Task 23 - User's Guide to GRI-SHOWFLOW

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Morgantown Site
P.O. Box 880
Morgantown, West Virginia 26507-0880

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Energy & Environmental Research Center
University of North Dakota
P. O. Box 9018
Grand Forks, North Dakota 58202-9018

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TABLE OF CONTENTS

LIST OF FIGURES	ii
ABBREVIATIONS AND ACRONYMS	iii
1.0 SUMMARY	1
2.0 SYSTEM REQUIREMENTS	2
3.0 INSTALLATION	2
4.0 WHAT IS GRI-SHOWFLOW?	3
4.1 Using GRI-ShowFlow	6
4.1.1 Model Selection	6
4.1.2 Source Type Selection	8
4.2 ShowFlow: The Windows™ Interface	10
4.3 The SSGPLUME Model	13
4.4 The 3DADE Model	20
4.5 The AT123D Model	23
4.6 Display Model Results	27
4.6.1 Transects	28
4.6.2 Contour Plots	28
4.6.3 Graph Interpretation	30
5.0 MODELING EXAMPLES	31
5.1 Steady-State Versus Transient Simulation	31
5.2 Plume Differences Due to Initial Source Dimensions	31
5.3 Comparison of a Point, a Plane, and a Cube Source	32
6.0 REFERENCES	42
GLOSSARY	Appendix A

LIST OF FIGURES

1	SSGPLUME, 3DADE, or AT123D model is chosen in this screen by clicking on the respective radio button	7
2	Source type selection screen with radio buttons to select source type and configuration in the three-dimensional models	8
3	Command Menu screen manages the input, execution, and output of the models	12
4	Input screen for the SSGPLUME model	14
5	Input screen for the 3DADE model with cube source	20
6	Input screen for the AT123D model with cube source	25
7	Graph information screen contains transect locations and contouring values that are used for visualization through slicing of the plume	29
8a	Input data for a test simulation with SSGPLUME with solute attenuation in the vadose zone and retardation and degradation in the saturated zone	32
8b	Output generated with data from Figure 8a	33
9a	Input data for a test simulation of AT123D with a horizontal plane source	34
9b	Transects generated by data from Figure 9a	35
9c	Contours generated by data from Figure 9a	36
10a	Input data for a test simulation of 3DADE with an initial cube source of 10 m ³	37
10b	Contour map and X-Transect for a 10-m ³ source based on input data from Figure 10a . . .	38
10c	Same graphs as in Figure 10b for a source of 100 m ³ and other parameters unchanged . . .	39
11a	Input data used in the AT123D cube source model to generate concentration profiles shown in Figure 11b	40
11b	Concentration profiles along the center line of a plume originating from different landfill representations	41

ABBREVIATIONS AND ACRONYMS

3DADE	Three-Dimensional Advection-Dispersion Equation
API	American Petroleum Institute
APIDSS	American Petroleum Institute Decision Support System
ARMOS	Areal Multiphase Organic Simulator
AT123D	Analytical Transient One-, Two-, and Three- Dimensional model
CFR	Code of Federal Register
DOS	Disk Operating System
EERC	Energy and Environmental Research Center
EPA	Environmental Protection Agency
EPACML	Environmental Protection Agency Composite Model for Landfills
EPRI	Electric Power Research Institute
GRI	Gas Research Institute
HPS	Horizontal Plane Source
HSSM	Hydrocarbon Spill Screening Model
MS	Microsoft
MULTIMED	Multimedia Exposure Assessment Model
MYGRT	Migration of organic and inorganic chemical in groundwater
NAPL	Non-Aqueous Phase Liquid
NRC	National Research Council
PC	Personal Computer
RAM	Random Access Memory
ROAM	Remedial Options Assessment Model
SSGPLUME	Steady-State Gaussian Plume
VGA	Video Graphics Array
VHS	Vertical Horizontal Spread

USER'S GUIDE TO GRI-SHOWFLOW

Version 1.0

1.0 SUMMARY

GRI-ShowFlow is a compilation of flow and transport groundwater models under one user-friendly, graphical interface in the Microsoft® Windows™ 3.1 environment. The groundwater models as well as the interface were derived from existing codes. The motivation behind the development of GRI-ShowFlow was twofold: 1) there is a need to compare and assess various analytical and screening-level models that are being used by regulatory agencies and 2) there is a need for the nonexpert to be able to use these screening-level models and the resulting information without expert interpretation.

GRI-ShowFlow was developed for use by gas industry environmental staff who may have little experience with hydrogeology or groundwater models but must be able to quickly determine whether there is sufficient chance of groundwater contamination and whether a site does or does not require a more extensive examination. Special attention was therefore given to the Help System in GRI-ShowFlow, which aids the development of the minimal amount of data required by the program and the interpretation of the resulting data.

Most of the analytical models used and developed by the U.S. Environmental Protection Agency (EPA) are designed to provide rough estimates of contaminant spreading. Such estimates are needed for classification rather than for a true representation of a contaminated groundwater scenario. The reasoning behind the use of simple screening models is that during the initial assessment, the quantity and the quality of available data do not warrant the use of computationally intensive simulations.

The more complex simulations are typically made by means of numerical models, while the groundwater models that are applied at the screening level are typically analytical models. The term "analytical" means that these models have been derived by algebraic analysis of the governing equation, which is the advection-dispersion transport equation, based on Darcy's law and the mass balance equation. That several analytical models exist is the result of the inherent assumptions required to obtain an analytical solution.

The critical difference between various analytical models is in the source description. For example, the source of a contaminant mass entering groundwater has been described as a point—Vertical Horizontal Spread model (VHS) (EPA, 1985); as a horizontal rectangle—Horizontal Plane Source model (HPS) (Bond and Hwang, 1988); and as a vertical plane with a Gaussian contaminant distribution—EPASMOD model (Huyakorn and others, 1986). In all instances, the source description remains an idealized view of reality, restricted to one or two dimensions.

The objective of GRI-ShowFlow is to bring together the existing EPA models in a user-friendly environment and to compare them to each other as well as to new models that contain analytical solutions to three-dimensional source descriptions. A three-dimensional body will more closely reflect the shapes of contaminant sources than one- or two-dimensional geometries. In the

real world, contaminant sources such as landfills, storage pits, and lagoons will, after all, occupy a three-dimensional space.

2.0 SYSTEM REQUIREMENTS

To run GRI-ShowFlow, the following minimum personal computer (PC) system configuration is needed: an IBM-compatible 386 PC with math coprocessor or better, a VGA monitor, a minimum of four megabytes of RAM, a mouse, a hard drive with a minimum of three megabytes of available space, and a floppy disk drive.

The operating system required by GRI-ShowFlow is Microsoft® Windows™ Version 3.1 or Windows™ for Workgroups Version 3.11. Note that both of the aforementioned Windows™ versions require MS-DOS Version 3.1 or higher.

3.0 INSTALLATION

The following files are found on the GRI-ShowFlow diskette:

3DADE.EXE
AT123D.EXE
BWCC.DLL
EXAM1.PAR
EXAM2.PRM
EXAM3.PFL
INSTALL.CFG
INSTALL.EXE
MANUAL.WP
README.TXT
SFGLOSS.HLP
SFHELP.HLP
SHOWFLOW.EXE
SHOWFLOW.ICO
SSGPLUME.EXE

It is advised to back up these files on another diskette and to write-protect the diskettes. The distributed diskette contains several system files that need to be copied to one subdirectory on the hard drive. A backup copy can be made either through DOS commands or through Windows™ using the File Manager in the MAIN program group. After creating a new subdirectory, the user copies all files from the distribution diskette into that subdirectory, either on the hard drive or on another diskette.

Installation of the software is done within the Windows™ environment. Using the File Manager from Windows™, the user selects the drive in which the distribution diskette is placed (presumably A:). The user selects the file INSTALL.EXE by pointing on it with the mouse cursor and clicking the left mouse button. The user runs the A:\INSTALL.EXE program by clicking on

the highlighted file name again (or double-clicking while pointing to the file name), and GRI-ShowFlow will be installed in a subdirectory as directed by the user.

After the installation of GRI-ShowFlow is completed, the program is executed by double-clicking on the GRI-ShowFlow icon or, alternately, through the Windows™ File Manager by double-clicking on the primary interface file called SHOWFLOW.EXE. The default location for the GRI-ShowFlow icon is the SHOWFLOW program group. It can be moved to any other location within the Windows™ Program Manager by simply dragging the icon to a new program group.

4.0 WHAT IS GRI-SHOWFLOW?

GRI-ShowFlow is a software package that executes a variety of analytical groundwater models that are commonly being used as screening-level tools by both industry groups and consortia (e.g., American Petroleum Institute [API], Electric Power Research Institute [EPRI]) and regulatory agencies (EPA). The typical application of a screening model is to estimate contaminant concentrations at the point of exposure relative to the concentrations at the point of compliance. The point of exposure is typically a well where groundwater is withdrawn and where public health can be affected, and the point of compliance is a monitoring well at the downstream boundary of a waste disposal unit. However, screening-level models may differ in their predictions of these concentrations as a result of the nonuniqueness of the solution to the governing equation describing the groundwater system.

