average molecular weight ≈170 g/mole)
JP-4	C_4 - C_{12} (average molecular weight ≈120 g/mole)
diesel oil	C_8 - C_{21} (average molecular weight ≈200 g/mole)
No. 6 Fuel Oil	C_9 - C_{31} (average molecular weight ≈280 g/mole)
Lube Oil (20 wt)	C_{20} - C_{40} (average molecular weight ≈420 g/mole)
condensate	C_5 - C_{12} (average molecular weight ≈120 g/mole)
crude oil	C_4 - C_{30} (average molecular weight ≈120 - 240 g/mole)

Table A-3. Organic carbon content of various aquifer sediments (API 1994)

Aquifer Name	Sediment Composition	Organic Carbon Fraction
Tirstrup 1	c. sand-2%, f.sand-94%, silt-2%, clay-3%	0.00048
Tirstrup 2	c. sand-18%, f.sand-79%, silt-0%, clay-2%	0.00035
Finderup 2	c. sand-34%, f.sand-63%, silt-2%, clay-0%	0.00213
Tylstrup	c. sand-42%, f.sand-52%, silt-2%, clay-4%	0.00159
Barksdale	sand-52.3%, silt-41.5%, clay-6.2%	0.00030
Allerod 2	c. sand-54%, f.sand-42%, silt-4%, clay-0%	0.00048
Vasby	c. sand-63%, f.sand-34%, silt-2%, clay-1%	0.00012
Gunderup 2	c. sand-74%, f.sand-22%, silt-4%, clay-0%	0.00021
Finderup 1	c. sand-77%, f.sand-18%, silt-1%, clay-1%	0.00006
Vejen 2	c. sand-77%, f.sand-21%, silt-0%, clay-3%	0.00032
Allerod 1	c. sand-78%, f.sand-17%, silt-3%, clay-2%	0.00071
155-21-cm	sand-83.7%, silt-6.8%, clay-9.5%	0.00039
Rabis	c. sand-84%, f.sand-15%, silt-0%, clay-1%	0.00016
Brande 2	c. sand-87%, f.sand-10%, silt-2%, clay-1%	0.00020
Vorbasse 1	c. sand-88%, f.sand-11%, silt-0%, clay-1%	0.00006
Vejen 1	c. sand-90%, f.sand-8%, silt-1%, clay-1%	0.00029
Vorbasse 3	c. sand-90%, f.sand-8%, silt-2%, clay-1%	0.00122
Lula	sand-91%, silt-5.6%, clay-3.4%	0.00020
Borris	c. sand-92%, f.sand-6%, silt-2%, clay-0%	0.00020
Gundrup1	c. sand-93%, f.sand-6%, silt-0%, clay-1%	0.00009
Herborg	c. sand-93%, f.sand-5%, silt-2%, clay-0%	0.00213
Vorbasse 2	c. sand-93%, f.sand-5%, silt-2%, clay-0%	0.00007
Branden 1	c. sand-94%, f.sand-3%, silt-2%, clay-1%	0.00010
350-450-m	black sands	0.00730

Source Dimensions

Source dimensions must be specified by the user, and are determined from chemical analysis of soil samples collected from the site. Source zones are often assumed to be roughly rectangular with similar lengths (L - parallel to groundwater flow) and widths (W - transverse to groundwater flow). Rough estimates are sufficient to produce reasonable DAF estimates for a given site.

For submerged sources, vertical spreading of the contaminant due to dispersion causes the effective thickness of a given source to be somewhat greater than the measured thickness based on soil analyses. In the absence of significant vertical gradients, the following equation should provide a reasonable estimate of the submerged source thickness H (USEPA 1996):

$$H = H_{soil} + \sqrt{2\alpha_v L}$$

where:

H = the effective source thickness [m]
H_{soil} = the measured source thickness [m]
L = the source length parallel to groundwater flow [m]
α_v = vertical dispersivity [m]

First-Order Biodegradation Rate Constant

Biodegradation of organic chemicals in the vadose and saturated zones is a complex phenomenon. The rate at which a chemical will biodegrade in the subsurface is dependent on the availability of microorganisms, nutrients, and electron acceptors. Rigorous mathematical models of biodegradation require difficult to obtain chemical and site-specific data, such as the availability of electron acceptors (oxygen, nitrate, sulfate or ferric ions) and electron donors (organic carbon), as well as the nutrient supply and hydrolysis constants. The majority of fate and transport models assume a first-order kinetic reaction rate and use empirically-determined data for the rate constant. Several publications have reported decay rates of hydrocarbons in the saturated zone (Chiang 1989, Buscheck 1992) obtained by performing material balances on contaminants over time. Reported values for first-order biodegradation rates of aromatic (benzene, toluene, ethylbenzene, and xylenes) compounds in the saturated zone range from 0.0006 to 0.01 d^{-1}.

Groundwater Seepage Velocity

The groundwater seepage velocity is related to the aquifer characteristics through Darcy's law, which is given by:

$$U_{GW} = \frac{K_L\, i}{n}$$

where:

U_{GW} = regional seepage velocity of the groundwater [m/d]
K_L = longitudinal hydraulic conductivity of the aquifer [m/d]
i = regional hydraulic gradient [m/m]
n = total soil porosity [L_{void}/L_{soil}]

If the aquifer characteristics are known, the groundwater velocity may be determined by Darcy's law. A range of seepage velocities was reported (Newell 1990) for various regional hydrogeological environments. The user may estimate aquifer characteristics, or groundwater velocity from these data, based on aquifer media type, geomorphology and hydrogeological environment. Table A-4 lists aquifer characteristics and groundwater velocities for 12 hydrogeological environments, as well as a national average.

Aquifer Thickness

Table A-4 gives saturated thickness of 12 hydrogeological environments, as well as a national average.

Separation of the Source and Saturated Zones

The separation of the source zone and saturated zone (H_s) is determined by subtracting the source thickness (D_s) from the depth to groundwater.

Dispersion Coefficients

Dispersion causes spreading and dilution of the contaminant plume, and is the result of both advective and diffusive processes. This parameter is a site- and scale-dependent property of the media, and is characterized by the dispersion coefficient [m^2/d]. Historically, this parameter has been considered very difficult to quantify. The dispersion coefficient (D) is a tensorial quantity, and, for one-dimensional flows, the dispersivity of the media (α_i) in each direction i and seepage velocity (U_{GW}) are related by:

$$D_L = \alpha_L U_{GW}$$

$$D_T = \alpha_T U_{GW}$$

$$D_V = \alpha_V U_{GW}$$

where the subscripts L, T, and V represent the longitudinal, horizontal and vertical directions with respect to the principal direction of groundwater flow. In the absence of user specified site specific values, EPA (1994) has used the following equation:

$$\alpha_L(L_R) = \alpha_L(L_R^{ref})\left[\frac{0.5L + L_R}{L_R^{ref}}\right]^{1/2}$$

where:

$\alpha_L(L_R)$ = dispersivity for a given receptor distance L_R [m]
$\alpha_L(L_R^{reff})$ = reference dispersivity value of 10 m
L = source length along the direction of groundwater flow [m]

This relationship is based on a reference dispersivity of 10 m, which is the seventieth percentile value of a national probabilistic distribution for a receptor located at 152.4 meters. The travel distance utilized by the above relationship is equal to the distance to the receptor plus half the source zone length.

A review of published dispersivity values indicated wide variations, due to testing scale and between measurement techniques. In general, dispersivities increase with distance, and decrease in the order:

$$\alpha_L > \alpha_T > \alpha_V$$

Gelhar (1992) performed a critical review of published field-scale dispersivities in saturated media at 59 sites, in which the data were placed in three classes of reliability: I (high), II (moderate) and III (low). Data from tests which ranked I and II in the reliability classification are listed in Table A-5.

In Chapter 4 it was necessary to adopt reasonable fixed dispersivity values to develop the graphical approach for vadose zone sources. The values selected are:

$$\alpha_L = L_R/10 \qquad \alpha_T = \alpha_L/3 \qquad \alpha_V = \alpha_L/10$$

Table A-4. Aquifer characteristics and groundwater velocities for various hydrogeological environments (Newell *et al.*, 1990).

Hydrogeological Environments	Saturated Thickness [m]	Saturated Conductivity [m/d]	Hydraulic Gradient [m/m]	Seepage Velocity [m/d]
National Average	13.45	4.32	0.006	0.108
Metamorphic / Igneous	13.45	0.26	0.019	0.063
Bedded Sedimentary Rock	15.70	0.26	0.009	0.049
Till over Sedimentary Rock	6.05	0.43	0.010	0.049
Sand and Gravel	13.45	6.91	0.005	0.139
River Valley with Overbank	11.43	5.18	0.004	0.157
River Valley without Overbank	16.82	17.28	0.005	0.538
Alluvial Basins, Valley & Fans	11.21	6.05	0.005	0.283
Outwash	27.35	40.61	0.002	0.628
Till and Till Over Outwash	11.21	0.78	0.010	0.359
Un & Semi-Consolidated	10.67	0.86	0.005	0.031
Coastal Beaches	15.70	5.62	0.004	0.040
Solution Limestone	26.50	3.46	0.006	0.121

Table A-5. Field-scale dispersivities in saturated media (Gelhar, 1992)

Aquifer Material	Test Scale [m]	Dispersivity $\alpha_L / \alpha_T / \alpha_V$ [m]	Reliability
poorly sorted sand and gravel	200	7.5/-/-	II
fractured granite	5	0.5/-/	II
glaciofluvial sand	90	0.43/0.039/-	I
medium to coarse sand and some gravel	250	0.96/0.018/0.0015	I
brecciated basalt interflow zone	17.1	0.6/-/-	I
Dolomite	250	6/-/-	II
sandstone with silt and clay	28	0.1-1.0	II
layered gravel and silty sand	4.4	1.1, 1.2/-/-	II
layered medium sand	38.3	4.0/-/-	I
alluvial deposits	40	3/1.5/-	II
glaciofluvial gravel	10	5,1.9/-/-	II
sand	5-6	0.18/-/-	II
fractures dolomite	22	44-110/-/-	II
fractures dolomite	21.3	2.1	II
limestone	27	2.7-27	II
limestone	41.5	20.8/-/-	II
sand and gravel with clay lenses	19	2-3/-/-	II
sand	≤6	0.012/-/-	II
sand , sandstone with some silt and clay	≤115	0.5-1.5/-/-	I
sand	13	0.79,1.27,0.72/-/-	I
sand	26	2.23/-/-	I
sand	33.2	1.94/0.11/-	I
sand	32.5	2.73/0.11	I
fluvial sand	40	0.06-0.16/ - / 0.0006-0.002	II
gravel with cobbles	54-59	1.4-11.5/0.1-3.3/ 0.04-0.1	II
alluvium (gravels)	25	0.3-1.5/-/0.06	II
sandstone	6	0.16,0.38	II

Table A-5. Field-scale dispersivities in saturated media (Gelhar, 1992)

Aquifer Material	Test Scale [m]	Dispersivity $\alpha_L / \alpha_T / \alpha_V$ [m]	Reliability
sandstone	3	0.31/-/-	II
sandstone	6	0.6/-/-	II
sandstone	3	0.6/-/-	II
medium to fine sand	57.3	1.5/-/-	II
glaciofluvial sand	90	0.5/0.05/0.0022	I
clay sand and gravel	9.3	6.9/-/-	II
clay sand and gravel	7.1	0.37/-/-	II
sand and gravel	150	12.5/-/-	II
sand	13	1.0/-/-	II
glaciofluvial sand	11	0.08/0.03/-	II
glaciofluvial sand	0.75	0.01/0.005/-	II
sand silt and clay	57.3	0.76/-/0.15	II
sand gravel and silt	16	1.0/0.1/-	I
sand and gravel	18.3	0.26/-/-	II
sand and gravel	1.52	0.015/-/-	II

Infiltration

Infiltration is the net recharge rate to groundwater. The range of infiltration values was determined by simulating conditions at several locations around the country with the HELP model (Schroeder 1989). Groundwater infiltration rates are listed in Table A-6 as a function of soil type and geography.

To achieve a level of site-specificity, the Hydrologic Evaluation of Landfill Performance (HELP) model is used to determine infiltration rates. The HELP model is a quasi-two-dimensional hydrologic model of water movement at landfill sites. The model accepts weather, soil and design data, and uses solution techniques which account for the effects of surface storage, runoff, snow melt, infiltration, evapotranspiration, vegetative growth, soil moisture storage, and unsaturated vertical drainage. While designed for landfill sites, HELP can be applied to waste sites to determine groundwater infiltration rates.

The model's water balance can be divided into two categories: surface water processes and subsurface processes. Surface processes include snow melt, interception of rainfall by vegetation, surface runoff, and surface evaporation. Subsurface processes of concern for common waste sites include evaporation from the soil, plant transpiration and unsaturated vertical drainage.

The model indirectly determines daily infiltration from a water balance which assumes that infiltration equals the sum of rainfall, surface storage and snow melt, minus the sum of runoff, additional storage in snow pack, and evaporation of the surface water. Snow pack is the only means by which liquid water may be held in storage from one day to the next unless the topsoil is saturated and runoff is not permitted. Available surface water for infiltration, evaporation, and runoff is determined daily from the surface storage, discharge from snowcap, and rainfall. Snowfall is added to the snow pack, which may be depleted by either evaporation or melting. Snow melt is added to the surface water and treated as rainfall, except it is not intercepted by vegetation. The free available surface water is used to compute the runoff by the SCS rainfall-runoff relationship. Interception is the amount of surface water available for evaporation. Interception in excess of the potential evaporation is added to infiltration. Surface evaporation is then computed. Potential evaporation from the surface is first applied to the interception and any excess is applied to the snow melt, then the snow pack, and finally to the ground melt. Potential evaporation in excess of the evaporation from the surface is applied to the soil column and plant transpiration. Snow melt and rainfall that does not evaporate or runoff is assumed to infiltrate into the soil.

In the subsurface, processes considered include soil evaporation and plant transpiration from the evaporative zone of the soil. A vegetative growth model determines daily growth and decay of surface vegetation, which is used to compute plant transpiration rates. After accounting for evaporative and plant transpiration losses, the infiltration rate is assumed to equal the unsaturated hydraulic conductivity of the soil computed as a function of the soil moisture content.

To achieve conservative estimates of infiltration, sites are modeled as consisting of bare ground with no vegetative cover, eliminating rainfall interception and evapotranspiration of soil water. Further, the shallowest evaporative depth recommended for each city is used, reducing soil evaporative losses, and sites are modeled with the mildest ground slope allowable (1 percent) to limit runoff of surface water. These measures provide a conservative site design which should slightly over-estimate groundwater infiltration.

The HELP model has a climatological database which can generate synthetic evapotranspiration, precipitation, temperature, and solar radiation data for many U.S. cities based on their location and historical record. In simulations run to develop infiltration estimates, twenty years of synthetic evapotranspiration, precipitation, temperature, and solar radiation data were generated and the model was run for different cities using six different USDA soil types. Sites were modeled with a surface area of one acre and a soil column ten feet deep. These parameters are arbitrary from the standpoint of percolation as long the soil column depth exceeds the evaporative depth of the soil. Table A-6 presents the results of the simulations run for this research.

Table A-6. Prediction of groundwater infiltration rates for various U.S. cities using the HELP model

State	City	Annual Precipitation (cm/year)	HELP Model Prediction of Annual Groundwater Infiltration by USDA Soil Type (cm/year)					
			Sand	Sandy Loam	Loam	Silty Loam	Clay Loam	Clay
Alabama	Montgomery	121.5	51.0	37.1	27.4	22.8	14.6	5.4
Alaska	Fairbanks	23.9	2.0	4.1	3.9	4.0	3.5	3.6
Arizona	Phoenix	17.8	1.3	1.2	0.9	1.0	0.7	0.6
Arkansas	Little Rock	119.5	53.9	40.2	30.5	25.7	17.5	7.4
California	Bakersfield	14.1	1.2	1.4	1.4	1.5	1.0	1.1
California	San Francisco	48.8	20.6	17.2	14.6	13.0	9.1	4.7
California	San Diego	22.4	4.7	4.2	3.1	2.6	2.0	1.3
Colorado	Denver	36.1	2.5	1.5	1.0	1.1	0.8	0.6
Delaware	Wilmington	104.0	35.7	25.5	19.4	16.2	10.8	4.7
Florida	Jacksonville	129.0	48.1	32.2	22.8	17.7	10.5	3.1
Florida	Miami	140.7	51.0	33.2	22.7	17.7	9.6	2.3
Florida	Tampa	114.4	40.0	25.3	17.2	12.8	7.3	2.1
Georgia	Atlanta	123.0	49.7	35.9	27.0	22.5	14.6	5.9
Idaho	Boise	28.3	1.6	1.1	1.0	1.1	0.8	0.7
Illinois	Chicago	83.5	21.4	14.5	10.9	8.7	6.1	2.8
Indiana	Indianapolis	97.1	28.1	20.3	15.8	13.1	9.5	4.7
Kansas	Wichita	70.1	19.7	13.3	9.6	7.8	5.6	2.7
Louisiana	New Orleans	145.0	62.0	43.0	30.7	24.7	15.1	4.7

Table A-6. Prediction of groundwater infiltration rates for various U.S. cities using the HELP model (continued)

State	City	Annual Precipitation (cm/year)	HELP Model Prediction of Annual Groundwater Infiltration by USDA Soil Type (cm/year)					
			Sand	Sandy Loam	Loam	Silty Loam	Clay Loam	Clay
Maine	Portland	107.9	31.0	23.9	19.6	17.1	12.4	6.5
Maryland	Baltimore	103.8	36.4	26.4	20.0	16.8	11.3	5.1
Massachusetts	Boston	110.0	33.4	25.3	19.8	16.9	11.8	5.4
Michigan	Detroit	77.7	17.9	12.5	9.7	8.2	6.2	3.3
Minnesota	Minneapolis	66.6	13.8	9.4	6.8	5.6	3.9	2.0
Mississippi	Jackson	128.5	58.6	44.7	34.2	29.3	19.6	8.1
Missouri	St. Louis	83.7	23.5	16.5	12.4	10.4	7.3	3.6
Montana	Helena	27.8	0.7	0.7	0.7	0.8	0.6	0.5
Nevada	Las Vegas	10.3	0.4	0.7	0.7	0.9	0.7	0.6
New Mexico	Albuquerque	20.8	0.9	0.8	0.9	0.9	0.7	0.6
New York	New York	106.7	36.0	26.9	21.1	17.9	12.6	6.0
North Carolina	Raleigh	104.8	39.3	29.3	22.5	18.8	12.4	4.9
North Dakota	Bismarck	37.6	4.0	2.9	2.4	2.0	1.5	1.0
Oklahoma	Oklahoma City	72.2	19.3	11.5	7.8	5.9	3.7	1.6
Oregon	Portland	95.4	56.8	53.9	49.4	46.8	39.7	26.6
Pennsylvania	Philadelphia	103.0	33.6	23.4	17.6	14.6	9.9	4.3
Pennsylvania	Pittsburgh	91.9	21.4	41.6	12.0	10.2	7.7	3.8
Rhode Island	Providence	112.4	34.9	25.7	20.2	17.1	12.2	5.7

Table A-6. Prediction of groundwater infiltration rates for various U.S. cities using the HELP model (continued)

State	City	Annual Precipitation (cm/year)	HELP Model Prediction of Annual Groundwater Infiltration by USDA Soil Type (cm/year)					
			Sand	Sandy Loam	Loam	Silty Loam	Clay Loam	Clay
South Carolina	Charleston	126.9	50.9	35.9	26.2	21.4	13.5	4.4
South Dakota	Rapid City	40.3	4.5	3.2	2.3	2.0	1.4	0.9
Tennessee	Nashville	121.3	52.1	40.6	32.2	28.1	20.0	9.5
Texas	Amarillo	45.1	8.8	5.6	3.7	3.4	2.4	1.7
Texas	Austin	74.9	23.2	14.0	9.5	7.1	4.6	2.0
Texas	Dallas	70.9	21.0	13.1	8.7	6.8	4.1	1.8
Texas	El Paso	18.4	1.3	1.1	0.9	1.0	0.6	0.6
Texas	Houston	105.8	41.3	28.3	20.0	16.1	10.0	3.4
Texas	San Antonio	67.6	22.1	14.5	10.0	7.7	5.0	1.8
Virginia	Richmond	112.0	44.3	32.4	24.8	21.0	14.1	5.7
Washington	Olympia	129.7	93.8	87.3	77.9	73.6	60.5	39.6
Wisconsin	Madison	77.5	19.9	12.7	9.4	7.4	5.1	2.6
Wyoming	Cheyenne	32.6	1.9	1.9	1.5	1.4	1.1	1.1

Table A-7. Chemical specific properties for selected organic compounds (based on EPA 1996)

Compound	S [mg/L]	K_H [L_{H2O}/L_{air}]	K_{oc} [L_{H2O}/kg_{soil}]	K_d [L_{H2O}/kg_{soil}]	γ^* [L_{H2O}/kg_{soil}]
Acenapthene	4.13e+00	7.50e-03	4.90e+03	9.80e+00	1.68e+01
Acetone	6.04e+05	1.20e-03	4.60e-01	9.20e-04	1.02e-01
Aldrin	7.84e-02	4.20e-03	4.84e+04	9.68e+01	1.65e+02
Anthracene	5.37e-02	4.60e-03	2.12e+04	4.24e+01	7.22e+01
Benzene	1.78e+03	2.20e-01	5.70e+01	1.14e-01	3.38e-01
Benzo(a)antreacene	2.18e-02	1.50e-04	3.57e+05	7.14e+02	1.21e+03
Benzo(b)fluoranthene	4.33e-03	2.50e-04	8.83e+05	1.77e+03	3.00e+03
Benzoic acid	3.13e+03	1.40e-05	6.00e-01	1.20e-03	1.02e-01
Benzo(a)pyrene	1.94e-03	3.40e-05	9.16e+05	1.83e+03	3.11e+03
Bis(2-chloroethyl)ether	1.18e+04	8.80e-04	7.60e+01	1.52e-01	3.59e-01
Bis(2-ethylhexyl)phthalate	3.96e-01	3.40e-04	8.74e+04	1.75e+02	2.97e+02
Bromodichloromethane	3.97e+03	1.30e-01	5.40e+01	1.08e-01	3.10e-01
Bromoform	3.21e+03	2.50e-02	1.26e+02	2.52e-01	5.33e-01
Butanol	7.47e+04	3.50e-04	5.00e+00	1.00e-02	1.17e-01
Butyl benzyl phthalate	2.58e+00	7.80e-05	3.41e+04	6.82e+01	1.16e+02
carbazole	7.21e-01	3.30e-03	2.44e+03	4.88e+00	8.40e+00
carbon disulfide	2.67e+03	5.20e-01	5.20e+01	1.04e-01	3.81e-01
carbon tetrachloride	7.92e+02	1.20e+00	1.64e+02	3.28e-01	8.98e-01
chlorodane	2.19e-01	2.70e-03	5.13e+04	1.03e+02	1.75e+02
p-chloroanaline	3.36e+03	4.80e-05	4.10e+01	8.20e-02	2.39e-01
chlorobenzene	4.09e+02	1.80e-01	2.04e+02	4.08e-01	8.30e-01
chlorodibromomethane	3.44e+03	1.00e-01	7.20e+01	1.44e-01	3.65e-01
chloroform	7.96e+03	1.60e-01	5.60e+01	1.12e-01	3.22e-01
2-chlorophenol	2.15e+04	6.80e-04	3.91e+02	7.82e-01	1.43e+00
chysene	1.94e-03	5.00e-05	3.12e+05	6.24e+02	1.06e+03
DDD	7.33e-02	2.00e-04	8.49e+04	1.70e+02	2.89e+02
DDE	1.92e-02	5.10e-03	8.64e+04	1.73e+02	2.94e+02
DDT	3.41e-03	2.20e-03	2.37e+05	4.74e+02	8.06e+02
dibenzo(a,h)anthracene	6.70e-04	4.60e-07	1.80e+06	3.60e+03	6.12e+03

Table A-7. Chemical specific properties for selected organic compounds (based on EPA 1994)

Compound	S [mg/L]	K_H [L_{H2O} /L_{air}]	K_{OC} [L_{H2O} /kg_{soil}]	K_d [L_{H2O} /kg_{soil}]	γ^* [L_{H2O} /kg_{soil}]
di-n-butyl phthalate	1.08e+01	5.90e-05	1.57e+03	3.14e+00	5.44e+00
1-2-dichlorobenzene	1.25e+02	8.60e-02	3.76e+02	7.52e-01	1.40e+00
1-4-dichlorobenzene	7.30e+01	1.20e-01	5.16e+02	1.03e+00	1.88e+00
3-3-dichlorobenzidine	3.52e+00	8.50e-07	2.44e+03	4.88e+00	8.40e+00
1,1-dichloroethane	5.16e+03	2.40e-01	5.20e+01	1.04e-01	3.25e-01
1-2-dichloroethane	8.31e+03	5.20e-02	3.80e+01	7.60e-02	2.40e-01
1-1-dichloroeththylene	3.00e+03	1.00e+00	6.50e+01	1.30e-01	5.21e-01
cis-1,2-dichloroethylene	4.94e+03	1.80e-01	2.90e+01	5.80e-02	2.35e-01
trans-1-2-dichloroethylene	8.03e+03	2.30e-01	5.00e+01	1.00e-01	3.16e-01
2-4-dichlorophenol	4.93e+03	9.80e-06	1.46e+02	2.92e-01	5.96e-01
1-2-dichloropropane	2.68e+03	1.20e-01	4.70e+01	9.40e-02	2.84e-01
1-3-dichloropropene	1.55e+03	1.20e-01	2.60e+01	5.20e-02	2.12e-01
dieldrin	1.87e-01	1.10e-04	1.09e+04	2.18e+01	3.72e+01
diethyl phthalate	8.83e+02	2.20e-05	8.20e+01	1.64e-01	3.79e-01
2,4, dimethylphenol	6.25e+03	1.30e-04	1.26e+02	2.52e-01	5.28e-01
dimethyl phthalate	4.19e+03	2.40e-05	4.60e+01	9.20e-02	2.56e-01
2-4-dinitrophenol	5.80e+03	2.00e-07	1.00e-02	2.00e-05	1.00e-01
2-4-dinitrotoluene	2.85e+02	6.00e-06	5.10e+01	1.02e-01	2.73e-01
2,6-dinitrotoluene	1.05e+03	5.30e-06	4.20e+01	8.40e-02	2.43e-01
di-n-octyl-phthalate	3.00e+00	3.10e-05	9.80e+08	1.96e+06	3.33e+06
endosulfan	2.31e-01	9.50e-04	7.38e+02	1.48e+00	2.61e+00
endrin	2.46e-01	4.90e-05	1.08e+04	2.16e+01	3.68e+01
ethylbenzene	1.73e+02	3.20e-01	2.21e+02	4.42e-01	9.15e-01
fluoranthene	2.32e-01	3.80e-04	4.91e+04	9.82e+01	1.67e+02
fluorene	1.86e+00	3.00e-03	7.96e+03	1.59e+01	2.72e+01
heptachlor	2.73e-01	2.40e-02	6.81e+03	1.36e+01	2.33e+01
heptachlor epoxide	2.68e-01	3.40e-04	7.24e+03	1.45e+01	2.47e+01
hexachlorobenzene	8.62e-03	2.20e-02	3.57e+04	7.14e+01	1.21e+02
hexachloro-1-3-butadiene	2.54e+00	9.80e-01	6.99e+03	1.40e+01	2.41e+01

Table A-7. Chemical specific properties for selected organic compounds (based on EPA 1994)

Compound	S [mg/L]	K_H [L_{H2O}/L_{air}]	K_{OC} [L_{H2O}/kg_{soil}]	K_d [L_{H2O}/kg_{soil}]	γ* [L_{H2O}/kg_{soil}]
hexachlorocyclopentadiene	1.53e+00	7.00e-01	9.59e+03	1.92e+01	3.28e+01
hexachloroethane	4.08e+01	1.50e-01	1.83e+03	3.66e+00	6.35e+00
indeno(1,2,3-c-d)pyrene	1.07e-01	2.00e-07	4.36e+06	8.72e+03	1.48e+04
isophorone	1.20e+04	2.50e-04	3.00e+01	6.00e-02	2.02e-01
methooxychlor	8.84e-02	2.60e-04	7.79e+04	1.56e+02	2.65e+02
methyl bromide	1.45e+04	5.80e-01	9.49e+00	1.90e-02	2.48e-01
methyl chloride	6.34e+03	1.90e+00	6.00e+00	1.20e-02	5.00e-01
methylene chloride	1.74e+04	9.70e-02	1.60e+01	3.20e-02	1.74e-01
2-methylphenol	2.77e+04	6.70e-05	5.40e+01	1.08e-01	2.84e-01
napthalene	3.11e+01	2.00e-02	9.64e+02	1.93e+00	3.38e+00
nitrobenzene	1.92e+03	8.40e-04	1.31e+02	2.62e-01	5.46e-01
n-nitrosodiphenylamine	3.74e+01	2.90e-02	3.27e+02	6.54e-01	1.22e+00
n-nitrosodi-n-propylamine	1.46e+04	1.70e-03	1.70e+01	3.40e-02	1.58e-01
pentachlorophenol	1.34e+01	5.80e-04	5.67e+02	1.13e+00	2.03e+00
phenol	9.08e+04	2.40e-05	2.20e+01	4.40e-02	1.75e-01
pyrene	1.37e-01	3.40e-04	6.82e+04	1.36e+02	2.32e+02
styrene	2.57e+02	1.40e-01	9.12e+02	1.82e+00	3.23e+00
1,1,2,2-tetrachloroethane	3.07e+03	1.50e-02	7.90e+01	1.58e-01	3.72e-01
tetrachloroethylene	2.32e+02	7.10e-01	3.00e+02	6.00e-01	1.26e+00
toluene	5.58e+02	2.50e-01	1.31e+02	2.62e-01	5.95e-01
toxaphene	6.79e-01	1.40e-04	5.01e+02	1.00e+00	1.80e+00
1,2,4-trichlorobenzene	3.07e+01	1.10e-01	1.54e+03	3.08e+00	5.36e+00
1,1,1-trichloroethane	1.17e+03	7.60e-01	9.90e+01	1.98e-01	5.89e-01
1,1,2-trichloroethane	4.40e+03	4.10e-02	7.60e+01	1.52e-01	3.67e-01
trichloroethylene	1.18e+03	4.30e-01	9.40e+01	1.88e-01	5.06e-01
2,4,5-trichlorophenol	9.65e+02	1.80e-04	1.40e+03	2.80e+00	4.86e+00
2,4,6-trichlorophenol	7.53e+02	1.70e-04	2.83e+02	5.66e-01	1.06e+00
vinyl acetate	2.24e+04	2.30e-02	5.00e+00	1.00e-02	1.22e-01
vinyl chloride	2.73e+03	3.50e+00	1.10e+01	2.20e-02	8.37e-01
xylenes (total)	1.86e+02	2.50e-01	2.60e+02	5.20e-01	1.03e+00

* Soil/water partitioning coefficients K_d and dissolved phase partitioning coefficients γ were determined for a soil with organic carbon content of 0.2%, total porosity of 30%, and moisture content 10%.

