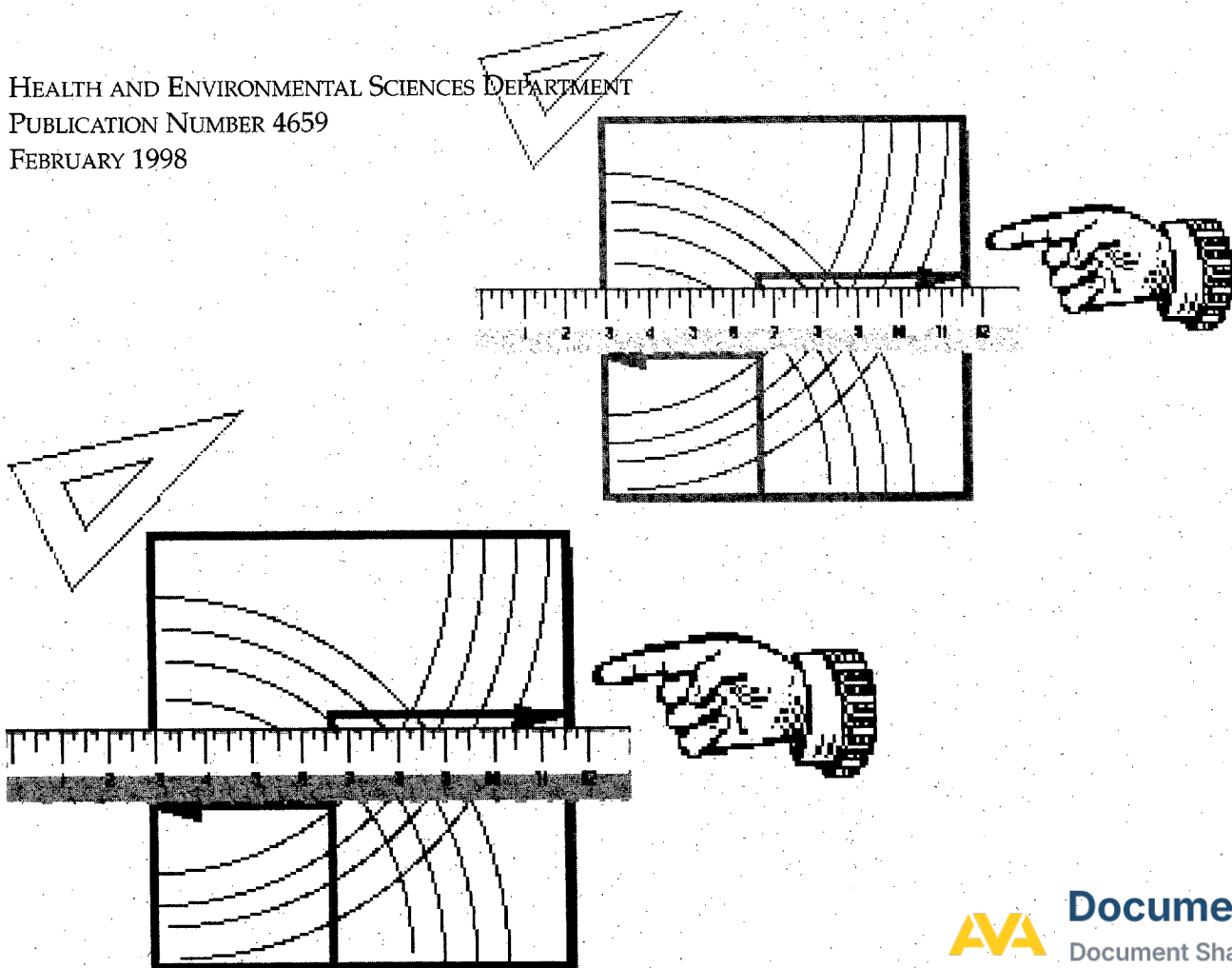


GRAPHICAL APPROACH FOR DETERMINING SITE-SPECIFIC DILUTION-ATTENUATION FACTORS (DAFs)

TECHNICAL BACKGROUND DOCUMENT

HEALTH AND ENVIRONMENTAL SCIENCES DEPARTMENT
PUBLICATION NUMBER 4659
FEBRUARY 1998



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August 6, 1998

To: Consumers of API's *Graphical Approach for Determining Site-Specific Dilution-Attenuation Factors (DAFs), Technical Background Document and User's Guide* Publication (Pub No. 4659)

From: The American Petroleum Institute: Health and Environmental Sciences Department

Enclosed is a replacement sheet for page A-20 of the *DAFfy Graphs User's Guide*. Please find the following three changes:

The date in the title above Table A-7 was changed to 1994 from 1996

The spelling of Benzo(a)antreacene was corrected to Benzo(a)anthracene

The number in the S [mg/L] column beside Benzo(a)anthracene was changed from 2.18e-02 to 1.28e-02.

Please remove the old page and insert the corrected version.

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

Compound	S [mg/L]	K_H [L_{H_2O}/L_{air}]	K_{OC} [L_{H_2O}/kg_{soil}]	K_d [L_{H_2O}/kg_{soil}]	γ^* [L_{H_2O}/kg_{soil}]
Acenaphthene	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)anthracene	1.28e-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-chloroaniline	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

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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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.

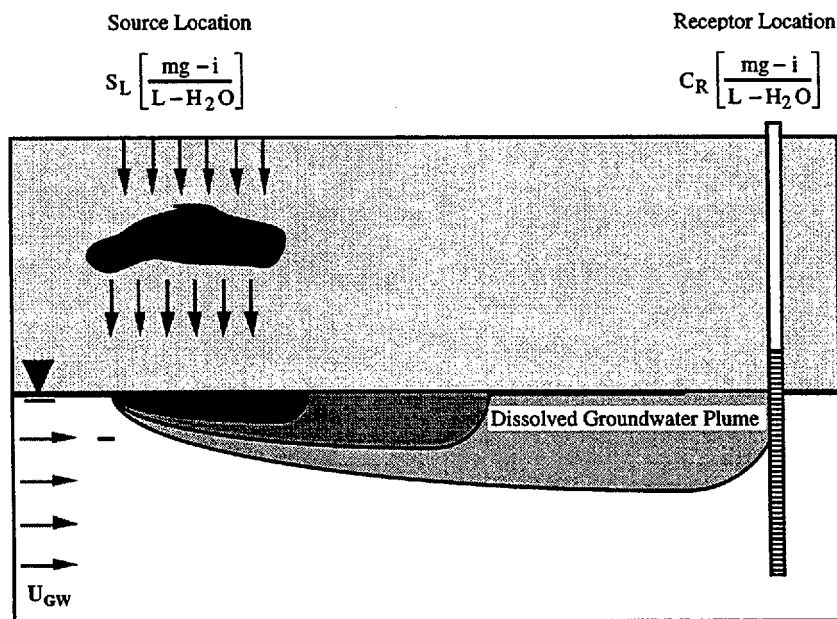


Figure 1-1. Soil-to-groundwater pathway schematic for compound “i”