GRI-ShowFlow is based on ShowFlow, a practical Windows™ interface for groundwater modeling, developed by John Tauxe (Tauxe, 1990). ShowFlow provides a user-friendly, intuitive environment for quick simulations and visualization of spatially distributed systems. Its use is not restricted to groundwater systems: ShowFlow is applicable to any type of Windows™ or DOS model that requires spatial visualization by means of contouring. It has been applied to groundwater flow and transport as represented by the advection-dispersion equation simulating the migration of a single solute through an idealized groundwater system. The original versions of ShowFlow (Versions 1.0 and 2.0) made use of the Steady-State Gaussian Plume (SSGPLUME) model developed by Smith and Charbeneau (1990). SSGPLUME is a steady-state, two-dimensional model requiring fixed concentration input. GRI-ShowFlow exploits and enhances the ShowFlow interface through the incorporation of two additional three-dimensional models and through inclusion of extensive on-line help.

The two new models included in the GRI-ShowFlow package are based on analytical solutions to the advection-dispersion equation as formulated by Yeh (1981) and by Leij and others (1991), respectively. These solutions have been used by the respective authors in building individual models known as AT123D (Analytical Transient 1-, 2-, and 3-Dimensional) and 3DADE (3-Dimensional Advection-Dispersion Equation). AT123D and 3DADE were selected because of their three-dimensional features, their transient mass transport capabilities, and their versatility in simulating a number of different geometric forms that can be used to describe the source of the solute. The addition of these two models into ShowFlow has, in effect, increased the number of modeling scenarios from one to twenty-one.

Numerous analytical models for predicting the transport and fate of solutes in the subsurface media are being used, for example, by the National Research Council (NRC), EPA, and EPRI. Typically, each model deals with a particular problem and, more or less, involves simplification in order to render a possible analytical solution to the governing equation. Because of the variability in problem definition, more than one solution is possible to the same governing equation. Recent analytical solutions have relaxed some of the assumptions, such as the requirement that all solute contamination is entering the groundwater system through one point or that the flow domain, or aquifer, is semi-infinite in all three dimensions.

The selected models AT123D and 3DADE were considered most suitable because they embrace a family of analytical solutions. They both can represent a number of source scenarios, such as point sources, plane sources, or rectangular parallelepiped (cube) sources. The geometry of the source can thus be selected to resemble the actual source as closely as desired. A correct representation of the source becomes critical, particularly in estimating concentrations close to the source. This can be the case in estimating solute concentrations at property lines or at downstream boundaries of disposal areas. Applying a point source to represent areal features can yield erroneous estimates regarding plume development, typically by overestimating the concentrations near the source. This is because in the initial stages of transport, the shape of the source rather than the hydraulic parameters determines the shape of a plume that emanates from that source. Only after prolonged periods of time during which the source was active will the plume be controlled by the advective and dispersive properties of the aquifer and become less dependent on the geometry of that source.

In addition to the geometry of a source, the process of how the source releases the solute into the aquifer will also affect the evolution of the plume (van Genuchten and Alves, 1982). Two types of sources can be distinguished: a constant concentration source and a solute flux source. Both types are now possible options in GRI-ShowFlow. In the case of the constant concentration condition, a solute concentration is maintained at a fixed level at the point(s) that make up the source geometry. The source is described by that geometry and by the concentration value, which has the units of mass per volume (mg/L), which, for dilute solutes in water, is equivalent to parts per million (ppm) (Freeze and Cherry, 1979). In the case of the solute flux source, the solute is introduced at a constant rate, representing a mass loading, for which the units are mass per time (kg/yr). The concentration may vary over time at the point(s) that make up the flux source geometry.

Existing solutions of the three-dimensional advection-dispersion equation can be further divided, based on the length of activity, or duration, of the source. A source can have an initial solute distribution that migrates instantly and in bulk with the groundwater flow. Migration occurs whether or not additional solute is added to the source. Since the source duration may be equal to zero, this type of scenario is called the initial value problem. An initial value scenario requires only the amount of solute released and its approximate distribution (shape and extent) at an arbitrary time. This is embodied in the 3DADE model that is best suited to simulate liquid waste sources. A second scenario is when the source is at a fixed position and only some solute is able to migrate away from the source. The bulk of the source does not move, while the solute dissipates from the source at a prescribed concentration or by a constant flux. This is the so-called inlet value problem. A solid or otherwise immobile waste source is best modeled with the inlet value model, AT123D. The bulk of the source remains at one location, for which the dimensions must be determined. The

length of time during which the source was active and the rate, or concentration, of solute release must also be known.

Although the initial value and the inlet value problems are mathematically related, the two three-dimensional models in GRI-ShowFlow have been derived and developed by different authors using different solution techniques. AT123D, which encompasses the inlet value scenarios, has been developed using Green's functions (Yeh, 1981). This technique suffers from singularity (solution remains undefined) when the duration of source activity equals zero. The 3DADE model, which encompasses the initial value scenarios, is based on the Gauss-Chebyshev quadrature formula and requires different expressions of the solution for every source configuration (Leij and others, 1991). The initial value solutions were developed more recently, and 3DADE is the only model that has been found for such a scenario.

The selection of source geometry, source type, and source duration is critical in modeling plumes because of the various waste depositions. Liquid (solution) wastes, solid wastes, and hydrocarbon or nonaqueous-phase liquid (NAPL) wastes typically require different modeling approaches (Kühnel and Schmit, 1992). A liquid waste source, such as the release of a brine, will be best modeled with the initial value model. A solid or otherwise immobile waste source, such as a sludge pit, is best modeled with the inlet value model. A NAPL waste source, if immobile with respect to the free phase (residual NAPL), will be best modeled as an inlet value source, but if the NAPL is mobile, very different three-phase flow models such as ARMOS or HSSM are required (Kaluvarachchi and others, 1990; Weaver and others, 1994).

The source type should match the waste deposition history. If an infiltration pond receives surface runoff and remains ponded for a period of time, a constant flux source is the appropriate source type. The same source applies to pipe discharges that can be measured over time. A landfarm that periodically receives a sludge with solutes of a concentration in the plow zone maintained at a fixed level is best modeled as a constant concentration source. This scenario also applies to waste pits that receive compounds such as residual NAPLs that slowly leach into groundwater.

The geometry of the source needs to be considered in selecting a model. For example, a solute spill from a leaky valve that dripped and affected a relatively small area can best be described as a point source. Alternately, a vertical line source can be used if the solute was disposed of in an auger hole or is suspected to have otherwise penetrated into the aquifer, for example, as a dense solute. A buried waste disposal trench can be represented by a vertical plane. In the available models, the orientation of this plane can be either in the direction of the groundwater flow or perpendicular to it. A plugged but leaking pipeline, or a duct section, can be approximated by a line, again, with the option of longitudinal or transverse orientation. A horizontal plane source can represent an infiltration pond, a lagoon, or a landfarm, while a three-dimensional source would typically be used to simulate contaminant spreading from a buried waste in the form of disposal pits, sumps, cribs, heaps and piles, caissons, and landfills.

GRI-ShowFlow illustrates the above differences in the source description, which may help clarify the implications of using the various screening models employed by the regulatory agencies and by industry representatives. EPA, for example, is using a point-source description, as well as the Gaussian plume source description (EPA models VHS, EPACML, MULTIMED, and HSSM).

On the other hand, both API and EPRI have incorporated a plane or a cube source description in their respective models (API decision support system [APIDSS] and EPRI MYGRT and ROAM models). Both API and EPRI models are based on the inlet value solutions from the AT123D model or a particular case of it. The application of any of these models may not be appropriate for a given site, particularly if the geometry and the type of the actual contaminant source is not correctly represented by the model. For this reason, GRI-ShowFlow includes all available source descriptions and source types to allow the selection of the best possible representation. The GRI-ShowFlow package brings together the existing models in a user-friendly environment and facilitates comparison between them as well as comparison to new models.

4.1 Using GRI-ShowFlow

Like other Windows™ applications, GRI-ShowFlow will appear in a Program Manager group as an icon and can be started simply by double-clicking with the mouse cursor on the icon. This action will activate introduction screens that provide information about the software. Clicking OK is the only option to continue.

Three steps are required in order generate output with GRI-ShowFlow: model selection, source type selection, and data entry. Model selection should be based on knowledge of the geometry of the contaminant source, for example, a waste pit, a trench, or an infiltration pond. Source type selection reflects the source history, for example, duration of existence, concentration, or discharge rate. Once these selections are made, data can be entered into model-specific input parameter screens. Only then can the selected model be executed.

The selection steps are explained and sample data sets are provided in this manual, as well as the Help System of the GRI-ShowFlow code. A glossary is accessible through the Help System that contains short explanations of the less familiar terms.

4.1.1 Model Selection

The first dialog screen allows the user to select one of three models: SSGPLUME, 3DADE, and AT123D (see Figure 1). The Help button can be clicked to obtain information on model selection and the purpose of individual models. Although different, these models have one thing in common: they use simple mathematical expressions to simulate the distribution of a solute in a groundwater system. The solute distribution is a plume described by concentrations that are calculated in space and time. The concentration distributions calculated by the three models will be different because the models employ different representations of the contaminant source and the aquifer.