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APPENDIX B

COMPARISON OF APPROXIMATE AND FULL SOLUTIONS TO THE GROUNDWATER TRANSPORT PROBLEM

B.1 INTRODUCTION

In §2.1, the dilution attenuation factor (DAF) for time-varying sources is defined by Equation (2-3) to be:

$$\mathrm{DAF}\left[\frac{(\mathrm{mg_i}\,/\,\mathrm{L_{H_2O}})_{\mathrm{source}}}{(\mathrm{mg_i}\,/\,\mathrm{L_{H_2O}})_{\mathrm{receptor}}}\right] = \frac{S_L^o}{<<C_R>_z>_{t,\max}} \tag{B-1}$$

where:

S_L° = dissolved concentration of compound i leaving source zone at time t=0 $[\mathrm{mg_i}/\mathrm{L_{H2O}}]$

$<<C_R>_z>_{t,\max}$ = maximum-time-averaged and vertically-averaged centerline dissolved concentration at the receptor location $x=L_R$ $[\mathrm{mg_i}/\mathrm{L_{H2O}}]$

Furthermore, §2.5 proposed a mathematical approximation that was used in developing the graphs presented in Chapter 3 and Chapter 4:

$$\mathrm{DAF} = \frac{1}{\left\{\frac{1}{T}\int_0^T \frac{S_L(t)}{S_L(0)}\,dt\right\} \times \left\{\frac{1}{H_w}\int_0^{H_w} C_{cs}^*(L_R, 0, z, \infty)\,dz\right\}} \tag{B-2}$$

where:

$S_L(t)$ = the time-varying source zone leachate concentration for chemical "i" $[\mathrm{mg_i}/\mathrm{L_{H2O}}]$

T = averaging time period (often the exposure duration upon which the receptor location tolerance criterion is based) [y]

H_w = well screen interval (screen interval is assumed to extend from the water table downwards) [m]

L_R = distance from the origin to the receptor [m]

$C^*_{cs}(L_R,0,z,\infty)$ = steady-state concentration at the receptor location for a steady source of strength unity [dimensionless]

In this appendix, the validity of this assumption is examined through the use of two computer codes - VADSAT (API, 1996) and HPS (UT, 1996). Each calculates the transient solution to the groundwater transport problem for time-varying sources.

B.2 COMPARISON WITH VADSAT OUTPUT

To conduct the comparison, the following approach was used:

- First the VADSAT code was used to compute the concentrations for a constant strength source, for receptors located 15 m, 30 m, and 150 m from the source zone. To simplify the exercise, concentrations at the water table were recorded (H_w->0). This concentration was then divided by the steady source zone leachate concentration to obtain the quantity:

  $$\frac{1}{H_W}\int_0^{H_W} C^*_{cs}(L_R, 0, z, \infty)\, dz$$

  appearing in Equation (B-2).

- Then, for all other parameters fixed, solutions were computed for cases where the source was allowed to decay exponentially.

- The exact DAF was calculated directly using Equation (B-1) and VADSAT model output. A 30-y averaging time was used in each of these calculations. The approximate DAF was calculated using the result of the first step and the normalized and time-averaged source leachate concentration as dictated by Equation (B-2).

Table B-1 summarizes parameter values that were held fixed during this analysis.

Table B-2 and Figure B-1 present results of this analysis for a range of source decay rates and groundwater velocities. For the range of parameters studied, the exact and approximate solutions agree to within ≈20%. As stated in Chapter 2, it is expected that approximate DAF values should be slightly less (or more conservative) than the full-solution results. This is the behavior observed in Table 2 for most cases, the exception being sources that decay fairly rapidly. In those cases, the agreement between approximate and exact solutions is still good, being within 10%. It is not clear why the approximate solution DAF exceeds the exact solution DAF for those cases, but it is likely to be caused by some numerical limitation of the VADSAT code.

B.3 COMPARISON WITH THE HPS MODEL

In this section, we present approximate and exact solutions calculated using the HPS model (see Chapter 4). The fundamental basis of the HPS code is similar to that of the VADSAT code.

The approach used to calculate approximate and exact solutions with the HPS code was similar to the approach described in §B.2 for the VADSAT code.

Table B-3 presents values of parameters that were held fixed during this exercise.

Table B-4 presents a summary of the results. In this evaluation, all parameters were held fixed, except the source decay rate. In this case, the quantitative agreement (0 - 50%) is not as good as in the case of the VADSAT results presented in Table 2; however, all of the approximate solution estimates are clearly conservative in that the approximate DAFs are all less than the exact solution DAFs, as expected. In general, differences between the exact and approximate solutions increase as the receptor distance increases.

Table B-1. Parameters held fixed during the VADSAT simulations

Parameter	Value
source length [m]	10
source width [m]	10
cover thickness [m]	30
initial mass fraction of chemical “I” in the mixture	0.01
total hydrocarbon concentration in soil [mg/kg]	10000
chemical “i”	benzene
molecular weight of species [g/mole]	78.1
average molecular weight of hydrocarbons [g/mole]	100
density of chemical “i” [g/cm^3]	0.896
average density of hydrocarbons [g/cm^3]	0.90
unsaturated zone decay coefficient [1/day]	0
depth to groundwater from source zone bottom [m]	0
vadose zone porosity	0.3
value of van Genuchten parameter	1.23
residual water content	0.1
saturated zone porosity	0.3
saturated zone organic carbon fraction	0.02
longitudinal dispersivity [m] (X = distance downgradient)	0.1 X
transverse dispersivity [m] (X = distance downgradient)	0.03 X
vertical dispersivity [m] (X = distance downgradient)	0.01 X
hydraulic gradient [m/m]	0.03
aquifer thickness [m]	10
infiltration rate [m/day]	0.001

Table B-2. VADSAT simulation results

Case #	GW Velocity [m/d]	1st-Order Decay Rate in Sat Zone [1/d]	Source Thickness [m]	Initial (t=0) Source Leachate Conc. [mg/L]	30-y Ave. Source Conc. [Normalized]	Distance to Receptor [m]	Constant Source Rec. Conc. [mg/L]	Max 30-y Ave. Conc. [mg/L]	DAF Exact Solution	DAF Approx. Solution	% Deviation from Exact Soln
1	0.03	0.00	10000	22.9193	1.0000	15.0000	2.7724	2.7724	8.3E+00	8.3E+00	0.00
	0.03	0.00	10000	22.9193	1.0000	30.0000	0.8865	0.8865	2.6E+01	2.6E+01	0.00
	0.03	0.00	10000	22.9193	1.0000	150.0000	0.0615	0.0615	3.7E+02	3.7E+02	0.00
2	0.03	0.00	30	22.9193	0.9770	15.0000	2.7724	2.6924	8.5E+00	8.5E+00	0.60
	0.03	0.00	30	22.9193	0.9770	30.0000	0.8865	0.8565	2.7E+01	2.6E+01	1.11
	0.03	0.00	30	22.9193	0.9770	150.0000	0.0615	0.0572	4.0E+02	3.8E+02	4.66
3	0.03	0.00	3	22.9193	0.7990	15.0000	2.7724	2.1724	1.1E+01	1.0E+01	1.93
	0.03	0.00	3	22.9193	0.7990	30.0000	0.8865	0.6815	3.4E+01	3.2E+01	3.78
	0.03	0.00	3	22.9193	0.7990	150.0000	0.0615	0.0397	5.8E+02	4.7E+02	19.26
4	0.03	0.00	0.3	22.9193	0.2040	15.0000	2.7724	0.6039	3.8E+01	4.1E+01	-6.78
	0.03	0.00	0.3	22.9193	0.2040	30.0000	0.8865	0.1919	1.2E+02	1.3E+02	-6.14
	0.03	0.00	0.3	22.9193	0.2040	150.0000	0.0615	0.0103	2.2E+03	1.8E+03	17.45
5	0.03	0.01	10000	22.9193	1.0000	15.0000	0.5156	0.5156	4.4E+01	4.4E+01	0.00
	0.03	0.01	10000	22.9193	1.0000	30.0000	0.0607	0.0607	3.8E+02	3.8E+02	0.00
	0.03	0.01	10000	22.9193	1.0000	150.0000	0.0000	0.0000	1.9E+06	1.9E+06	0.00
6	0.03	0.01	30	22.9193	0.9770	15.0000	0.5156	0.5019	4.6E+01	4.5E+01	0.37
	0.03	0.01	30	22.9193	0.9770	30.0000	0.0607	0.0590	3.9E+02	3.9E+02	0.51
	0.03	0.01	30	22.9193	0.9770	150.0000	0.0000	0.0000	1.9E+06	1.9E+06	0.95
7	0.03	0.01	3	22.9193	0.7990	15.0000	0.5156	0.4073	5.6E+01	5.6E+01	1.13
	0.03	0.01	3	22.9193	0.7990	30.0000	0.0607	0.0477	4.8E+02	4.7E+02	1.66
	0.03	0.01	3	22.9193	0.7990	150.0000	0.0000	0.0000	2.4E+06	2.3E+06	3.62
8	0.03	0.01	0.3	22.9193	0.2040	15.0000	0.5156	0.1126	2.0E+02	2.2E+02	-7.00
	0.03	0.01	0.3	22.9193	0.2040	30.0000	0.0607	0.0132	1.7E+03	1.9E+03	-6.83
	0.03	0.01	0.3	22.9193	0.2040	150.0000	0.0000	0.0000	8.6E+06	9.2E+06	-5.98
9	0.30	0.00	10000	22.9193	1.0000	15.0000	0.2773	0.2773	8.3E+01	8.3E+01	0.00
	0.30	0.00	10000	22.9193	1.0000	30.0000	0.0887	0.0887	2.6E+02	2.6E+02	0.00
	0.30	0.00	10000	22.9193	1.0000	150.0000	0.0062	0.0062	3.7E+03	3.7E+03	0.00
10	0.30	0.00	30	22.9193	0.9770	15.0000	0.2773	0.2706	8.5E+01	8.5E+01	0.13
	0.30	0.00	30	22.9193	0.9770	30.0000	0.0887	0.0865	2.6E+02	2.6E+02	0.14
	0.30	0.00	30	22.9193	0.9770	150.0000	0.0062	0.0060	3.8E+03	3.8E+03	0.49
11	0.30	0.00	3	22.9193	0.7990	15.0000	0.2773	0.2210	1.0E+02	1.0E+02	0.25
	0.30	0.00	3	22.9193	0.7990	30.0000	0.0887	0.0706	3.2E+02	3.2E+02	0.30
	0.30	0.00	3	22.9193	0.7990	150.0000	0.0062	0.0049	4.7E+03	4.6E+03	1.54
12	0.30	0.00	0.3	22.9193	0.2040	15.0000	0.2773	0.0606	3.8E+02	4.1E+02	-7.20
	0.30	0.00	0.3	22.9193	0.2040	30.0000	0.0887	0.0194	1.2E+03	1.3E+03	-7.21
	0.30	0.00	0.3	22.9193	0.2040	150.0000	0.0062	0.0013	1.7E+04	1.8E+04	-6.91
13	0.30	0.01	10000.0	22.9193	1.0000	15.0000	0.2279	0.2279	1.0E+02	1.0E+02	0.00
	0.30	0.01	10000.0	22.9193	1.0000	30.0000	0.0633	0.0633	3.6E+02	3.6E+02	0.00
	0.30	0.01	10000.0	22.9193	1.0000	150.0000	0.0015	0.0015	1.6E+04	1.6E+04	0.00
14	0.30	0.01	30.0	22.9193	0.9770	15.0000	0.2279	0.2224	1.0E+02	1.0E+02	0.11
	0.30	0.01	30.0	22.9193	0.9770	30.0000	0.0633	0.0617	3.7E+02	3.7E+02	0.14
	0.30	0.01	30.0	22.9193	0.9770	150.0000	0.0015	0.0014	1.6E+04	1.6E+04	0.32
15	0.30	0.01	3.0	22.9193	0.7990	15.0000	0.2279	0.1817	1.3E+02	1.3E+02	0.22
	0.30	0.01	3.0	22.9193	0.7990	30.0000	0.0633	0.0504	4.5E+02	4.5E+02	0.30
	0.30	0.01	3.0	22.9193	0.7990	150.0000	0.0015	0.0012	2.0E+04	2.0E+04	0.93
16	0.30	0.01	0.3	22.9193	0.2040	15.0000	0.2279	0.0499	4.6E+02	4.9E+02	-7.24
	0.30	0.01	0.3	22.9193	0.2040	30.0000	0.0633	0.0138	1.7E+03	1.8E+03	-7.20
	0.30	0.01	0.3	22.9193	0.2040	150.0000	0.0015	0.0003	7.2E+04	7.7E+04	-7.04

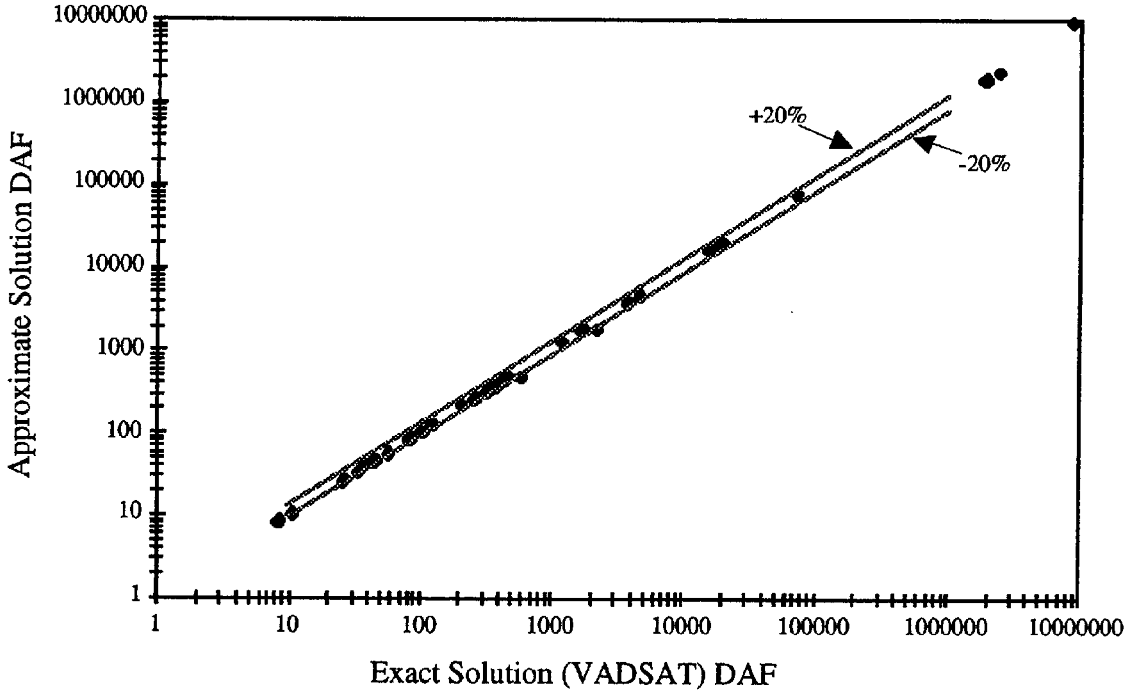

Figure B-1. Comparison of approximate and full (VADSAT) solution DAF calculations

Table B-3. Parameters held fixed during the HPS simulations

Parameter	Value
source length [m]	10
source width [m]	10
source thickness [m]	1
cover thickness [m]	3
initial leachate concentration [mg/L]	5.874
unsaturated zone decay coefficient [1/day]	0
infiltration rate [m/d]	0.25
aquifer first-order degradation rate constant [1/d]	0
aquifer seepage velocity [m/y]	10
longitudinal dispersivity [m]	10
transverse dispersivity [m]	1
vertical dispersivity [m]	0.5
hydraulic gradient [m/m]	0.03
aquifer thickness [m]	10
well thickness [m]	1

Table B-4. HPS simulation results

Source Decay Rate (1/y)	Receptor Distance (m)	Exact 30-y Peak Conc. (mg/L)	Exact Peak DAF	Approximate Peak Conc. (mg/L)
0.000	15	1.0228	5.8	1.0228
0.000	50	0.1231	47.8	0.1231
0.000	150	0.0336	175.0	0.0336
0.005	15	0.9667	6.1	1.02259
0.005	50	0.1065	55.3	0.1230
0.005	150	0.0249	236.8	0.0336
0.010	15	0.9269	6.4	1.0225
0.010	50	0.0967	60.9	0.1230
0.010	150	0.0205	287.2	0.0336
0.020	15	0.8659	6.8	1.0225
0.020	50	0.0833	70.7	0.1230
0.020	150	0.0155	380.3	0.0336
0.100	15	0.6080	9.7	1.02252
0.100	50	0.0428	137.4	0.1230
0.100	150	0.0053	1107.5	0.0336

Source Decay Rate (1/y)	Receptor Distance (m)	Exact 30-y Average Conc. (mg/L)	Exact Average DAF	Approximate 30-y Average Conc. (mg/L)	Approximate Average DAF	Exact and Approximate Difference (%)
0.000	15	1.0226	5.8	1.0226	5.8	0.0
0.000	50	0.1230	47.8	0.1230	47.8	0.0
0.000	150	0.0329	178.8	0.0329	178.8	0.0
0.005	15	0.9240	6.4	0.9500	6.2	3.1
0.005	50	0.1043	56.4	0.1143	51.9	8.0
0.005	150	0.0247	238.5	0.0306	194	18.7
0.010	15	0.8484	6.9	0.8794	6.74	2.3
0.010	50	0.0929	63.4	0.1058	56.0	11.7
0.010	150	0.0202	291.0	0.0289	205	30.0
0.020	15	0.7327	8.0	0.7680	7.72	3.5
0.020	50	0.0771	76.3	0.0925	64.1	16.0
0.020	150	0.0151	389.4	0.0252	235	39.7
0.100	15	0.3142	18.7	0.3240	18.3	2.1
0.100	50	0.0325	181.1	0.0390	152	16.1
0.100	150	0.0050	1178.2	0.0107	554	53.0

APPENDIX C

ASSESSMENT OF THE SIGNIFICANCE OF DIFFUSIVE TRANSPORT RELATIVE TO INFILTRATION ON GROUNDWATER IMPACTS

C.1 ISSUE

During the development of the graphical approach described in this document, a question arose concerning the need to include both advective and diffusive transport when estimating contaminant fluxes to groundwater from vadose zone sources.

This issue has arisen because conventional leaching models that consider only advective transport predict no potential for impact to groundwater in the limit as the infiltration rate becomes zero. However, results published by Mendoza and McAlary (1990) suggest that diffusive transport can be significant in some cases. In particular, diffusive transport can contribute to groundwater effects by:

a) contributing to the overall flux to groundwater in the vertical direction, and

b) increasing the effective source size through the lateral spreading of vapors.

C.2 SUMMARY AND RECOMMENDATION

The first-order analysis below indicates that diffusive transport may be significant when the following conditions are met:

a) the vertical distance between the source zone and groundwater is less than the horizontal width of the source area (i.e. the transport is roughly one-dimensional), and

b) the rate of infiltration is ≤ 1 inch/year.

Here 1 inch/year is a rough order-of-magnitude approximation. The expected qualitative dependence of contaminant flux to groundwater on the infiltration rate is as follows:

- at infiltration rates in excess of ≈1 inch/year, it is expected that the contaminant flux to groundwater changes linearly with changes in infiltration rate, and

- at infiltration rates less than ≈1 inch/year, the contaminant flux is relatively constant and dependent only on diffusive parameters.

The following three options were considered as resolutions for this issue:

A) model vadose zone transport by the traditional advective-transport approach, recognizing that this approach will underpredict groundwater impact when users select infiltration rates less than about 1 inch/year.

B) model vadose zone transport by the traditional advective-transport approach, but constrain users to infiltration rates greater than about 1 inch/year, unless the vertical separation between the source and groundwater is much larger than the horizontal source width (assuming that the asymptotic diffusive flux contribution is roughly equivalent to the advective-transport flux contribution when the infiltration rate is 1 inch/year).

C) model vadose zone transport with a screening level model that incorporates diffusive transport, first-order decay, and advection.

For simplicity, and to avoid the use of models that appear significantly different from traditional approaches, the compromise option B was adopted.

C.3 BRIEF DESCRIPTION OF ANALYSIS

Consider the scenario depicted in Figure C-1, where a source zone is located some distance h_v [cm] above the capillary fringe of thickness h_c [cm].

Limiting the discussion to one-dimensional transport, steady infiltration, homogeneous conditions, and first-order decay, the steady-state transport of contaminants from the source to groundwater can be described mathematically as follows:

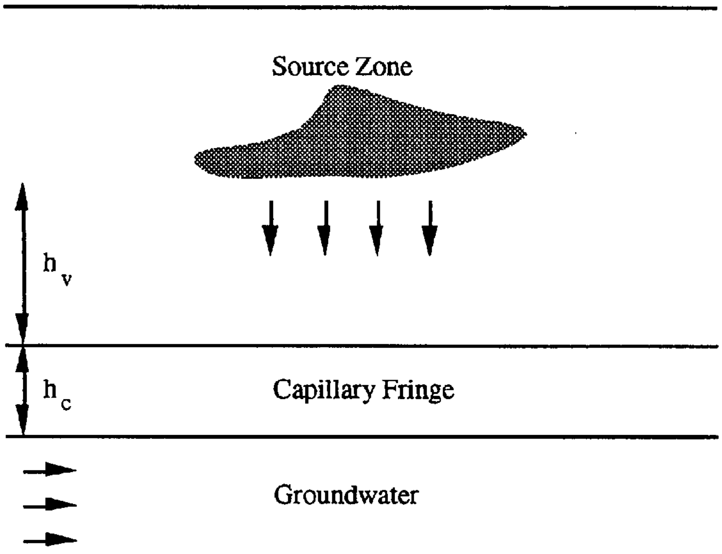

Figure C-1. Soil-to-groundwater pathway schematic

$$I\frac{\partial C_w}{\partial z} = D_v^{eff}\frac{\partial^2 C_v}{\partial z^2} + D_w^{eff}\frac{\partial^2 C_w}{\partial z^2} - \lambda\theta_w C_w \tag{C-1}$$

$$C_v = HC_w \tag{C-2}$$

$$C_w = C_L^o \quad ; \; z = 0 \tag{C-3}$$

$$D_v^{eff}\frac{\partial C_v}{\partial z} + D_w^{eff}\frac{\partial C_w}{\partial z} = -\frac{D_c^{eff}\, C_w}{h_c} \quad ; \; z = h_v \tag{C-4}$$

where:

C_w = dissolved contaminant concentration [mg_i /cm^3-H_2O]
C_v = vapor concentration of contaminant [mg_i /cm^3-vapor]
I = infiltration rate (Darcy velocity) [(cm^3-H_2O/s)/cm^2-soil]
z = vertical distance measured from the source zone [cm]
D_v^{eff} = effective porous medium vapor phase diffusion coefficient [cm^2/s]
D_w^{eff} = effective porous medium dissolved phase diffusion coefficient [cm^2/s]

D_c^{eff} = effective porous medium dissolved phase diffusion coefficient in the capillary fringe [cm^2/s]

h_c = capillary fringe thickness [cm]

h_v = distance between the source bottom and top of capillary fringe [cm]

C_L^o = source zone leachate concentration [mg_i/cm^3-H_2O]

λ = first-order degradation rate constant [s^{-1}]

θ_w = moisture content [cm^3-H_2O/cm^3-soil]

H = Henry's Law constant [(mg_i/cm^3-vapor)/(mg_i/cm^3-H_2O)]

Here, Equation (C-1) is the simplified general transport equation, Equation (C-2) is an equilibrium relationship, and Equation (C-3) is the boundary condition at the source zone. Boundary condition (C-4) was derived from a mass balance around the capillary fringe, assuming no degradation in the capillary zone and continuity of water infiltration through this zone. It implicitly assumes that resistance to diffusion through the capillary fringe is greater than resistance to dispersion in the saturated zone. This was verified in the course of this work, but will not be elaborated on further here.

Analytical solutions can be obtained for Equations (C-1) through (C-4). For brevity, the complete solution is omitted. Instead, a limiting case is examined where the first-order degradation constant is zero. In this case, one uses the solution to Equations (C-1) through (C-4) to develop an expression for the total contaminant flux F [mg/cm^2-s] to groundwater:

$$F^* = \frac{F}{I\,C_L^o} = \frac{1}{1 - \frac{(D_c^{eff}/Ih_c)}{[1+(D_c^{eff}/Ih_c)]}\,e^{-(Ih_s/D^{eff}H)}} \qquad \text{(C-5)}$$

where the dimensionless flux F* has been scaled by the flux for the case where only infiltration is considered. The focus is to identify cases where the diffusive flux is significant (relative to infiltration), so conditions are sought under which $F^*>1$. This occurs when:

$$\frac{(D_c^{eff}/Ih_c)}{[1+(D_c^{eff}/Ih_c)]}\,e^{-(Ih_s/D^{eff}H)} \approx 1 \qquad \text{(C-6)}$$

which requires that the following be satisfied:

$$(D_c^{eff}/Ih_c) >> 1 \qquad \text{(C-7)}$$

and

$$(Ih_s / D^{eff} H) << 1 \qquad \text{(C-8)}$$

In Equations (C-6) through (C-8):

$$D^{eff} = D_v^{eff} + \frac{D_w^{eff}}{H} \qquad \text{(C-9)}$$

Now, Equations (C-7) and (C-8) can be used to identify a critical infiltration rate, below which diffusive transport is important relative to advection. Assume the following reasonable parameter values (note that these have been selected to minimize diffusive transport):

$D_c^{eff} \approx D^{H2O} * \varepsilon^{1.33} \approx 2.8 \text{ x } 10^{-6}$ cm²/s (ε = porosity)
$h_c \approx$ 50 cm
$H \approx$ 0.01 (cm³-H_2O/s)/cm²-soil
$D^{eff} \approx D^{air} * \theta_a^{3.33} / \varepsilon^2 \approx 0.01$ cm²/s (θ_a = air filled porosity)
$h_s \approx$ 10 m

Using these parameter values and Equations (C-7) and (C-8), it can be seen that diffusive transport is important relative to advection if:

$$I << 5.6 \text{ x } 10^{-8} \text{ cm/s} \approx 1.8 \text{ cm/y} \approx 0.7 \text{ inch/year} \qquad \text{(C-10)}$$

and

$$I << 10^{-5} \text{ cm/s} \approx 300 \text{ cm/y} \approx 100 \text{ inch/year} \qquad \text{(C-11)}$$

Thus, conditions (C-10) and (C-11) indicate that the diffusive transport begins to be significant relative to infiltration when the infiltration rate is less than approximately 1 inch/year.

APPENDIX D

HPS MODEL FORTRAN CODE

D.1 BACKGROUND

In order to generate solutions to the equations presented in Chapter 4 for vadose zone sources, three Fortran codes were created. One was the HPS (horizontal plane source) code, which solves the general problem outlined in Chapter 4, and incorporates source decay, transient transport through the vadose and saturated zones. It can be used to find the “exact” solution to the governing equations, and will calculate the maximum time-, and vertically-averaged concentration at user-specified locations along the plume centerline (y=0).

The other two Fortran codes (OMEGA and SIGMA) solve for the functions Ω and σ which are components of the approximate DAF solution technique.

In §D.3, §D.4, and §D.5, listings of each code are provided. These are preceded by §D.2, which contains a discussion of the procedure used to validate the HPS code.

D.2 VERIFICATION OF THE HPS MODEL

In order to ensure that the HPS code produces accurate results, it was compared to three other solute transport models. First, the HPS model was compared to the three-dimensional point source model presented by Hunt (1983). In the Hunt solution, mass is introduced into an aquifer of infinite thickness at a single point, whereas the horizontal plane source model evenly distributes mass over the entire source area. Inputting mass at a single point requires that the solute entering the aquifer have an infinite concentration. This requirement leads the point source model to overestimate of solute concentrations very near the source point.

After modifying the Hunt solution to consider mass input at the water table, the point source solution was compared to the HPS model using a source length, L=10 meters, and varying source widths, W. Simulations were run for receptor points located at the water table (z = 0) along the centerline of the plume (y = 0) using the same base scenario: an infinitely thick aquifer; steady-state conditions; total mass input = 1000 g/y; $\alpha_L = 10$ m, $\alpha_T = 1$ m, $\alpha_V = 1$ m, n = 0.43; $U_{GW} = 10$ m/y, and R = 1. Figure D1 contains the results of these simulations and shows that the HPS model always predicts receptor concentrations that are less than or equal to those predicted using the point source solution. At locations near the source, the difference between the two models is significant and the limitation of using a point source model is revealed. As the distance from the source area increases, the geometry of the source becomes less important and the HPS model and the point source model yield similar results. Also, as the source length and width used in the HPS model decrease, the HPS model and point source model yield identical results because the horizontal plane source begins to approximate a point.