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:

$$\text{DAF} \left[\frac{(\text{mg}_i / \text{L}_{\text{H}_2\text{O}})_{\text{source}}}{(\text{mg}_i / \text{L}_{\text{H}_2\text{O}})_{\text{receptor}}} \right] = \frac{S_L}{C_R} \quad (2-1)$$

where:

S_L = concentration of compound “i” dissolved in leachate leaving the source zone [$\text{mg}_i / \text{L}_{\text{H}_2\text{O}}$]

C_R = dissolved concentration of compound “i” at the receptor [$\text{mg}_i / \text{L}_{\text{H}_2\text{O}}$]

As defined by Equation (2-1), the DAF must take on values greater than or equal to one ($\text{DAF} \geq 1$). 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:

$$DAF \left[\frac{(mg_i / L_{H_2O})_{source}}{(mg_i / L_{H_2O})_{receptor}} \right] = \frac{S_L^o}{\langle\langle C_R \rangle\rangle_{z,t,max}} \quad (2-2)$$

where:

S_L^o = dissolved concentration of compound i leaving source zone at time $t=0$
[mg_i / L_{H_2O}]

$\langle\langle C_R \rangle\rangle_{z,t,max}$ = maximum-time-averaged and vertically-averaged centerline dissolved concentration of compound i at the receptor location $x=L_R$ [mg_i / L_{H_2O}]

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 $\langle\langle C_R \rangle\rangle_{z,t,max}$ 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 $\langle\langle C_R \rangle\rangle_{z,t,max}$ 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 $\langle\langle C_R \rangle\rangle_{z,t,max}$ 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:

$$\frac{\partial(\rho_b C_T)}{\partial t} = \sum_j \nabla \cdot \phi_j D_j \cdot \nabla C_j - \sum_j \phi_j u_j \cdot \nabla C_j - \sum_j \beta_j \phi_j C_j \quad (2-3)$$

In Equation (2-3):

C_T = total concentration of compound i per unit mass of soil = $\sum C_j \phi_j / \rho_b$ [mg_i / kg_{soil}]
 C_j = concentration of contaminant i in phase j [$mg_i / L_{phase-j}$]
 ρ_b = soil bulk density [kg_{soil} / L_{soil}]
 D_j = hydrodynamic dispersion tensor for phase j [m^2/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 [$L_{\text{phase-j}}/L_{\text{soil}}$]
β_j	=	decay coefficient of the contaminant in phase j [d^{-1}]
$\underline{\nabla}$	=	del differential vectorial operator, ($i \partial/\partial x + j \partial/\partial y + k \partial/\partial z$) [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 $\langle\langle C_R \rangle_z \rangle_{t,\max}$ 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 :

$$\langle\langle C_R \rangle_z \rangle_{t,\max} = \max \left\{ \frac{1}{T} \int_{\tau}^{\tau+T} \left\{ \frac{1}{H_w} \int_h^{h+H_w} C(L_R, 0, z, t) dz \right\} dt \right\} \quad (2-4)$$

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, Javandel *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 $S_L^0 = 1$):

$$C_{cs}^*(x,y,z,t) = C(x,y,z,t) \quad (\text{for constant-strength sources with } S_L^0 = 1) \quad (2-5)$$

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):

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

where:

$$\begin{aligned} S_L(t) &= \text{time-varying source zone leachate concentration [mg}_i/\text{L}_{\text{H}_2\text{O}}] \\ \omega &= \text{dummy integration variable} \\ C_{cs}^*(x,y,z,t) &= \text{normalized solution for a constant strength source [unitless]} \end{aligned}$$

Thus, if the constant source solution (C_{cs}^*) for a given set of boundary conditions is known, then $\langle\langle C_R \rangle\rangle_{z,t,\max}$ 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:

$$C(x,y,z,t) \approx H(t - \tau_d) S_L(t - \tau_d) C_{cs}^*(x,y,z,\infty) \quad (2-7)$$

where:

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

- $C_{CS}^*(x,y,z,\infty)$ = steady-state normalized solution for a constant-strength source [unitless]
 $S_L(t - \tau_d)$ = time-varying source zone leachate concentration [$\text{mg}_i / \text{L}_{\text{H}_2\text{O}}$]
 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:

$$\langle\langle C_R \rangle\rangle_{z,t,\max} \approx \left\{ \frac{1}{T} \int_0^T S_L(t) dt \right\} \times \left\{ \frac{1}{H_w} \int_h^{h+H_w} C_{CS}^*(L_R, 0, z, \infty) dz \right\} \quad (2-8)$$

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:

$$\text{DAF} = \frac{1}{\left\{ \frac{1}{T} \int_0^T \frac{S_L(t)}{S_L(0)} dt \right\} \times \left\{ \frac{1}{H_w} \int_h^{h+H_w} C_{CS}^*(L_R, 0, z, \infty) dz \right\}} \quad (2-9)$$