The SSGPLUME model should be selected only if a steady-state condition of a plume is required as output. The term "steady state" is used to describe a condition when the plume does not appear to be migrating with the groundwater flow. The amount of solute that leaves the source is equal to the amount of solute diluting and dissipating in the plume, without moving the source's boundaries. This model may be best suited for cases where a solute has been released for long periods of time and where the solute affects the full thickness of an aquifer. The source is a vertical plane with a Gaussian distribution of the solute concentration. SSGPLUME also contains a module to simulate transport processes in the unsaturated zone.

Figure 1. SSGPLUME, 3DADE, or AT123D model is chosen in this screen by clicking on the respective radio button.

The AT123D model simulates groundwater plume development for an inlet value source in the form of a point, a line, a plane, or a cube. The source itself cannot move. AT123D is, therefore, suited to simulate solutes leaching from immobile sources such as solids or sludges, including residual hydrocarbons. It is not suited for simulation of migrating sources that originate from liquids, such as discharges of brines or produced water. The aquifer in AT123D may be infinite in three dimensions, or it may have a finite width, a finite depth, or both. This model is, therefore, suited for modeling of bounded aquifers where the plume size may be affected by the aquifer dimensions.

3DADE is the initial value model in which the solute residing in a given space is allowed to move along with the groundwater flow. An example of an initial value scenario is a soil column that received concentrated solute in the center of the top of that column. After injection of the solute, water is applied uniformly to the top of the column, and the entire solute source is tracked as it disperses from the moving source. A typical application of 3DADE would be for liquid sources in a horizontally flowing groundwater system, such as surface runoff or wastewater

discharges into infiltration pits or trenches. The source configuration is either a vertical plane or a cube. The aquifer is assumed to be infinite in the x, y, and z dimensions.

After selecting one of the three available models and confirming the selection by clicking on OK, the user can proceed by entering site-specific data. This is done through the menu item Edit in the command line of the initial window. This menu also features the Help menu, which can be used to obtain on-screen information regarding the selection. The Edit item contains two selections: Select Source and Edit Parameters. The 3DADE and AT123D models offer various source configurations. The user is prompted to select the source prior to entering data through the Edit Parameters command when using either of these models.

4.1.2 Source Type Selection

The three analytical models in GRI-ShowFlow use a orthogonal (x, y, z, or Cartesian) coordinate system to describe the dimensions and location of a source as well as points of interest in determining concentration. The x-dimension, or longitudinal axis, is the direction of the one-dimensional groundwater flow velocity in the aquifer. The z-dimension is the vertical direction measured positive downwards, with a value of zero at the water table. The horizontal direction perpendicular to the direction of the flow is the transverse direction, represented by the y-axis. All three models assume groundwater to flow parallel to the x-axis. To visualize a plume on the screen and on printed graphs, the models place the source on the left side of the screen while the plume is moving with the flow to the right.

Together, the models under the GRI-ShowFlow interface allow nine geometric source configurations. Specific configurations may be available only in one or two models. The models and their corresponding choices of source configurations are shown in the Source Type Selection screen, Figure 2. The selected configuration source should match the shape of the actual contaminant source as closely as possible. In the following configurations, the subscript p refers to

SOURCE TYPE SELECTION				
<p>Point</p> <p>SOURCE</p> <p>☒ Solute Flux</p> <p>☐ Constant Conc.</p>	<p>2 Dimensional vertical rectangular</p> <p>SOURCE</p> <p>☐ Solute Flux</p> <p>☐ Constant Conc.</p>	<p>2 Dimensional horizontal rectangular</p> <p>SOURCE</p> <p>☐ Solute Flux</p> <p>☐ Constant Conc.</p>	<p>2 Dimensional parallel plane</p> <p>SOURCE</p> <p>☐ Solute Flux</p> <p>☐ Constant Conc.</p>	<p>3 Dimensional cube</p> <p>SOURCE</p> <p>☐ Solute Flux</p> <p>☐ Constant Conc.</p>
<p>OK Help</p>				

Figure 2. Source type selection screen with radio buttons to select source type and configuration in the three-dimensional models.

an arbitrary point of reference (origin), which is typically zero; the subscripts 1 and 2 refer to points on the orthogonal axes other than the origin:

1. A point source specified by the coordinates (x_p, y_p, z_p)
2. A line source parallel to the x-axis specified by the pair of coordinates (x_1, y_p, z_p) and (x_2, y_p, z_p)
3. A line source parallel to the y-axis specified by the pair of coordinates (x_p, y_1, z_p) and (x_p, y_2, z_p)
4. A line source parallel to the z-axis specified by the pair of coordinates (x_p, y_p, z_1) and (x_p, y_p, z_2)
5. A plane source perpendicular to the x-axis, specified by width from (x_p, y_1, z_p) to (x_p, y_2, z_p) and depth from (x_p, y_p, z_1) to (x_p, y_p, z_2)
6. A plane source perpendicular to the y-axis, specified by length from (x_1, y_p, z_p) to (x_2, y_p, z_p) and depth from (x_p, y_p, z_1) to (x_p, y_p, z_2)
7. A plane source perpendicular to the z-axis, specified by length from (x_1, y_p, z_p) to (x_2, y_p, z_p) and width from (x_p, y_1, z_p) to (x_p, y_2, z_p)
8. A rectangular parallelepiped (cube) source specified by length from (x_1, y_p, z_p) to (x_2, y_p, z_p) , width from (x_p, y_1, z_p) to (x_p, y_2, z_p) , and depth from (x_p, y_p, z_1) to (x_p, y_p, z_2) .
9. A vertical plane source, perpendicular to the x-axis, specified by point coordinates (x_p, y_p, z_p) of concentration maximum and standard deviation. This distribution represents a Gaussian source.

Selection is aided by the sketches on the model selection and the source selection screens depicting the source geometry and the direction of groundwater flow in the orthogonal coordinate system. The source configuration should be selected to fit the scenario to be modeled most closely. For example, for a sump or a spill from a leaky valve that dripped and affected a relatively small area, a point geometry (Configuration 1) may describe the source most closely. Alternately, a vertical line source (Configuration 4) can be used if the solute was disposed of in an auger hole, an injection well, or the solute is suspected to have otherwise penetrated into the aquifer, for example, as a dense solute. If no borders can be drawn around a spill area, but only the center or hot spot can be pinpointed, the contaminant distribution may be best described by a Gaussian plume source (Configuration 9).

If a surface spill was large and sudden and an area was flooded before the contaminant infiltrated, the horizontal plane source (Configuration 7) may be the best source geometry to choose. This configuration is suited for containment lagoons and infiltration ponds collecting surface runoff or water from hydrostatic pressure tests. A buried waste disposal trench can be represented by a vertical plane (Configuration 5 or 6, depending on trench orientation), while a plugged but leaking pipeline section will correspond to a line source (Configuration 2 or 3,

depending on pipeline orientation). A three-dimensional source (Configuration 8) would typically be used to simulate contaminant spreading from buried waste in the form of disposal pits, cribs, heaps, piles, caissons, and landfills. Note that the lengths of the lattices of a "cube" source can be varied independently so that any three-dimensional body with rectangular faces can be described as a cube source.

Not all source geometries are available in all the three models. In SSGPLUME, there is only one source geometry, which is a vertical plane with a Gaussian distribution of the solute concentration corresponding to source Configuration 9. For AT123D, the source configuration can be any one of 1 through 8. In 3DADE, the available source configurations are for 5 and 8. Furthermore, Configurations 1 to 8 have two alternative types, a constant concentration source and a solute flux source. These must be selected by clicking on the radio buttons under the respective sketches of the source configuration (see Figure 2).

A constant concentration should be selected if the solute is entering the groundwater system at some constant, limiting value. The solubility of a compound is typically associated with such a limiting value. The source definition required as input for this scenario is in units of concentration (mg/L or ppm). A solute flux condition is selected if the contaminant release occurred at a fixed rate over a given period of time. The flux source is defined, in this case, in units of mass per time (kg/yr), and the duration of the release is determined by the time the release began and the time the release ended.

The user should select one of the three models based on the knowledge of how the solute contaminant is introduced into the environment. Particular attention should be given to the type of the solute source, whether it is sharply delineated, such as berms or trench walls, or it has vague boundaries such as "stained areas" or nondescript "pit locations." SSGPLUME can be used for the latter, while AT123D or 3DADE provide for more accurate source descriptions. If a source is fixed at one place from which only the solute leaches, the AT123D model is probably the most suitable. This is typically a scenario for solid or semisolid sources, which by themselves do not move, but they release a solute from a fixed location over a prolonged period of time. If, on the other hand, the source is a liquid, for example a brine deposited into a disposal pit, the bulk of the source can flow with the groundwater as a contaminant pulse while the solute disperses from the source along the way. This scenario is better simulated with the 3DADE model.

After selecting the appropriate source configuration and type, the user can proceed with data input through the Edit Parameters window. This window appears automatically when OK is clicked in the Source Type Selection window. It can be also activated from the main Model Selection window by pulling down the Edit menu. Since the models differ slightly in the respective input requirements, data entry will be discussed separately for the three models. Three sample input data sets are provided in this manual, and three additional data sets are discussed in the GRI-ShowFlow Help System.