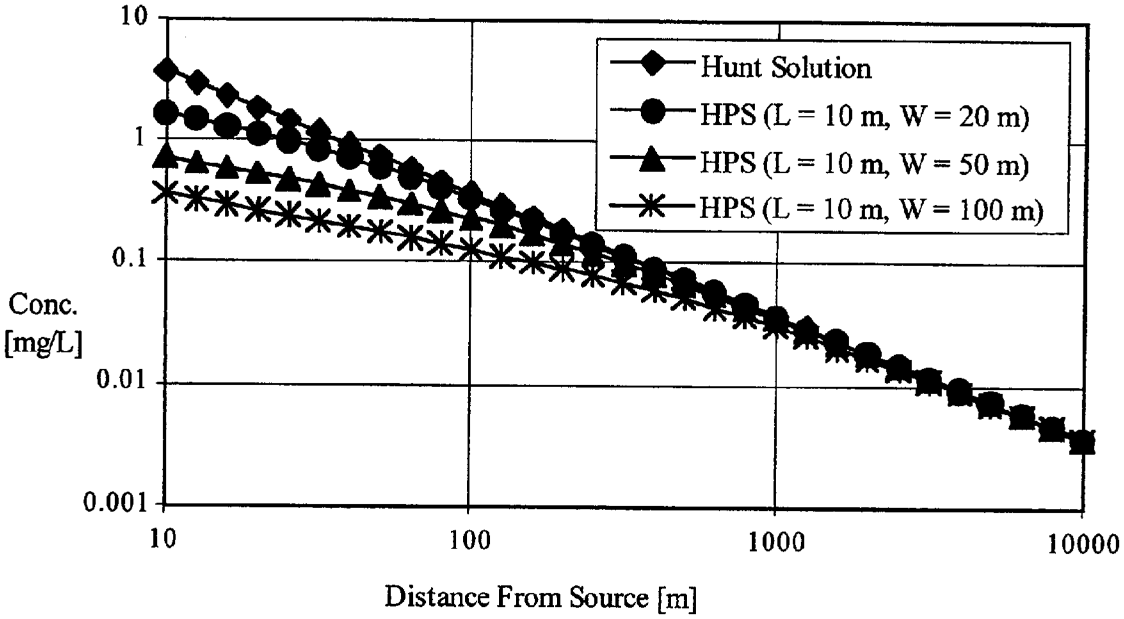

Figure D1. Comparison of the HPS model to the Hunt point source model

Next, the horizontal plane source model was compared to a simple two-dimensional steady-state plume model (Charbeneau, 1995). This model assumes a uniform concentration throughout the aquifer thickness and considers only advection and transverse mixing. The HPS model was compared to the simple plume model using the scenario outlined in the point source model comparison, except with an aquifer thickness, b, of ten meters. This comparison (Figure D2), shows the concentrations predicted by the models for different receptor distances.

Near the source, the HPS model predicts higher concentrations and the two models converge as the distance from the source increases. This is because mass is introduced at the water table in the HPS model and then becomes vertically mixed as the distance from the source increases. The simple plume model assumes that contaminants are initially mixed throughout the aquifer thickness, and therefore predicts lower concentrations near the source than the HPS model. The two solutions converge at a distance from the source where the mass in the HPS model becomes completely mixed throughout the aquifer depth.

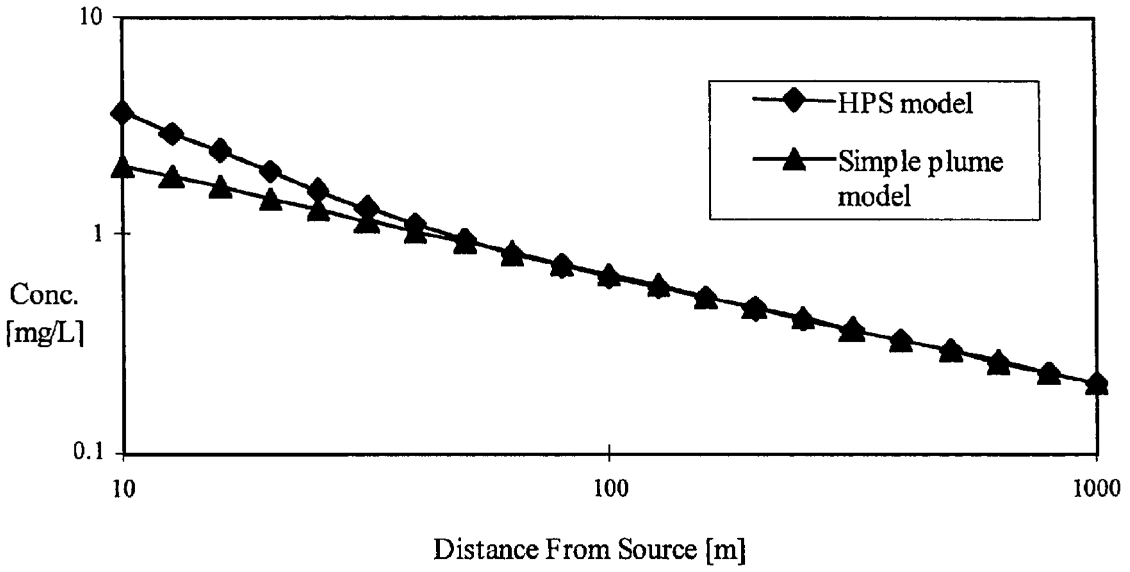

Figure D2. Comparison of the HPS and simple plume models

Finally, the HPS model was compared to the ESGP model developed by Charbeneau and Johnson (1992). The ESGP model is a two-dimensional model that considers longitudinal dispersion, advection, and transverse mixing. The model computes a leachate penetration depth and uses this result in a mixing zone model that determines solute concentrations beneath the source. Using an aquifer thickness of ten meters, centerline concentrations at the water table were obtained from the two models for a receptor distance of one hundred meters. As a further check, the HPS model was modified to mimic the two-dimensional ESGP model by setting the aquifer thickness equal to the leachate penetration depth computed by the ESGP model. The results obtained from these comparisons are shown in Figure D3.

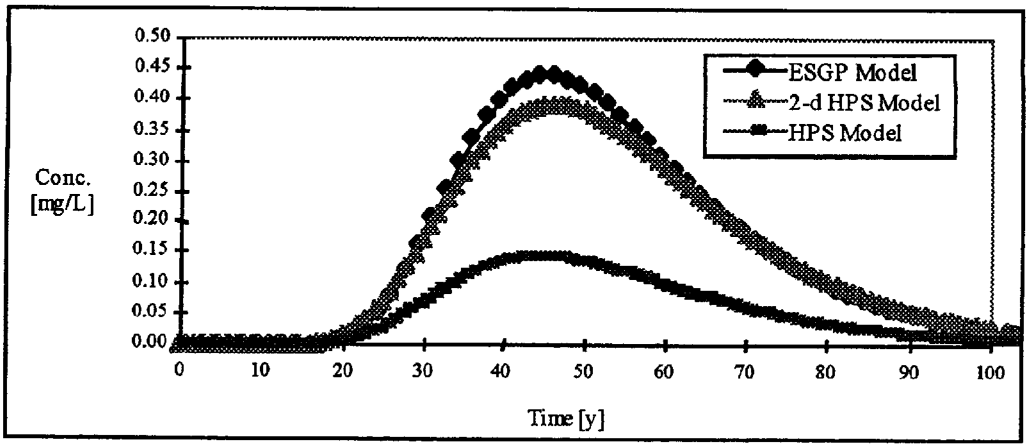

Figure D3. Comparison of the HPS and ESGP models

As seen in Figure D3, the concentration predicted by the HPS model is much lower than that predicted by the ESGP model. This is because the ESGP model does not consider vertical mixing and concentrations are uniform only over the leachate penetration depth, computed to be 1.979 m in this comparison. However, at a distance of 100 meters, the solute in the HPS model spreads throughout the entire 10 m aquifer thickness, resulting in greater dilution of the solute.

With the 2-d modification, the HPS model predicts concentrations that are only slightly lower than those predicted by the ESGP model. This is because concentrations beneath the source zone in the ESGP model are given a gaussian distribution, with centerline concentrations higher than those beneath the edges of the source zone. However, the HPS model assumes a uniform concentration profile under the source area, resulting in centerline concentrations less than those observed with the ESGP model. Of particular note, the shape of the concentration curves are consistent and maximum concentrations are observed at the same time.

With these comparisons, it is clear that the horizontal plane source model performs as expected and yields aquifer concentrations comparable with other models. In addition, the HPS model provides more realistic estimates of concentrations near the source.