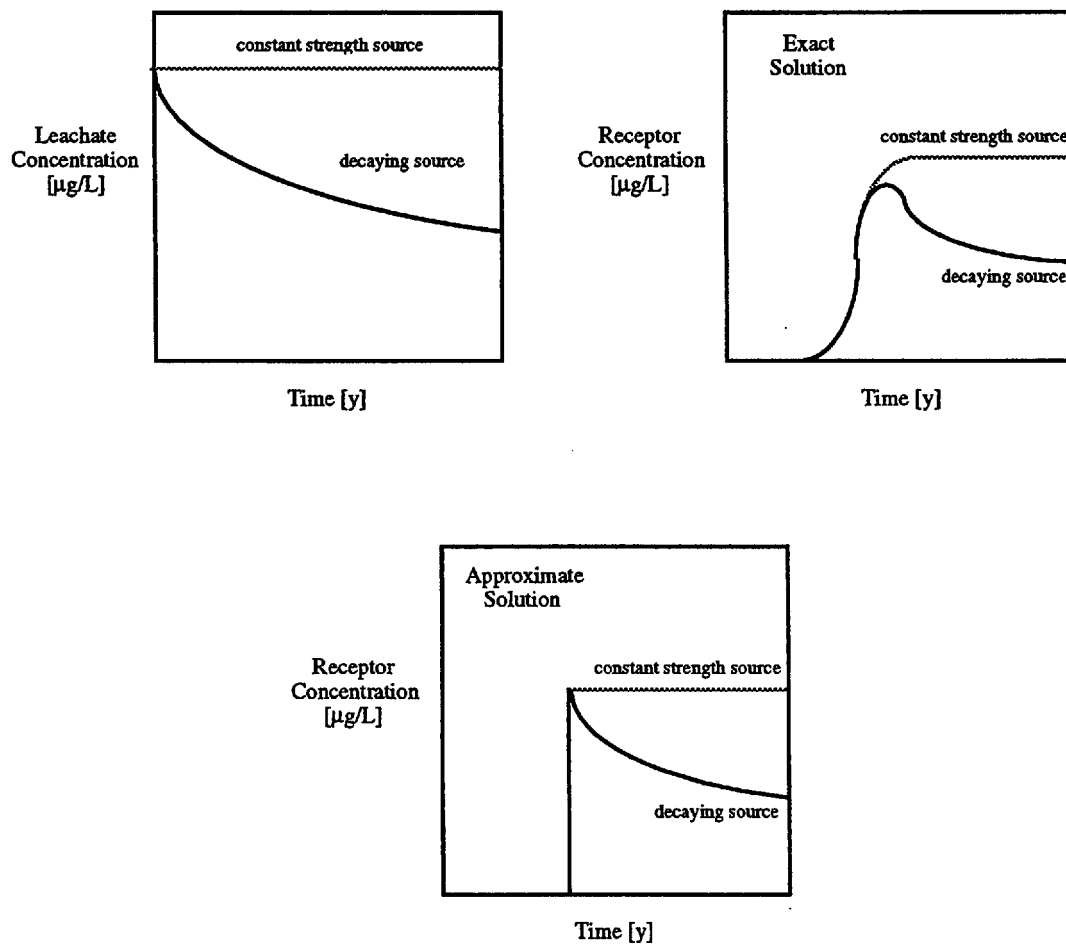


Figure 2-2. Qualitative comparison of exact and approximate solutions

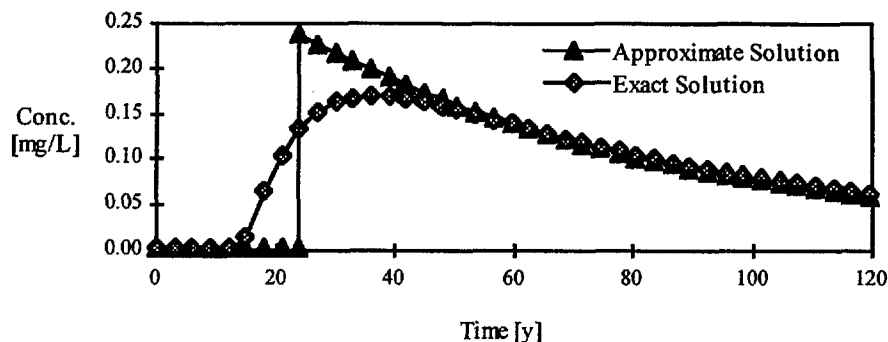


Figure 2-3. Comparison of receptor concentrations at $x = 30$ m (distance downgradient from center of source zone) obtained from the approximate and exact solutions for an exponentially-decaying source, using the HPS model discussed in Chapter 4

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.

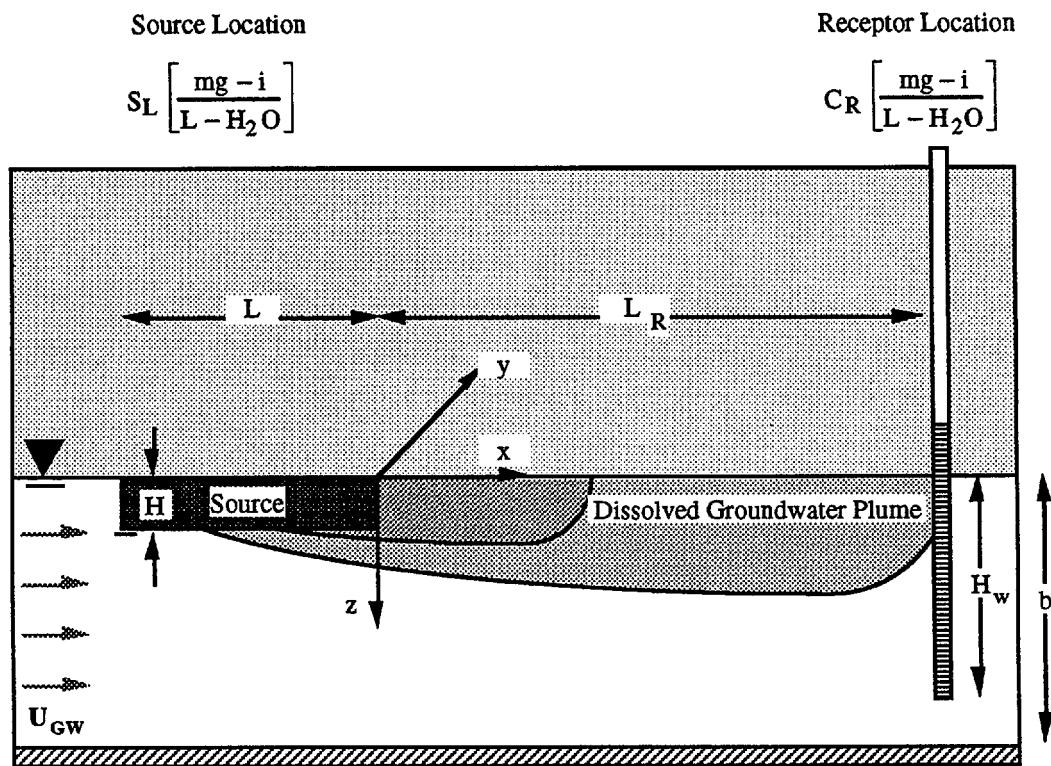


Figure 3-1. Generalized submerged source schematic

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:

$$\begin{aligned}
C_{cs}^*(x, y, z, t) = & \frac{1}{8} \exp \left\{ \frac{x}{2\alpha_L} \left[1 - \sqrt{1 + \frac{4\beta_s \alpha_L}{U_{GW}}} \right] \right\} \\
& \times \operatorname{erfc} \left\{ \frac{x - U_{GW}t \sqrt{1 + \frac{4\beta_s \alpha_L}{U_{GW}}}}{2\sqrt{\alpha_L U_{GW}t}} \right\} \\
& \times \left\{ \operatorname{erf} \left\{ \frac{y + \frac{W}{2}}{2\sqrt{\alpha_T x}} \right\} - \operatorname{erf} \left\{ \frac{y - \frac{W}{2}}{2\sqrt{\alpha_T x}} \right\} \right\} \\
& \times \left\{ \operatorname{erf} \left\{ \frac{z + H}{2\sqrt{\alpha_V x}} \right\} - \operatorname{erf} \left\{ \frac{z - H}{2\sqrt{\alpha_V x}} \right\} \right\}
\end{aligned} \tag{3-1}$$

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

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

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:

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

where all the parameters are defined as above, except:

$$\begin{aligned} t^* &= t/R \text{ [d]} \\ R &= \text{saturated zone retardation factor} = 1 + K_d \rho_b / \phi_m \text{ [dimensionless]} \end{aligned}$$

- K_d = soil-water partitioning coefficient $[(mg_i / kg_{soil}) / (mg_i / L_{H_2O})]$
 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:

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

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:

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

or:

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

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:

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

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

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

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:

$$h^* = h_{inf}^*\left(\frac{\sqrt{\alpha_V L_R}}{H}, \frac{H}{H_w}\right) + h_{cor}^*\left(\frac{\sqrt{\alpha_V L_R}}{b}, \frac{H}{b}, \frac{H}{H_w}\right) \quad (3-11)$$

where:

$$h_{inf}^* \left(\frac{H}{\sqrt{\alpha_v L_R}}, \frac{H}{H_W} \right) = \frac{1}{2} \int_0^1 \left[\operatorname{erf} \left\{ \frac{Z (H_W / H) + 1}{2(\sqrt{\alpha_v L_R} / H^2)} \right\} - \operatorname{erf} \left\{ \frac{Z (H_W / H) - 1}{2(\sqrt{\alpha_v L_R} / H^2)} \right\} \right] dZ \quad (3-12)$$

and:

$$\begin{aligned} h_{cor}^* \left(\frac{\sqrt{\alpha_v L_R}}{b}, \frac{H}{b}, \frac{H}{H_W} \right) &= \frac{1}{2} \sum_{n=1}^{\infty} \int_0^1 \operatorname{erf} \left\{ \frac{2n + Z \left(\frac{H}{b} \right) \left(\frac{H_W}{H} \right) + \left(\frac{H}{b} \right)}{2 \left(\frac{\sqrt{\alpha_v L_R}}{b} \right)} \right\} dZ \\ &- \frac{1}{2} \sum_{n=1}^{\infty} \int_0^1 \operatorname{erf} \left\{ \frac{2n + Z \left(\frac{H}{b} \right) \left(\frac{H_W}{H} \right) - \left(\frac{H}{b} \right)}{2 \left(\frac{\sqrt{\alpha_v L_R}}{b} \right)} \right\} dZ + \frac{1}{2} \sum_{n=1}^{\infty} \int_0^1 \operatorname{erf} \left\{ \frac{2n - Z \left(\frac{H}{b} \right) \left(\frac{H_W}{H} \right) + \left(\frac{H}{b} \right)}{2 \left(\frac{\sqrt{\alpha_v L_R}}{b} \right)} \right\} dZ \\ &- \frac{1}{2} \sum_{n=1}^{\infty} \int_0^1 \operatorname{erf} \left\{ \frac{2n - Z \left(\frac{H}{b} \right) \left(\frac{H_W}{H} \right) - \left(\frac{H}{b} \right)}{2 \left(\frac{\sqrt{\alpha_v L_R}}{b} \right)} \right\} dZ \end{aligned} \quad (3-13)$$

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):

$$\lim \left(\frac{\sqrt{\alpha_v L_R}}{b} \ll 1 \right); \quad h_{cor}^* \left(\frac{\sqrt{\alpha_v L_R}}{b}, \frac{H}{b}, \frac{H}{H_W} \right) \ll h_{inf}^* \left(\frac{\sqrt{\alpha_v L_R}}{H}, \frac{H}{H_W} \right) \quad (i.e. \ h^* \approx h_{inf}^*) \quad (3-14)$$

$$\lim \left(\frac{\sqrt{\alpha_v L_R}}{b} \gg 1 \right); \quad h_{cor}^* \left(\frac{\sqrt{\alpha_v L_R}}{b}, \frac{H}{b}, \frac{H}{H_W} \right) \rightarrow \left(\frac{H}{b} \right) \quad (i.e. \ h^* \approx h_{cor}^*) \quad (3-15)$$

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

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:

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

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

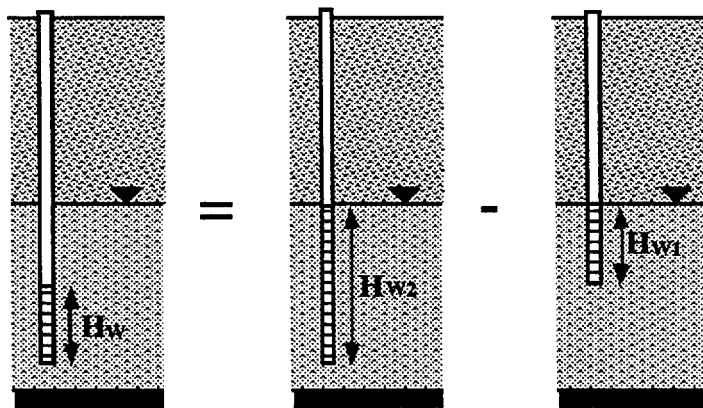


Figure 3-2. Alternate well construction configuration and graphical representation of calculation method given in Equation (3-17)

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 $\alpha_T \approx 0.03 L_R$ (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 decrease 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 $h_{cor}^* \rightarrow (H/b)$ 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 $((\alpha_v L_R)^{1/2}/b) < 1$.