4.2 ShowFlow: The Windows™ Interface

Many potentially useful models involve sophisticated mathematics and rudimentary computer programming, often resulting in a program that is as practically unapproachable as it is theoretically sophisticated. In part, this is because theoreticians often write their own program code, focusing

not so much on the user as on the results, which are often no more than an array of numbers. Furthermore, computer languages not conducive to producing a user-friendly interface are still in heavy use.

The use of models, however, has been generally adopted by groundwater scientists and engineers, because models are relatively inexpensive and, through multiple sensitivity simulations, offer an insight into the application of physical models to natural systems and help to strengthen one's intuition about the processes involved. As groundwater models grow in interest and application, so does the need for programs that can be used and understood by a broader audience. Industry managers, policy makers, and researchers can all benefit from more productive groundwater modeling software. The development of such software has been made easier by new operating systems and graphical environments such as that of Microsoft® Windows™.

The Windows™ graphical environment and ShowFlow make the development, analysis, and application of groundwater modeling programs a more productive and efficient process. Since the ShowFlow program is distinct from the model it is executing, a modeler can make changes to a developing scenario and run it from ShowFlow to see its effects. Different versions of the model can be compared easily. Once a particular scenario has been developed, ShowFlow facilitates the process of examining sensitivities to changes in parameters or of conducting sensitivity simulations. This is easily accomplished by displaying more than one simulation on one screen. This feature and its ease of use make ShowFlow a visual teaching tool with greater potential than that of conventional modeling interfaces.

The original Windows™ application (ShowFlow Version 1.0) was designed generally for analytical groundwater models and specifically for the groundwater contamination model SSGPLUME. It was written by John Tauxe (Tauxe, 1990) as a thesis requirement for the M.S. degree in Engineering at the University of Texas at Austin. Version 2.0 of the ShowFlow code (Tauxe, 1991) has been designed specifically to allow for adding other models, which is what this work encompassed. ShowFlow was intended to be generalized, and instructions were provided to enable a user to perform the necessary modifications. Without the advanced design, flexibility, and documentation of ShowFlow, the development of the present package would be an order of magnitude more complex.

In the present package, ShowFlow acts as a shell for the models described in Section 4.1 and performs four basic functions: file management, preprocessing of input data, model execution, and postprocessing of data generated by the models. Most of the original ShowFlow code operates the key items on the initial menu: FILE, EDIT, and MODEL (see Figure 3). With the addition of three-dimensional and transient models, certain sections of the code had to be modified as follows:

1. Three-dimensional scenarios require slicing in three directions to fully visualize a plume. ShowFlow 2.0 accommodated only two orientations.
2. Transient models require data input on solute release and the timing of that release. ShowFlow, using a steady-state model, did not provide for time-variable input.

Figure 3. Command Menu screen manages the input, execution, and output of the models. Edit, Model, and Graph are the respective menu items for these modeling functions.

3. Significant Help information had to be provided to assist the user in matching a scenario to a model. ShowFlow did have a Help function, but it did not consider multiple options for the description of a contaminant setting.

Other changes, such as an icon-driven source selection process, context-sensitive help, and the inclusion of a glossary, are some of the further enhancements to the original code. The concept, however, is based on the code by John Tauxe, and due credit is given.

GRI-ShowFlow requires model-specific input to execute any of the available groundwater models. Some input, such as contaminant behavior parameters, can be obtained from literature, and some input, such as type of contaminant and source description, requires site-specific information. Literature sources for some of the contaminant-specific input are Rai and Zachara (1984) for partitioning coefficients of inorganic constituents; Lyman and others (1982) for partitioning coefficients of organic constituents; Gherini and others (1988, 1989), for degradation rate constants; Gelhar and others (1985) for dispersion coefficients of various scenarios; Harju and Schmit (1993) for selected physicochemical constants; and Freeze and Cherry (1979) for various

groundwater flow and porosity ranges. The typical ranges of the input parameters are also provided through the Help system throughout the program.

The input requirements differ somewhat for the individual models. The Edit Parameter screens of GRI-ShowFlow are, therefore, discussed separately for each model in the following sections.

4.3 The SSGPLUME Model

The Steady-State Gaussian Plume model (SSGPLUME) is the model used by the original ShowFlow interface. SSGPLUME uses straightforward algebraic solutions of steady-state, two-dimensional flow, and transport equations, requiring few computational resources. The theoretical and mathematical basis for SSGPLUME has been developed by Smith and Charbeneau (1990) for an uncertainty analysis required by an exposure assessment procedure. They have demonstrated that SSGPLUME is a useful tool for uncertainty analyses when examining the relative importance of various site parameters.

The basis for SSGPLUME is a deterministic model that ultimately predicts single-phase contaminant concentrations using a one-dimensional vertical soil-water solute transport model coupled with a two-dimensional, horizontal groundwater flow, single-solute fate and transport model used by EPA (Huyakorn and others, 1986). The solution is, therefore, a quasi-three-dimensional model, representing the aqueous-phase concentration of a contaminant underlying a specified area and a two-dimensional groundwater plume in the saturated zone extended in the direction of the groundwater flow.

Contaminant transport, as represented by SSGPLUME and described by Smith and Charbeneau (1990), can be applied to problems associated with land treatment or the disposal of organic compounds. The aqueous-phase concentration of an organic constituent is traced as leachate from a zone of contamination in the upper part of the vadose zone, through adsorption and further degradation as it travels vertically through the lower (initially uncontaminated) part of the vadose zone, and, finally, to its distribution within the saturated zone below. Mixing of the constituent upon reaching groundwater is assumed to produce a Gaussian concentration distribution beneath the source. The contaminant further disperses as the plume is transported horizontally in the flow direction.

ShowFlow execution of SSGPLUME enables visualization of only the solute concentrations in the saturated zone. The unsaturated module, although executed, does not lend itself to the graphing of profiles or contour maps, mainly because of the one-dimensional nature of the flow. Since SSGPLUME was the original model in the ShowFlow interface, the code was left as is, although newer transient models have been developed for the Gaussian source (Huyakorn and others 1986, 1987). These transient models for a Gaussian plume source have been incorporated in the latest release of EPA's multimedia exposure assessment model, MULTIMED Version 2.0 (Salhotra and others, 1993). The inclusion and comparison in GRI-ShowFlow of these new models may be considered as a future task.

When the SSGPLUME model is selected, the source is automatically set to the Gaussian plane source, since this is the only source available in this model. The interface presents to the user the Edit Parameter screen as shown in Figure 4. This screen serves as the input field for all

Parameter File Editor for SSGPlume			
Current File: EXAM1.PAR		<input type="button" value="OK"/>	
Run Title:		<input type="button" value="Cancel"/>	
INPUT SCREEN FOR SSGPLUME		<input type="button" value="Help"/>	
SITE DESCRIPTION:		CONTAMINANT CHARACTERISTICS:	
X minimum point (m)	<input type="text"/>	Loading rate (g/m ² -d)	<input type="text"/>
X maximum point (m)	<input type="text"/>	Water bulk partition coefficient	<input type="text"/>
X resolution (number of points)	<input type="text"/>	Henry's Law constant (no dim)	<input type="text"/>
Y minimum point (m)	<input type="text"/>	Schmidt number	<input type="text"/>
Y maximum point (m)	<input type="text"/>	(Range 0.2 to 5.0; 1.0 typical)	
Y resolution (number of points)	<input type="text"/>	AQUIFER CHARACTERISTICS:	
Width of facility (m)	<input type="text"/>	Seepage velocity along X (m/d)	<input type="text"/>
Area of facility (m ²)	<input type="text"/>	Dispersivity in X (m)	<input type="text"/>
10-meter wind velocity (m/s)	<input type="text"/>	Dispersivity in Y (m)	<input type="text"/>
Water infiltration rate (m/d)	<input type="text"/>	Retardation factor (no dim)	<input type="text"/>
VADOSE ZONE CHARACTERISTICS:		First-order decay rate (1/d)	<input type="text"/>
Vadose zone thickness (m)	<input type="text"/>	Regional infiltration rate (m/d)	<input type="text"/>
Contaminated zone thickness (m)	<input type="text"/>	Saturated thickness (m)	<input type="text"/>
First-order decay rate (1/d)	<input type="text"/>	Porosity	<input type="text"/>

Figure 4. Input screen for the SSGPLUME model. The Help button will guide the user to a typical range for every parameter.

parameters required by the model. A valid value must be entered in each field. Typical ranges are provided for each parameter, and an error check is made by the code to prevent input of impossible values. The input fields have been grouped into four categories:

1. Site Description:

X minimum point [m]: X_{min} , typical range: 0-100
 X maximum point [m]: X_{max} , typical range: 1-2000

These limits specify the range of area over which SSGPLUME will calculate contaminant concentrations, with X measured in the direction of groundwater flow. The range from X_{min} to X_{max} can be envisioned as the viewing window in which the plume can be examined.

X resolution (number of points), typical range: 25-100, default 100

This is the number of points in the X direction of the solution grid. More points will result in smoother graphs, but also in larger files and slower executions. On 486 PC computers or higher, a resolution value of 100 can be easily accomplished.

Y minimum point [m]: Y_{min} , typical range: 0-100
 Y maximum point [m]: Y_{max} , typical range: 1-2000

Y resolution (number of points), typical range: 25-100, default 100

These parameters are identical to the above, but they relate to the transverse axis (y-dimension). The resolution can be set to 100 for most fast computers.