D.3 HPS Source Code

```
PROGRAM HPS16
C *********************************************************************
C                 HORIZONTAL PLANE SOURCE (HPS) MODEL
C             ANALYTICAL THREE DIMENSIONAL SOLUTION FOR
C                 GROUND-WATER CONTAMINANT TRANSPORT
C
C                    ROMBERG INTEGRATION SCHEME
C                WITH VERTICAL AVERAGING OVER THE
C                       DEPTH OF THE WELL
C
C
C                  LAST MODIFIED MARCH 30, 1996
C
C     WRITTEN BY:     TIM HEMSTREET, UNIVERSITY OF TEXAS AT AUSTIN
C
C     LANGUAGE:       FORTRAN 77
C
C     SUBROUTINES:    WELLCONC, CONC, CS, ERF, INFO, USERIN
C
C     P U R P O S E :   E X A C T    M O D E L
C
C     THIS PROGRAM EVALUATES THE HPS MODEL WITH ROMBERG INTEGRATION
C     TO FIND THE CONCENTRATION AT ANY POINT IN THE AQUIFER AT
C     A GIVEN TIME.  INDIVIDUAL CONCENTRATIONS AT A LOCATION ARE
C     VERTICALLY AVERAGED TO GIVE THE CONCENTRATION THAT WOULD
C     APPEAR IN A WELL PLACED AT THAT LOCATION.  IN ADDITION, THIS
C     VERSION GIVES THE 30-YEAR TIME-AVERAGED CONCENTRATION FOUND AT
C     A POINT OR IN A WELL.  DISPERSIVITIES ARE COMPUTED INTERNALLY
C     IF THE LONGITUDINAL DISPERSIVITY IS SET TO ZERO (ALPHX = 0).
C
C     DILUTION ATTENUATION FACTORS ARE ALSO COMPUTED
C
C     I N P U T    P A R A M E T E R S :
C
C     T         TIME OF CONCENTRATION CALCULATION (YEARS)
C     NUMPT     NUMBER OF CALCULATION POINTS
C     BLKMO     INITIAL CHEMICAL CONSTITUENT BULK CONCENTRATION (MG/LITER)
C     QIN       SOURCE INFILTRATION (METERS/YEAR)
C     DSPILL    DEPTH OF CONTAMINATED SOIL (METERS)
C     THKVZ     THICKNESS OF THE VADOSE ZONE (METERS)
C     XS        X LOCATION OF I SOURCE AREA CENTER (METERS)
C     YS        Y LOCATION OF I SOURCE AREA CENTER (METERS)
C     ZS        Z LOCATION OF I SOURCE AREA CENTER (METERS)
C     SLEN      LENGTH (METERS IN X DIRECTION) OF SOURCE AREA
C     SWID      WIDTH  (METERS IN Y DIRECTION) OF SOURCE AREA
C     X(K)      X LOCATION FOR CONCENTRATION CALCULATION (METERS)
C     Y(K)      Y LOCATION FOR CONCENTRATION CALCULATION (METERS)
C     Z1(K)     Z LOCATION OF TOP OF WELL SCREEN (METERS)
C     Z2(K)     Z LOCATION OF BOTTOM OF WELL SCREEN (METERS)
C                      (= Z1(K) FOR A POINT RECEPTOR)
C     POR       AQUIFER AND SOIL POROSITY (-)
```

```
C       B          AQUIFER THICKNESS (METERS) (=99999 FOR INFINITE THICKNESS)
C       U          GROUNDWATER PORE VELOCITY (Darcy/porosity)(METERS/YEAR)
C       WATCR      IRREDUCIBLE WATER CONTENT (-)
C       HYDCR      RESIDUAL HYDROCARBON CONTENT (-)
C       PSDI       BROOKS-COREY PORE SIZE DISTRIBUTION INDEX
C       XKSVZ      SATURATED VERTICAL HYDRAULIC CONDUCTIVITY (METERS/YEAR)
C       AHALF      CONTAMINANT HALF-LIFE IN THE AQUIFER (YEARS)
C       VHALF      CONTAMINANT HALF-LIFE IN THE VADOSE ZONE (YEARS)
C       XKD        SOIL-WATER PARTITION COEFFICIENT (M^3/KG)
C       XK0        HYDROCARBON-WATER PARTITION COEFFICIENT (-)
C       XKH        HENRYís LAW PARTITION COEFFICIENT (-)
C       ALPHX      LONGITUDINAL DISPERSIVITY (METERS)
C       ALPHY      TRANSVERSE HORIZONTAL DISPERSIVITY (METERS)
C       ALPHZ      TRANSVERSE VERTICAL DISPERSIVITY (METERS)
C
C       O U T P U T   P A R A M E T E R S :
C
C       DHALF      THE LEACHATE SOURCE 'HALF-LIFE' (YR)
C       TAQF       LEACHATE TRAVEL TIME TO AQUIFER (YR)
C       BLKDEN     SOIL BULK DENSITY (KG/M^3)
C       WATC       VADOSE ZONE WATER CONTENT (-)
C       BW         BULK WATER PARTITION COEFFICIENT (-)
C       R          RETARDATION FACTOR IN THE AQUIFER (-)
C       XFLUX      INITIAL LEACHATE FLUX TO AQUIFER (G/YR)
C       WCONC      CONSTITUENT CONCENTRATION IN THE 'WELL'
C       DAF        DILUTION ATTENUATION FACTOR
C
C ***********************************************************************
C ***********************************************************************
      INTEGER IN, OUT
      PARAMETER (IN = 4, OUT = 8)
      DIMENSION TYM(200), WELC(200,100), XMS(200), CPEAK(100),TPEAK(100)
      DIMENSION DAF(100), AVCONC(100), AVDAF(100)
      REAL XSUM, AVCONC, FTIM
C
      COMMON /SIMU/ T, NUMPT, XS, YS, EPS, JSTEP
      COMMON /SRCE/ BLKMO, QIN, CTIME, DSPILL, SLEN, SWID
      COMMON /PART/ XKD, XKO, XKH, WATCR, HYDCR
      COMMON /VADZ/ POR, PSDI, THKVZ, XKSVZ, VHALF
      COMMON /AQUF/ B, U, AHALF, ALPHX, ALPHY, ALPHZ
      COMMON /RECP/ X(200), Y(200), Z1(200), Z2(200), IPT
      COMMON /CAL1/ BLKDEN, SATW, BW, R, TAQF, XFLUX, SHALF
      COMMON /CAL2/ SLAM, VLAM, ALAM, SMASS, CINIT
      COMMON /GRN1/ C1, CX1, CX2, CX3, CX4, CY1, CY2, CY3
      COMMON /GRN2/ CZ1, CZ2, DZ
C
      WRITE(*,10)
   10 FORMAT(////
     +      '          HORIZONTAL PLANE SOURCE (HPS) MODEL'/
     1      '        ANALYTICAL THREE DIMENSIONAL SOLUTION FOR'/
     2      '           GROUNDWATER CONTAMINANT TRANSPORT'////
     3      '                   VERSION 16.0'//
     4      '                 MARCH 26,  1995'//////////)
C
```

```
      CALL INFO
      FTIM = T
C
C     CALCULATE COEFFICIENTS FOR CALCULATION
      C1 = 1. / ( R * POR )
      CX1 = 1. / ( 2. * SLEN )
      CX2 = SLEN / 2.
      CX3 = U / R
      CY1 = 1. / ( 2. * SWID )
      CY2 = SWID / 2.
C
      PRINT*
      PRINT*, 'START COMPUTATIONS'
      PRINT*
C
C     BEGIN DO LOOP FOR NUMPT CALCULATION POINTS
      DO 50 K = 1, NUMPT
      PRINT*
      PRINT*, 'RECEPTOR NUMBER: ', K
      PRINT*
C
      IF(ALPHX .EQ. 0.) THEN
        PRINT*, 'INTERNALLY COMPUTED DISPERSION'
        DX = 0.1 * (X(K)- SLEN/2) * U
        DY = 0.03 * (X(K)- SLEN/2) * U
        DZ = 0.001 * (X(K)- SLEN/2) * U
      ELSE
        PRINT*, 'MANUALLY ENTERED DISPERSION'
        DX = ALPHX * U
        DY = ALPHY * U
        DZ = ALPHZ * U
      ENDIF
C
      CX4 = 4. * DX / R
      CY3 = 4. * DY / R
      CZ1 = 4. * DZ / R
      CZ2 = 3.1416 * DZ / R
C
C     BEGIN DO LOOP FOR YEARLY CONCENTRATION POINTS
      DO 50 J = 0, FTIM, JSTEP
C
C     LET THE EVALUATION TIME, T, VARY IN ORDER TO PRODUCE
C     CONCENTRATION PROFILES
      T = J
C
C     CALCULATE SOURCE MASS FLUX, XMS, AT TIMESTEP TAU
      IF(T .GE. CTIME) THEN
          XMS(J) = XFLUX * EXP(-SLAM*(T-CTIME)) * EXP(-VLAM*TAQF)
      ELSE
          XMS(J) = XFLUX * EXP(-VLAM*TAQF)
      ENDIF
C
      PRINT*, 'Time = ', J
      WCONC = 0.
```

```
C
C     COMPUTE DISTANCE BETWEEN RECEPTOR AND SOURCE AREA CENTER
      XC = X(K) - XS
      YC = Y(K) - YS
      ZT = Z1(K)
      IF(Z2(K) .EQ. Z1(K)) THEN
        ZB = -99
      ELSE
        ZB = Z2(K)
      ENDIF
C
C     SOLVE THE INTEGRAL FOR THE CURRENT WELL LOCATION AND STORE THE
C     CONCENTRATION FOR THE REAL TIME.
      CALL WELLCONC(XC,YC,ZT,ZB,WCONC)
      WELC(J,K) = WCONC
      TYM(J) = T
C
C     END OF DO LOOP(S) FOR CALCULATIONS
   50 CONTINUE
C
C     PRINT MATRIX OF CONCENTRATION PROFILES OVER TIME
      WRITE(OUT,100)
  100 FORMAT('  -------------------'/,
     +       '  BREAKTHROUGH CURVES'/,
     +       '  -------------------'/
     + '   YEAR    RECEPTOR 1   RECEPTOR 2   RECEPTOR 3'
     + '   RECEPTOR 4   RECEPTOR 5'/)
      DO 125 M = 0, FTIM, JSTEP
      WRITE(OUT,130) TYM(M), (WELC(M,N), N = 1, NUMPT)
  125 CONTINUE
  130 FORMAT(F6.1,3X,E11.5,2X,E11.5,2X,E11.5,2X,E11.5,2X,E11.5)
C
C     FIND THE PEAK CONCENTRATION(S) AND TIME(S)
      DO 150 K = 1, NUMPT
      DO 140 N = 0, FTIM
      IF(WELC(N,K) .GT. CPEAK(K)) THEN
        CPEAK(K) = WELC(N,K)
        TPEAK(K) = TYM(N)
      ENDIF
  140 CONTINUE
  150 CONTINUE
C
C     CALCULATE AND PRINT MATRIX OF PEAK DAFs OVER TIME
      WRITE(OUT,370)
  370 FORMAT(/'---------------------------------'/,
     +       'PEAK DILUTION ATTENUATION FACTORS'/,
     +       '---------------------------------'/
     + 'RECEPTOR #     PEAK CONC. (MG/L)      PEAK TIME (YR)      DAF')
      DO 385 M = 1, NUMPT
      DAF(M) = (CINIT)/CPEAK(M)
      WRITE(OUT,390) M, CPEAK(M), TPEAK(M), DAF(M)
  385 CONTINUE
  390 FORMAT(I5,9X,E11.5,10X,F6.1,13X,F6.1)
C
```

```
C     DO LOOP TO AVERAGE THE CONCENTRATION OVER A CERTAIN
C     NUMBER OF YEARS
      AVSUM = 0.
      DO 190 K = 1, NUMPT
      AVCONC(K) = 0.
C
      DO 200 J = 0, FTIM-30
      XSUM = 0.
      DO 80 N = J, J+29
        XSUM = XSUM + 0.5 * (WELC(N,K) + WELC(N+1,K))
   80 CONTINUE
C
      AVSUM = XSUM/30
      IF(AVSUM .GT. AVCONC(K)) AVCONC(K) = AVSUM
  200 CONTINUE
  190 CONTINUE
C
C     CALCULATE AND PRINT MATRIX OF PEAK DAFs OVER TIME
      WRITE(OUT,371)
  371 FORMAT(/'----------------------------------'/,
     +        '30-YR DILUTION ATTENUATION FACTORS'/,
     +        '----------------------------------'/
     + 'RECEPTOR #      AVG CONC. (MG/L)       30-YR DAF')
      DO 386 M = 1, NUMPT
      AVDAF(M) = (CINIT)/AVCONC(M)
      WRITE(OUT,391) M, AVCONC(M), AVDAF(M)
  386 CONTINUE
  391 FORMAT(I5,9X,E11.5,13X,F6.1)
C
C     PRINT MATRIX OF SOURCE MASS FLUX OVER TIME
      WRITE(OUT,400)
  400 FORMAT(/,'----------------------'/,
     +         '   SOURCE MASS FLUX '/,
     +         '----------------------'/
     + '   TIME (YRS)     MASS FLUX (G/YR)'/)
      DO 500 J = 0, FTIM, JSTEP
        WRITE(OUT,410) TYM(J), XMS(J)
  410 FORMAT(8X,F5.1,7X,F9.3)
  500 CONTINUE
C
C     STOP AND END THE PROGRAM
      PRINT*
      PRINT*, 'SIMULATION COMPLETED'
      PRINT*
      CLOSE(OUT)
      STOP
      END
C
      SUBROUTINE WELLCONC(XC,YC,ZT,ZB,WCONC)
C     *********************************************************************
C     *********************************************************************
C     **  P U R P O S E                                                  **
C     **                                                                 **
C     **   THIS ROUTINE PEFORMS A NUMERICAL INTEGRATION BASED ON A       **
```

```
C     **   ROMBERG ALGORITHM. POINT CONCENTRATIONS ARE VERTICALLY          **
C     **   AVERAGED OVER THE DEPTH OF THE WELL SCREEN TO APPROXIMATE       **
C     **   A WELL.                                                         **
C     **                                                                   **
C     **  I N P U T    P A R A M E T E R S                                 **
C     **                                                                   **
C     **       XC .... THE X-COORDINATE                                    **
C     **       YC .... THE Y-COORDINATE                                    **
C     **       ZT..... THE Z-COORDINATE OF THE TOP OF THE WELL SCREEN      **
C     **       ZB..... THE Z-COORDINATE OF THE BOTTOM OF THE WELL SCREEN   **
C     **                                                                   **
C     **  O U T P U T    P A R A M E T E R S                               **
C     **                                                                   **
C     **       CINT....THE SOLUTION TO THE CONCENTRATION INTEGRAL          **
C     **               OVER THE LENGTH OF THE WELL SCREEN                  **
C     **       WCONC...THE AVERAGE CONCENTRATION IN THE WELL AT A GIVEN    **
C     **               TIME                                                **
C     **                                                                   **
C     **  O T H E R   P A R A M E T E R S                                  **
C     **                                                                   **
C     **       TA1.... REAL ARRAY CONTAINING INTEGRAL APPROXIMATIONS       **
C     **       EPS ... REAL VARIABLE. THE RELATIVE ERROR FOR WHICH         **
C     **               CONVERGENCE IS CHECKED                              **
C     **       A  .... REAL VARIABLE. THE LOWER BOUND OF INTEGRATION       **
C     **                                                                   **
C     **   REQUIRED ROUTINES: CONC                                         **
C     ***********************************************************************
C     ***********************************************************************
      INTEGER IN, OUT
      PARAMETER (IN = 4, OUT = 8)
      REAL TA1(25,25)
      COMMON /SIMU/ T, NUMPT, XS, YS, EPS, JSTEP
C
C     TEST TO SEE IF THE RECEPTOR IS A WELL LENGTH TO BE AVERAGED OR A
C     POINT TO BE EVALUATED.  IF RECEPTOR IS A POINT THEN SKIP VERTICAL
C     AVERAGING ALGORITHM AND SIMPLY CALCULATE THE POINT CONCENTRATION.
      IF(ZB .EQ. -99) THEN
         WCONC = CONC(XC,YC,ZT)
         GOTO 45
      ENDIF
C
C     SET MAXIMUM ITERATIONS
      NUMITS=23
C
C     LOWER BOUND OF INTEGRATION IS ALWAYS THE BOTTOM OF THE WELL SCREEN
      Z2=ZB
C
C     UPPER BOUND OF INTEGRATION IS ALWAYS THE TOP OF THE WELL SCREEN
      Z1=ZT
C
C     CALCULATE THE LENGTH OF THE SCREEN, HW
      HW = ZB - ZT
C
C     CALCULATE THE AVERAGE LENGTH VALUE BETWEEN UPPER AND LOWER BOUND
```

```
C     OF INTEGRATION
      ZAV = (Z2+Z1)/2.
C
C     CALCULATE THE FIRST SET OF INTEGRAL 'PANELS'
C     AT THE LOWER BOUND, AVERAGE LENGTH, AND UPPER BOUND

      TA1(1,1)=(Z2-Z1)/2.*(CONC(XC,YC,Z1)+CONC(XC,YC,Z2))
      TA1(1,2)=TA1(1,1)/2.+(Z2-Z1)/2.*(CONC(XC,YC,ZAV))
      TA1(2,1)=1./3.*(4.*TA1(1,2)-TA1(1,1))
C
C     BEGIN ITERATION TO GET BEST APPROXIMATION FOR THE INTEGRAL
      DO 30 J=3,25
C
C     SET THE INTERVAL DISTANCE
         DLM=(Z2-Z1)/(2**(J-1))
C
C     CALCULATE ANOTHER 'PANEL' LOCATION
         XLAM=Z1-DLM
         N=2**(J-2)
C
C     BEGIN INTEGRATION
         SUM=0.
         DO 10 I=1,N
C
C     CALCULATE THE STEP SIZE
            XLAM=XLAM+2.*DLM
            SUM=SUM+CONC(XC,YC,XLAM)
10       CONTINUE
C
C     CALCULATE NEW PANELS
         TA1(1,J)=TA1(1,J-1)/2.+DLM*SUM
         DO 20 L=2,J
            K = J + 1 - L
            TA1(L,K)=(4**(L-1)*TA1(L-1,K+1)-TA1(L-1,K))/(4**(L-1)-1.)
20       CONTINUE
C
C     CHECK FOR CONVERGENCE BASED ON RELATIVE ERROR CRITERIA
C     IF CONVERGENCE IS MET THE INTEGRAL VALUE HAS BEEN
C     DETERMINED AND RETURN THE SOLUTION
C
C     THIS NEXT STATEMENT CAUSES ERRORS IF TA1(J,1) = 0.
         IF ( ABS( TA1(J,1)-TA1(J-1,1) ) .LE. EPS*ABS(TA1(J,1)) ) THEN
            CINT=TA1(J,1)
            GO TO 40
         ELSE
            ITS=J
         ENDIF
 30   CONTINUE
C
C     IF CONVERGENCE WAS NEVER ACHIEVED FOR THIS TIME STEP
C     (STOP THE PROGRAM RUN)
      IF (ITS.GE.NUMITS) THEN
         WRITE(OUT,*)'CONVERGENCE WAS NOT FOUND...'
         STOP
```

```
      ENDIF
 40   CONTINUE
C
C     CALCULATE CONCENTRATION
      WCONC = CINT/HW
 45   RETURN
      END
C
      FUNCTION CONC(XC,YC,ZC)
C     ***********************************************************************
C     ***********************************************************************
C     **  P U R P O S E                                                   **
C     **                                                                  **
C     **   THIS ROUTINE PEFORMS A NUMERICAL INTEGRATION BASED ON A        **
C     **   ROMBERG ALGORITHM. THE FUNCTION CS IS INTEGRATED OVER TIME.    **
C     **                                                                  **
C     **  I N P U T   P A R A M E T E R S                                 **
C     **                                                                  **
C     **       XC .... THE X-COORDINATE                                   **
C     **       YC .... THE Y-COORDINATE                                   **
C     **       ZC .... THE Z-COORDINATE                                   **
C     **                                                                  **
C     **      (THE OTHER PARAMETERS PASSED THROUGH COMMON BLOCKS ARE      **
C     **       THE SAME AS IN THE ABOVE ROUTINES)                         **
C     **                                                                  **
C     **  O U T P U T   P A R A M E T E R S                               **
C     **                                                                  **
C     **       CP   ....THE INTEGRAL OF THE GREEN'S FUNCTIONS OVER TIME   **
C     **       CONC....THE CONCENTRATION AT THE GIVEN LOCATION AND TIME   **
C     **                                                                  **
C     **  O T H E R   P A R A M E T E R S                                 **
C     **                                                                  **
C     **       TA1.... REAL ARRAY CONTAINING INTEGRAL APPROXIMATIONS      **
C     **       EPS ... REAL VARIABLE. THE RELATIVE ERROR FOR WHICH        **
C     **               CONVERGENCE IS CHECKED                             **
C     **       T1 .... REAL VARIABLE. THE LOWER BOUND OF INTEGRATION      **
C     **       T2 .... REAL VARIABLE. EQUALS THE UPPER TIME LIMIT OF      **
C     **               INTEGRATION                                        **
C     **                                                                  **
C     **   REQUIRED ROUTINES: CS                                          **
C     ***********************************************************************
C     ***********************************************************************
      INTEGER IN, OUT
      PARAMETER (IN = 4, OUT = 8)
      REAL TA1(25,25)
C
      COMMON /SIMU/ T, NUMPT, XS, YS, EPS, JSTEP
      COMMON /CAL1/ BLKDEN, SATW, BW, R, TAQF, XFLUX, SHALF
      COMMON /CAL2/ SLAM, VLAM, ALAM, SMASS, CINIT
      COMMON /GRN1/ C1, CX1, CX2, CX3, CX4, CY1, CY2, CY3
C
C     SET MAXIMUM ITERATIONS
      NUMITS=23
C
```

```
C     SET INTEGRATION LIMITS.  THE LOWER BOUND OF INTEGRATION (T1) IS ALWAYS
C     TIME = ZERO.  TIME 'ZERO' IS THE TIME AT WHICH MASS REACHES THE
C     WATER TABLE.  T2 IS THE UPPER TIME LIMIT OF INTEGRATION.
      T1 = 0.
      T2 = T
C
C     CALCULATE THE AVERAGE TIME VALUE BETWEEN ZERO AND
C     UPPER BOUND OF INTEGRATION.
      TAV=(T2+T1)/2.
C
C     CALCULATE THE FIRST SET OF INTEGRAL 'PANELS'
C     AT THE LOWER BOUND, AVERAGE TIME, AND UPPER BOUND
      TA1(1,1)=(T2-T1)/2.*(CS(XC,YC,ZC,T1)+CS(XC,YC,ZC,T2))
      TA1(1,2)=TA1(1,1)/2.+(T2-T1)/2.*(CS(XC,YC,ZC,TAV))
      TA1(2,1)=1./3.*(4.*TA1(1,2)-TA1(1,1))
C
C     BEGIN ITERATION TO GET BEST APPROXIMATION FOR THE INTEGRAL
      DO 30 J=3,25
C
C     SET THE INTERVAL DISTANCE
         DLM=(T2-T1)/(2**(J-1))
C
C     CALCULATE ANOTHER 'PANEL' LOCATION
         XLAM=T1-DLM
         N=2**(J-2)
C
C     BEGIN INTEGRATION
         SUM=0.
         DO 10 I=1,N
C
C     CALCULATE THE STEP SIZE
            XLAM=XLAM+2.*DLM
            SUM=SUM+CS(XC,YC,ZC,XLAM)
10       CONTINUE
C
C     CALCULATE NEW PANELS
         TA1(1,J)=TA1(1,J-1)/2.+DLM*SUM
         DO 20 L=2,J
            K = J + 1 - L
            TA1(L,K)=(4**(L-1)*TA1(L-1,K+1)-TA1(L-1,K))/(4**(L-1)-1.)
20       CONTINUE
C
C     CHECK FOR CONVERGENCE BASED ON RELATIVE ERROR CRITERIA
C     IF CONVERGENCE IS MET THE INTEGRAL VALUE HAS BEEN
C     DETERMINED AND RETURN TO SOLN
C
C     THIS NEXT STATEMENT CAUSES ERRORS IF TA1(J,1) = 0.
         IF ( ABS( TA1(J,1)-TA1(J-1,1) ) .LE. EPS*ABS(TA1(J,1)) ) THEN
            CP=TA1(J,1)
            GO TO 40
         ELSE
            ITS=J
         ENDIF
30    CONTINUE
```

```
C
C      IF CONVERGENCE WAS NEVER ACHIEVED FOR THIS TIME STEP
C      (STOP THE PROGRAM RUN)
       IF (ITS.GE.NUMITS) THEN
          WRITE(OUT,*)'CONVERGENCE WAS NOT FOUND...'
          STOP
       ENDIF
40     CONTINUE
C
C      CALCULATE CONCENTRATION
       CONC = C1 * CP
       RETURN
       END
C
C
       FUNCTION CS(XC,YC,ZC,TAU)
C      **********************************************************************
C      **********************************************************************
C      **  P U R P O S E                                                   **
C      **                                                                  **
C      **  THIS ROUTINE EVALUATES THE FUNCTION (INTEGRAND) AT A GIVEN      **
C      **  TIME AND LOCATION.  THE FUNCTION INCLUDES THE DIMENSIONAL       **
C      **  GREENS FUNCTIONS AND A DEGRADATION FUNCTION.                    **
C      **                                                                  **
C      **  I N P U T    P A R A M E T E R S                                **
C      **                                                                  **
C      **       XC .... REAL VARIABLE. THE X-COORDINATE                    **
C      **       YC .... REAL VARIABLE. THE Y-COORDINATE                    **
C      **       ZC .... REAL VARIABLE. THE Z-COORDINATE                    **
C      **       TAU.... REAL VARIABLE. THE TIME FOR WHICH THE FUNCTION     **
C      **               IS TO BE EVALUATED                                 **
C      **                                                                  **
C      **  O U T P U T    P A R A M E T E R S                              **
C      **                                                                  **
C      **       CS .... REAL VARIABLE. THE VALUE OF THE FUNCTION FOR       **
C      **               THE INPUT PARAMETERS                               **
C      **                                                                  **
C      **   REQUIRED ROUTINES: ERF                                         **
C      **********************************************************************
C      **********************************************************************
       INTEGER IN, OUT
       PARAMETER (IN = 4, OUT = 8)
C
       COMMON /SIMU/ T, NUMPT, XS, YS, EPS, JSTEP
       COMMON /SRCE/ BLKMO, QIN, CTIME, DSPILL, SLEN, SWID
       COMMON /PART/ XKD, XKO, XKH, WATCR, HYDCR
       COMMON /VADZ/ POR, PSDI, THKVZ, XKSVZ, VHALF
       COMMON /AQUF/ B, U, AHALF, ALPHX, ALPHY, ALPHZ
       COMMON /RECP/ X(200), Y(200), Z1(200), Z2(200), IPT
       COMMON /CAL1/ BLKDEN, SATW, BW, R, TAQF, XFLUX, SHALF
       COMMON /CAL2/ SLAM, VLAM, ALAM, SMASS, CINIT
       COMMON /GRN1/ C1, CX1, CX2, CX3, CX4, CY1, CY2, CY3
       COMMON /GRN2/ CZ1, CZ2, DZ
C
```

```
C     CALCULATE SOURCE STRENGTH AT TIMESTEP TAU
      IF(TAU .GE. CTIME) THEN
          SMASS = XFLUX * EXP(-SLAM*(TAU-CTIME)) * EXP(-VLAM*TAQF)
      ENDIF
      IF(TAU .LT. CTIME) THEN
          SMASS = XFLUX * EXP(-VLAM*TAQF)
      ENDIF
C
C     CALULATE TTAU, THE TIME FOR THE CONVOLUTION
      TTAU = T - TAU
      IF(TTAU .LE. 0.) THEN
          CS = 0.
          GOTO 800
      ENDIF
C
C     CALCULATE X-DIRECTION GREEN'S FUNCTION
      XG1 = ( CX2 + XC - CX3 *TTAU ) / ( CX4 * TTAU )**0.5
      IF ( ABS(XG1) .LT. 0.00001 ) THEN
       XG1 = 0.
      ELSEIF ( XG1 .LT. -6. ) THEN
       XG1 = -1.
      ELSEIF ( XG1 .GT. 6. ) THEN
       XG1 = 1.
      ELSE
       XG1 = ERF(XG1)
      ENDIF
      XG2 = ( CX2 - XC + CX3 *TTAU ) / ( CX4 * TTAU )**0.5
      IF ( ABS(XG2) .LT. 0.00001 ) THEN
       XG2 = 0.
      ELSEIF ( XG2 .LT. -6. ) THEN
       XG2 = -1.
      ELSEIF ( XG2 .GT. 6. ) THEN
       XG2 = 1.
      ELSE
       XG2=ERF(XG2)
      ENDIF
      XG = CX1 * ( XG1 + XG2 )
C
C CALCULATE Y-DIRECTION GREEN'S FUNCTION
      YG1 = ( CY2 + YC ) / ( CY3 * TTAU )**0.5
      IF ( ABS(YG1) .LT. 0.00001 ) THEN
       YG1 = 0.
      ELSEIF ( YG1 .LT. -6. ) THEN
       YG1 = -1.
      ELSEIF ( YG1 .GT. 6. ) THEN
       YG1 = 1.
      ELSE
       YG1 = ERF(YG1)
      ENDIF
      YG2 = ( CY2 -YC ) / ( CY3 * TTAU )**0.5
      IF ( ABS(YG2) .LT. 0.00001 ) THEN
       YG2 = 0.
      ELSEIF ( YG2 .LT. -6. ) THEN
       YG2 = -1.
```

```
      ELSEIF ( YG2 .GT. 6. ) THEN
       YG2 = 1.
      ELSE
       YG2 = ERF(YG2)
      ENDIF
      YG = CY1 * ( YG1 + YG2 )
C
C CALCULATE Z-DIRECTION GREEN'S FUNCTION FOR AQUIFER OF FINITE THICKNESS
      ZIP = ZC + 0.
      IF (B.EQ.99999) GO TO 700
      PHI = DZ * TTAU / ( R * B**2 )
      IF ( PHI .GT. 1. ) THEN
        ZG = 1./B
      ELSE
        FUN = 0.
        DO 600 J = -5,5
          FUN = FUN + EXP( - (2.* J * B - ZIP)**2 / (CZ1 *TTAU) )
 600    CONTINUE
        ZG = FUN / (CZ2*TTAU)**0.5
      ENDIF
      GO TO 750
C
C CALCULATE Z-DIRECTION GREEN'S FUNCTION FOR AQUIFER OF INFINITE THICKNESS
 700  CZ6 = ( ZC**2 ) / ( CZ1 * TTAU )
      IF ( CZ6 .GT. 25. ) THEN
       CZ6 = 0.
      ELSE
       CZ6 = EXP(-CZ6)
      ENDIF
      CZ7 = ( ZIP + 0. )**2 / ( CZ1 * TTAU )
      IF ( CZ7 .GT. 25. ) THEN
       CZ7 = 0.
      ELSE
       CZ7 = EXP(-CZ7)
      ENDIF
      ZG = ( CZ6 + CZ7 ) / ( 4. * CZ2 * TTAU )**0.5
C
C     COMBINE GREENS FUNCTIONS,SOURCE STRENGTH, AND DEGRADATION FUNCTION
C     TO COMPUTE CS FUNCTION
 750  CS = SMASS * XG * YG * ZG * EXP(-ALAM*TTAU)
C
 800  RETURN
      END
C
C
      FUNCTION ERF(ARG)
C     *******************************************************************
C     *******************************************************************
C     **  P U R P O S E                                                **
C     **                                                               **
C     **   THIS ROUTINE EVALUATES THE ERROR FUNCTION OF A GIVEN        **
C     **   ARGUMENT (ARG).                                             **
C     **                                                               **
C     **  REQUIRED ROUTINES: NONE                                      **
```

```
C     ******************************************************************
C     ******************************************************************
      REAL P, A1, A2, A3, A4, A5
      DATA P,A1,A2,A3,A4,A5/.3275911,.254829592,-.284496736,
     +     1.421413741,-1.453152027,1.061405429/
      TE = 1/(1+ABS(P*ARG))
      ERF = 1-((((A5*TE+A4)*TE+A3)*TE+A2)*TE+A1)*TE*EXP(-(ARG*ARG))
      IF (ARG.LT.0) ERF=-ERF
      RETURN
      END
C
C
      SUBROUTINE INFO
C     ******************************************************************
C     ******************************************************************
C     **  P U R P O S E                                               **
C     **                                                              **
C     **   THIS ROUTINE READS THE INPUT DATA INTO THE PROGRAM         **
C     **                                                              **
C     **  REQUIRED ROUTINES:  USERIN                                  **
C     ******************************************************************
C     ******************************************************************
      CHARACTER*14  INFILE, OUTFILE
      CHARACTER*5  ANSWER
      CHARACTER*60  TITLE
      INTEGER IN, OUT
      PARAMETER (IN = 4, OUT = 8)
C
      COMMON /SIMU/ T, NUMPT, XS, YS, EPS, JSTEP
      COMMON /SRCE/ BLKMO, QIN, CTIME, DSPILL, SLEN, SWID
      COMMON /PART/ XKD, XKO, XKH, WATCR, HYDCR
      COMMON /VADZ/ POR, PSDI, THKVZ, XKSVZ, VHALF
      COMMON /AQUF/ B, U, AHALF, ALPHX, ALPHY, ALPHZ
      COMMON /RECP/ X(200), Y(200), Z1(200), Z2(200), IPT
      COMMON /CAL1/ BLKDEN, SATW, BW, R, TAQF, XFLUX, SHALF
      COMMON /CAL2/ SLAM, VLAM, ALAM, SMASS, CINIT
C
C     DETERMINE SOURCE OF INPUT
      PRINT*
      PRINT*, 'DO YOU WISH TO READ AN INPUT FILE OR CREATE A NEW ONE?'
      PRINT*, 'ENTER Y IF YOU WISH TO READ AN EXISTING FILE - '
      READ(*,12) ANSWER
      IF (ANSWER .EQ. 'Y' .OR. ANSWER .EQ. 'y') THEN
       PRINT*
       PRINT*, 'ENTER NAME OF INPUT FILE - '
       READ(*,14) INFILE
       OPEN (UNIT=IN,FILE=INFILE,STATUS='OLD')
       PRINT*
       PRINT*, 'ENTER NAME OF OUTPUT FILE - '
       READ(*,14) OUTFILE
       OPEN (UNIT=OUT,FILE=OUTFILE,STATUS='UNKNOWN')
       READ(IN,20) TITLE
   20  FORMAT(15A)
       READ(IN,*) T, NUMPT, XS, YS, EPS, JSTEP
```

```
         READ(IN,*) BLKMO, QIN, CTIME, DSPILL, SLEN, SWID
         READ(IN,*) XKD, XKO, XKH, WATCR, HYDCR
         READ(IN,*) POR, PSDI, THKVZ, XKSVZ, VHALF
         READ(IN,*) B, U, AHALF, ALPHX, ALPHY, ALPHZ
         READ(IN,*) (X(I),Y(I),Z1(I),Z2(I), I=1,NUMPT)
        ELSE
         PRINT*
         PRINT*, 'ENTER NAME TO SAVE INPUT FILE WHICH IS CREATED -'
         READ(*,14) INFILE
         OPEN (UNIT=IN,FILE=INFILE,STATUS='UNKNOWN')
         CALL USERIN
         CLOSE(IN)
         PRINT*
         PRINT*, 'ENTER NAME TO SAVE OUTPUT FILE WHICH IS CREATED - '
         READ(*,14) OUTFILE
         OPEN (UNIT=OUT,FILE=OUTFILE,STATUS='UNKNOWN')
        ENDIF
   12   FORMAT(A5)
   14   FORMAT(A14)
C
        PRINT*, 'ENTER SLAM [-] - '
        READ(*,*) SLAM
        PRINT*, 'ENTER CINIT [MG/L] - '
        READ(*,*) CINIT

C
C       CALCULATE SIMULATION PARAMETERS
C       --ASSUME SOIL DENSITY = 2650. KG/M**3
        BLKDEN = 2650. * (1. - POR)
C
C       --WATER SATURATION FROM BROOKS-COREY MODEL AND AIR CONTENT
        WATC = WATCR + (POR - WATCR)*(QIN/XKSVZ)**(PSDI/(3.*PSDI+2.))
        AIRC = POR - WATC - HYDCR
C
C       --PARTITION AND RETARDATION COEFFICIENTS
        BW = WATC + HYDCR*XKO + BLKDEN*XKD + AIRC*XKH
        R = 1. + BLKDEN * XKD / POR
C
C       --TIME FOR THE SOLUTE LEACHATE TO REACH THE WATER TABLE
        TAQF = (WATC + BLKDEN*XKD) * (THKVZ - DSPILL) / QIN
C
C       --INITIAL SOLUTE FLUX TO THE AQUIFER
        XFLUX = SLEN * SWID * QIN * CINIT
C
C       --LEACHATE HALF-LIFE
        SHALF = ALOG(2.) * BW * DSPILL / QIN
C
C       CALCULATE DIMENSIONLESS DECAY-RATE COEFFICIENTS
        IF (AHALF .NE. 0.) THEN
           ALAM = ALOG(2.) / AHALF
        ELSE
           ALAM = 0.
        ENDIF
C
```

```
      IF (VHALF .NE. 0.) THEN
         VLAM = ALOG(2.) / VHALF
      ELSE
         VLAM = 0.
      ENDIF
C
      PRINT*, SLAM
      IF(SLAM .GT. 0.) THEN
        SHALF = ALOG(2.)/SLAM
      ELSE
        SHALF = 0.
      ENDIF
C
C     WRITE OUTPUT DATA
      PRINT*
      PRINT*, 'WRITE OUTPUT FILE'
      WRITE (OUT,40)
      WRITE (OUT,30) TITLE
      WRITE (OUT,45) T, EPS, JSTEP
      WRITE (OUT,50) THKVZ, QIN, POR, WATCR, PSDI, XKSVZ, VHALF
      WRITE (OUT,60) B, U, ALPHX, ALPHY, ALPHZ
      WRITE (OUT,70) CTIME, SLEN, SWID, DSPILL, BLKMO, HYDCR
      WRITE (OUT,80) XKD, XKO, XKH, AHALF
      WRITE (OUT,90) BLKDEN, WATC, BW, R, TAQF, CINIT, SHALF
C
  30  FORMAT(2X,A60)
  40  FORMAT('  *************************************************** '/,
     +       '          HORIZONTAL PLANE SOURCE (HPS) MODEL '/,
     +       '       ANALYTICAL THREE DIMENSIONAL SOLUTION FOR'/
     +       '           GROUNDWATER CONTAMINANT TRANSPORT'//
     +       '                      VERSION 16.0'/
     +       '  *************************************************** '/)
  45  FORMAT(/'  ---------------------'/,
     +  '  SIMULATION PARAMETERS'/,
     +  '  ---------------------'/,
     +  '  LENGTH OF SIMULATION                    (YR)     = ',F9.3/,
     +  '  ROMBERG CONVERGENCE TOLERANCE           (-)      = ',F9.3/,
     +  '  LENGTH OF TIMESTEPS                     (YR)     = ',6X,I3/)
  50  FORMAT(/'  ------------------------------------   '/,
     +  '  SOIL AND VADOSE ZONE CHARACTERISTICS   '/,
     +  '  ------------------------------------   '/,
     +  '  VADOSE ZONE THICKNESS                   (M)      = ',F9.3/,
     +  '  AVERAGE INFILTRATION RATE               (M/YR)   = ',F9.3/,
     +  '  TOTAL SOIL POROSITY                     (-)      = ',F9.3/,
     +  '  IRREDUCIBLE WATER CONTENT               (-)      = ',F9.3/,
     +  '  PORE SIZE DISTRIBUTION INDEX            (-)      = ',F9.3/,
     +  '  SAT. VERTICAL HYDRAULIC CONDUCTIVITY    (M/YR)   = ',F9.3/,
     +  '  CONSTITUENT HALF-LIFE IN VADOSE ZONE    (YR)     = ',F9.3/)
  60  FORMAT('  ----------------------- '/,
     +  '  AQUIFER CHARACTERISTICS '/,
     +  '  ----------------------- '/,
     +  '  AQUIFER SATURATED THICKNESS             (M)      = ',F9.3/,
     +  '  GROUNDWATER SEEPAGE VELOCITY (q/n)      (M/YR)   = ',F9.3/,
     +  '  LONGITUDINAL DISPERSIVITY               (M)      = ',F9.3/,
```

```
     +  '  TRANSVERSE DISPERSIVITY                         (M)       = ',F9.3/,
     +  '  VERTICAL DISPERSIVITY                           (M)       = ',F9.3/)
  70  FORMAT('  ---------------------------------------'/,
     +  '  CONTAMINATED SOIL SOURCE CHARACTERISTICS'/,
     +  '  ---------------------------------------'/,
     +  '  DURATION OF CONSTANT SOURCE STRENGTH            (YR)      = ',F9.3/,
     +  '  LENGTH OF SOURCE CONTAMINATION                  (M)       = ',F9.3/,
     +  '  WIDTH OF SOURCE CONTAMINATION                   (M)       = ',F9.3/,
     +  '  THICKNESS OF SOIL CONTAMINATION                 (M)       = ',F9.3/,
     +  '  INITIAL CONSTITUENT BULK CONCENTRATION          (MG/L)    = ',F9.3/,
     +  '  RESIDUAL HYDROCARBON CONTENT                    (-)       = ',F9.3/)
  80  FORMAT('  --------------------------'/,
     +  '  CONSTITUENT CHARACTERISTICS'/,
     +  '  --------------------------'/,
     +  '  SOIL-WATER PARTITION COEFFICIENT                (M^3/KG)  = ',E9.3/,
     +  '  HYDROCARBON-WATER PARTITION COEFFICIENT         (-)       = ',E9.3/,
     +  '  HENRYS LAW PARTITION COEFFICIENT                (-)       = ',E9.3/,
     +  '  CONSTITUENT HALF-LIFE IN AQUIFER                (YR)      = ',F9.3/)
  90  FORMAT('  -----------------------------------'/,
     +  '  CALCULATED PARAMETERS AND VARIABLES'/,
     +  '  -----------------------------------'/,
     +  '  SOIL BULK DENSITY                               (KG/M^3)  = ',F9.3/,
     +  '  WATER CONTENT                                   (-)       = ',F9.3/,
     +  '  BULK WATER PARTITION COEFFICIENT                (-)       = ',F9.3/,
     +  '  RETARDATION FACTOR (AQUIFER)                    (-)       = ',F9.3/,
     +  '  LEACHATE TRAVEL TIME TO AQUIFER                 (YR)      = ',F9.3/,
     +  '  INITIAL LEACHATE CONCENTRATION                  (MG/L)    = ',F9.3/,
     +  '  LEACHATE SOURCE HALF-LIFE                       (YR)      = ',F9.3/)
C
      WRITE(OUT,100)
 100  FORMAT('  -------------'/,
     +       '  RECEPTOR DATA'/,
     +       '  -------------'/,
     +  '  RECEPTOR #     X (M)     Y (M)     Z1 (M)     Z2 (M)'/,
     +  '  ----------    -------   -------   --------   --------')
C
      WRITE(OUT,110) (I,X(I),Y(I),Z1(I),Z2(I), I=1,NUMPT)
 110  FORMAT(2X,I5,9X,F5.1,5X,F5.1,6X,F5.1,6X,F5.1)
C
      WRITE(OUT,310)
 310  FORMAT(//'  ---------------'/,
     +         '  PROGRAM RESULTS'/,
     +         '  ---------------'/)
C
      RETURN
      END
C
      SUBROUTINE USERIN
C     *****************************************************************
C     *****************************************************************
C     **  P U R P O S E                                              **
C     **                                                             **
C     **    THIS ROUTINE READS THE INPUT DATA INTO THE PROGRAM IF    **
C     **    THE DATA HAS NOT PREVIOUSLY BEEN ENTERED INTO A DATA FILE **
```

```
C     **                                                                  **
C     **  REQUIRED ROUTINES:   NONE                                       **
C     **********************************************************************
C     **********************************************************************
      CHARACTER*60 TITLE
      INTEGER IN, OUT
      REAL POR, PSDI
      PARAMETER (IN = 4, OUT = 8)
C
      COMMON /SIMU/ T, NUMPT, XS, YS, EPS, JSTEP
      COMMON /SRCE/ BLKMO, QIN, CTIME, DSPILL, SLEN, SWID
      COMMON /PART/ XKD, XKO, XKH, WATCR, HYDCR
      COMMON /VADZ/ POR, PSDI, THKVZ, XKSVZ, VHALF
      COMMON /AQUF/ B, U, AHALF, ALPHX, ALPHY, ALPHZ
      COMMON /RECP/ X(200), Y(200), Z1(200), Z2(200), IPT
C
      WRITE(*,10)
   10 FORMAT(//
     +      ' ENTER A TITLE FOR THE SIMULATION (UP TO 60 CHARACTERS)')
      READ(*,15)  TITLE
      WRITE(IN,15) TITLE
   15 FORMAT(60A)
C
      WRITE(*,20)
   20 FORMAT(///
     +  '      GENERAL SIMULATION DATA'//
     +  '      T         TIME OF CONCENTRATION CALCULATION  (YR)'/
     +  '      NUMPT     NUMBER OF RECEPTOR LOCATIONS'/
     +  '      XS        X-LOCATION OF SOURCE AREA CENTER   (M)'/
     +  '      YS        Y-LOCATION OF SOURCE AREA CENTER   (M)'/
     +  '      EPS       THE TOLERANCE OF CONVERGENCE       (-)'/
     +  '      JSTEP     LENGTH OF TIMESTEPS                (YR)'//
     +  '   => PLEASE ENTER THE ABOVE PARAMETERS'//
     +  '   T = ?, NUMPT = ?, XS = ?, YS = ?, EPS = ?, JSTEP = ?',/)
      READ (*,*)    T, NUMPT, XS, YS, EPS, JSTEP
      WRITE(IN,30) T, NUMPT, XS, YS, EPS, JSTEP
   30 FORMAT(F6.2, 2X, I5, F6.2, 2X, F6.2, 2X, F7.4, I5)
C
      WRITE (*,40)
   40 FORMAT(/////,
     + '      SOURCE CHARACTERISTIC DATA'//
     + '      BLKMO     CONSTITUENT BULK CONCENTRATION         (MG/L)'/
     + '      QIN       SOURCE INFILTRATION RATE               (M/YR)'/
     + '      CTIME     DURATION OF CONSTANT SOURCE STRENGTH   (YR)'/
     + '      DSPILL    THICKNESS OF CONTAMINATED SOURCE ZONE  (M)'/
     + '      SLEN      SOURCE LENGTH IN X DIRECTION           (M)'/
     + '      SWID      SOURCE WIDTH IN Y DIRECTION            (M)'/
     + '   => PLEASE ENTER THE ABOVE PARAMETERS'//
     + '  BLKMO = ?, QIN = ?, CTIME = ?, DSPILL = ?,'
     + ' SLEN = ?, SWID = ?',/)
      READ (*,*)    BLKMO, QIN, CTIME, DSPILL, SLEN, SWID
        WRITE (IN,50) BLKMO, QIN, CTIME, DSPILL, SLEN, SWID
   50 FORMAT(6F12.3)
C
```

```
      WRITE(*,65)
   65 FORMAT(/////
     +  '    CONTAMINANT PARTITIONING AND SPILL DATA'//
     +  '    XKD      SOIL-WATER PARTITION COEFFICIENT           (M^3/KG)'/
     +  '    XKO      HYDROCARBON-WATER PARTITION COEFFICIENT    (-)'/
     +  '    XKH      HENRYS LAW PARTITION COEFFICIENT           (-)'/
     +  '    WATCR    IRREDUCIBLE WATER SATURATION OF SOIL       (-)'/
     +  '    HYDCR    RESIDUAL HYDROCARBON CONTENT               (-)'/
     +  '  => PLEASE ENTER THE ABOVE PARAMETERS'//)
      READ (*,*)     XKD, XKO, XKH, WATCR, HYDCR
      WRITE(IN,71) XKD, XKO, XKH, WATCR, HYDCR
   71 FORMAT(5F12.6)
C
      WRITE (*,80)
   80 FORMAT(/////
     +  '     VADOSE ZONE CHARACTERISTICS'//
     +  '     POR      SOIL AND AQUIFER POROSITY                 (-)'/
     +  '     PSDI     B. C. PORE SIZE DISTRIBUTION INDEX        (-)'/
     +  '     THKVZ    THICKNESS OF THE VADOSE ZONE              (M)'/
     +  '     XKSVZ    SAT. VERTICAL HYDRAULIC CONDUCTIVITY      (M/YR)'/
     +  '     VHALF    VADOSE ZONE CONSTITUENT HALF-LIFE         (YR)'/
     +  '  => PLEASE ENTER THE ABOVE PARAMETERS'//
     +  '  POR = ?, PSDI = ?, THKVZ = ?, XKSVZ = ?, VHALF = ?',/)
      READ(*,*)     POR, PSDI, THKVZ, XKSVZ, VHALF
      WRITE(IN,90) POR, PSDI, THKVZ, XKSVZ, VHALF
   90 FORMAT(5F12.3)
C
      WRITE(*,100)
  100 FORMAT(/////
     +  '    AQUIFER CHARACTERISTICS (2)'//
     +  '    B        AQUIFER THICKNESS                          (M)'/
     +  '    U        GROUNDWATER PORE VELOCITY (q/n)            (M/YR)'/
     +  '    AHALF    CONTAMINANT HALF-LIFE IN THE AQUIFER       (YR)'/
     +  '    ALPHX    LONGITUDINAL DISPERSIVITY                  (M)'/
     +  '    ALPHY    HORIZONTAL DISPERSIVITY                    (M)'/
     +  '    ALPHZ    VERTICAL DISPERSIVITY                      (M)'/
     +  ' => PLEASE ENTER THE ABOVE PARAMETERS'//
     +  '    B = ?, U = ?, AHALF = ?, ALPHX = ?, ALPHY = ?, ALPHZ = ?'/)
      READ(*,*)      B, U, AHALF, ALPHX, ALPHY, ALPHZ
      WRITE(IN,110) B, U, AHALF, ALPHX, ALPHY, ALPHZ
  110 FORMAT(6F12.3)
C
      WRITE (*,120)
  120 FORMAT(/////,
     1  '     RECEPTOR DATA'//
     2  '     X(I)     X-LOCATION OF RECEPTOR                         (M)'/
     3  '     Y(I)     Y-LOCATION OF RECEPTOR                         (M)'/
     4  '     Z1(I)    Z-LOCATION OF THE TOP OF THE WELL SCREEN       (M)'/
     5  '     Z2(I)    Z-LOCATION OF THE BOTTOM OF THE WELL SCREEN    (M)'//
     6  '     ENTER NUMPT VALUES'///
     7  '  => PLEASE ENTER THE ABOVE PARAMETERS'//
     8  '  (X(I) = ?, Y(I) = ? ,Z1(I) = ?, Z2(I) = ?, I=1,NUMPT)'/)
      READ (*,*) (X(I), Y(I), Z1(I), Z2(I), I=1,NUMPT)
      WRITE (IN,130) (X(I), Y(I), Z1(I), Z2(I), I=1,NUMPT)
```

```
 130  FORMAT(4F10.2)C
      RETURN
      END
```