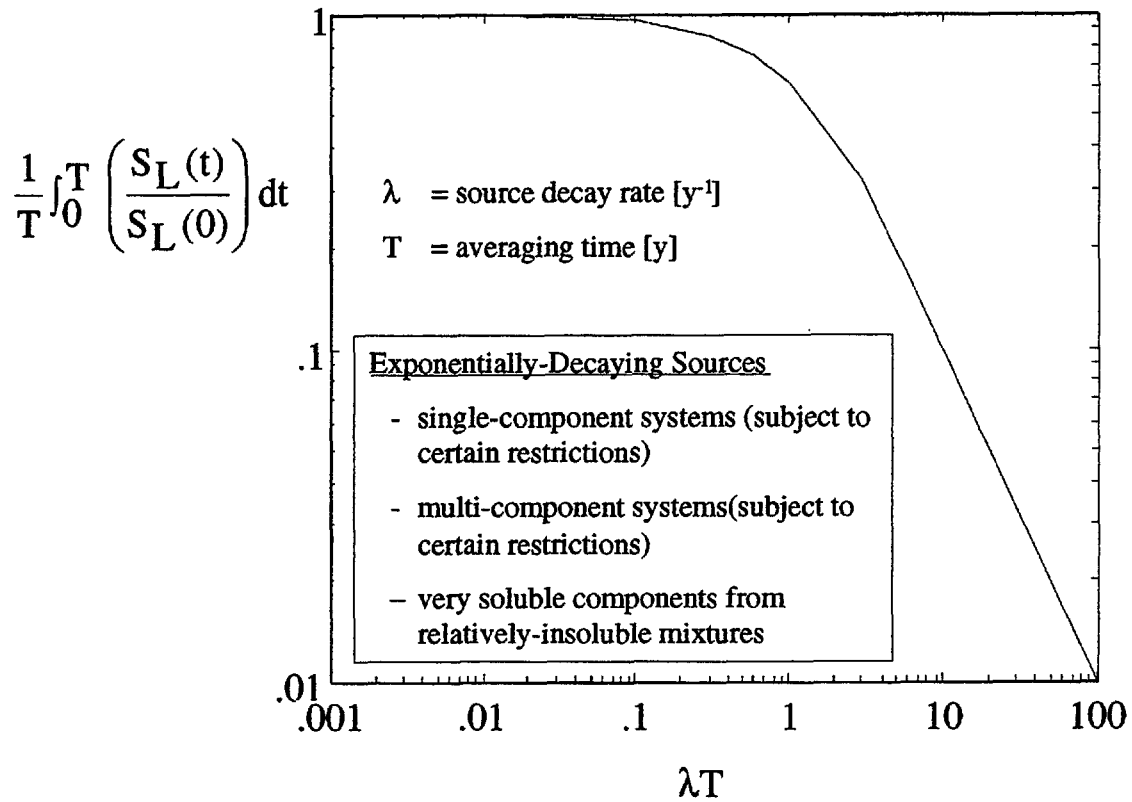
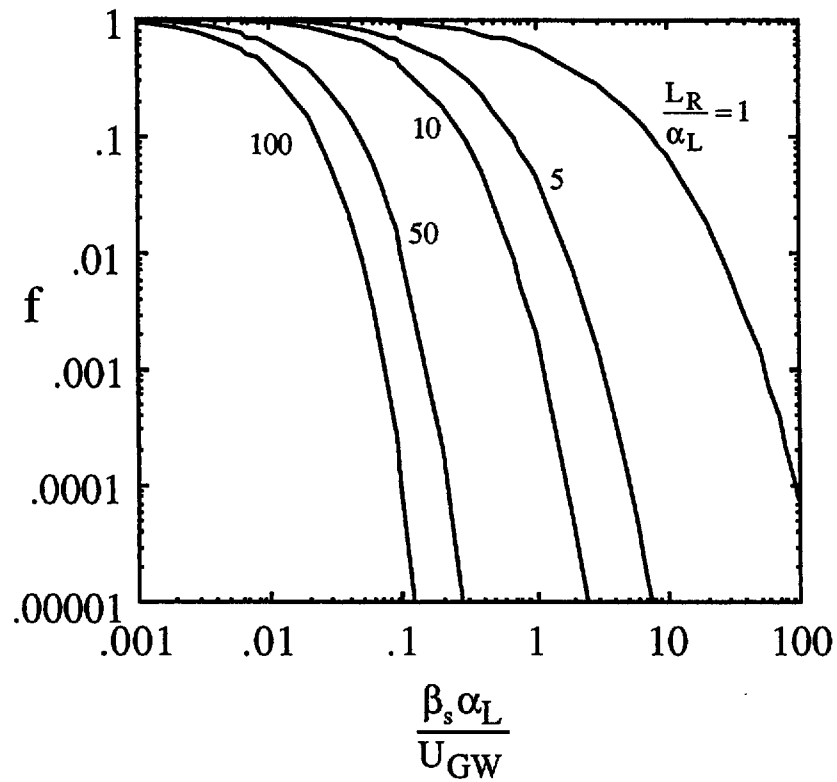
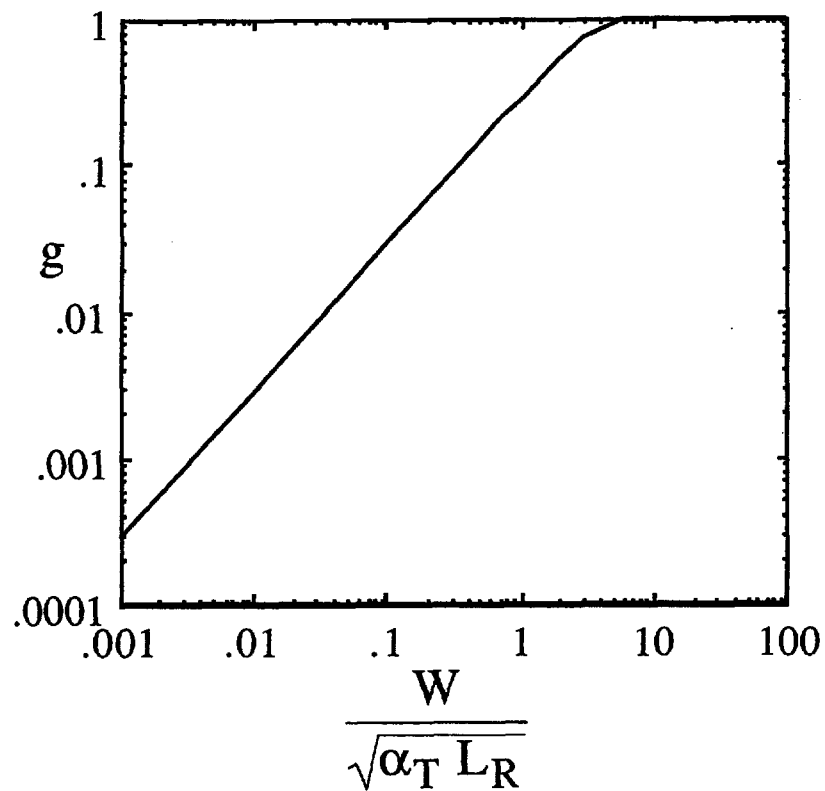


Figure 3-3. Source decay factor for exponentially-decaying sources (see Chapter 6 for calculation of decay rates and similar graphs for other idealized source decay models)



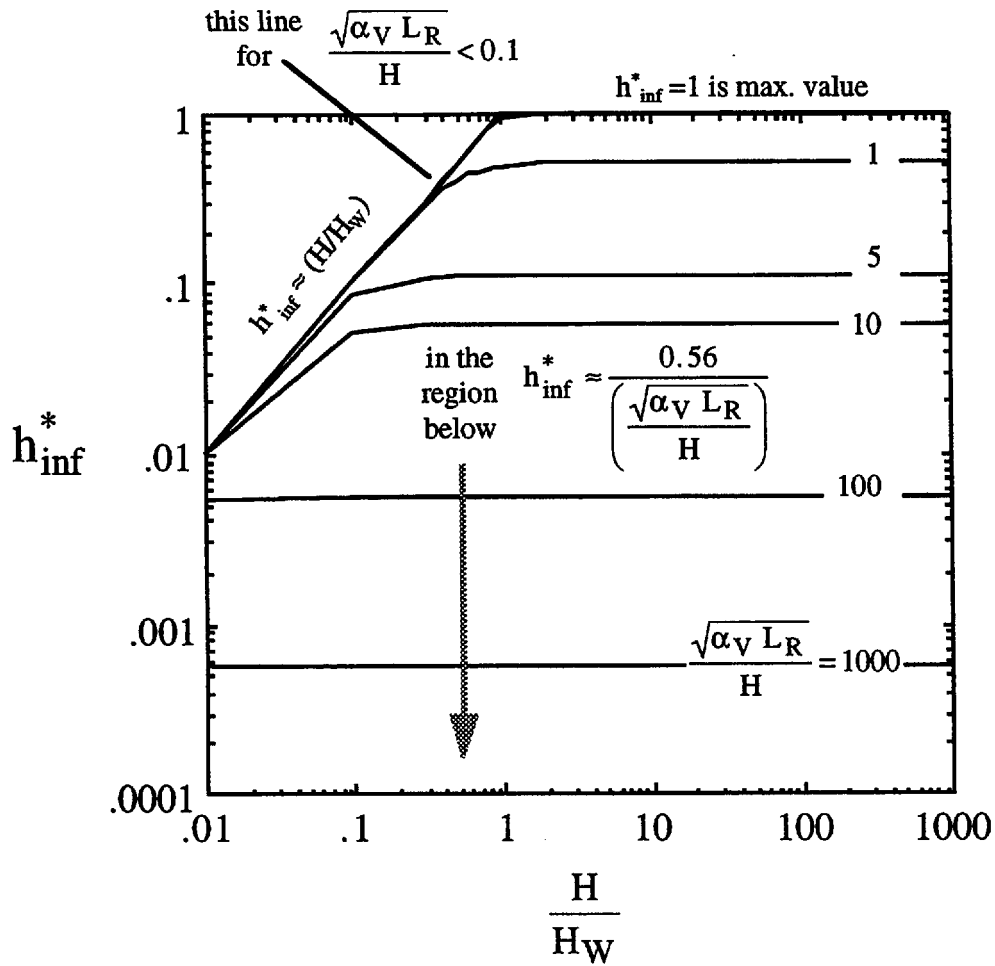
β_s	= first-order biodegradation rate constant [d ⁻¹]
α_L	= longitudinal dispersivity ($\approx L_R/10$) [m]
U_{GW}	= groundwater seepage velocity [m/d]
L_R	= distance to receptor [m]