Width of facility [m]: W , typical range: 1-1000

Area of facility [m^2]: A_f , typical range: 1-1,000,000

The areal size of the facility or disposal site is defined by its width W , measured in the transverse direction to the groundwater flow, and its area A_f on the land surface. It assumes a rectangular shape.

10-meter wind velocity [m/s]: U_{10} , typical range: 2.5-6.5 [m/s]

This is the average wind velocity at the site, measured in meters per second at a height of 10 meters from the ground surface.

Water infiltration rate at the facility [m/d]: I_f , typical range: 0-0.03 [m/d]

I_f is the net (effective) infiltration rate of water at the site. I_f generally ranges from one-tenth to one-half of the total rainfall.

2. Vadose Zone Characteristics:

Vadose zone thickness [m]: L_v , typical range: 0-50

This is the thickness of the entire vadose (unsaturated) zone.

Contaminated zone thickness [m]: L_u , typical range: 0.1-50

This is the thickness of the upper part of the vadose zone, which contains the initial contamination.

Degradation rate constant in the vadose zone [d^{-1}]: λ_v , typical range: 0-10

This is the first-order degradation rate constant for the constituent in the vadose zone. A different constant can be effective in the saturated zone. Substances that do not degrade because of chemical, physical, or biological processes will have $\lambda_v = 0$. Substances that do transfer or degrade will have a λ greater than zero. This parameter is comparable to half-life (t_{half} , in days) of radioactive materials. Half-life is the time necessary for a compound to lose half of its (radio)activity or concentration and is related to λ through:

$$\lambda = \frac{0.693}{t_{half}}$$

This equation is also very useful when converting half-life values from [d^{-1}] to [yr^{-1}] and in reverse.

3. Contaminant Characteristics:

Loading rate per area [$\text{g}/\text{m}^2/\text{d}$]: m_L , typical range: 0.1–100,000

The mass-loading rate is calculated as mass flux per unit area. The units employed here determine those of the final groundwater concentration. If m_L is expressed in $\text{g}/\text{m}^2\text{-d}$, the resultant concentrations will be in g/m^3 , which, for solutes, is equivalent to mg/L . If concentration units of g/L are desired, then m_L should be given in $\text{kg}/\text{m}^2\text{-d}$, although the graph labels would still read mg/L .

Water bulk partitioning coefficient [no dim.]: B_w , typical range: 0.0–1.0

This is the volume of pollutant in the aqueous phase divided by the total volume. It is defined as:

$$B_w = \theta_w + \theta_g K_H + \theta_o K_o + \rho_b K_s$$

where:

θ_w is the volumetric water content [no dim.].

θ_g is the volumetric gas content [no dim.].

K_H is Henry's Law constant [no dim.].

θ_o is the volumetric oil content, if free phase present [no dim.].

K_o is the oil–water partitioning coefficient [no dim.].

ρ_b is the soil bulk density [g/cm^3].

K_s is the soil–water partitioning coefficient [cm^3/g].

Note that K_s in this equation is the partitioning in the uncontaminated soil only. By definition, its value cannot exceed unity: K_s = concentration in soil ($\mu\text{g}/\text{g}$) divided by concentration in water ($\mu\text{g}/\text{mL}$). This is because the number of sorption sites in the soil is limited, while the amount of solute in the percolating water is assumed to be unlimited. In steady-state systems, this condition is plausible.

Henry's Law constant [no dim.]: K_H , typical range: 0.000001–0.1

This Henry's Law constant is calculated as the pollutant concentration in the gaseous phase divided by that in the water phase.

Substances with K_H around or below 10^{-6} are less volatile than water. They tend to partition into the aqueous phase and can be considered essentially nonvolatile. An example in this class is ethylene glycol.

Substances with K_H in the range from 10^{-6} to 10^{-2} volatilize significantly. Most polycyclic aromatic and halogenated hydrocarbons lie in this range.

For substances with K_H of 10^{-2} and above, volatilization is the dominant mass transfer mechanism. Most of the compound will partition into the gaseous phase. An example in this class is octane.

Schmidt number [no dim.]: v_g/D_g , typical range: 0.2–5.0

The Schmidt number is the dimensionless ratio of the kinematic viscosity v_g and the diffusivity D_g in water of a gaseous phase of the constituent. D_g and v_g may be expressed in any identical units. The typical value is 1.0.

4. Aquifer Characteristics:

Seepage velocity along X [m/d]: v , typical range: 0.001–10

This is the groundwater longitudinal (or linear) seepage velocity. Note that the linear seepage velocity (v) is related to the so-called Darcy velocity (V) through $v = V/n$, where n is the aquifer porosity.

Dispersivity in X (longitudinal) [m]: a_L , typical range: 0.1–100

Dispersivity in Y (transverse) [m]: a_T , typical range: 0.01–10

Yeh (1981) suggests the following values:

	Sand	Silt	Clay
a_L [m]	10 to 100	1 to 10	0.1 to 1
a_T [m]	1 to 10	0.1 to 1.0	0.1 to 0.1

Gelhar and others (1985) give the following equations to obtain estimates of the dispersivities:

$$a_L = L/10$$

$$a_T = a_L/8$$

where L is the simulation length or the length of the suspected travel path of the solute.

Retardation factor [no dim.]: R , typical range: 1–100,000

The retardation factor is used to quantify processes that inhibit migration of the pollutant through the porous medium. A value of $R = 1$ implies no retardation, and values of $R > 1$ imply retardation.

The retardation factor is defined as follows:

$$R = 1 + \frac{\rho_b K_d}{n}$$

where:

n = effective porosity for the saturated zone [cm^3/cm^3]

ρ_b = bulk density of the porous media [g/cm^3]

K_d = distribution coefficient [cm^3/g]

Degradation rate constant in the aquifer [d^{-1}]: λ , typical range: 0–10

This is the first-order degradation rate constant for the constituent in the saturated zone. A different constant can be effective in the vadose zone. Substances that do not degrade because of chemical, physical, or biological processes will have $\lambda = 0$. Substances that do transfer or degrade will have a λ greater than zero. This parameter is comparable to half-life of, for example, radioactive materials. Half-life is the time necessary for a compound to lose half of its (radio)activity or concentration and is related to λ through:

$$\lambda = \frac{0.693}{t_{\text{half}}}$$

Regional infiltration rate [m/d]: I_R , typical range: 0–0.01

The regional infiltration rate to the aquifer enables the dilution of the contaminant plume by recharge water to be calculated. In general, this will be less than one-fourth of the total rainfall, but this also depends upon whether the site is mostly paved and other local site conditions.

Saturated thickness [m]: b , typical range: 1–100

This is the average saturated thickness of the aquifer.

Porosity [no dim.]: n , typical range: 0.05–0.50

This is the porosity of the saturated aquifer.

Several references can be consulted for data that are not site-specific. A number of sources that are also given in the Help System include the following :

- Water infiltration rates
American Petroleum Institute, 1996, Estimation of infiltration and recharge for environmental site assessment: Health and Environmental Sciences Department, API Publication Number 4643, Washington D.C.

- Partitioning coefficients of inorganic constituents
Rai, D., and Zachara, J., 1984, Chemical attenuation rates, coefficients, and constants in leachate migration, vl. 1, a critical review: Electric Power Research Institute, Report EA-3356, Palo Alto, California, 336 p.
- Partitioning coefficients of organic constituents
Lyman, W.J., Reeho, W.F., and Rosenblatt, D.H., 1982, Handbook of chemical property estimation methods - environmental behavior of organic compounds: New York, McGraw-Hill Book Company.
- Compilation of various physicochemical constants for organic constituents
Harju, J.A., and Schmit, C.R., 1993, An overview of the subsurface transport and fate of constituents associated with gas industry operations: Gas Research Institute, Topical Report GRI-92/0477, Chicago, Illinois.
- Partitioning constants, degradation rates, and retardation factors
Olson, R.L., and Davis, A., 1990, Predicting the fate of organic compounds, part 1, Hazardous Materials Control, v. 3, May-June, p. 39-64.

Olson, R.L., and Davis, A., 1990, Predicting the fate of organic compounds, part 2, Hazardous Materials Control, v. 3, July-August, p. 18-37.
- Degradation rate constants
Gherini, S.A., Summers, K.V., Munson, R.K. and Mills, W.B., 1988, Chemical data for predicting the fate of organic compounds in water. vl.1 (Technical basis) and v. 2 (Database): Electric Power Research Institute, Report EA-5818, Palo Alto, California.
- Dispersion coefficients
Gelhar, L.W., Mantoglou, A., Welty, C., and Rehfeldt, K.R., 1985, A review of field-scale physical solute transport processes in saturated and unsaturated porous media: Electric Power Research Institute, Report EA-4190, Palo Alto, California.
- 10-m wind velocity
United States Environmental Protection Agency, 1985, Rapid assessment of exposure to particulate emissions from surface contamination sites: Office of Health and Environmental Assessment, EPA/600/6-86/002, Washington, D.C.
- Drinking water standards and other solute concentration limits
Maximum concentration limits (MCLs) have been established for the United States by the EPA. However, these MCLs are subject to change and the list of chemicals for which MCLs have been set is growing. One way to find recent MCLs is to search the Internet. Both EPA and the Government Printing Office have World Wide Web sites. Consult these sources for concentration limits of the chemicals of interest.
U.S. EPA: <http://www.epa.gov/ow/regs/>
U.S. GPO: http://www.access.gpo.gov/su_docs/

4.4 The 3DADE Model

The solutions to 3DADE have been published by Leij and others (1991) for five relatively simple scenarios of solute transport in semi-infinite, homogeneous, porous media. Three of these solutions were derived for sources in a orthogonal coordinate system, while two solutions considered a cylindrical system. The solutions in the orthogonal system include a semi-infinite horizontal plane, a finite horizontal plane, and a cube source, while in the cylindrical system, the solutions are derived for a vertical circular plane and a horizontal cylindrical source. GRI-ShowFlow includes only the finite horizontal plane and the cube source in the orthogonal coordinate system. The semi-infinite plane and the cylindrical sources were left out of the present package because they do not represent groundwater scenarios found in actual solute release settings.