D.4 OMEGA SOURCE CODE

```
PROGRAM OMEGA
C ***********************************************************************
C ***********************************************************************
C                   HORIZONTAL PLANE SOURCE (HPS) MODEL
C               ANALYTICAL THREE DIMENSIONAL SOLUTION FOR
C                   GROUND-WATER CONTAMINANT TRANSPORT
C                      ROMBERG INTEGRATION SCHEME
C
C                    LAST MODIFIED JANUARY 18, 1996
C
C     LANGUAGE:        FORTRAN 77
C
C     SUBROUTINES:     CONC, CS, ERF
C
C     P U R P O S E :  N O N - D I M E N S I O N A L    M O D E L
C
C     THIS PROGRAM EVALUATES THE NON-DIMENSIONALIZED SOLUTION OF THE
C     HORIZONTAL PLANE SOURCE (HPS) MODEL FOR A POINT RECEPTOR LOCATED
C     AT THE WATER TABLE (ZETAW = 0), NO WELL. THIS PROGRAM IS USED
C     TO GENERATE THE NOMOGRAPH FOR THE FUNCTION OMEGA.  DISPERSIVITIES
C     ARE RELATED TO THE RECEPTOR DISTANCE.
C
C     I N P U T    P A R A M E T E R S :

C
C     AOB2      RATIO OF THE SOURCE AREA TO THE AQUIFER THICKNESS
C               SQUARED (A/B2)
C     X2OB2     RATIO OF THE RECEPTOR DISTANCE (X) TO THE AQUIFER
C               THICKNESS, SQUARED (X/B)**2
C
C     O U T P U T    P A R A M E T E R S :
C
C     OMEGA(AOX2, X2OB2)
C ***********************************************************************
C ***********************************************************************
      INTEGER IN, OUT
      PARAMETER (IN = 4, OUT = 8)
      DIMENSION  XPHI(110,110), XI(100), YJ(100)
      CHARACTER*14  OUTFILE
      REAL AOX2, X2OB2, X2OB2LOG, AOB2LOG
C
      COMMON /GRN1/ ALPH1, ALPH2, ALPH3, CX1, CY1, CZ1, EPS
C
      WRITE(*,10)
   10 FORMAT(////
```

```
     +        '          HORIZONTAL PLANE SOURCE (HPS) MODEL'/
     1        '       ANALYTICAL THREE DIMENSIONAL SOLUTION FOR'/
     2        '           GROUNDWATER CONTAMINANT TRANSPORT'////
     3        '                      VERSION 25D.0'//
     4        '                   JANUARY 18,  1996'//////////)
C
C     DETERMINE NAME OF OUTPUT FILE
      PRINT*, 'ENTER IMIN, IMAX, AND XFRAC VALUES - '
      READ(*,*) IMIN, IMAX, XFRAC
      PRINT*
      PRINT*, 'ENTER JMIN, JMAX, AND YFRAC VALUES - '
      READ(*,*) JMIN, JMAX, YFRAC
      PRINT*
      PRINT*, 'ENTER EPS VALUE - '
      READ(*,*) EPS
      PRINT*
      PRINT*
      PRINT*, 'ENTER NAME OF OUTPUT FILE - '
      READ(*,14) OUTFILE
      OPEN (UNIT=OUT,FILE=OUTFILE,STATUS='UNKNOWN')
   14 FORMAT(A14)
      PRINT*
C
C     CALCULATE COEFFICIENTS FOR CALCULATION
      ALPH1 = 0.1
      ALPH2 = ALPH1/3.
      ALPH3 = 0.01
      CX1 =  4 * ALPH1
      CY1 = 16 * ALPH2
      CZ1 =  4 * ALPH3
      ISTEP = 1
      JSTEP = 1
      ZETA = 0.
      PRINT*
      PRINT*, 'START COMPUTATIONS'
      PRINT*
C
C     BEGIN DO LOOP FOR X2/B2 VALUES
      DO 50 I = IMIN, IMAX, ISTEP
      X2OB2LOG = 0.1 * I
      X2OB2 = 10**X2OB2LOG
C
C     BEGIN DO LOOP FOR A/B2 VALUES
      DO 50 J = JMIN, JMAX, JSTEP
      AOB2LOG = 0.1 * J
      AOB2 = 10**AOB2LOG
C
      AOX2 = AOB2 * (1/X2OB2)
      PRINT*, I, J
C
C     SOLVE THE INTEGRAL FOR THE CURRENT WELL LOCATION AND STORE THE
C     CONCENTRATION FOR THE REAL TIME.
      WTCONC = CONC(AOX2, X2OB2, ZETA)
      XPHI(I-IMIN,J-JMIN) = WTCONC
```

```
      XI(I-IMIN) = X2OB2LOG
      YJ(J-JMIN) = AOB2LOG
C
C     END OF DO LOOP(S) FOR CALCULATIONS
  50  CONTINUE
C
C     WRITE INPUT DATA TO THE OUTPUT FILE
      WRITE(OUT, 91) EPS,IMIN,IMAX,XFRAC,JMIN,JMAX,YFRAC
  91  FORMAT(/,
     + 'EPS     = ',F12.6/
     + 'IMIN    = ',I5/
     + 'IMAX    = ',I5/
     + 'XFRAC   = ',F12.6/
     + 'JMIN    = ',I5/
     + 'JMAX    = ',I5/
     + 'YFRAC   = ',F12.6/)
C
C     PRINT MATRIX OF OMEGA VALUES
      WRITE(OUT,100)
 100  FORMAT('  --------------------'/,
     +        '  MATRIX OF PHI VALUES'/,
     +        '  --------------------'//)
      DO 125 J = 0, JMAX-JMIN, JSTEP
      WRITE(OUT,130)(XPHI(I,J), I = 0, IMAX-IMIN, ISTEP)
 125  CONTINUE
 130  FORMAT(101(E9.3,2X))
C
C     PRINT MATRIX OF OMEGA VALUES FOR SURFER PLOTTING
      WRITE(OUT,200)
 200  FORMAT('  -------------------------'/,
     +        '  SURFER PLOT OF PSI VALUES'/,
     +        '  -------------------------'//
     +        'X2/B2       A/B2          PHI'/)
      DO 225 I = 0, IMAX-IMIN, ISTEP
      DO 225 J = 0, JMAX-JMIN, JSTEP
      WRITE(OUT,230) XI(I), YJ(J), XPHI(I,J)
 225  CONTINUE
 230  FORMAT(E10.3,3X,E10.3,3X,E12.5)
C
C     STOP AND END THE PROGRAM
      PRINT*
      PRINT*, 'SIMULATION COMPLETED'
      PRINT*
      CLOSE(OUT)
      STOP
      END
C
      FUNCTION CONC(AOX2, X2OB2, ZETA)
C     *********************************************************************
C     *********************************************************************
C     **  P U R P O S E                                                  **
C     **                                                                 **
C     **   THIS ROUTINE PEFORMS A NUMERICAL INTEGRATION BASED ON A       **
C     **   ROMBERG ALGORITHM. THE FUNCTION IS INTEGRATED FOR EACH GIVEN  **
```

```
C      **   TIME (UPPER BOUND OF INTEGRATION) AND LOCATION IN SPACE           **
C      **                                                                     **
C      **  I N P U T     P A R A M E T E R S                                  **
C      **                                                                     **
C      **        AOX2... THE RATIO OF AREA TO RECEPTOR DISTANCE SQUARED       **
C      **        X2OB2.. THE RATIO OF RECEPTOR DISTANCE TO AQUIFER            **
C      **                THICKNESS SQUARED                                    **
C      **        ZETA... THE DEPTH OF THE WELL SCREENING INTERVAL (= 0 )      **
C      **                                                                     **
C      **       (THE OTHER PARAMETERS PASSED THROUGH COMMON BLOCKS ARE        **
C      **        THE SAME AS IN THE ABOVE ROUTINES)                           **
C      **                                                                     **
C      **  O U T P U T     P A R A M E T E R S                                **
C      **                                                                     **
C      **        CP   ....THE INTEGRAL OF THE GREEN'S FUNCTIONS OVER TIME     **
C      **        CONC....THE CONCENTRATION AT THE GIVEN LOCATION AND TIME     **
C      **                                                                     **
C      **  O T H E R    P A R A M E T E R S                                   **
C      **                                                                     **
C      **        TA1.... REAL ARRAY CONTAINING INTEGRAL APPROXIMATIONS        **
C      **        EPS ... REAL VARIABLE. THE RELATIVE ERROR FOR WHICH          **
C      **                CONVERGENCE IS CHECKED                               **
C      **        A  .... REAL VARIABLE. THE LOWER BOUND OF INTEGRATION        **
C      **        B  .... REAL VARIABLE. EQUALS THE UPPER BOUND OF             **
C      **                INTEGRATION                                          **
C      **                                                                     **
C      **   REQUIRED ROUTINES: CS                                             **
C      ***********************************************************************
C      ***********************************************************************
       INTEGER IN, OUT
       PARAMETER (IN = 4, OUT = 8)
       REAL TA1(25,25)
C
       COMMON /GRN1/ ALPH1, ALPH2, ALPH3, CX1, CY1, CZ1, EPS
C
C      SET MAXIMUM ITERATIONS
       NUMITS=23
C
C      SET INTEGRATION LIMITS.  THE LOWER BOUND OF INTEGRATION (A) IS ALWAYS
C      TIME = ZERO.  THE UPPER BOUND, B, IS A NON-DIMENSIONAL TIME WHICH
C      CORRESPONDS TO A STEADY-STATE TIME.
       A = 0.
       B = 20.
C
C      CALCULATE THE AVERAGE TIME VALUE BETWEEN ZERO AND
C      UPPER BOUND OF INTEGRATION
       ABAV=(B+A)/2.
C
C      CALCULATE THE FIRST SET OF INTEGRAL 'PANELS'
C      AT THE LOWER BOUND, AVERAGE TIME, AND UPPER BOUND
       TA1(1,1)=(B-A)/2.*(CS(AOX2,X2OB2,ZETA,A)+CS(AOX2,X2OB2,ZETA,B))
       TA1(1,2)=TA1(1,1)/2.+(B-A)/2.*(CS(AOX2,X2OB2,ZETA,ABAV))
       TA1(2,1)=1./3.*(4.*TA1(1,2)-TA1(1,1))
C
```

```
C     BEGIN ITERATION TO GET BEST APPROXIMATION FOR THE INTEGRAL
      DO 30 J=3,25
C
C     SET THE INTERVAL DISTANCE
         DLM=(B-A)/(2**(J-1))
C
C     CALCULATE ANOTHER 'PANEL' LOCATION
         XLAM=A-DLM
         N=2**(J-2)
C
C     BEGIN INTEGRATION
         SUM=0.
         DO 10 I=1,N
C
C     CALCULATE THE STEP SIZE
            XLAM=XLAM+2.*DLM
            SUM=SUM+CS(AOX2,X2OB2,ZETA,XLAM)
10       CONTINUE
C
C     CALCULATE NEW PANELS
         TA1(1,J)=TA1(1,J-1)/2.+DLM*SUM
         DO 20 L=2,J
            K = J + 1 - L
            TA1(L,K)=(4**(L-1)*TA1(L-1,K+1)-TA1(L-1,K))/(4**(L-1)-1.)
20       CONTINUE
C
C     CHECK FOR CONVERGENCE BASED ON RELATIVE ERROR CRITERIA.
C     IF CONVERGENCE IS MET THE INTEGRAL VALUE HAS BEEN
C     DETERMINED AND RETURN TO SOLN
C
C     THIS NEXT STATEMENT CAUSES ERRORS IF TA1(J,1) = 0.
         IF ( ABS( TA1(J,1)-TA1(J-1,1) ) .LE. EPS*ABS(TA1(J,1)) ) THEN
            CP=TA1(J,1)
            GO TO 40
         ELSE
            ITS=J
         ENDIF
30    CONTINUE
C
C     IF CONVERGENCE WAS NEVER ACHIEVED FOR THIS TIME STEP
C     (STOP THE PROGRAM RUN)
      IF (ITS.GE.NUMITS) THEN
         WRITE(OUT,*)'CONVERGENCE WAS NOT FOUND...'
         STOP
      ENDIF
40    CONTINUE
C
C     CALCULATE CONCENTRATION
      CONC = CP
      RETURN
      END
C
      FUNCTION CS(AOX2,X2OB2,ZETA,TAU)
C     ********************************************************************
```

```
C     ********************************************************************
C     **  P U R P O S E                                                 **
C     **                                                                **
C     **  THIS ROUTINE EVALUATES THE FUNCTION (INTEGRAND) AT A GIVEN    **
C     **  TIME AND LOCATION.  THE FUNCTION INCLUDES THE DIMENSIONAL     **
C     **  GREENS FUNCTIONS AND A DEGRADATION FUNCTION.                  **
C     **                                                                **
C     **  I N P U T    P A R A M E T E R S                              **
C     **                                                                **
C     **       AOX2... THE RATIO OF AREA TO RECEPTOR DISTANCE SQUARED   **
C     **       X2OB2.. THE RATIO OF RECEPTOR DISTANCE TO AQUIFER        **
C     **               THICKNESS SQUARED                                **
C     **       ZETA... THE DEPTH OF THE WELL SCREENING INTERVAL (= 0 )  **
C     **       TAU.... THE NON-DIMENSIONAL TIME FOR WHICH THE FUNCTION  **
C     **               IS TO BE EVALUATED                               **
C     **                                                                **
C     ** O U T P U T    P A R A M E T E R S                             **
C     **                                                                **
C     **       CS .... REAL VARIABLE. THE VALUE OF THE FUNCTION FOR     **
C     **               THE INPUT PARAMETERS                             **
C     **                                                                **
C     **   REQUIRED ROUTINES: ERF                                       **
C     ********************************************************************
C     ********************************************************************
      INTEGER IN, OUT
      PARAMETER (IN = 4, OUT = 8)
C
      COMMON /GRN1/ ALPH1, ALPH2, ALPH3, CX1, CY1, CZ1, EPS
C
      IF(TAU .LE. 0.) THEN
          CS = 0.
          GOTO 800
      ENDIF
C
C     CALCULATE TERMS INSIDE THE INTEGRAL
      W1 = (1/(ALPH3*TAU))**0.5 * 1/(2*(3.14159**0.5)
C
C     CALCULATE X-DIRECTION GREEN'S FUNCTION
      XND1 = (AOX2/(4*CX1*TAU))**0.5
      XND2 = (1/(CX1*TAU))**0.5
      XND3 = (TAU/CX1)**0.5
      XG1 = XND1 + XND2 - XND3
      IF ( ABS(XG1) .LT. 0.00001 ) THEN
       XG1 = 0.
      ELSEIF ( XG1 .LT. -6. ) THEN
       XG1 = -1.
      ELSEIF ( XG1 .GT. 6. ) THEN
       XG1 = 1.
      ELSE
       XG1 = ERF(XG1)
      ENDIF
      XG2 = XND1 - XND2 + XND3
      IF ( ABS(XG2) .LT. 0.00001 ) THEN
       XG2 = 0.
```

```
      ELSEIF ( XG2 .LT. -6. ) THEN
       XG2 = -1.
      ELSEIF ( XG2 .GT. 6. ) THEN
       XG2 = 1.
      ELSE
       XG2=ERF(XG2)
      ENDIF
      XG = XG1 + XG2
C
C     CALCULATE Y-DIRECTION GREEN'S FUNCTION
      YG1 = ( AOX2/(CY1 * TAU) )**0.5
      IF ( ABS(YG1) .LT. 0.00001 ) THEN
       YG1 = 0.
      ELSEIF ( YG1 .LT. -6. ) THEN
       YG1 = -1.
      ELSEIF ( YG1 .GT. 6. ) THEN
       YG1 = 1.
      ELSE
       YG1 = ERF(YG1)
      ENDIF
      YG = YG1
C
C     CALCULATE Z-DIRECTION GREEN'S FUNCTION FOR AQUIFER OF FINITE THICKNESS
      IF(X2OB2 .EQ. 0.) THEN
        ZG = 0.
        GOTO 750
      ENDIF
      FUN = 0.
      DO 600 J = -5,5
         FUN = FUN + EXP( -(2*J - ZETA)**2/(CZ1 * X2OB2 * TAU) )
 600  CONTINUE
      ZG = FUN
C
C     COMBINE GREENS FUNCTIONS TO COMPUTE CS FUNCTION
 750  CS = W1 * XG * YG * ZG
C
 800  RETURN
      END
C
      FUNCTION ERF(ARG)
C     ********************************************************************
C     ********************************************************************
C     **  P U R P O S E                                                 **
C     **                                                                **
C     **   THIS ROUTINE EVALUATES THE ERROR FUNCTION OF A GIVEN         **
C     **   ARGUMENT (ARG).                                              **
C     **                                                                **
C     **  REQUIRED ROUTINES: NONE                                       **
C     ********************************************************************
C     ********************************************************************
      REAL P, A1, A2, A3, A4, A5
      DATA P,A1,A2,A3,A4,A5/.3275911,.254829592,-.284496736,
     1     1.421413741,-1.453152027,1.061405429/
      TE=1/(1+ABS(P*ARG))
```

```
      ERF=1-((((A5*TE+A4)*TE+A3)*TE+A2)*TE+A1)*TE*EXP(-(ARG*ARG))
      IF (ARG.LT.0) ERF=-ERF
C
      RETURN
      END
```

D.5 SIGMA SOURCE CODE

```
PROGRAM SIGMA
C ************************************************************************
C ************************************************************************
C                   HORIZONTAL PLANE SOURCE (HPS) MODEL
C               ANALYTICAL THREE DIMENSIONAL SOLUTION FOR
C                   GROUND-WATER CONTAMINANT TRANSPORT
C
C                    LAST MODIFIED FEBRUARY 27, 1996
C
C     LANGUAGE:         FORTRAN 77
C
C     SUBROUTINES:      WELLCONC, CONC, CS, ERF
C
C     P U R P O S E :   N O N - D I M E N S I O N A L    M O D E L
C
C     THIS PROGRAM EVALUATES THE NON-DIMENSIONALIZED SOLUTION OF THE
C     HORIZONTAL PLANE SOURCE (HPS) MODEL AND CALCULATES THE CORRECTION
C     FACTOR FUNCTION, SIGMA.  THE VALUE OF A/B2 IS HELD CONSTANT AND
C     THE VERTICALLY-AVERAGED SOLUTION IS DIVIDED BY THE POINT SOLUTION
C     AT THE WATER TABLE (Z = 0) TO DETERMINE THE VALUE OF SIGMA FOR
C     NOMOGRAPH CONSTRUCTION.  DISPERSIVITIES ARE RELATED TO THE
C     RECEPTOR DISTANCE.
C
C     I N P U T    P A R A M E T E R S :

C
C     AOB2       RATIO OF THE SOURCE AREA TO THE AQUIFER THICKNESS
C                SQUARED (A/B2)
C     X2OB2      RATIO OF THE RECEPTOR DISTANCE (X) TO THE AQUIFER
C                THICKNESS, SQUARED (X/B)**2
C
C     O U T P U T    P A R A M E T E R S :
C
C     SIGMA(A/B2, X/B, ZETAW)
CC ***********************************************************************
C ***********************************************************************
      INTEGER IN, OUT
      PARAMETER (IN = 4, OUT = 8)
      DIMENSION  XPHI(1000,1000), XI(1000), YJ(1000)
      CHARACTER*14  OUTFILE
      REAL X2OB2, XFRAC, YFRAC
C
```

```
      COMMON /GRN1/ ALPH1, ALPH2, ALPH3, CX1, CY1, CZ1, EPS, AOX2
C
      WRITE(*,10)
   10 FORMAT(////
     +        '          HORIZONTAL PLANE SOURCE (HPS) MODEL'/
     1        '       ANALYTICAL THREE DIMENSIONAL SOLUTION FOR'/
     2        '           GROUNDWATER CONTAMINANT TRANSPORT'////
     3        '                      VERSION 27D.0'//
     4        '                   FEBRUARY 27, 1996'//////////)
C     DETERMINE NAME OF OUTPUT FILE
      PRINT*, 'ENTER AOB2 VALUE - '
      READ(*,*) AOB2
      PRINT*
      PRINT*, 'ENTER IMIN, IMAX, AND XFRAC VALUES - '
      READ(*,*) IMIN, IMAX, XFRAC
      PRINT*
      PRINT*, 'ENTER JMIN, JMAX, AND YFRAC VALUES - '
      READ(*,*) JMIN, JMAX, YFRAC
      PRINT*
      PRINT*, 'ENTER EPS VALUE - '
      READ(*,*) EPS
      PRINT*
      PRINT*
      PRINT*, 'ENTER NAME OF OUTPUT FILE - '
      READ(*,14) OUTFILE
      OPEN (UNIT=OUT,FILE=OUTFILE,STATUS='UNKNOWN')
   14 FORMAT(A14)
C
C     CALCULATE COEFFICIENTS FOR CALCULATION
      EPS1 = EPS
      ALPH1 = 0.1
      ALPH2 = ALPH1/3.0
      ALPH3 = 0.01
      CX1 =  4 * ALPH1
      CY1 = 16 * ALPH2
      CZ1 =  4 * ALPH3
      ISTEP = 1
      JSTEP = 1
C
C     PRINT INPUT DATA
      WRITE(OUT, 91) AOB2,EPS1,IMIN,IMAX,XFRAC,JMIN,JMAX,YFRAC
   91 FORMAT(//,'INTEGRATION CORRECTION FACTORS'//,
     + 'AOB2   = ', F12.6/
     + 'EPS    = ',F12.6/
     + 'IMIN   = ',I5/
     + 'IMAX   = ',I5/
     + 'XFRAC  = ',F12.6/
     + 'JMIN   = ',I5/
     + 'JMAX   = ',I5/
     + 'YFRAC  = ',F12.6/)
C
      WRITE(OUT,200)
  200 FORMAT('  ---------------------------'/,
     +       '  SURFER PLOT OF SIGMA VALUES'/,
```

```
     +       '  ---------------------------'//,
     +       '     X/B          A/B2          SIGMA'/)
      PRINT*
      PRINT*, 'START COMPUTATIONS'
      PRINT*
C     BEGIN DO LOOP FOR X/B VALUE
      DO 50 I = IMIN, IMAX, ISTEP
      X2OB2LOG = 2. * XFRAC * I
      X2OB2 = 10**X2OB2LOG
C
C     SINCE CORRECTION FACTORS ARE SIMILAR AT LARGE RECEPTOR DISTANCES,
C     LOOSEN UP THE INTEGRATION TOLERANCE FOR EFFICIENCY
      IF(X2OB2LOG .GT. 2) THEN
        EPS = .01
      ENDIF
C
C     CALCULATE AOX2
      AOX2 = AOB2 * (1/X2OB2)
C
C     BEGIN DO LOOP FOR ZETAw VALUES
      DO 50 J = JMIN, JMAX, JSTEP
      ZETAWLOG = YFRAC * J
      ZETAW = 10**ZETAWLOG
      PRINT*, I, J
C
C     SOLVE THE INTEGRAL FOR THE CURRENT WELL LOCATION AND STORE THE
C     CONCENTRATION FOR THE REAL TIME.
      WPNTCONC = CONC(X2OB2, ZETAP)
      CALL ZETACONC(X2OB2, ZETAW, ZCONC)
      XPHI(I-IMIN,J-JMIN) = ZCONC/WPNTCONC
      XI(I-IMIN) = 0.5*X2OB2LOG
      YJ(J-JMIN) = ZETAWLOG
      WRITE(OUT,229) XI(I-IMIN), ZETAWLOG, XPHI(I-IMIN,J-JMIN)
 229  FORMAT(E10.3,3X,E10.3,3X,E12.5)
C
C     END OF DO LOOP(S) FOR CALCULATIONS
  50  CONTINUE
C
C     PRINT MATRIX OF CONCENTRATION PROFILES OVER TIME
      WRITE(OUT,100)
 100  FORMAT(//'  ----------------------'/,
     +        '  MATRIX OF SIGMA VALUES'/,
     +        '  ----------------------'//)
      DO 125 J = 0, JMAX-JMIN, JSTEP
      WRITE(OUT,130)(XPHI(I,J), I = 0, IMAX-IMIN, ISTEP)
 125  CONTINUE
 130  FORMAT(101(E9.3,2X))
C
C     STOP AND END THE PROGRAM
      PRINT*
      PRINT*, 'SIMULATION COMPLETED'
      PRINT*
      CLOSE(OUT)
      STOP
```

```
      END
C
      SUBROUTINE ZETACONC(X2OB2, ZETAW, ZCONC)
C     ***********************************************************************
C     ***********************************************************************
C     **  P U R P O S E                                                    **
C     **                                                                   **
C     **   THIS ROUTINE PEFORMS A NUMERICAL INTEGRATION BASED ON A         **
C     **   ROMBERG ALGORITHM. THE CONCENTRATION FUNCTION IS INTEGRATED     **
C     **   OVER THE LENGTH OF THE WELL SCREEN TO ARRIVE AT AN AVERAGE      **
C     **   CONCENTRATION IN THE WELL.                                      **
C     **                                                                   **
C     **  I N P U T   P A R A M E T E R S                                  **
C     **                                                                   **
C     **       X2OB2.. THE RATIO OF RECEPTOR DISTANCE TO AQUIFER           **
C     **               THICKNESS SQUARED                                   **
C     **       ZETAW.. THE RELATEIVE WELL SCREENING INTERVAL DEPTH         **
C     **                                                                   **
C     **  O U T P U T   P A R A M E T E R S                                **
C     **                                                                   **
C     **       CINT... THE SOLUTION TO THE INTEGRAL OF CONCENTRATION       **
C     **               OVER THE LENGTH OF THE SCREEN                       **
C     **       ZCONC.. THE AVERAGE CONCENTRATION IN THE WELL AT A GIVEN    **
C     **               TIME                                                **
C     **                                                                   **
C     **  O T H E R   P A R A M E T E R S                                  **
C     **                                                                   **
C     **       TA1.... REAL ARRAY CONTAINING INTEGRAL APPROXIMATIONS       **
C     **       EPS ... REAL VARIABLE. THE RELATIVE ERROR FOR WHICH         **
C     **               CONVERGENCE IS CHECKED                              **
C     **       A  .... REAL VARIABLE. THE LOWER BOUND OF INTEGRATION       **
C     **                                                                   **
C     **   REQUIRED ROUTINES: CONC                                         **
C     ***********************************************************************
C     ***********************************************************************
      INTEGER IN, OUT
      PARAMETER (IN = 4, OUT = 8)
      REAL TA1(25,25)
      COMMON /GRN1/ ALPH1, ALPH2, ALPH3, CX1, CY1, CZ1, EPS, AOX2
C
C     SET MAXIMUM ITERATIONS
      NUMITS=23
      ZEPS = 10.* EPS
C
      IF(ZETAW .EQ. 0.) THEN
          ZCONC = CONC(X2OB2, ZETAW)
          GOTO 45
      ENDIF
C
C     LOWER BOUND OF INTEGRATION IS ALWAYS THE BOTTOM OF THE WELL SCREEN
      B = ZETAW
C
C     UPPER BOUND OF INTEGRATION IS ALWAYS THE TOP OF THE WELL SCREEN
      A = 0.
```

```
C
C     CALCULATE THE AVERAGE LENGTH VALUE BETWEEN UPPER AND LOWER BOUND
C     OF INTEGRATION
      ABAV = (B+A)/2.
C
C     CALCULATE THE FIRST SET OF INTEGRAL 'PANELS'
C     AT THE LOWER BOUND, AVERAGE LENGTH, AND UPPER BOUND
      TA1(1,1)=(B-A)/2.*(CONC(X2OB2,A)+CONC(X2OB2,B))
      TA1(1,2)=TA1(1,1)/2.+(B-A)/2.*(CONC(X2OB2,ABAV))
      TA1(2,1)=1./3.*(4.*TA1(1,2)-TA1(1,1))
C
C     BEGIN ITERATION TO GET BEST APPROXIMATION FOR THE INTEGRAL
      DO 30 J=3,25
C
C     SET THE INTERVAL DISTANCE
         DLM=(B-A)/(2**(J-1))
C
C     CALCULATE ANOTHER 'PANEL' LOCATION
         XLAM=A-DLM
         N=2**(J-2)
C
C     BEGIN INTEGRATION
         SUM=0.
         DO 10 I=1,N
C
C     CALCULATE THE STEP SIZE
            XLAM=XLAM+2.*DLM
            SUM=SUM+CONC(X2OB2,XLAM)
10       CONTINUE
C
C     CALCULATE NEW PANELS
         TA1(1,J)=TA1(1,J-1)/2.+DLM*SUM
         DO 20 L=2,J
            K = J + 1 - L
            TA1(L,K)=(4**(L-1)*TA1(L-1,K+1)-TA1(L-1,K))/(4**(L-1)-1.)
20       CONTINUE
C
C     CHECK FOR CONVERGENCE BASED ON RELATIVE ERROR CRITERIA
C     IF CONVERGENCE IS MET THE INTEGRAL VALUE HAS BEEN
C     DETERMINED AND RETURN TO SOLN
C
C     THIS NEXT STATEMENT CAUSES ERRORS IF TA1(J,1) = 0.
         IF ( ABS( TA1(J,1)-TA1(J-1,1) ) .LE. ZEPS*ABS(TA1(J,1)) ) THEN
            CINT=TA1(J,1)
            GO TO 40
         ELSE
            ITS=J
         ENDIF
 30   CONTINUE
C
C     IF CONVERGENCE WAS NEVER ACHIEVED FOR THIS TIME STEP
C     (STOP THE PROGRAM RUN)
      IF (ITS.GE.NUMITS) THEN
         WRITE(OUT,*)'CONVERGENCE WAS NOT FOUND...'
```

```
         STOP
      ENDIF
 40   CONTINUE
C
C     CALCULATE CONCENTRATION AS THE AVERAGE CONCENTRATION OVER THE LENGTH
C     OF THE WELL SCREEN.
      ZCONC = CINT/(B-A)
 45   RETURN
      END
C
      FUNCTION CONC(X2OB2,ZETA)
C     **********************************************************************
C     **********************************************************************
C     **  P U R P O S E                                                   **
C     **                                                                  **
C     **   THIS ROUTINE PEFORMS A NUMERICAL INTEGRATION BASED ON A        **
C     **   ROMBERG ALGORITHM. THE FUNCTION IS INTEGRATED FOR EACH GIVEN   **
C     **   TIME (UPPER BOUND OF INTEGRATION) AND LOCATION IN SPACE        **
C     **                                                                  **
C     **  I N P U T     P A R A M E T E R S                               **
C     **                                                                  **
C     **       X2OB2.. THE RATIO OF RECEPTOR DISTANCE TO AQUIFER          **
C     **               THICKNESS SQUARED                                  **
C     **       ZETA... THE DEPTH OF THE WELL SCREENING INTERVAL (= 0 )    **
C     **                                                                  **
C     **      (THE OTHER PARAMETERS PASSED THROUGH COMMON BLOCKS ARE      **
C     **       THE SAME AS IN THE ABOVE ROUTINES)                         **
C     **                                                                  **
C     **  O U T P U T     P A R A M E T E R S                             **
C     **                                                                  **
C     **       CP  ....THE INTEGRAL OF THE GREEN'S FUNCTIONS OVER TIME    **
C     **       CONC....THE CONCENTRATION AT THE GIVEN LOCATION AND TIME   **
C     **                                                                  **
C     **  O T H E R   P A R A M E T E R S                                 **
C     **                                                                  **
C     **       TA1.... REAL ARRAY CONTAINING INTEGRAL APPROXIMATIONS      **
C     **       EPS ... REAL VARIABLE. THE RELATIVE ERROR FOR WHICH        **
C     **               CONVERGENCE IS CHECKED                             **
C     **       A  .... REAL VARIABLE. THE LOWER BOUND OF INTEGRATION      *
C     **       B  .... REAL VARIABLE. EQUALS THE UPPER BOUND OF           **
C     **               INTEGRATION                                        **
C     **                                                                  **
C     **   REQUIRED ROUTINES: CS                                          **
C     **********************************************************************
C     **********************************************************************
      INTEGER IN, OUT
      PARAMETER (IN = 4, OUT = 8)
      REAL TA1(25,25)
      COMMON /GRN1/ ALPH1, ALPH2, ALPH3, CX1, CY1, CZ1, EPS, AOX2
C
C     SET MAXIMUM ITERATIONS
      NUMITS=23
C
C     SET INTEGRATION LIMITS.  THE LOWER BOUND OF INTEGRATION (A) IS ALWAYS
```

```
C     TIME = ZERO.
      A = 0.
      B = 10.
C     CALCULATE THE AVERAGE TIME VALUE BETWEEN ZERO AND
C     UPPER BOUND OF INTEGRATION
      ABAV=(B+A)/2.
C
C     CALCULATE THE FIRST SET OF INTEGRAL 'PANELS'
C     AT THE LOWER BOUND, AVERAGE TIME, AND UPPER BOUND
      TA1(1,1)=(B-A)/2.*(CS(X2OB2,ZETA,A)+CS(X2OB2,ZETA,B))
      TA1(1,2)=TA1(1,1)/2.+(B-A)/2.*(CS(X2OB2,ZETA,ABAV))
      TA1(2,1)=1./3.*(4.*TA1(1,2)-TA1(1,1))
C
C     BEGIN ITERATION TO GET BEST APPROXIMATION FOR THE INTEGRAL
      DO 30 J=3,25
C
C     SET THE INTERVAL DISTANCE
         DLM=(B-A)/(2**(J-1))
C
C     CALCULATE ANOTHER 'PANEL' LOCATION
         XLAM=A-DLM
         N=2**(J-2)
C
C     BEGIN INTEGRATION
         SUM=0.
         DO 10 I=1,N
C
C     CALCULATE THE STEP SIZE
            XLAM=XLAM+2.*DLM
            SUM=SUM+CS(X2OB2,ZETA,XLAM)
10       CONTINUE
C
C     CALCULATE NEW PANELS
         TA1(1,J)=TA1(1,J-1)/2.+DLM*SUM
         DO 20 L=2,J
            K = J + 1 - L
            TA1(L,K)=(4**(L-1)*TA1(L-1,K+1)-TA1(L-1,K))/(4**(L-1)-1.)
20       CONTINUE
C
C     CHECK FOR CONVERGENCE BASED ON RELATIVE ERROR CRITERIA
C     IF CONVERGENCE IS MET THE INTEGRAL VALUE HAS BEEN
C     DETERMINED AND RETURN TO SOLN
C
C     THIS NEXT STATEMENT CAUSES ERRORS IF TA1(J,1) = 0.
         IF ( ABS( TA1(J,1)-TA1(J-1,1) ) .LE. EPS*ABS(TA1(J,1)) ) THEN
            CP=TA1(J,1)
            GO TO 40
         ELSE
            ITS=J
         ENDIF
30    CONTINUE
C
C     IF CONVERGENCE WAS NEVER ACHIEVED FOR THIS TIME STEP
C     (STOP THE PROGRAM RUN)
```

```
      IF (ITS.GE.NUMITS) THEN
         WRITE(OUT,*)'CONVERGENCE WAS NOT FOUND...'
         STOP
      ENDIF
40    CONTINUE
C
C     CALCULATE CONCENTRATION
      CONC = CP
      RETURN
      END
C
C
      FUNCTION CS(X2OB2,ZETA,TAU)
C     ******************************************************************
C     ******************************************************************
C     **  P U R P O S E                                               **
C     **                                                              **
C     **  THIS ROUTINE EVALUATES THE FUNCTION (INTEGRAND) AT A GIVEN   **
C     **  TIME AND LOCATION.  THE FUNCTION INCLUDES THE DIMENSIONAL    **
C     **  GREENS FUNCTIONS AND A DEGRADATION FUNCTION.                **
C     **                                                              **
C     **  I N P U T    P A R A M E T E R S                            **
C     **                                                              **
C     **       XC .... REAL VARIABLE. THE X-COORDINATE                **
C     **       YC .... REAL VARIABLE. THE Y-COORDINATE                **
C     **       ZC .... REAL VARIABLE. THE Z-COORDINATE                **
C     **       TAU.... REAL VARIABLE. THE TIME FOR WHICH THE FUNCTION  **
C     **               IS TO BE EVALUATED                             **
C     **                                                              **
C     **  O U T P U T    P A R A M E T E R S                          **
C     **                                                              **
C     **       CS .... REAL VARIABLE. THE VALUE OF THE FUNCTION FOR    **
C     **               THE INPUT PARAMETERS                           **
C     **                                                              **
C     **   REQUIRED ROUTINES: ERF                                     **
C     ******************************************************************
C     ******************************************************************
      INTEGER IN, OUT
      PARAMETER (IN = 4, OUT = 8)
C
      COMMON /GRN1/ ALPH1, ALPH2, ALPH3, CX1, CY1, CZ1, EPS, AOX2
C
      IF(TAU .LE. 0.) THEN
         CS = 0.
         GOTO 800
      ENDIF
C
C     CALCULATE VALUES INSIDE INTEGRAL
      W1 = (1/(ALPH3*TAU))**0.5 * 1/(2*(3.14159**0.5)
C
C     CALCULATE X-DIRECTION GREEN'S FUNCTION
      XND1 = (AOX2/(4*CX1*TAU))**0.5
      XND2 = (1/(CX1*TAU))**0.5
      XND3 = (TAU/CX1)**0.5
```

```
      XG1 = XND1 + XND2 - XND3
      IF ( ABS(XG1) .LT. 0.00001 ) THEN
       XG1 = 0.
      ELSEIF ( XG1 .LT. -6. ) THEN
       XG1 = -1.
      ELSEIF ( XG1 .GT. 6. ) THEN
       XG1 = 1.
      ELSE
       XG1 = ERF(XG1)
      ENDIF
      XG2 = XND1 - XND2 + XND3
      IF ( ABS(XG2) .LT. 0.00001 ) THEN
       XG2 = 0.
      ELSEIF ( XG2 .LT. -6. ) THEN
       XG2 = -1.
      ELSEIF ( XG2 .GT. 6. ) THEN
       XG2 = 1.
      ELSE
       XG2=ERF(XG2)
      ENDIF
      XG = XG1 + XG2
C
C CALCULATE Y-DIRECTION GREEN'S FUNCTION
      YG1 = ( AOX2/(CY1 * TAU) )**0.5
      IF ( ABS(YG1) .LT. 0.00001 ) THEN
       YG1 = 0.
      ELSEIF ( YG1 .LT. -6. ) THEN
       YG1 = -1.
      ELSEIF ( YG1 .GT. 6. ) THEN
       YG1 = 1.
      ELSE
       YG1 = ERF(YG1)
      ENDIF
      YG = YG1
C
C CALCULATE Z-DIRECTION GREEN'S FUNCTION FOR AQUIFER OF FINITE THICKNESS
      IF(X2OB2 .EQ. 0.) THEN
        ZG = 0.
        GOTO 750
      ENDIF
      FUN = 0.
      DO 600 J = -5,5
         FUN = FUN + EXP( -(2*J - ZETA)**2/(CZ1 * X2OB2 * TAU) )
 600  CONTINUE
      ZG = FUN
C
C     COMBINE GREENS FUNCTIONS TO COMPUTE CS FUNCTION
 750  CS = W1 * XG * YG * ZG
C
 800  RETURN
      END
C
C
      FUNCTION ERF(ARG)
```