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 $\geq (H/b)$

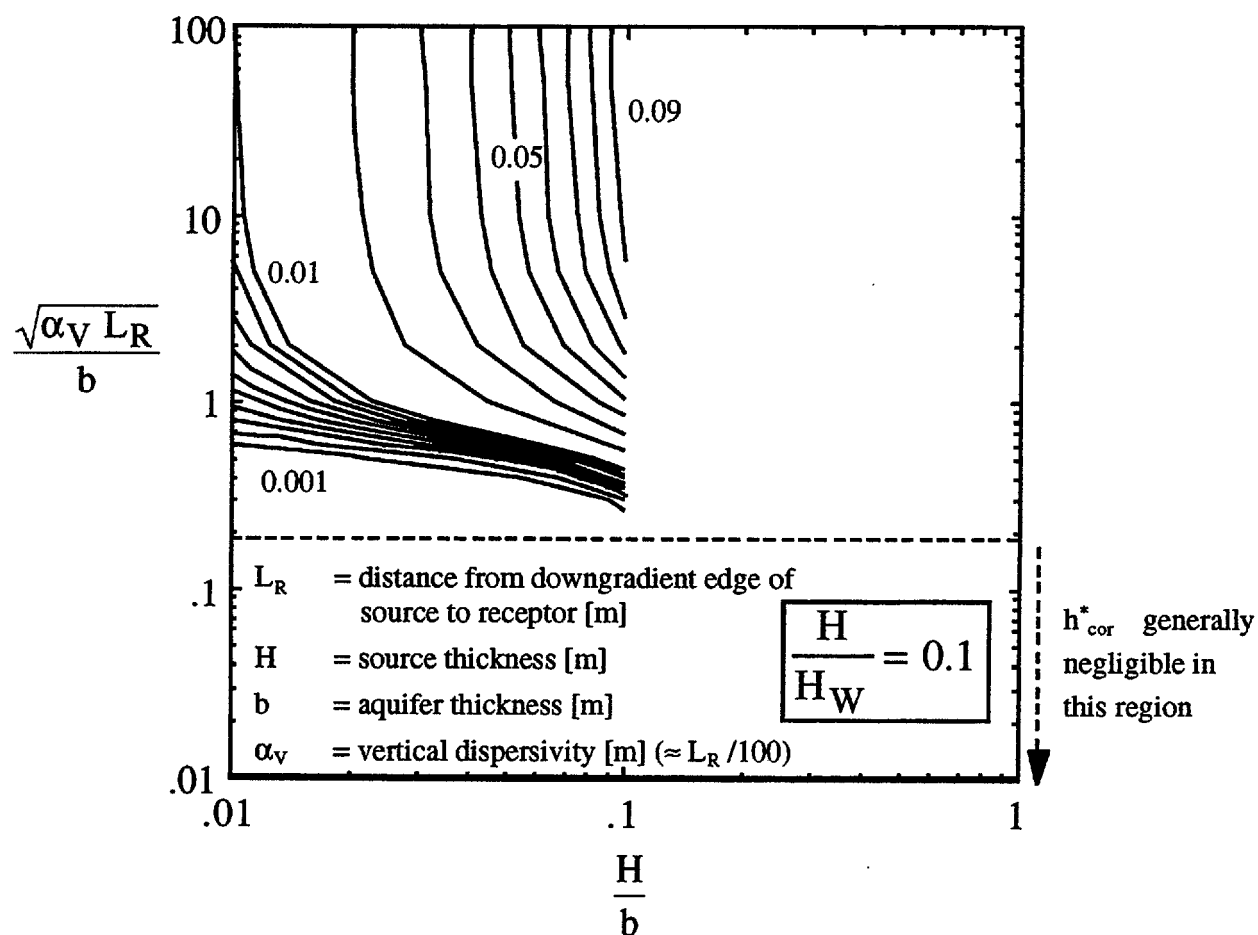


Figure 3-7. Vertical mixing correction factor (h_{cor}^*) for finite thickness aquifers, for $H/H_w=0.1$.
 Note that $h^* = h_{inf}^* + h_{cor}^*$ must be $\geq (H/b)$