Transient transport can be simulated with the 3DADE solutions. Although the groundwater flow has to be uniform and steady state at all times, the solutes that are entering the groundwater system can be "turned on" and "turned off" at arbitrary times set by the user. This transient solute loading is expressed as the duration of the solute source. An infinite duration will result in a steady-state transport simulation, and a finite duration results in a pulse-type injection that originates from a fixed point. This is the so-called inlet value problem. If the duration is set to zero, a step displacement is simulated, which appears as a drifting source. This is the initial value problem. Each case has been solved by Leij and others (1991) for a continuous concentration at the inlet and for a prescribed solute flux at the inlet.

The user is prompted in the Source Type Selection window (Figure 2) to select one of the four options describing the shape of the source and its type. By clicking on one of the respective radio buttons, the user is directed to the Edit Parameters screen (Figure 5). This screen groups the

Parameter File Editor for 3DADE Cube Source

Run Title: File Name:

Contaminant Setting:

Source length in X (m)

Source width in Y (m)

Source depth in Z (m)

Viewing Window Area Definition:

Offset in X dimension (m)

Start X value for viewing (m)

End X value for viewing (m)

Contamination Release Timing:

Duration waste release (yr) ..

Source flux (kg/yr)

Time of observation (yr)

Contaminant Movement Parameters:

Groundwater seepage velocity in the X or flow direction (m/yr).....

Dispersivity in X (m).....

Dispersivity in Y (m).....

Dispersivity in Z (m).....

Contaminant Behavior Parameters:

Retardation factor (no dim)

First-order decay rate (1/yr).....

Figure 5. Input screen for the 3DADE model with cube source. The Help button will guide the user to a typical range for every parameter.

input parameters into five categories. Since no vadose zone modeling is performed by this model, the parameters pertain only to information about the saturated subsurface.

1. Contaminant Setting:

Source width in Y [m]: W, typical range: 1-1000

Source depth in Z [m]: D, typical range: 0.1-50

The width (W) and depth (D) describe the vertical plane source perpendicular to the groundwater flow. Note that the x-axis is positioned at the center of W and that D is measured from the water table downward.

Source length in X [m]: L, typical range: 1-1000

By the addition of this dimension to width and depth, a cube source is defined. This field appears only if a cube source has been selected.

2. Viewing Window Area Definition:

Offset in X dimension [m]: X_{off} , typical range: 0-100

For most scenarios, the value for X_{off} can be set to zero. Only if the advection is low compared to the dispersion can the solute actually migrate upgradient from the source. The offset allows the user to view that portion of the aquifer that is X_{off} meters "upstream" from the source to view the full plume development.

Start X value for viewing [m]: X_1 , typical range: 0-100

End X value for viewing [m]: X_2 , typical range: 1-2000

These two values define the window into which the plume will be plotted. Typically, $X_1 = 0$, and X_2 corresponds to the approximate length of the plume. The values can be decreased in subsequent simulations to zoom in at a certain section of the plume.

3. Contamination Release Timing:

Duration of waste release [yr]: T_d

A value is entered here that describes the length of the contaminant pulse in years. Note that 3DADE allows T_d to be set to zero, for which case an initial value scenario is obtained.

Source concentration [mg/L]: C_0 , typical range: 0-10,000 [mg/L]

This is the solute concentration entering the aquifer. Concentrations above 10,000 mg/L (equivalent to 1%) are possible, but at these concentrations the solute affects the density of the groundwater. This effect is not simulated by any of these analytical models. Therefore, caution should be taken when using them to simulate plumes of highly concentrated solutes.

Solute flux [kg/yr]: F_0 , typical range: 0–1,000,000

F_0 is the amount of solute that enters, at a constant rate, the groundwater system per year. The solute enters the aquifer evenly through every point of the selected source configuration. Depending on the source configuration, the flux is expressed either per area (plane source) or per volume (cube source). The numerical values for the flux must be greater than zero. For very high fluxes (causing solute concentrations greater than 1%), caution must be taken so that density effects are not neglected.

Time of observation [yr]: T_{obs} , typical range: 0–500

Because transient solutions are employed by 3DADE, the time of observation T_{obs} for which output is desired must be specified. Two particular times of interest can be distinguished: $T_{obs} < T_d$ and $T_{obs} > T_d$, where T_d is the duration of waste release. The first condition shows a plume at a time when the source is still producing solutes, and the second condition shows a plume for which the source has been terminated.

4. Contaminant Movement Parameters

Average groundwater velocity in the X, or flow direction [m/yr]: V , typical range: 1–500

This is the groundwater front (or Darcy) velocity. Note that the Darcy velocity (V) is related to the seepage velocity (v) through $V = v \cdot n$, where n is the aquifer porosity.

Dispersivity in X [m]: a_L

Dispersivity in Y [m]: a_T

Dispersivity in X [m]: a_v

These are the longitudinal, transversal, and vertical dispersivities in an isotropic aquifer. Typical ranges are from 0.01 to 100 [m]. Various methods can be used to estimate a dispersivity. Yeh (1981) suggests the following values:

	Sand	Silt	Clay
a_L [m]	10 to 100	1 to 10	0.1 to 1
a_T [m]	10 to 10	0.1 to 1.0	0.01 to 0.1
a_v [m]	1 to 10	0.1 to 1.0	0.01 to 0.1

Gelhar and others (1985) gives the following equations to obtain estimates of the dispersivities:

$$\begin{aligned}a_L &= L/10 \\a_T &= a_L/8 \\a_v &= a_L/160\end{aligned}$$

where L is the simulation length or the length of the suspected travel path of the solute.

5. Contaminant Behavior Parameters

Retardation factor [no dim.]: R , typical range: 1–100,000

Retardation is used to quantify processes that inhibit migration of the pollutant through the porous medium. A value of $R = 1$ implies no retardation, and values of $R > 1$ imply retardation.

The retardation factor is as follows:

$$R = 1 + \frac{\rho_b K_d}{n}$$

where:

n = effective porosity for the saturated zone [no dim.].

ρ_b = bulk density of the porous media [g/cm³].

K_d = distribution coefficient [cm³/g].

First-order decay rate in the aquifer [yr⁻¹]: λ , typical range: 0–100

This is the first-order degradation rate constant for the constituent in the saturated zone. Substances that do not degrade because of chemical, physical, or biological processes will have $\lambda = 0$. Substances that do transfer or degrade will have a λ greater than zero. This parameter is comparable to half-life (t_{half} , in years) of radioactive materials. Half-life is the time necessary for a compound to lose half of its (radio)activity or concentration and is related to λ through:

$$\lambda = \frac{0.693}{t_{\text{half}}}$$

Note that in contrast to the SSGPLUME model, 3DADE does not consider the regional infiltration rate (I_R). This means that no dilution of the plume is allowed by groundwater recharge. The present solutions limit the use of 3DADE to plumes in confined aquifers that do not receive influx of water from the surface. However, there is a production term in the original 3DADE solution that represents a zero-order process (a constant source throughout the aquifer). This term has been used in the original 3DADE program to represent generation of a by-product. Recharge and production are both zero-order processes, represented by constant coefficients. The 3DADE solutions could be modified for unconfined aquifers. The applicability of such an option should be investigated further.

4.5 The AT123D Model

The AT123D model has been developed by Professor Gour-Tsyh Yeh at Oak Ridge National Laboratory, Oak Ridge, Tennessee. The model fully exploits the capacity of analytical solutions to the advection–dispersion equation, and their use has been demonstrated through simulations of solute transport, heat flow, and radioactive decay (Yeh, 1981).

Only the solute transport version of AT123D has been incorporated into the GRI-ShowFlow interface. In this form, AT123D simulates groundwater plume development from eight different source configurations, of which seven are a special case of the cube source geometry. For all sources, the solute can be introduced into the aquifer by one of two methods: as a constant concentration or as a constant flux. The solutions of the AT123D model simulate transient solute transport, for which the duration of the pulse must be entered. This duration cannot be equal to zero. This is a major difference between the 3DADE and AT123D models. Whereas the 3DADE model allows a pulsed contaminant source to migrate with the plume, the sources in AT123D cannot move. AT123D is, therefore, only suited to simulate immobile sources from which the solutes are leaching but that leave the bulk contamination in place. Typical examples of such scenarios are solid wastes, sludges, or residual hydrocarbons.