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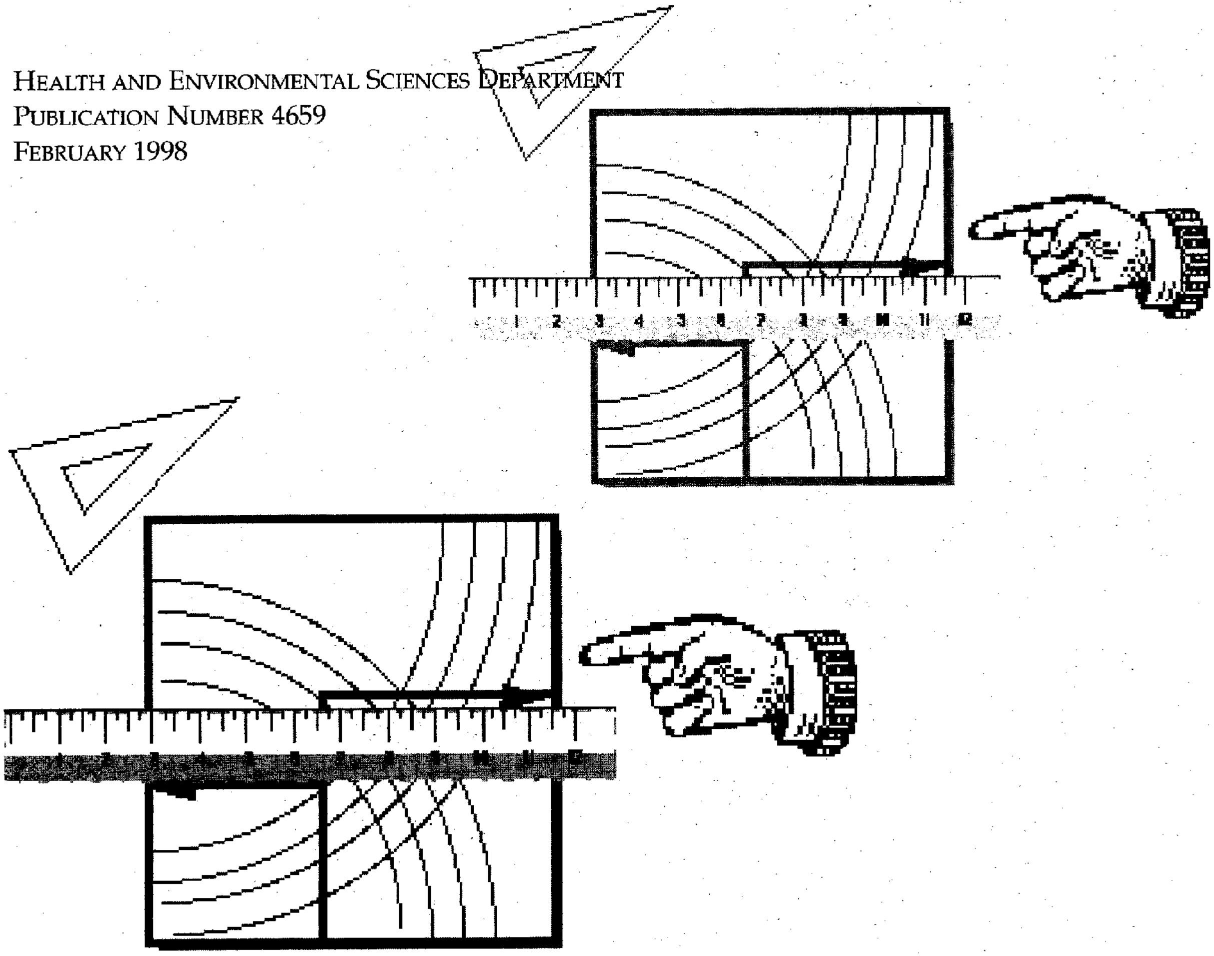
Strategies for Today's Environmental Partnership

GRAPHICAL APPROACH FOR DETERMINING SITE-SPECIFIC DILUTION-ATTENUATION FACTORS (DAFS)

TECHNICAL BACKGROUND DOCUMENT AND USER'S GUIDE

HEALTH AND ENVIRONMENTAL SCIENCES DEPARTMENT
PUBLICATION NUMBER 4659
FEBRUARY 1998



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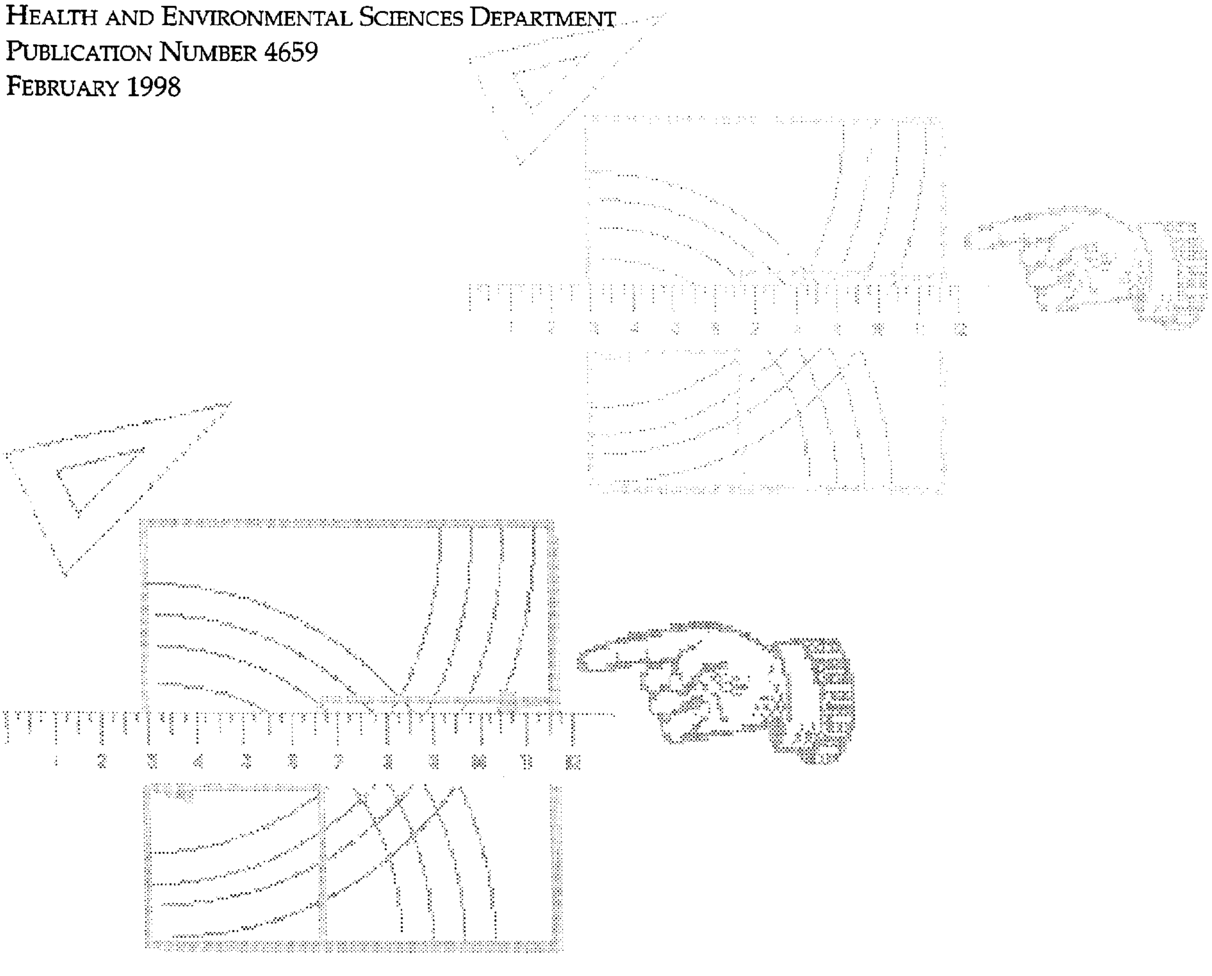

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American Petroleum Institute Environmental, Health, and Safety Mission and Guiding Principles

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- To promote these principles and practices by sharing experiences and offering assistance to others who produce, handle, use, transport or dispose of similar raw materials, petroleum products and wastes.

Graphical Approach for Determining Site-Specific Dilution-Attenuation Factors (DAFs)

User's Guide

Health and Environmental Sciences Department

API PUBLICATION NUMBER 4659

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Table of Contents

1.0 Introduction

This *User's Guide* provides instructions for determining soil-to-groundwater dilution attenuation factors (DAFs) using a graphically-based approach. The derivation and basis for this approach are discussed in more detail in the accompanying *Technical Background Document for the Graphical Approach for Determining Site-Specific Dilution Attenuation Factors* (Johnson *et al.*, 1997).

This graphically-based approach can be used for hydrocarbon-contaminated soils located above or within an aquifer. This approach accounts for attenuation with distance and time due to advection, dispersion, finite sources, and biodegradation (modeled as a first-order reaction).

This approach is both unique and attractive relative to other options because:

- The user can move away from fixed generic DAF values without having to resort to complex numerical simulations.

- It allows for varying degrees of site-specific information. Therefore, the same series of graphs can be used to provide an initial DAF estimate with minimal data and also to refine that DAF estimate when more site-specific data become available.

- Unlike the available numerical models and fixed generic values, this graphical approach is applicable to both vadose zone and submerged sources.

- The graphs visually indicate the sensitivity to various parameters, which is valuable information not easily gleaned from most numerical software simulators.

Users, however, should understand that the approach described in this guide is not appropriate for all situations; it should not be used to estimate chemical concentrations in active groundwater supply wells (unless the pumping rate does not affect the local groundwater flow field), or for very complex hydrogeologic settings (e.g., fractured geology).

2.0 Definition of the Dilution Attenuation Factor (DAF)

In the general release scenario shown in Figure 1, chemicals leach from the source zone, travel down to groundwater and then are transported horizontally by groundwater flow.

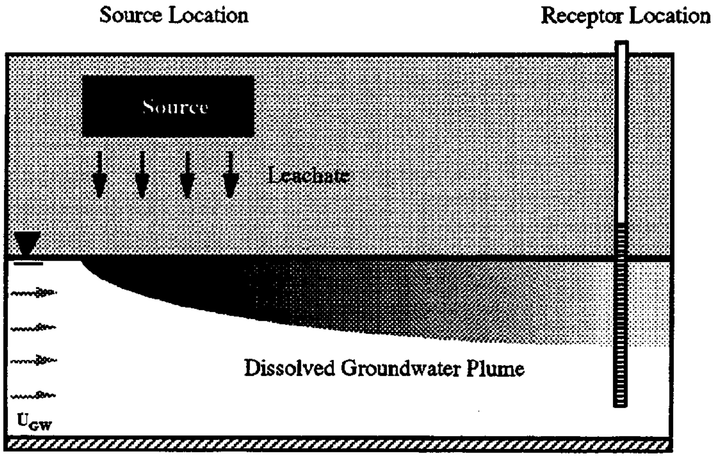

Figure 1. Generalized soil-to-groundwater pathway schematic

The DAF is defined to be the ratio of the initial source zone leachate concentration (time=0) divided by the maximum-time-average of the estimated well concentration at the point of interest (the receptor location):

$$\mathrm{DAF} = \frac{S_L^o}{<< C_R >_z>_{t,\max}} \tag{2.1}$$

where:

DAF = the dilution attenuation factor [dimensionless]

S^o_L= = the initial source zone leachate concentration [mg/L_{H20}]

$<<C_R>_z>_{t,max}$ = the maximum-time-average of the well concentration at the selected location [mg/L_{H20}] (note that the concentration is vertically-averaged over the well screen interval)

Thus, the DAF is always greater than or equal to one, and larger DAF values are indicative of increased attenuation. The DAF is generally a chemical-specific parameter; however, if chemical degradation and source decay are considered to be negligible, then the DAF value is the same for all chemicals at a given site.

While the DAF provides an estimate of the potential downgradient impact, it does not indicate when that impact might occur. In cases where:

- groundwater moves very slowly,
- the distance from the source to the receptor location is large,
- infiltration rates are low,
- the distance from the source to groundwater is very large, or
- compounds are strongly sorbing

the expected travel time between the source and receptor may be many decades or even centuries. Because of this, it is recommended that users of this graphical approach also estimate the travel time T_{travel} [y] necessary for chemical migration from the source to the receptor location. Guidance for making this estimate appears in §7.0. From a risk-based decision making perspective, some users may opt not to be concerned in situations where the estimated travel time exceeds some very long practical time frame (e.g., 10,000 years).

3.0 Using the Graphical Approach

Figures 3 and 4 present flow charts that outline sequences of data gathering exercises, calculations, and decisions involved with this graphical approach. There are two different flow charts because, at any given site, the source may be located above, or within, an aquifer, as shown in Figure 2.

When using this graphical approach, the user must first select the source type that is appropriate for his or her site. The user should then proceed to the instructions specific to that source type (either section 4.0 or 5.0 of this *User's Guide*).

If the source zone is partially submerged (i.e., it lies across both the vadose and saturated zones), the approach prescribed for submerged sources is recommended.

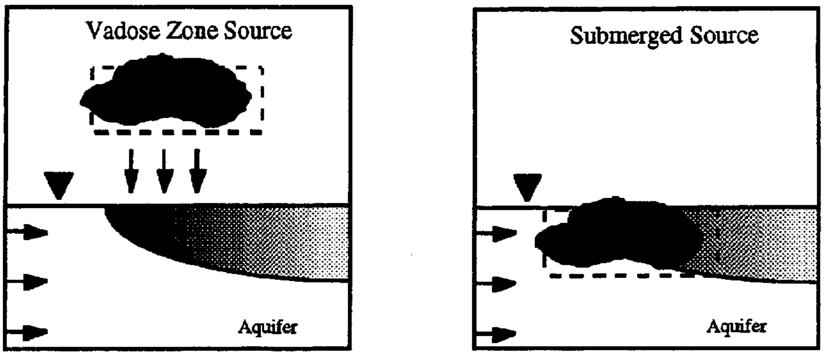

Figure 2. Conceptual pictures of vadose zone and submerged sources

4.0 Submerged Sources

For the case of submerged sources the DAF can be calculated from:

$$\mathrm{DAF} = \frac{1}{< S_L^* > \times f \times g \times \left(h_{inf}^* + h_{cor}^*\right)} \tag{4.1}$$

where:

g = attenuation factor for transverse dispersion [unitless] - Graph 1

h^*_{inf} = attenuation factor for vertical dispersion in an infinitely thick aquifer, averaged over the well screen interval [unitless] - Graph 2

h^*_{cor} = vertical dispersion correction term to account for a finite aquifer thickness [unitless] - Graph 3

f = attenuation factor for longitudinal dispersion and chemical reaction [unitless] - Graph 4

$<S_L^*>$ = maximum-time-averaged and normalized source zone leachate concentration [mg/L_{H2O}] - Graph 5

Values for g, h^*_{inf}, h^*_{cor}, f, and $<S_L^*>$ are determined as described below from Graphs 1 through 5. The graphs are attached at the end of the *User's Guide*.

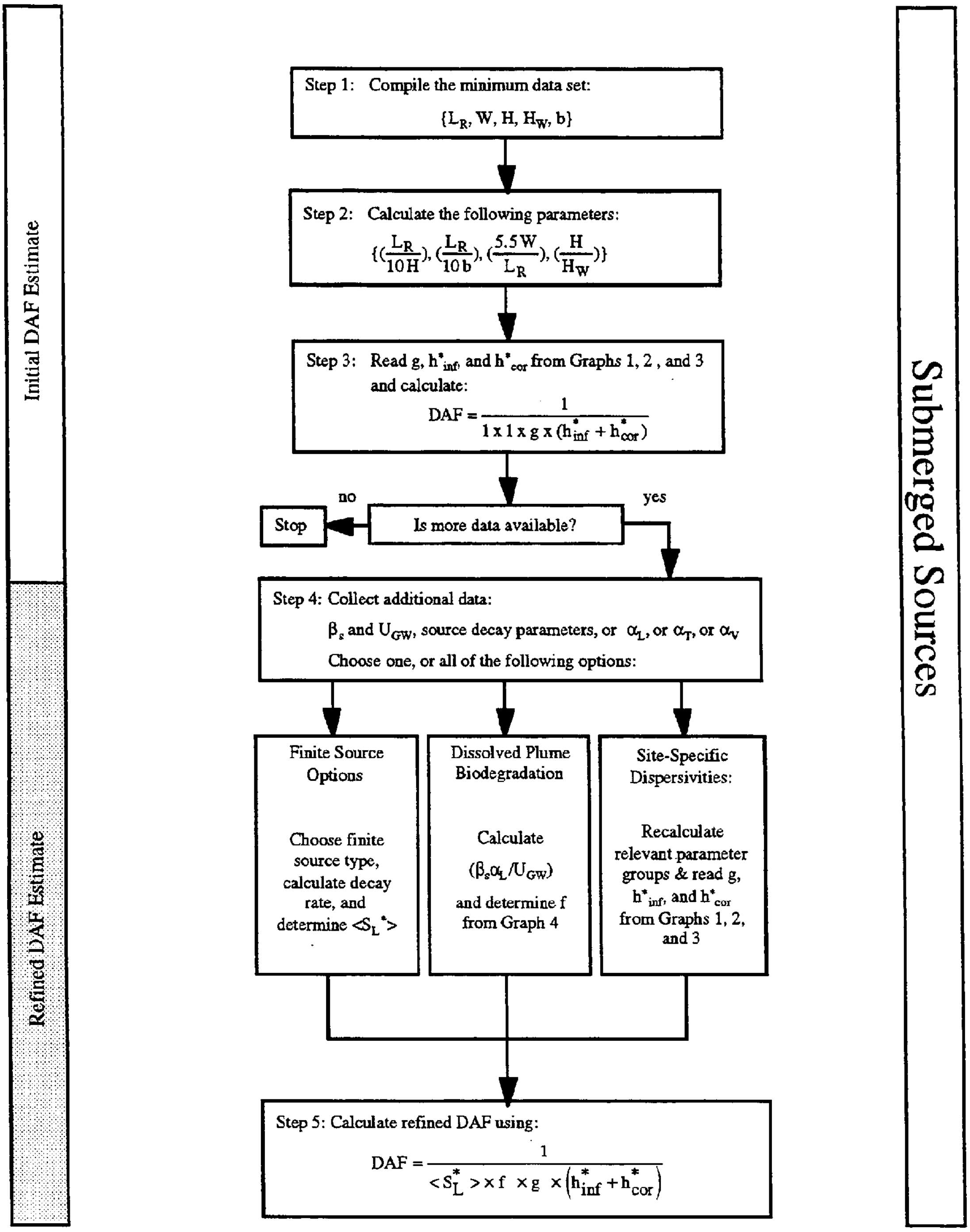

Figure 3. Flow chart outlining data gathering and DAF calculations for submerged sources

4.1 Submerged Sources - Initial Estimate

Initial DAF estimates require only a minimum data set defined entirely by the geometry of the release scenario:

b = aquifer thickness [m]
H = penetration depth (or vertical thickness) of source zone [m]
H_W = well screen thickness - (starting at the groundwater table) [m]
L_R = distance to receptor along the groundwater flow direction measured from the down-gradient edge of the source zone [m]
W = plan view width of source zone perpendicular to groundwater flow direction [m]

In making the initial DAF estimate, source decay and biodegradation are neglected. Under these conditions f and $<S_L^*>$ become:

$$f = 1 \qquad <S_L^*> = 1 \tag{4.2}$$

Site-specific dispersivity values $\{\alpha_L, \alpha_T, \text{and } \alpha_V\}$ are rarely available; thus, generic dispersivity values are used at this stage:

$$\alpha_L = L_R/10 \qquad \alpha_T = \alpha_L/3 \qquad \alpha_V = \alpha_L/10 \tag{4.3}$$

The user is free to change these if site-specific data or experience suggests other values are more appropriate. Thus, when using Graphs 1 through 5, the relevant parameter groups become:

$$\frac{W}{\sqrt{\alpha_T L_R}} = \frac{5.5\,W}{L_R}, \qquad \frac{\sqrt{\alpha_V L_R}}{H} = \frac{L_R}{10\,H}, \quad \text{and} \quad \frac{\sqrt{\alpha_V L_R}}{b} = \frac{L_R}{10\,b} \tag{4.4}$$

and the initial DAF estimate is then calculated by the following four-step procedure:

<u>STEP 1</u>: Based on site-specific data, choose appropriate values for H, H_W, L_R, and b. For submerged sources, the distance L_R should be measured from the down-gradient edge of the source zone to the receptor location.

STEP 2: Calculate the following five parameters:

$$\frac{W}{\sqrt{\alpha_T L_R}} = \frac{5.5\,W}{L_R}, \quad \frac{\sqrt{\alpha_V L_R}}{b} = \frac{L_R}{10\,b}, \quad \frac{\sqrt{\alpha_V L_R}}{H} = \frac{L_R}{10\,H}, \quad \frac{H}{H_W}, \text{ and } \frac{H}{b}$$

STEP 3: Obtain values for g, h^*_{inf}, and h^*_{cor} from Graphs 1, 2 and 3, respectively.

Note that Graph 3 corresponds to $(H/H_W)=1$ and that your value is likely to be different. In the *Technical Background Document for the Graphical Approach for Determining Site-Specific Dilution Attenuation Factors (DAFs)*, Figures 3-7 through 3-9 present graphs for other (H/H_W) values. These other graphs may be used; however it was determined that h^*_{cor} values are not very sensitive to changes in (H/H_W). Also, if $(L_R/10b) \ll 1$ then h^*_{cor} can be neglected; if $(L_R/10b) \gg 1$ then $h^*_{cor} = (H/b)$ and h^*_{inf} can be neglected.

STEP 4: Calculate the DAF according to:

$$\mathrm{DAF} = \frac{1}{1 \times 1 \times g \times \left(h^*_{inf} + h^*_{cor}\right)} \tag{4.5}$$

4.2 Refined DAF Estimates - Submerged Sources

As more site characterization data become available, users may opt to refine the DAF estimate. Additional site-specific data can be used to justify the incorporation of:

4.2.1) decaying (finite) sources;
4.2.2) biodegradation of the dissolved plume; or
4.2.3) site-specific dispersivity values.

Procedures for incorporating each of these processes are given below.

4.2.1 Finite Submerged Sources

Source decay can occur as a result of dissolution, degradation, and volatilization. Users should only consider accounting for source decay in cases where the source strength is expected to diminish significantly over the time period of interest. Otherwise, including this effect will only result in minor changes to the initial DAF estimate.

In the following section, exponentially-decaying sources with known first-order decay rates λ [d^{-1}] are discussed. Readers are referred to Chapter 6 of this *User's Guide*, and Chapter 6 of the companion *Technical Background Document for the Graphical Approach for Determining Site-Specific Dilution Attenuation Factors (DAFs)* for further discussion of source depletion models.

STEP 1: Calculate the first-order source decay rate constant λ [d^{-1}] (see Chapter 6 of the technical background document for guidance).

STEP 2: Choose an appropriate averaging time period T [d]. For example, 30 years is a common averaging period when concerned about chronic effects associated with prolonged exposures to low levels of dissolved chemicals. Calculate the value for the parameter λT, then use this value to determine $<S_L^*>$ from the attached Graph 5.