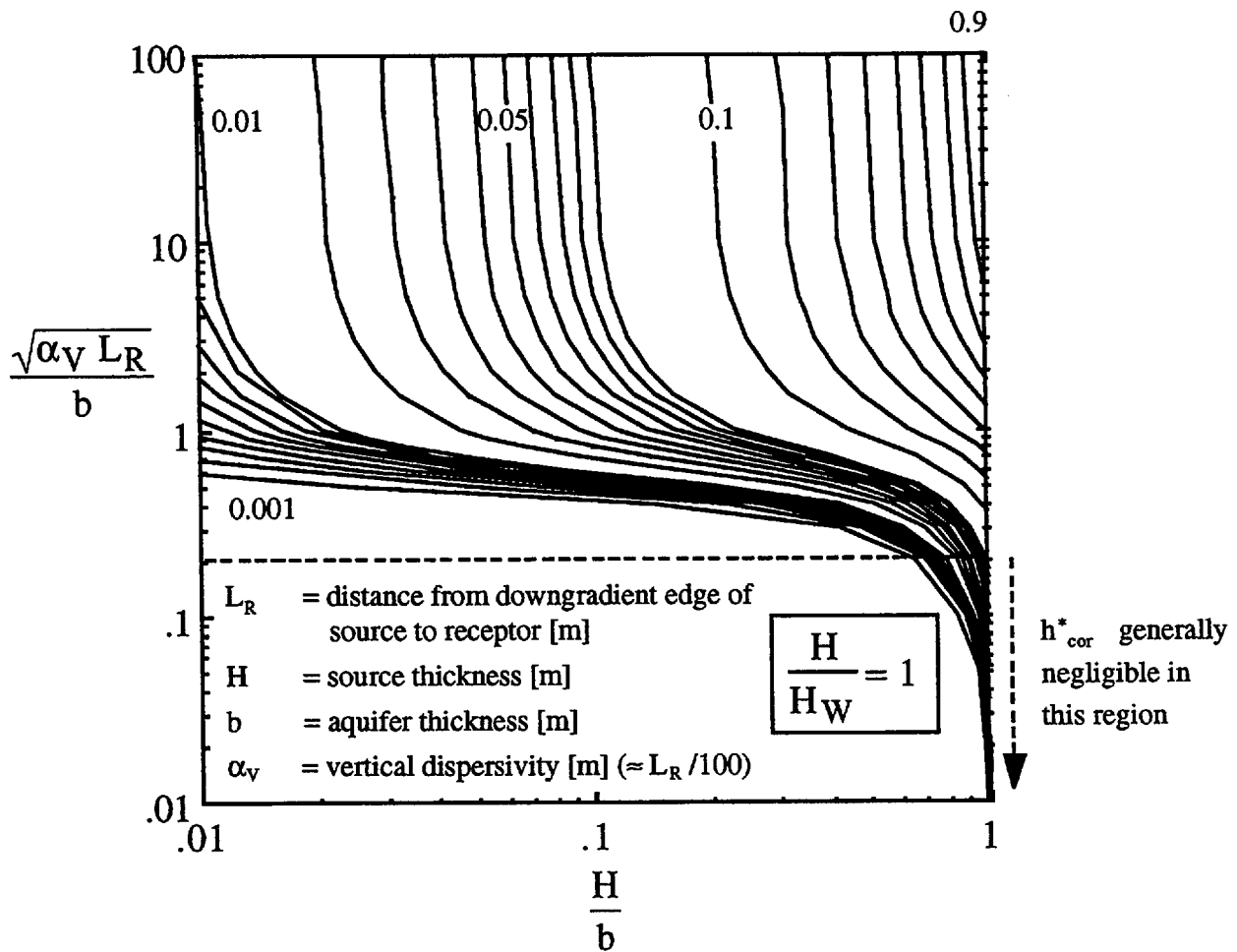


Figure 3-8. Vertical mixing correction factor (h_{cor}^*) for finite thickness aquifers, for $H/H_w=1.0$. Note that $h^* = h_{inf}^* + h_{cor}^*$ must be $\geq (H/b)$

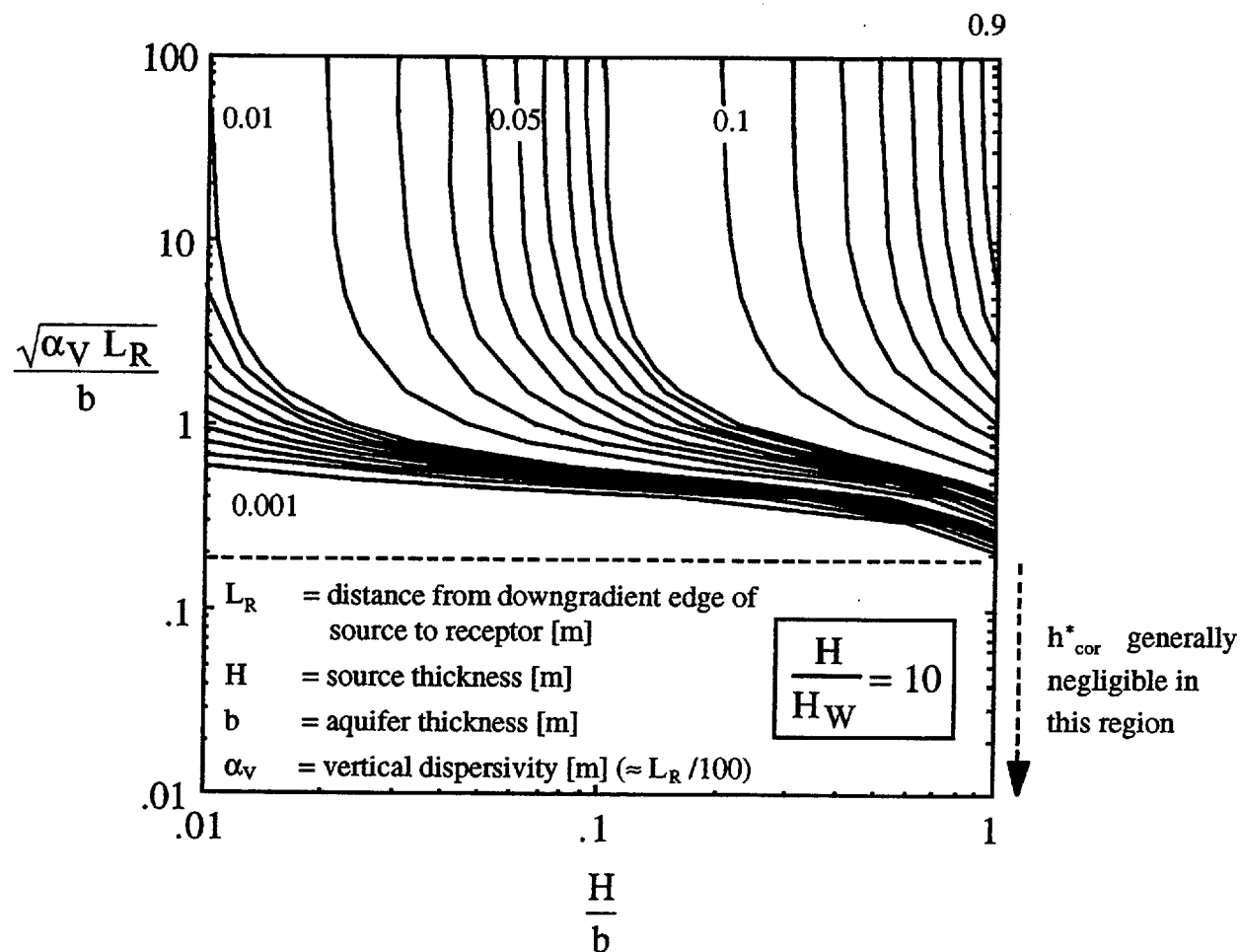
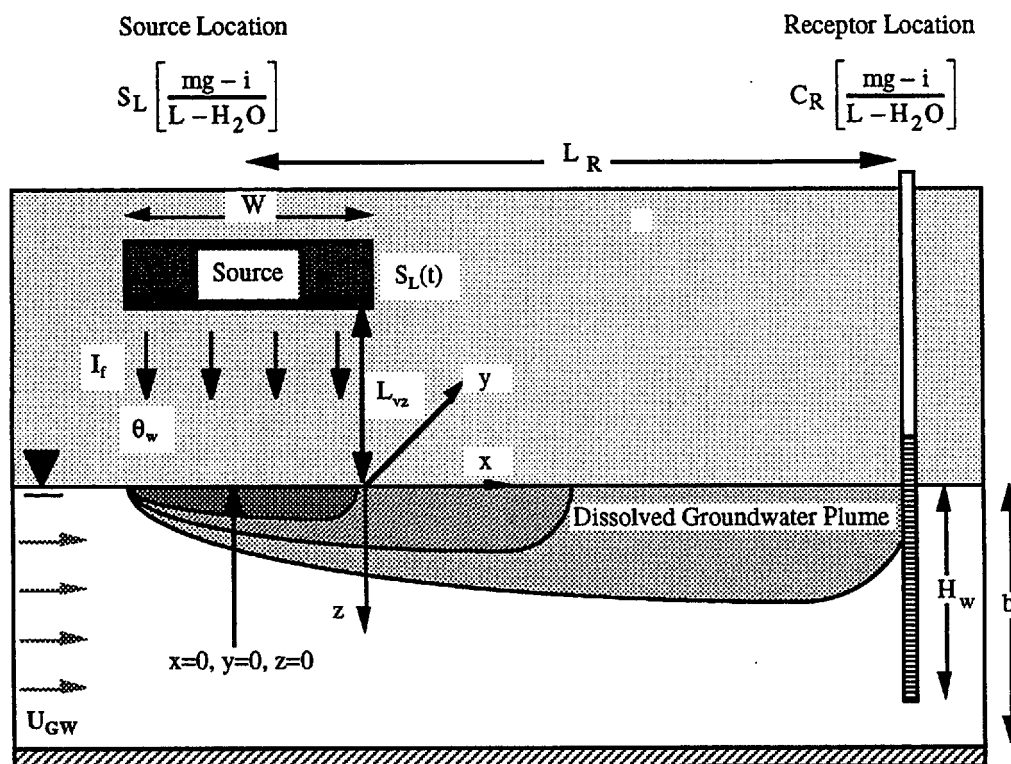