A feature that the other models do not have is that the aquifer in AT123D does not have to be infinite in its width and depth. The aquifer may have a finite width, a finite depth, or both. This model is, therefore, suited for modeling of small aquifers where the plume size may be affected by the aquifer dimensions. These so-called boundary effects are visible on the plume shape only when the depth or the width of the aquifer is of the same order of magnitude as the depth and the width of the waste facility, expressed in source dimensions.

Note that AT123D does not have a zero-order sink or source term, so that infiltration of recharging water into the plume is not considered. This means that the AT123D model is suited only for the simulation of confined aquifers where a plume is not being diluted by recharge. When used for modeling of transport in unconfined aquifers, the plume concentrations are typically overestimated. This has been one of the reasons that the EPA's model, VHS, which is a special case of the AT123D model (a point source), did not withstand criticism, and its use as a delisting model has been discontinued (NRC, 1990).

The input data required by the AT123D model are entered in the Edit Parameters screen as shown in Figure 6. The data are grouped in five blocks:

1. Contaminant Setting:

Source length in X [m]: L, typical range: 1-1000

Source width in Y [m]: W, typical range: 1-1000

Source depth in Z [m]: D, typical range: 0.1-50

These dimensions describe the cube source. If a plane source or a point source is chosen, the fields that do not require input will be hidden, and the values for W, D, or L will be automatically set to zero. A line source is a special case of the plane source where either width, depth, or length is set to zero.

Note that the x-axis is positioned at the center of W and that D is measured from the water table downward.

Aquifer thickness [m]: Z_m , typical range: 5-100

Aquifer width [m]: Y_m , typical range: 100-2000

Parameter File Editor for AT123D Cube Source			
Run Title: INPUT SCREEN FOR AT123D MODEL		File Name: EXAM2.PRM	
Contaminant Setting:		Contaminant Movement Parameters:	
Source length in X (m)		Groundwater seepage velocity in the X or flow direction (m/yr)	
Source width in Y (m)		Dispersivity in X (m)	
Source depth in Z (m)		Dispersivity in Y (m)	
Aquifer thickness (m) (0=∞)		Dispersivity in Z (m)	
Aquifer width (m) (0=∞)			
Viewing Window Area Definition:		Contaminant Behavior Parameters:	
Offset in X dimension (m)		Retardation factor (no dim)	
Start X value for viewing (m) ..		First-order decay rate (1/yr)	
End X value for viewing (m) ..			
Contamination Release Timing:			
Duration waste release (yr) ...		<div style="display: flex; justify-content: space-around;"> <div style="border: 1px solid black; padding: 5px 15px;">OK</div> <div style="border: 1px solid black; padding: 5px 15px;">Cancel</div> <div style="border: 1px solid black; padding: 5px 15px;">Help</div> </div>	
Source concentration (mg/L) ..			
Time of observation (yr)			

Figure 6. Input screen for the AT123D model with cube source. The Help button will guide the user to a typical range for every parameter.

These two values enable the user to specify the thickness and/or the width of the aquifer. For an aquifer that can be considered as infinite in width, $Y_m = 0$ is entered. For an aquifer that can be considered as infinite in depth, $Z_m = 0$ is entered.

2. Viewing Window Area Definition

Offset in X dimension [m]: X_{off} , typical range: 0-100

For most scenarios, the value for X_{off} can be set to zero. Only if the advection is low compared to the dispersion can the solute actually migrate upgradient from the source. The offset allows the user to view that portion of the aquifer that is X_{off} meters "upstream" from the source to view the full plume development.

Start X value for viewing [m]: X_1 , typical range: 0-100

End X value for viewing [m]: X_2 , typical range: 1-2000

These two values define the window into which the plume will be plotted. Typically, $X_1 = 0$, and X_2 corresponds to the approximate length of the plume. The values can be decreased in subsequent simulations to zoom in at a certain section of the plume.

3. Contaminant Release Timing

Duration of waste release [yr]: T_d

A value is entered here that describes the length of the contaminant pulse in years. Note that AT123D does not allow T_d to be set to zero. Only inlet value scenarios can be modeled with AT123D.

Source concentration [mg/L]: C_0 , typical range: 0–10,000 [mg/L]

This is the solute concentration entering the aquifer. Concentrations above 10,000 mg/L (equivalent to 1%) are possible, but at these concentrations, the solute affects the density of the groundwater. This effect is not simulated by any of these analytical models. Therefore, caution should be taken when using them to simulate plumes of highly concentrated solutes.

Solute flux [kg/yr]: F_0 , typical range: 0–100,000

F_0 is the amount of solute that enters, at a constant rate, the groundwater system per year. The solute enters the aquifer evenly through every point of the selected source configuration. Depending on the source configuration, the flux is expressed either as is (point source) or per length (line source), per area (plane source), or per volume (cube source). The numerical values for the flux must be greater than zero. For very high fluxes (causing solute concentrations greater than 1%), caution must be taken so that density effects are not neglected.

Time of observation [yr]: T_{obs} , typical range: 0–500

Because transient solutions are employed by AT123D, the time of observation T_{obs} for which output is desired must be specified. Two particular times of interest can be distinguished: $T_{obs} < T_d$ and $T_{obs} > T_d$, where T_d is the duration of waste release. The first condition shows a plume at a time when the source is still producing solutes, and the second condition shows a plume for which the source has been terminated.

4. Contaminant Movement Parameters

Average groundwater velocity in the X, or flow direction [m/yr]: V , typical range: 1–500

This is the groundwater front (or Darcy) velocity. Note that the Darcy velocity (V) is related to the linear seepage velocity (v) through $V = v \cdot n$, where n is the aquifer porosity.

Dispersivity in X [m]: a_L

Dispersivity in Y [m]: a_T

Dispersivity in X [m]: a_v

These are the longitudinal, transversal, and vertical dispersivities in an isotropic aquifer. Typical ranges are from 0.01 to 100 [m]. Various methods can be used to estimate a dispersivity. Yeh (1981) suggests the following values:

	Sand	Silt	Clay
a_L [m]	10 to 100	1 to 10	0.1 to 1
a_T [m]	1 to 10	0.1 to 1.0	0.01 to 0.1
a_v [m]	1 to 10	0.1 to 1.0	0.01 to 0.1

Gelhar and others (1985) give the following equations to obtain estimates of the dispersivities:

$$\begin{aligned}a_L &= L/10 \\a_T &= a_L/8 \\a_v &= a_L/160\end{aligned}$$

where L is the simulation length or the length of the suspected travel path of the solute.

5. Contaminant Behavior Parameters

Retardation factor [no dim.]: R, typical range: 1-100,000

Retardation is used to quantify processes which inhibit migration of the pollutant through the porous medium. A value of $R = 1$ implies no retardation, and values of $R > 1$ imply retardation.

The retardation factor is as follows:

$$R = 1 + \frac{\rho_b K_d}{n}$$

where:

n = effective porosity for the saturated zone [no dim.].

ρ_b = bulk density of the porous media [g/cm^3].

K_d = distribution coefficient [cm^3/g].

First-order decay rate in the aquifer [yr^{-1}]: λ , typical range: 0-100

This is the first-order degradation rate constant for the constituent in the saturated zone. Substances that do not degrade because of chemical, physical, or biological processes will have $\lambda = 0$. Substances that do transfer or degrade, will have a λ greater than zero. This parameter is comparable to half-life (t_{half} , in years) of radioactive materials. Half-life is the time necessary for a compound to lose half of its (radio)activity or concentration and is related to λ through:

$$\lambda = \frac{0.693}{t_{\text{half}}}$$

4.6 Display Model Results

Model output is accessed through the Graph item in the Command Menu. This item contains information only after a model has been run or after a previously executed scenario has been loaded through the File and Open commands. The Graph pull-down menu has four options: Graph Information, Graph Results, Copy Graph, and Print Graph. A function is activated by clicking on

the desired item. Copy Graph and Print Graph are only valid after Graph Results has been chosen. This is because the user should view the output graphs prior to printing or processing.

A graph window that has been displayed on the screen can now be printed on a Windows™-supported printer. From the Graph menu, choose the Print Graph option, which is available once a graph has been displayed. The size of the printed image will be of the same size as the image on the screen. A print of the desired size can be made by resizing the graph window on the screen prior to printing.

Graph Results directs the user to the Display Graph dialog box where the user specifies which graphs are to be drawn. The user can suppress the generation of one or more graphs. This may save time and will save space on the screen for the generation of the remaining plot(s). More commonly, however, the user will generate all available graphs. The Display Graph dialog box also contains the input file name that was used to generate these graphs. The user selects the graphs by clicking with the mouse cursor on the respective boxes. A cross appears in the selected box; to unselect a box, the user simply clicks on the box again.

Two types of graphs are generated: Transects and Contours. The two-dimensional model (SSGPLUME) generates two Transects (in X and Y dimension) and one Contour map (in the X-Y plane). The three-dimensional models (3DADE and AT123D) generate three transects and three contours in all three orthogonal directions and planes.