4.2.2 Dissolved Chemical Biodegradation

Attenuation of chemicals in groundwater due to biodegradation (or any other first-order reaction) may also be included in the refined DAF estimate:

STEP 1: Determine appropriate values for the groundwater seepage velocity U_{GW} [m/d] and the first-order biodegradation rate constant β_s [d^{-1}].[1]

STEP 2: Calculate the values for the following parameter groups:

$$\frac{\beta_s \alpha_L}{U_{GW}} \quad \text{and} \quad \frac{L_R}{\alpha_L}$$

---

[1] See Appendix A, page A9 of the *Technical Background Document for the Graphical Approach for Determining Site-Specific Dilution Attenuation Factors (DAFs)* for guidance on reasonable dissolved-phase biodegradation rates.

In the absence of site-specific dispersivity values, it is reasonable to assume that $\alpha_L = L_R/10$ and therefore $(L_R/\alpha_L)=10$ and $(\beta_s\alpha_L/U_{GW})=(\beta_s L_R/10U_{GW})$.

STEP 3: Obtain the value of the longitudinal dispersion/bio-decay attenuation factor f from the attached Graph 4.

4.2.3 Site-Specific Dispersivities

Site-specific dispersivities are rarely determined, except at field study sites. The generic values used in the initial DAF estimates are representative of the available literature data[2]. If site-specific dispersivities are known, they may be used in the calculation of the parameter groups required to obtain the attenuation factors f, g, h^*_{inf}, and h^*_{cor} from Graphs 1 through 4.

4.3 Refined DAF Calculation

Once the user has refined the estimates of the individual attenuation factors as described in §4.2.1 through §4.2.3, a refined DAF value is calculated using Equation 4.1:

$$\mathrm{DAF} = \frac{1}{< S_L^* > \times f \times g \times \left(h_{inf}^* + h_{cor}^*\right)} \tag{4.1}$$

If the user chooses not to include source decay, then $<S_L^*>=1$. If the user chooses not to include dissolved-phase biodegradation then f=1. If the default dispersivities are used, the function values g, h^*_{inf}, and h^*_{cor} determined for the initial DAF estimate will not have changed and may be substituted directly into Equation 4.1.

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[2] See Appendix A, pages A-11 through A-13 of the *Technical Background Document for the Graphical Approach for Determining Site-Specific Dilution Attenuation Factors (DAFs)* for guidance on reasonable dispersivities.

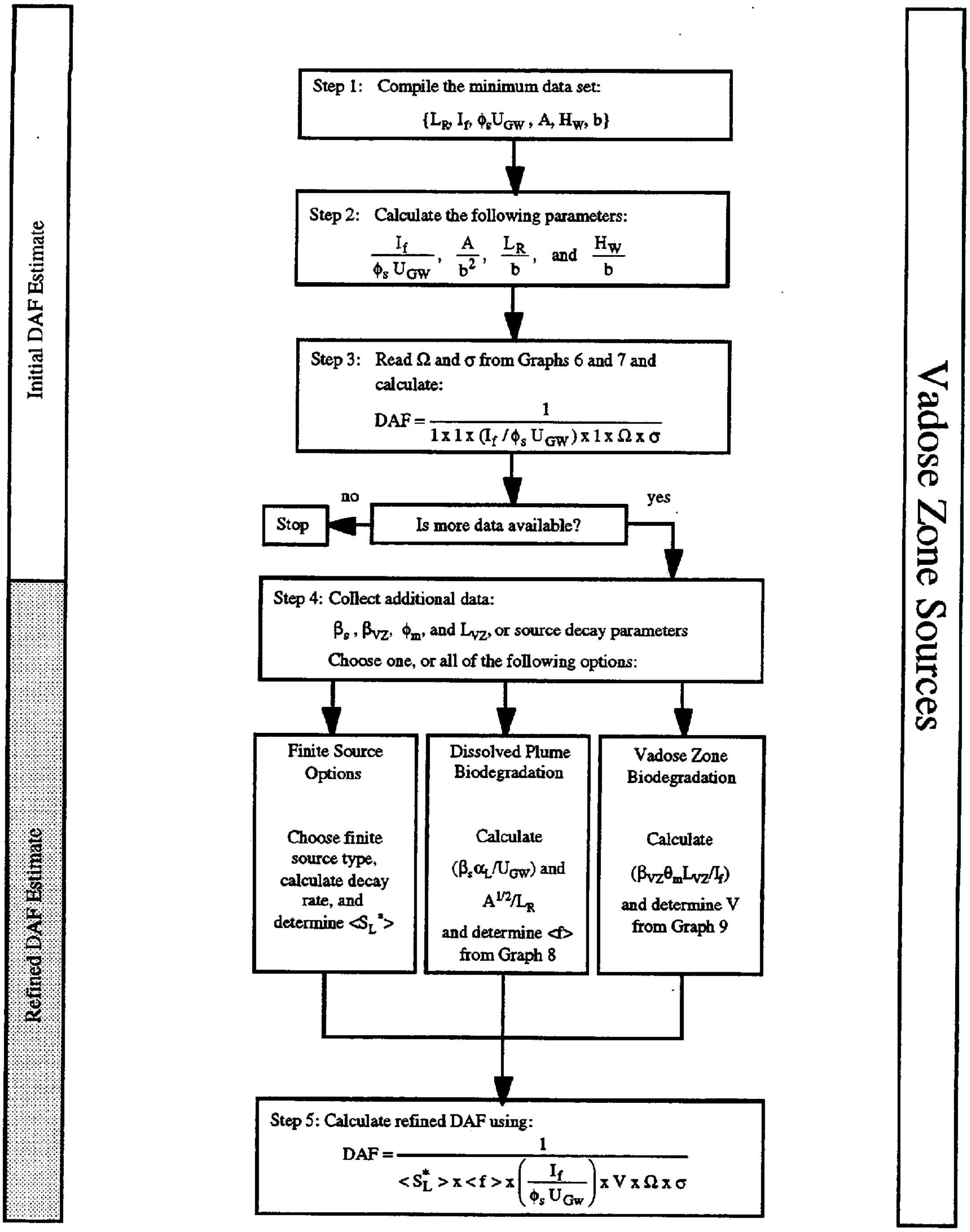


Figure 4. Flow chart outlining data gathering and DAF calculations for vadose zone sources

5.0 Vadose-Zone Sources

For the case of vadose zone sources (see Figure 4), the DAF can be calculated from:

$$\mathrm{DAF} = \frac{1}{< S_L^* > x < f > x \left(\frac{I_f}{\phi_s U_{Gw}} \right) x\ V\ x\ \Omega\ x\ \sigma} \quad (5.1)$$

where:

I_f = time-averaged water infiltration rate per unit area [m/d]
U_{GW} = groundwater seepage velocity [m/d]
ϕ_s = aquifer porosity [L-voids/L-soil]
$<S_L^*>$ = maximum-time-averaged and normalized source zone leachate concentration [mg/L_{H2O}] - Graph 5
Ω = attenuation factor for centerline concentrations at the groundwater table [unitless] - Graph 6
σ = attenuation factor correction term accounting for vertical averaging [unitless] - Graph 7
$<f>$ = attenuation factor for longitudinal dispersion and chemical reaction [unitless] - Graph 8
V = attenuation factor for vadose zone transport [unitless] - Graph 9

5.1 Vadose Zone Sources - Initial Estimate

Initial DAF estimates require only a minimum data set {b, A, H_W, L_R, I_f, and $\phi_s U_{GW}$ }, where:

b = aquifer thickness [m]
A = plan view area of the source zone [m^2]
H_W = vertical averaging depth (starting at the groundwater table) [m]
L_R = distance to receptor along the groundwater flow direction measured from the center of the source zone [m]
I_f = time-averaged infiltration rate [m/d]
$\phi_s U_{GW}$ = groundwater specific discharge [m/d]

With the exception of the groundwater specific discharge ($\phi_s U_{GW}$) and time-averaged *infiltration* rate (I_f), this minimum set of parameters is defined entirely by the geometry of the release scenario.

In making the initial DAF estimate, source decay and chemical degradation in the saturated and vadose zones are assumed not to occur. Under these conditions, the functions <f>, V, and $<S_L^*>$ become:

$$<f> = 1 \qquad V = 1 \qquad <S_L^*> = 1 \tag{5.2}$$

Unlike the submerged source case described previously, this analysis uses fixed generic dispersivity values $\{\alpha_L, \alpha_T, \text{and } \alpha_V\}$:

$$\alpha_L = L_R/10 \qquad \alpha_T = \alpha_L/3 \qquad \alpha_V = \alpha_L/10 \tag{5.3}$$

and the initial DAF estimate is calculated by the following procedure:

STEP 1: Based on site-specific data, choose appropriate values for $\{b, A, H_W, L_R, I_f, \text{and } \phi_s U_{GW}\}$. For vadose zone sources, the distance L_R is measured from the center of the source zone to the receptor location of interest.

STEP 2: Calculate the following four parameters:

$$\frac{I_f}{\phi_s U_{GW}}, \ \frac{A}{b^2}, \ \frac{L_R}{b}, \ \text{and} \ \frac{H_W}{b}$$

STEP 3: Obtain values for Ω and σ from Graphs 6 and 7.

Graph 7 corresponds to $(A/b^2)=1$ and the value calculated by the user is likely to be different. In the *Technical Background Document for the Graphical Approach for Determining Site-Specific Dilution Attenuation Factors (DAFs)*, Figures 4-8 through 4-13 present graphs $(A/b^2)=0.001, 0.01, 0.1, 1, 10$, and 100. These graphs may be used; however, it was determined that σ values are not very sensitive to changes in (A/b^2).

STEP 4: Calculate the DAF according to:

$$\mathrm{DAF} = \frac{1}{1 \times 1 \times \left(\frac{I_f}{\phi_s \, U_{GW}}\right) \times 1 \times \Omega \times \sigma} \qquad (5.4)$$

5.2 Vadose Zone Sources - Refined DAF Estimates

As more site characterization data become available, users may opt to refine their DAF estimates. Additional site-specific data can be used to justify the incorporation of:

5.2.1) decaying (finite) sources;
5.2.2) chemical degradation of the dissolved plume; or
5.2.3) chemical degradation in the vadose zone.

The procedures for incorporating each of these processes are given below.

5.2.1 Finite Vadose Zone Sources

Users should only consider accounting for source decay in cases where the source strength is expected to diminish significantly over the time period of interest. Otherwise, including this effect will only result in minor changes to the initial DAF estimate.

The following steps illustrate how to account for exponentially-decaying sources with known first-order decay rates λ [d^{-1}]. Readers are referred to Chapter 6 of this *User's Guide*, and Chapter 6 of the companion *Technical Background Document for the Graphical Approach for Determining Site-Specific Dilution Attenuation Factors (DAFs)* for further discussion of source depletion models.

STEP 1: Calculate the first-order source-strength decay rate constant λ [d^{-1}] (see Chapter 6 of the technical background document for guidance).

STEP 2: Choose an appropriate averaging time period T [d]. For example, 30 years is a common averaging period when concerned about chronic effects associated with prolonged exposures to low levels of dissolved chemicals. Calculate the value for the parameter λT, and then use this value to determine $<S_L^*>$ from Graph 5.

5.2.2 Dissolved Chemical Biodegradation in Aquifer

Attenuation of dissolved chemicals due to biodegradation (or any other first-order reaction) may be included in the refined DAF estimate by following the following steps:

STEP 1: Determine appropriate values for the groundwater seepage velocity U_{GW} [m/d] and the first-order biodegradation rate constant β_s [d^{-1}].[3]

STEP 2: Calculate the values for the following parameter groups:

$$\frac{\beta_s L_R}{U_{GW}} \quad \text{and} \quad \frac{\sqrt{A}}{L_R}$$

STEP 3: Obtain the value of the longitudinal dispersion/bio-decay attenuation factor <f> from Graph 8.

5.2.3 Chemical Degradation in the Vadose Zone

Chemical degradation in the vadose zone is a process known to occur, but few data are currently available to guide mathematical descriptions or input parameters for this process. Here, the chemical degradation is described by a first-order decay process characterized by a first-order degradation rate constant β_{VZ} [d^{-1}] and a travel time in the vadose zone T_{VZ} [d]. The travel time in the vadose zone can be estimated by $(L_{VZ}\ \phi_m/I_f)$, where L_{VZ} is the distance from the bottom of the source to groundwater and ϕ_m is the vadose zone moisture content [L-H_2O/L-soil].

STEP 1: Determine appropriate values for the infiltration rate I_f [m/d], first-order biodegradation rate constant β_{VZ} [d^{-1}], distance from the base of the source zone to groundwater L_{VZ} [m], and vadose zone soil moisture content ϕ_m [L_{H2O}/L_{soil}].

---

[3] See Appendix A, page A9 of the *Technical Background Document for the Graphical Approach for Determining Site-Specific Dilution Attenuation Factors (DAFs)* for guidance on reasonable dissolved-phase biodegradation rates.

STEP 2: Calculate the value for the following parameter group:

$$\beta_{VZ}\, T_{VZ} = \frac{\beta_{VZ}\, \phi_m\, L_{VZ}}{I_f}$$

STEP 3: Obtain the value of the vadose zone attenuation factor V from Graph 9.

5.3 Refined DAF Calculation

Once the user has refined the estimates of the individual attenuation factors as described in §5.2.1 through §5.2.3, a refined DAF value is calculated using Equation 5.1:

$$\mathrm{DAF} = \frac{1}{< S_L^* > \mathrm{x} < f > \mathrm{x} \left(\dfrac{I_f}{\phi_s\, U_{Gw}} \right) \mathrm{x}\ V\ \mathrm{x}\ \Omega\ \mathrm{x}\ \sigma} \qquad (5.1)$$

If the user chooses not to include source decay, then $<S_L^*>=1$. If the user chooses not to include dissolved-phase biodegradation, then $<f>=1$. If the user chooses not to include chemical degradation in the unsaturated zone, then $V=1$.

6.0 Finite/Decaying Sources

Chapter 6 of the companion *Technical Background Document for the Graphical Approach for Determining Site-Specific Dilution Attenuation Factors (DAFs)* discusses a range of possible source types. Here, the focus is on exponentially-decaying source types, since this is likely to be the predominant choice of most users. The reader is encouraged to read this section of the background technical document to ensure that all restrictions are met. This discussion is applicable to both submerged and vadose zone source types.

The leachate concentration dependence on time, $S_L(t)$ [mg/L_{H2O}] and the maximum time-averaged normalized leachate concentration $<S_L^*>$ (used in the DAF calculation), for an exponentially-decaying source are given by:

$$S_L(t) \;=\; S_L^o\, e^{-\lambda t} \qquad \text{and} \qquad < S_L^* > = \frac{(1 - e^{-\lambda T})}{\lambda T} \qquad (6.1)$$

where:

S_L^o = initial source zone normalized leachate concentration [mg/L_{H2O}]
λ = first-order decay rate of source zone leachate strength [d^{-1}]
T = averaging time [d]

The challenge is to estimate the first-order leachate source-strength decay constant λ [d^{-1}] using available site-specific information. Two different cases are discussed below, and these result in exponentially-decaying sources. In each case the equation for the source-strength decay constant λ [d^{-1}] is derived from mass balance and equilibrium partitioning relations.

6.1 Single or Multi-Component Mixtures without Immiscible Phase Present

At very low soil concentrations (<100 mg total hydrocarbons/kg-soil), one may assume that an immiscible hydrocarbon phase is not present. In this case, the following expression for λ [d^{-1}] can be derived:

$$\lambda = \frac{\left(\frac{I_f}{H} + \frac{K_H D^{eff}}{H L_d} + \beta_{source} \phi_m\right)}{\phi_m + \phi_A K_H + \rho_b K_d} \quad \textit{immiscible phase not present} \qquad (6.2)$$

Here:

K_H = Henry's Law coefficient [$(mg/L_{air})/(mg/L_{H2O})$]
K_d = Freundlich soil/water partition coefficient [$(mg/kg_{soil})/(mg/L_{H2O})$]
ϕ_m = volumetric soil moisture content [L_{H2O}/L_{soil}]
ϕ_A = air-filled soil porosity [L_{void}/L_{soil}]
ρ_b = soil bulk density [kg_{soil}/L_{soil}]
I_f = water infiltration rate [m/d]
H = source zone thickness (vertical dimension) [m]
D^{eff} = effective porous medium diffusion coefficient [m^2/d]
L_d = diffusion path length [m]
β_{source} = first-order biodegradation coefficient for dissolved constituents [d^{-1}]

Equation (6.2) above is specific for vadose zone sources; for submerged sources replace (I_f/H) with ($U_{GW}\phi_m/L$). For many chemicals and soil conditions, the following equation provides a reasonable approximation to Equation (6.2):

$$\lambda = \frac{(\frac{I_f}{H})}{\rho_b K_d} \tag{6.3}$$

Again, Equation (6.3) is specific for vadose zone sources; for submerged sources replace (I_f/H) with ($U_{GW}\phi_m/L$). The technical background document provides guidance for the selection of these chemical- and site-specific values. For these same conditions (no immiscible phase present), the relationship between the initial source zone leachate concentration, S°_L [mg/L_{H2O}], and initial soil concentration, C°_T [mg/kg_{soil}], of any compound is given by:

$$C^{o}_{T} = S^{o}_{L}\left(\frac{\phi_m}{\rho_b} + \frac{\phi_A K_H}{\rho_b} + K_d\right) \textit{ provided that } \sum_{i=1}^{i=n}\left(\frac{S^{o}_{L}}{S}\right)_i < 1 \tag{6.4}$$

where S [mg/L] is the pure component solubility for the compound(s) of interest.

6.2 Single or Multi-Component Mixtures with Immiscible Phase Always Present

When an immiscible hydrocarbon phase is present in the soil, as is often the case for spills involving oily wastes, the total mass of any compound is distributed among the pore water, soil air, soil particle surfaces, and immiscible phase in the soil matrix, and the source decay rate λ is given by:

$$\lambda = \left[\left(\frac{I_f}{H} + \beta_{source}\,\phi_m\right) + \frac{D^{eff}}{H\,L_d}K_H\right]\left(\frac{S}{\rho_b\,C_{T,mix}}\right)\left(\frac{M_{w,avg}}{M_w}\right) \textit{immiscible phase present} \tag{6.5}$$

where:

K_H = Henry's Law coefficient [$(mg/L_{air})/(mg/L_{H2O})$]
ϕ_m = volumetric soil moisture content [L_{H2O}/L_{soil}]
ρ_b = soil bulk density [kg_{soil}/L_{soil}]

I_f = water infiltration rate (groundwater specific discharge for submerged sources) [m/d]

H = source zone thickness (vertical dimension for vadose-zone sources; horizontal width of source zone for submerged sources) [m]

D^{eff} = effective porous medium diffusion coefficient [m^2/d]

L_d = diffusion path length [m]

β_{source} = first-order biodegradation coefficient for dissolved constituents [d^{-1}]

S = pure component solubility [mg/L_{H2O}]

$C_{T,mix}$ = total concentration of mixture (sum of all compounds) in the soil matrix [$mg_{mixture}/kg_{soil}$]

C_T = total concentration of compound i in the soil matrix [mg/kg_{soil}]

M_W = molecular weight of component i [$g/mole_i$]

$M_{W,avg}$ = mixture average molecular weight [$g_{mixture}/mole_{mixture}$]

Again, Equation (6.5) is specific for vadose zone sources; for submerged sources replace (I_f/H) with ($U_{GW}\phi_m/L$). A reasonable and conservative approximation of Equation (6.5) is:

$$\lambda = [(\frac{I_f}{H})]\left(\frac{S}{\rho_b\, C_{T,mix}}\right)\left(\frac{M_{w,avg}}{M_w}\right) \qquad (6.6)$$

For these same conditions (immiscible phase present), the relationship between the initial source zone leachate concentration, S°_L [mg/L_{H2O}], and initial soil concentration, C°_T [mg/kg_{soil}], of any compound is given by:

$$C^o_T = \frac{M_W}{M_{W,avg}}\left(\frac{S^o_L}{S}\right)C_{T,mix} \quad \textit{provided that} \quad \sum_{i=1}^{i=n}\left(\frac{S^o_L}{S}\right)_i = 1 \qquad (6.7)$$

7.0 A Note on Time Frames and Strongly Sorbing Compounds

As mentioned previously, the graphical approach provides an estimate of the maximum time-averaged down-gradient groundwater concentrations; however, it does not provide an estimate of when that maximum occurs. In cases where:

- groundwater moves very slowly,
- the distance from the source to the receptor location is large,
- infiltration rates are low,
- the distance from the source to groundwater is very large, or
- compounds are strongly sorbing,

the expected travel time between the source and receptor may be many decades or even centuries. Because of this, it is recommended that users of this graphical approach also estimate the travel time T_{travel} [y] necessary for chemical migration from the source to the receptor location. From a risk-based decision making perspective, some users may opt not to be concerned in situations where the estimated travel time exceeds some very long practical time frame (e.g., 10,000 years).

An estimate of the total travel time T_{travel} [d] is given by:

$$T_{travel} = T_V + T_S = \frac{R_{VZ}\,\phi_m\,L_{VZ}}{I_f} + \frac{R_S\,L_S}{U_{GW}} \tag{7.1}$$

where:

$$R_{VZ} = 1 + \frac{\phi_A\,K_H}{\phi_m} + \frac{\rho_b K_{d,VZ}}{\phi_m} \approx 1 + \frac{\rho_b K_{d,VZ}}{\phi_m} \quad \textit{(for many chemicals \& scenarios)} \tag{7.2}$$

$$R_S = 1 + \frac{\rho_b K_{d,S}}{\phi_S} \tag{7.3}$$

and

T_{travel} = total travel time from source to receptor [d]
T_V = travel time for the front to move from the source to groundwater [d]
T_S = travel time for the front to move through the aquifer to the receptor [d]

L_{VZ} = distance from the base of the source zone to the aquifer [m]

L_S = distance chemicals travel through the aquifer to reach the receptor [m]

I_f = infiltration rate [m/d]

ϕ_m = volumetric soil moisture content in the vadose zone [L_{H2O}/L_{soil}]

ϕ_S = volumetric soil moisture content in the aquifer [L_{H2O}/L_{soil}]

K_H = Henry's law coefficient [$(mg/L_{air})/(mg/L_{H2O})$]

$K_{d,VZ}$ = Freundlich soil/water partition coefficient in the vadose zone [$(mg/kg_{soil})/(mg/L_{H2O})$]

$K_{d,S}$ = Freundlich soil/water partition coefficient in the aquifer [$(mg/kg_{soil})/(mg/L_{H2O})$]

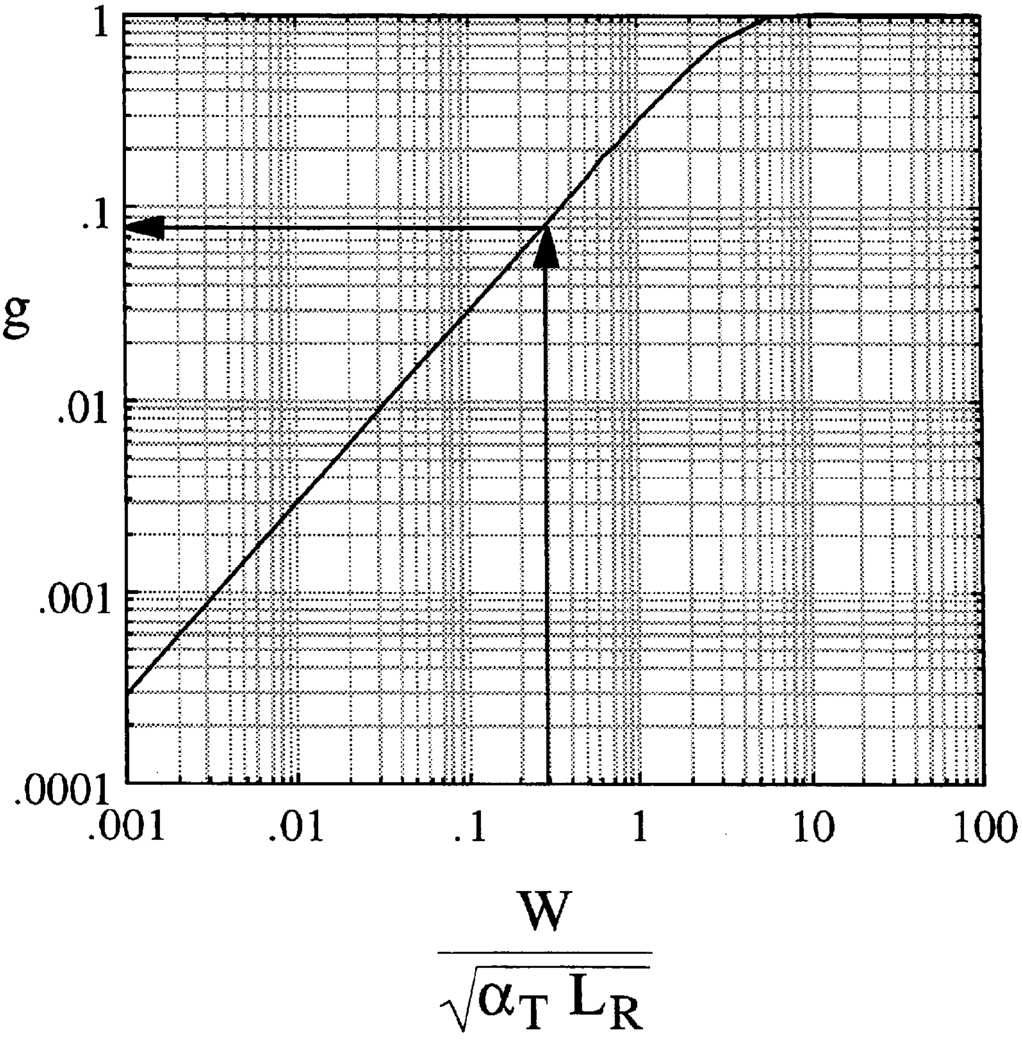
ϕ_A = air-filled soil porosity in the vadose zone [L_{void}/L_{soil}]

ρ_b = soil bulk density [kg_{soil}/L_{soil}]

U_{GW} = groundwater seepage velocity [m/d]

8.0 References

Johnson, P. C., R. J. Charbeneau, D. Abranovic, T. Hemstreet. 1997. *Technical Background Document for the Graphical Approach for Determining Site-Specific Dilution Attenuation Factors (DAFs).* API Publication 4659. American Petroleum Institute. Washington D.C.