Figure 3-9. Vertical mixing correction factor (h^*_{cor}) for finite thickness aquifers, for $H/H_w=10$.
 Note that $h^* = h^*_{inf} + h^*_{cor}$ must be $\geq (H/b)$

VADOSE ZONE SOURCES

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.



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 $M_i(t)$ [mg_i/m²-d] of chemical "i" into the aquifer is given by:

$$M_i(t) = L W I_f S_L(t - R_{vz} T_{vz}) H(t - R_{vz} T_{vz}) e^{-\beta_{vz} T_{vz}} \quad (4-1)$$

where:

- $M_i(t)$ = mass flux of solute "i" reaching the groundwater table at time t [mg_i/m²-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/m³-H₂O]
 $H(t - T_{vz} R_{vz})$ = 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} :

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

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 [m³-water/m³-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:

$$I_f = K_{sv} k_{rw} \quad (4-3)$$

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:

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

where ϕ_{mr} is the irreducible water content [$\text{m}^3\text{-water}/\text{m}^3\text{-soil}$] 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:

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

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:

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

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 [$\text{kg}_{\text{soil}}/\text{m}^3$] is the soil bulk density; K_{oc} [$(\text{mg}_i/\text{kg}_{\text{soil}})/(\text{mg}_i/\text{L-H}_2\text{O})$] is the chemical-specific soil-organic carbon partition coefficient (see Appendix A); and f_{oc} [$\text{kg}_{\text{organic carbon}}/\text{kg}_{\text{soil}}$] 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.

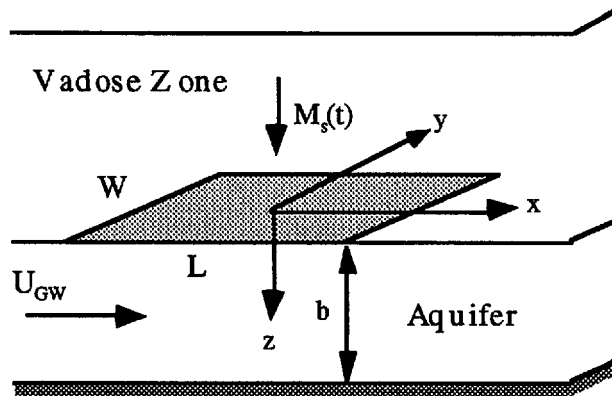


Figure 4-2. Horizontal Plane Source (HPS) Model geometry

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:

$$C(x, y, z, t) = \frac{1}{\phi_s R_s} \int_0^t M_s(\tau) X_o(x, t-\tau) Y_o(y, t-\tau) Z_o(z, t-\tau) T(t-\tau) d\tau \quad (4-7)$$

where:

$$X_o(x, t) = \frac{1}{2L} \left[\operatorname{erf} \left(\frac{\frac{L}{2} + x - \frac{U_{GW} t}{R_s}}{\sqrt{4\alpha_L U_{GW} t / R_s}} \right) + \operatorname{erf} \left(\frac{\frac{L}{2} - x - \frac{U_{GW} t}{R_s}}{\sqrt{4\alpha_L U_{GW} t / R_s}} \right) \right] \quad (4-8)$$

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

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

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

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:

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

where:

- T = averaging time [d]
 $S_L(t)$ = source zone leachate strength at time t [$\text{mg}_i/\text{L-H}_2\text{O}$]
 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:

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

and:

$$\begin{aligned} \frac{1}{H_w} \int_0^{H_w} C_{cs}^*(L_R, 0, z, \infty) dz = \\ \frac{I_f e^{-\beta_{vz} T_{vz}}}{H_w \phi_s} \int_0^{H_w} \int_0^{\infty} \left\{ \frac{1}{2} \left[\operatorname{erf} \left(\frac{\frac{L}{2} + L_R - U_{GW} \tau}{\sqrt{4 \alpha_L U_{GW} \tau}} \right) + \operatorname{erf} \left(\frac{\frac{L}{2} - L_R - U_{GW} \tau}{\sqrt{4 \alpha_L U_{GW} \tau}} \right) \right] \cdot \right. \\ \left. \left[\operatorname{erf} \left(\frac{W}{\sqrt{\alpha_T U_{GW} \tau}} \right) \right] \cdot \frac{1}{\sqrt{\pi \alpha_V U_{GW} \tau}} \sum_{n=-\infty}^{\infty} \left[\exp \left(\frac{-(2nb - z)^2}{4 \alpha_V U_{GW} \tau} \right) \right] e^{-\beta_s \tau} \right\} d\tau dz \end{aligned} \quad (4-14)$$

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 $(t-\tau)$ 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:

$$Z = z/H_w \quad (4-15a)$$

$$\tau^* = \tau U_{GW}/L_R \quad (4-15b)$$