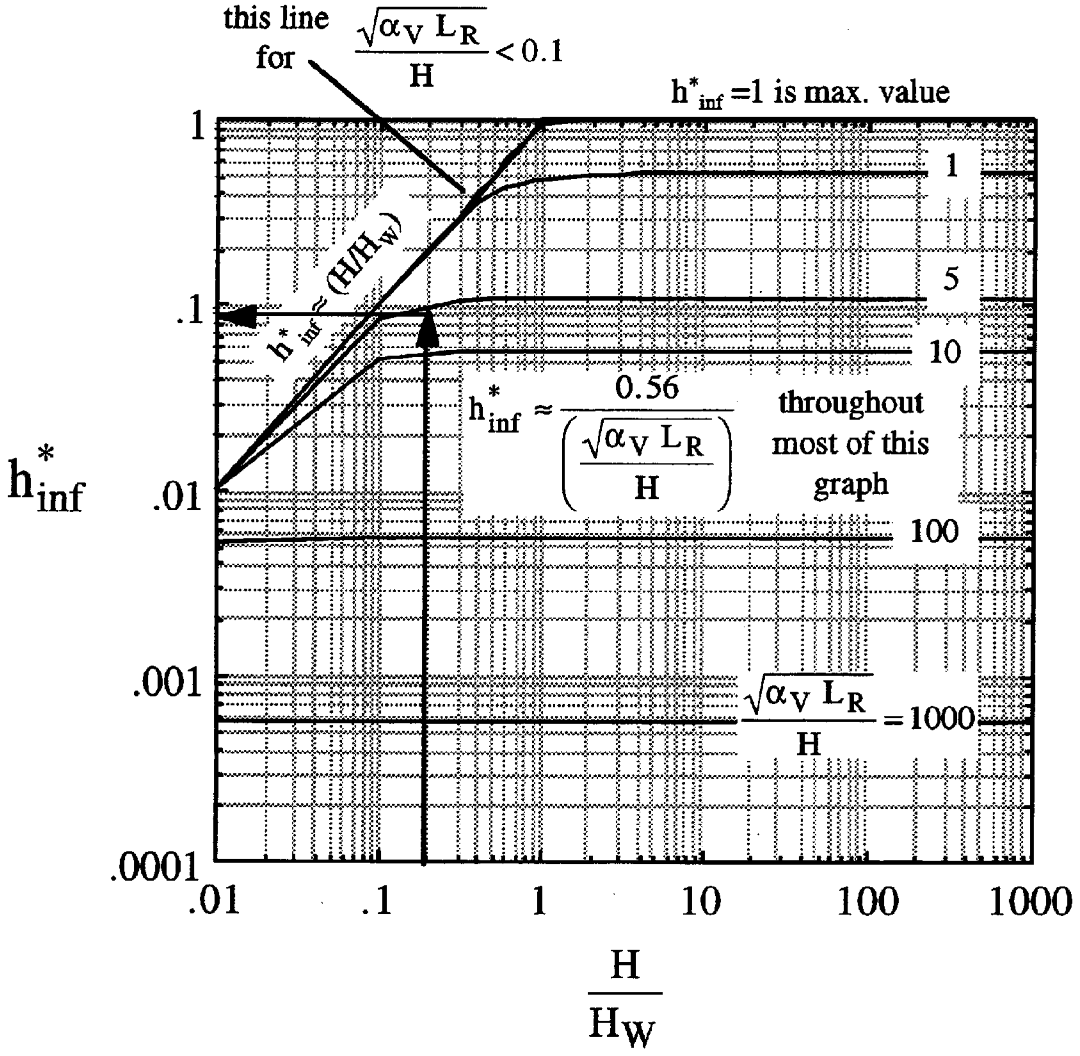


W = plan view source width perpendicular to groundwater flow [m]

α_T = transverse dispersivity ($\approx L_R/30$) [m]

L_R = distance to receptor [m]

Graph 1. Transverse dispersion (lateral spreading) factor (g) for submerged sources. Sample lines show use of the graph for the case of $W/(\alpha_T L_R)^{1/2}=0.3$ *and* $g \approx 0.08$



H = vertical source thickness [m]

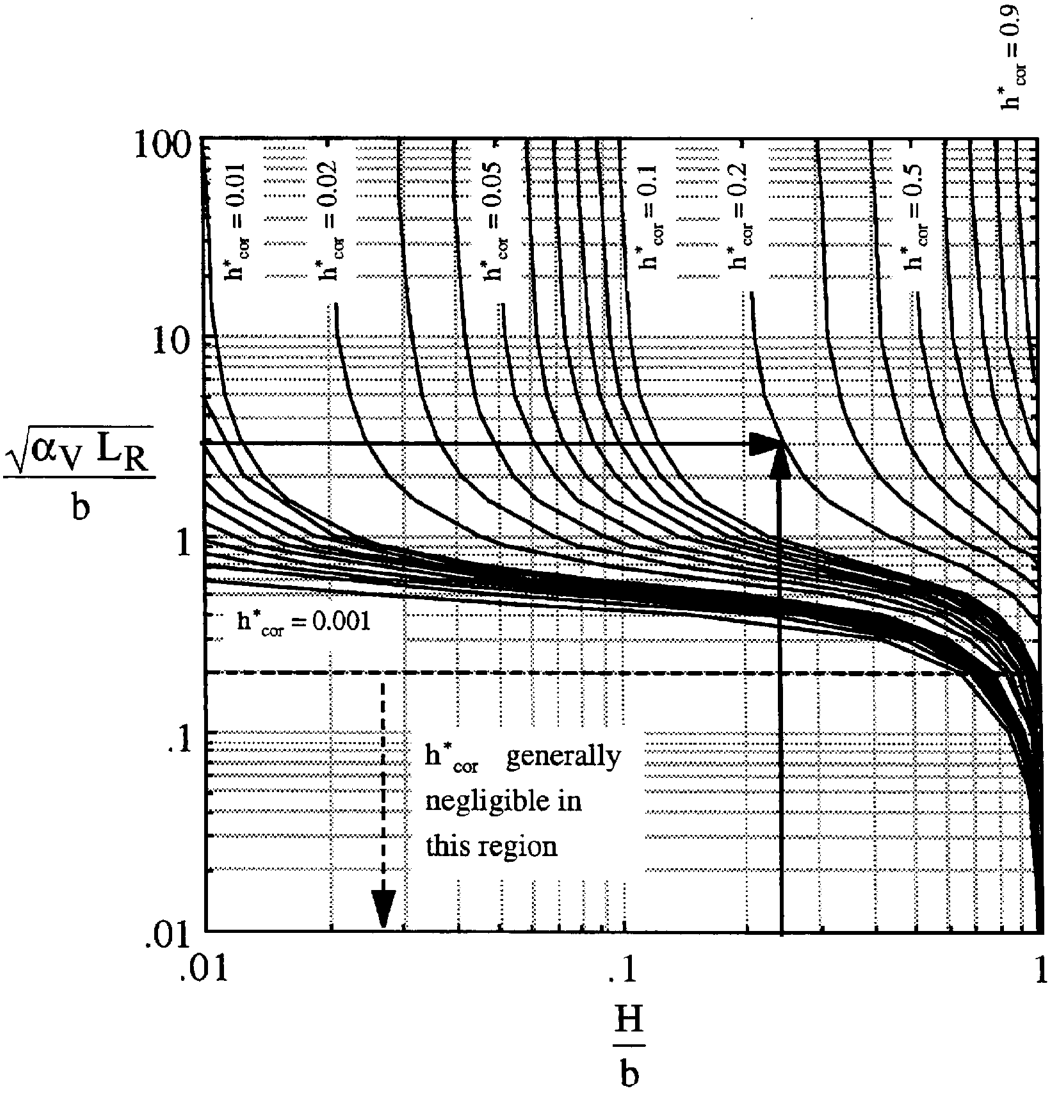
α_V = vertical dispersivity ($\approx 0.01\ L_R$) [m]

H_W = well screen interval thickness [m]

L_R = distance to receptor [m]

b = aquifer thickness [m]

Graph 2. Vertical mixing factor (h^*_{inf}) for an infinitely thick aquifer. Note that $h^* = h^*_{inf} + h^*_{cor}$ must be $\geq (H/b)$. Sample lines illustrate use of the graph for the case $H/H_W = 0.2$ and $(\alpha_V L_R)^{1/2}/H = 5$, which yields a value $h^*_{inf} \approx 0.09$



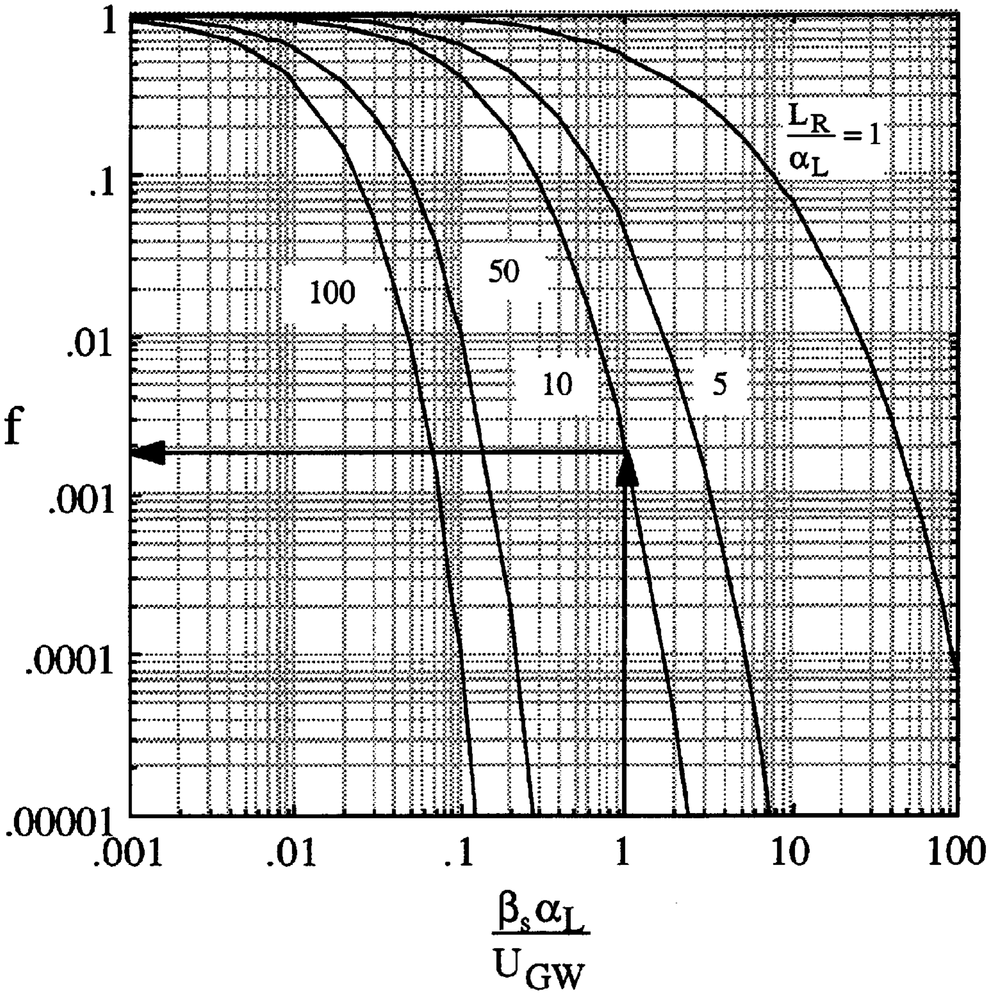
L_R = distance from downgradient edge of source to receptor [m]

H = source thickness [m]

b = aquifer thickness [m]

α_V = vertical dispersivity [m] (≈ L_R/100)

Graph 3. Contours of the vertical mixing correction factor (h^*_{cor}) for finite thickness aquifers, for $H/H_w=1.0$. Note that $h^* = h^*_{inf} + h^*_{cor}$ must be $\geq (H/b)$. Sample lines illustrate use of the graph for $(H/b)=0.24$ and $(\alpha_V L_R)^{1/2}/b=3$, which yields a value $h^*_{cor} \approx 0.2$



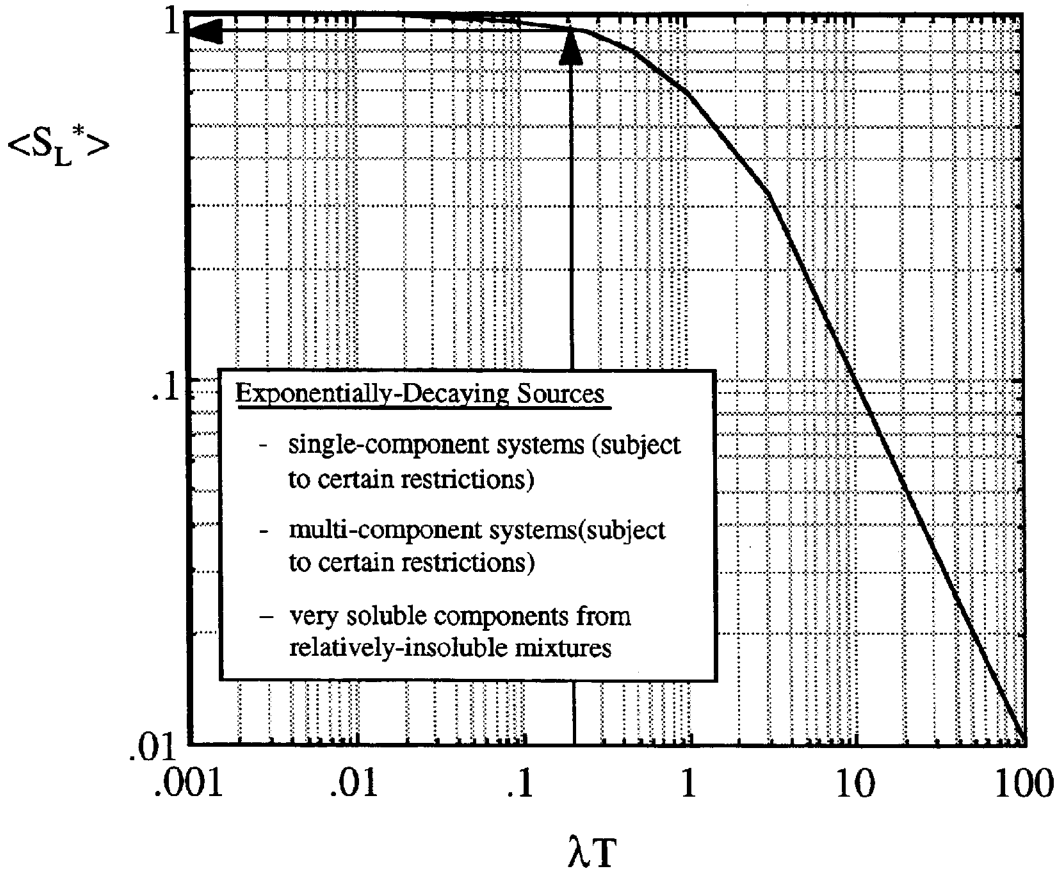
β_s = first-order biodegradation rate constant [d^{-1}]

α_L = longitudinal dispersivity ($\approx L_R/10$) [m]

U_{GW} = groundwater seepage velocity [m/d]

L_R = distance to receptor [m]

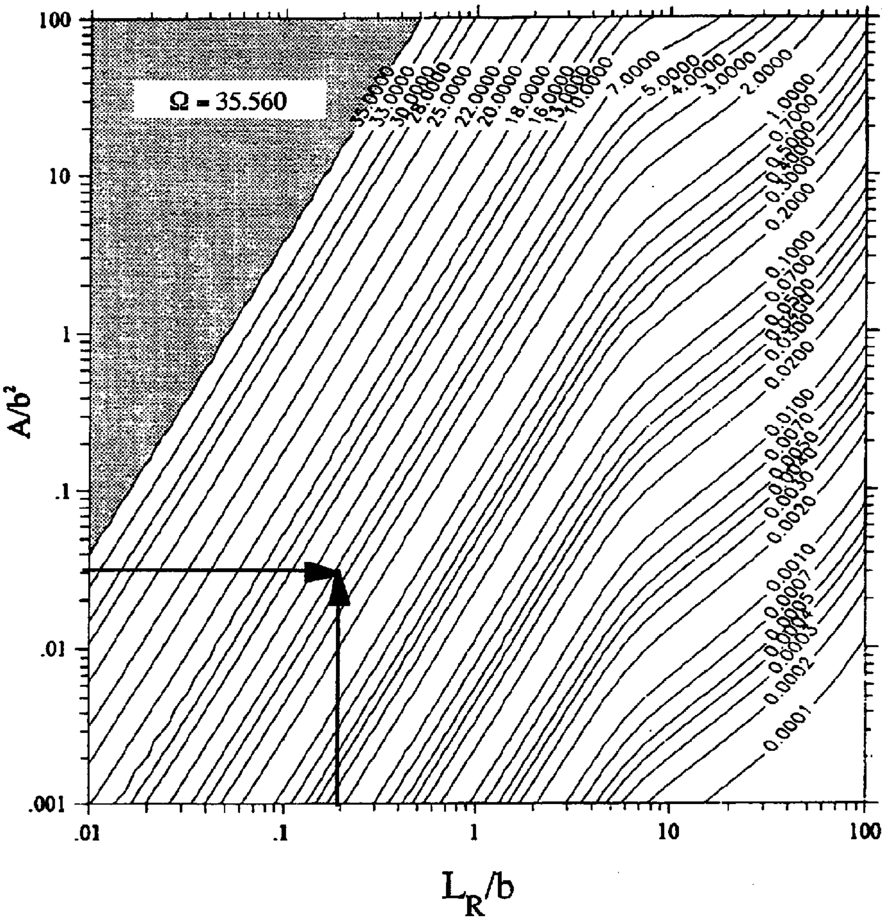
Graph 4. Longitudinal dispersion/bio-decay factor (f) for submerged sources. Sample lines illustrate use of the graph for ($\beta_s\alpha_L/U_{GW}$)=1 and L_R/α_L=10, which yields a value $f \approx 0.002$



λ = overall source decay rate [y^{-1}]

T = averaging time [y]

Graph 5. Source decay factor for exponentially-decaying sources (see Chapter 6 of the technical document for calculation of decay rates and similar graphs for other idealized source decay models). Sample lines illustrate use of the graph for $\lambda T=0.2$*, which yields* $<S_L{}^*> \approx 0.9$

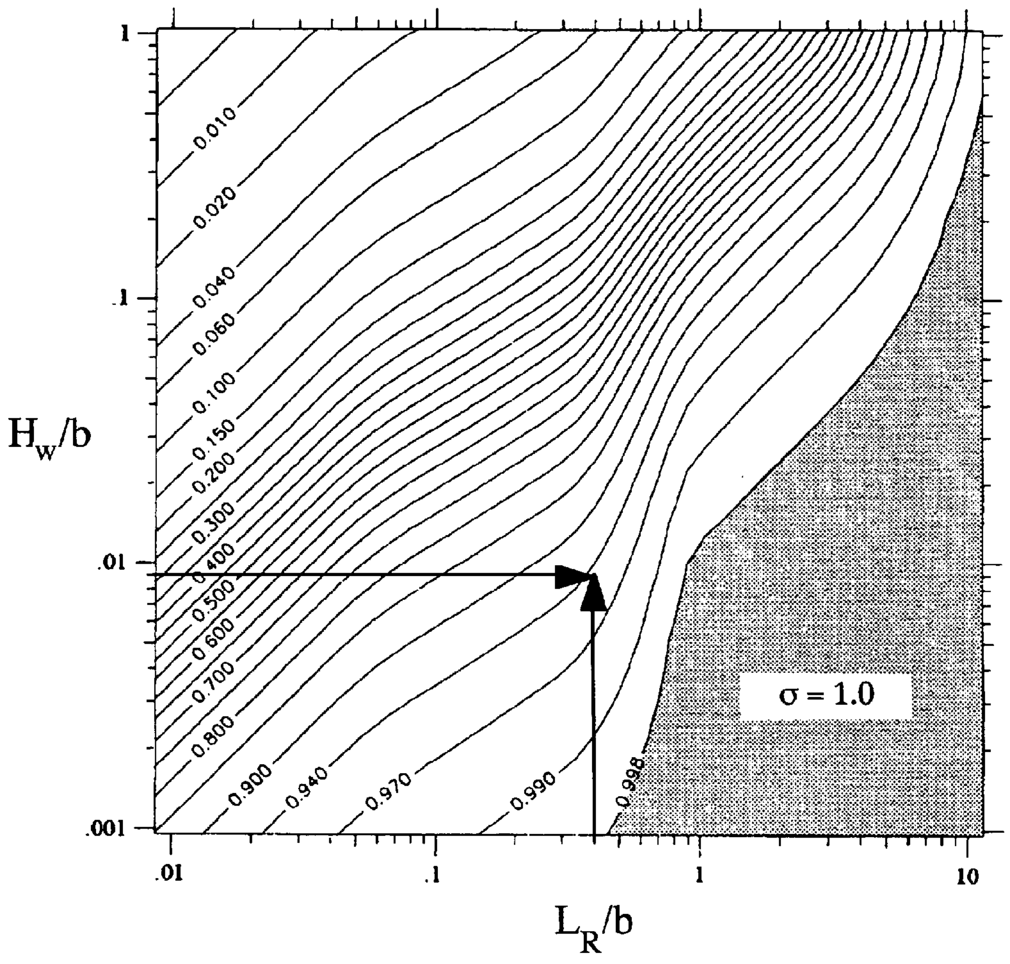


L_R = distance from center of source to receptor [m]

A = plan view source area [m^2]

b = aquifer thickness [m]

Graph 6. Contours of the function Ω. Sample lines illustrate use of the graph for the case $L_R/b=0.2$ and $A/b^2=0.03$, which yields $\Omega \approx 4.5$

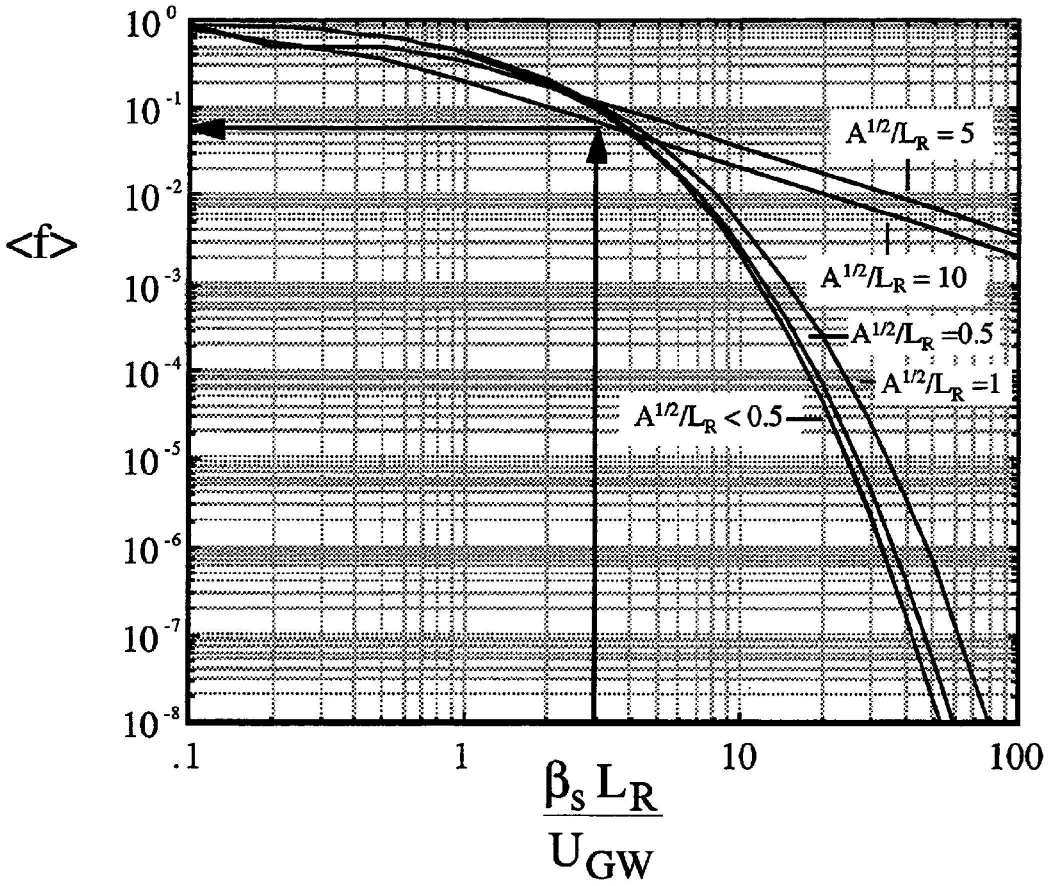


L_R = distance to receptor [m]

b = aquifer thickness [m]

H_W = well screen thickness [m]

Graph 7. Nomograph of the function σ *for* $A/b^2=1$*. See Chapter 6 of the technical document for calculation of decay rates and similar graphs for other idealized source decay models. Sample lines show use of the graph for the case of* $L_R/b=0.4$ *and* $H_W/b=0.009$*, which yields* $\sigma \approx 0.94$



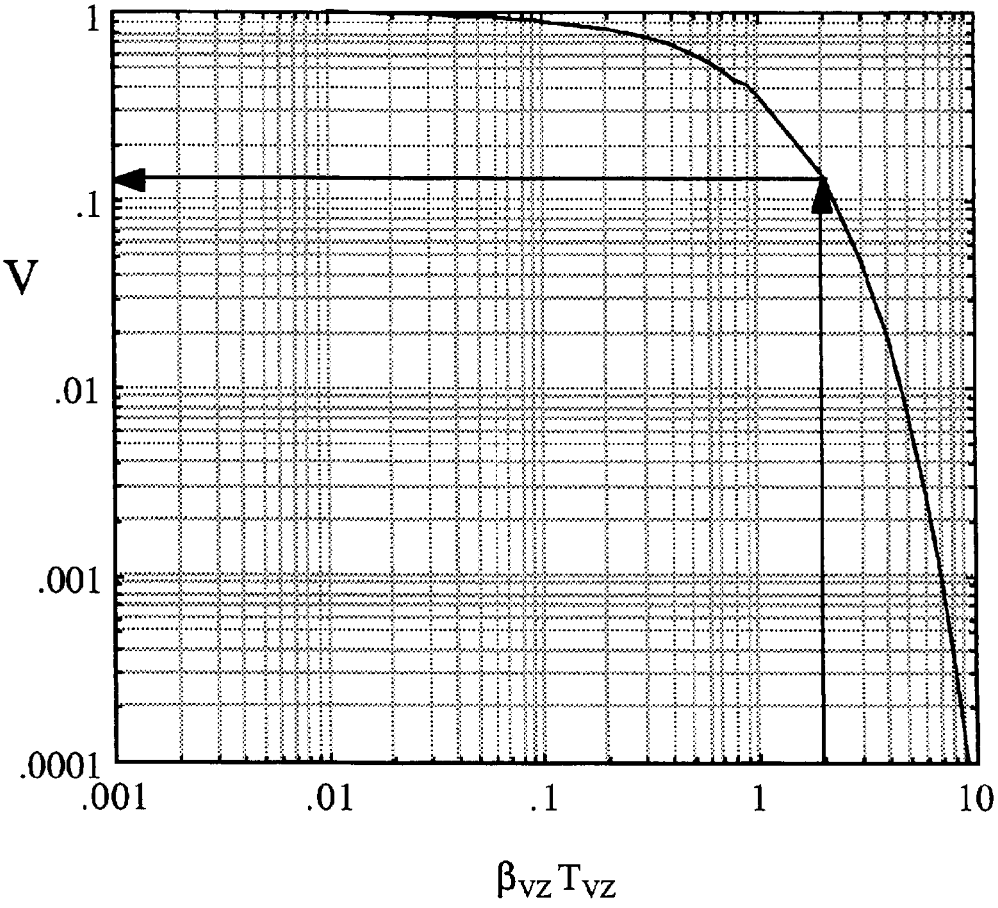
β_s = first-order biodegradation rate constant [d^{-1}]

U_{GW} = groundwater seepage velocity [m/d]

L_R = distance to receptor [m]

A = plan view source area [m^2]

Graph 8. Nomograph of the vadose zone source aquifer degradation factor <f>. Sample lines show use of the graph for ($\beta_s L_R/U_{GW}$)=3 and $A^{1/2}/L_R$=10, which yields <f>≈0.06



β_{VZ} = first-order biodegradation rate constant in vadose zone [d^{-1}]

T_{VZ} = time for soil moisture to travel from the source zone to the water table [d]

Graph 9. Nomograph of the vadose zone attenuation function V. Sample lines show use of the graph for the case $\beta_{VZ}T_{VZ}=2$, which yields $V\approx0.13$

Worksheets for the Graphical Approach for Determining Site-Specific Dilution-Attenuation Factors (DAFs)

Submerged Source DAF Estimation Worksheet.

INITIAL DAF ESTIMATE		REFINED DAF ESTIMATE	
Parameter [units]	Value	Parameter [units]	Value
L_R - receptor distance [m] (measured from the downgradient submerged source edge)		L_R - receptor distance [m] (measured from the downgradient source edge)	
W - source width [m]		W - source width [m]	
H - source thickness [m]		H - source thickness [m]	
H_W - well screen thickness [m]		H_W - well screen thickness [m]	
b - aquifer thickness [m]		b - aquifer thickness [m]	
α_L - longitudinal dispersivity [m]	$L_R/10$	α_L - longitudinal dispersivity [m]	
α_T - transverse dispersivity [m]	$\alpha_L/3$	α_T - transverse dispersivity [m]	
α_V - vertical dispersivity [m]	$\alpha_L/10$	α_V - vertical dispersivity [m]	
β_s - dissolved-phase bio-decay rate [d^{-1}]	NR	β_s - dissolved-phase bio-decay rate [d^{-1}]	
U_{GW} - seepage velocity [m/d]	NR	U_{GW} - seepage velocity [m/d]	
λ - first-order source decay rate [d^{-1}]	NR	λ - first-order source decay rate [d^{-1}]	
T - averaging time [d]	NR	T - averaging time [d]	

INITIAL DAF ESTIMATE		REFINED DAF ESTIMATE	
Graph Parameters	Value	Graph Parameters	Value
$5.5W/L_R$		$W/[\alpha_T L_R]^{1/2}$	
$L_R/10H$		$[\alpha_V L_R]^{1/2}/H$	
H/H_W		H/H_W	
H/b		H/b	
$L_R/(10b)$		$[\alpha_V L_R]^{1/2}/b$	
$\beta\alpha_L/U_{GW}$	NR	$\beta_s\alpha_L/U_{GW}$	
L_R/α_L	10	L_R/α_L	
λT	NR	λT	

INITIAL DAF ESTIMATE		REFINED DAF ESTIMATE	
Attenuation Factors (from Graphs 1 - 5)	Value	Attenuation Factors (from Graphs 1 - 5)	Value
g		g	
h^*_{inf}		h^*_{inf}	
h^*_{cor}		h^*_{cor}	
f	1	f	
$<S_L^*>$	1	$<S_L^*>$	

INITIAL DAF ESTIMATE		REFINED DAF ESTIMATE	
$DAF = 1/[<S_L^*> \times f \times g \times (h^*_{inf} + h^*_{cor})]$		$DAF = 1/[<S_L^*> \times f \times g \times (h^*_{inf} + h^*_{cor})]$	

NR - information not required

Vadose Zone Source DAF Estimation Worksheet.

INITIAL DAF ESTIMATE		REFINED DAF ESTIMATE	
Parameter [units]	Value	Parameter [units]	Value
L_R - source-receptor distance [m] (measured from the source center for vadose sources)		L_R - source-receptor distance [m] (measured from the source center for vadose sources)	
A - source area [m^2]		A - source area [m^2]	
H_W - well screen thickness [m]		H_W - well screen thickness [m]	
b - aquifer thickness [m]		b - aquifer thickness [m]	
U_{GW} - aquifer seepage velocity [m/d]		U_{GW} - aquifer seepage velocity [m/d]	
ϕ_s - effective aquifer porosity [L/L-soil]		ϕ_s - effective aquifer porosity [L/L-soil]	
I_f - infiltration rate [m/d]		I_f - infiltration rate [m/d]	
β_s - dissolved-phase bio-decay rate [d^{-1}]	NR	β_s - dissolved-phase bio-decay rate [d^{-1}]	
ϕ_m - vadose zone moisture content [L/L-soil]	NR	ϕ_m - vadose zone moisture content [L/L-soil]	
β_{VZ} - vadose zone bio-decay rate [d^{-1}]	NR	β_{VZ} - vadose zone bio-decay rate [d^{-1}]	
L_{VZ} - source zone - aquifer separation [m]	NR	L_{VZ} - source zone - aquifer separation [m]	
λ - first-order source decay rate [d^{-1}]	NR	λ - first-order source decay rate [d^{-1}]	
T - averaging time [d]	NR	T - averaging time [d]	

INITIAL DAF ESTIMATE		REFINED DAF ESTIMATE	
Graph Parameters	Value	Graph Parameters	Value
$I_f/\phi_s U_{GW}$		$I_f/\phi_s U_{GW}$	
A/b^2		A/b^2	
L_R/b		L_R/b	
H_W/b		H_W/b	
$\beta_s L_R/U_{GW}$	NR	$\beta_s L_R/U_{GW}$	
$\beta_{VZ}\,\phi_m\,L_{VZ}/I_f$	NR	$\beta_{VZ}\,\phi_m\,L_{VZ}/I_f$	
λT	NR	λT	

NR - Information Not Required

INITIAL DAF ESTIMATE		REFINED DAF ESTIMATE	
Attenuation Factors (from Graphs 6 - 7)	Value	Attenuation Factors (from Graphs 5 - 9)	Value
<f>	1	<f>	
$<S_L^*>$	1	$<S_L^*>$	
Ω		Ω	
σ		σ	
V	1	V	

INITIAL DAF ESTIMATE		REFINED DAF ESTIMATE	
$DAF = 1/[1 \times 1 \times (I_f/\phi_s U_{GW}) \times 1 \times \Omega \times \sigma]$		$DAF = 1/[<S_L^*> \times <f> \times (I_f/\phi_s U_{GW}) \times V \times \Omega \times \sigma]$	

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