4.6.1 Transects

Transects are concentration profiles where concentration is plotted against length in one dimension (x, y, or z). When concentration is plotted against the x dimension, the typical concentration profile is obtained. This graph shows the concentrations directly downstream from the source. The X-Transect is located along the center line of the source; therefore, the maximum concentration of the entire system will be found on this transect.

The Y- and Z-Transects are concentration profiles at given distances along the x-axis. These transects slice the plume at five equidistant intervals across the full length of the viewing window. The transects are parallel to the y-axis and/or z-axis and are drawn at x-locations that correspond to 0.00, 0.25, 0.50, 0.75, and 1.00 times the maximum value of X. It is possible that these transects will show less than five curves. This is because the viewing window is smaller than the plume. To see five curves in the transects, the size of the viewing window must be changed to fit approximately the full length of the plume, from source to toe.

4.6.2 Contour Plots

Contour plots are graphs where the concentration is mapped against two dimensions (x-y, x-z, or y-z). When concentration is mapped in x and y dimensions, the typical contour map is obtained. Contour maps of plumes typically feature "hot spots" or "bull's-eyes" that indicate highest concentrations. Because of spatial symmetry of the solutions used in these analytical models, only half-maps are generated by the contour plots. The contour plots are always symmetrical with respect to the axes that are perpendicular to the groundwater flow, that is, with respect to y- and/or z-axis.

To obtain a full contour map showing the entire plume, the user can copy the graph into Clipboard (using the Alt-Print Screen command) and then paste (Paste command) the graph into a software package that can receive bitmaps. To run another Windows™ application, the user does not have to exit GRI-ShowFlow, provided sufficient memory is available to run a second software package. The most common package to process graphical output is Paintbrush, which is distributed with Windows™. In Paintbrush, an image can be mirrored using the Pick and Flip or Pick and Rotate functions. Paintbrush can also be used to add information to a graph, for example, to add text regarding contour labels or to add location indicators such as landmarks or the north arrow.

A two-dimensional plume (SSGPLUME) is fully visualized by two Transects and one Contour plot. A three-dimensional plume (3DADE or AT123D) is fully visualized by three Transects and three Contour plots, all of which are preset by the program. The plots contain the necessary information to interpret the shape of the contaminant plume calculated by the selected models. Information on the calculated concentrations in the plume are contained in the Graph Information screen (See Figure 7).

Graph Information	
<p>TRANSECTS</p> <p>Transects are concentration profiles created by slicing the plume along the orthogonal axes. Three transects are generated:</p> <p>X-Transect: Concentration profile through the center of the plume along the x-axis. The maximum of 1.000e+00 [mg/L] in this system is shown by this transect.</p> <p>Y-Transect: Set of concentration profiles parallel to the y-axis at five equidistant intervals.</p> <p>Z-Transect: Set of concentration profiles parallel to the z-axis at five equidistant intervals.</p> <p>X LOCATIONS OF Y AND Z TRANSECTS</p> <p>The profiles are drawn from left to right at the following X values representing the viewing window of 1.300e+02 [m]:</p> <p>and X = 0.000e+00 [m] and X = 3.250e+01 [m] and X = 6.500e+01 [m] and X = 9.750e+01 [m] and X = 1.300e+02 [m]</p>	<p>CONTOURS</p> <p>Contour graphs are maps showing lines that connect points of equal concentration in three orthogonal planes. Three contour graphs are generated:</p> <p>X-Y Contours: A half-image of equal concentration lines in the horizontal plane.</p> <p>X-Z Contours: A half-image of equal concentration lines in the vertical plane parallel to the flow.</p> <p>Y-Z Contours: A half-image of equal concentration lines through the plume center at X= 4.940e+01 [m] in the vertical plane perpendicular to the flow.</p> <p>CONTOURING VALUES</p> <p>The concentrations represented by the contours are from high (inside) to low (outside) of the plume:</p> <p>(innermost) 9.000e-01 [mg/L] 7.000e-01 [mg/L] 5.000e-01 [mg/L] 3.000e-01 [mg/L] (outermost) 1.000e-01 [mg/L]</p>
OK	Help

Figure 7. Graph information screen contains transect locations and contouring values that are used for visualization through slicing of the plume.

4.6.3 Graph Interpretation

Each graphical output screen can be identified by the information in the plot window. The caption bar of the output window contains the name of the input file that was used to generate the results, and the header of each generated graph contains the title of the simulation. This is useful when similar graphs from different simulations are compared next to each other. Note that output from more than one model run can be displayed simultaneously. Two preset arrangements are available to display more than one window from the Windows™ pull-down menu: Cascade and Tile. Cascade configuration shows all the files stacked behind each other so that only the caption bar is visible, while the tile configuration displays all the graphs fully, using all the space available on the screen. The tile arrangement is the default setting in this program.

A graph window can be moved to a desired position by pointing the mouse cursor over the caption bar at the top of each window. The user presses the left mouse button and drags the window across the screen. When the button is released, the graph window will be redrawn in its new position. A graph window can be removed by either closing it (double-click on the upper left box of the window) or minimizing it (click on the down-arrow box in the upper right). To redraw a closed graph window, the Graph Results menu has to be used to reload the output information. To redraw a minimized graph window, the user double-clicks on the icon with the appropriate caption bar text. The function Close All in the Windows™ pull-down menu is used to close all the graph windows at once and to clear the screen.

The graphical output is scaled automatically by the program. The only scaling parameter that the user controls is the length of the x-axis that will be viewed in the X-Transect and, subsequently, in the X-Y and X-Z Contour maps. The other axes are scaled so that the range of all calculated values fits into a graph window. This means that every simulation may have different ranges represented by the two axes in each of the generated plots. Particularly for the contour graphs, different scales of the two axes can distort the shape of the actual plume. To an inexperienced user, the plume shapes may appear unrealistic. The scales of the vertical and horizontal axes can be modified on-screen without rerunning the model.

To adjust the scale along one or both of the axes, the graph window can be stretched or squeezed using the mouse cursor to drag the border lines of individual plots. First, the plot must be selected by simply clicking on it. The Title Bar of a selected plot is then highlighted. Placing the mouse cursor on the edge or corner border of the selected graph window will cause the cursor arrow to change to a small double-headed arrow, indicating the allowed directions of movement. Holding the left mouse button down permits the border to be dragged in the allowed direction, changing the length of the plotted axes as well as their scale. When the mouse button is released, the window will be redrawn to fill the new size. On an X-Y contour map, the scale can be adjusted in such a way that a unit length on the x-axis is the same as a unit length on the y-axis. The concentration contours will now represent the true shape of the plume.

The concentration value at a particular point can be determined by examining the generated graphs. For example, for locations directly downgradient and on the center line of the source, the concentrations can be read directly from the X-Transect. The distance from the source is read from the x-axis, and the corresponding concentration is read from the y-axis. By resizing the window

(through stretching or clicking on the maximize button), the scales may be maximized to obtain the highest resolution on the axes.

For concentration at a point that is not on the x-axis, the user must interpolate using the Concentration Contour graphs and/or the Y- or Z-Transects. Using the Contour graphs, the coordinates of the point of interest will indicate the contour interval in which the desired concentration will be. The contour intervals are always at 90%, 70%, 50%, 30%, and 10% of the maximum concentration, and the actual contour line concentrations are listed in the Graph Information window. The user estimates the percentage from the contour pattern and multiplies by the maximum concentration to obtain the concentration at the off-axis location.

A concentration at an off-axis location can also be read off the Y- or Z-Transects. The user has control of the positions of the transects which are at 0, 25%, 50%, 75%, and 100 % of the X-value determining the size of the viewing window. By choosing this X-value in Edit Parameters to coincide with the x-location of the point of interest, the corresponding concentration will be read directly from the Y- or Z-Transect for the known y- or z-location. The user maximizes the transect graph window prior to reading the concentration of the vertical axis to obtain better accuracy.

5.0 MODELING EXAMPLES

The following examples show some of the differences between various solute source definitions and plume evolutions that can be illustrated by GRI-ShowFlow. The possibility of displaying more than one window on the screen is used to place output from several models next to each other. To print an individual screen, the Print command from the File Menu can be used. To obtain a printed copy of a multiwindow screen, the screen must be copied to the Clipboard (by pressing the keys Alt-Print Screen simultaneously) and pasted into a package that supports Clipboard graphic files, such as Paintbrush, MS-Word, or WordPerfect.

5.1 Steady-State Versus Transient Simulation

Figures 8a and 8b demonstrate the application of a solute source of 10 m² of surface area that would apply to, for example, a disposal pit receiving liquid wastes. The steady-state simulation (Figure 8b) shows a plume originating from a Gaussian source and extending over more than 50 meters in the flow direction. This scenario considers attenuation in the vadose zone. Figures 9a-9c represent the same scenario, but the solute is assumed to enter the aquifer directly, without attenuation in the vadose zone. The transient model AT123D predicts the plume to develop from such a source within two years. Both models agree in the limit of solute migration to approximately 50 meters from the source because of degradation of the compound. The three-dimensional model also provides estimates of the depth of the plume that is not available from the steady-state Gaussian plume model. The estimated plume depth is 1.3 meters, as shown in Figure 9c.

5.2 Plume Differences Due to Initial Source Dimensions

Figure 10a illustrates two plumes that develop from cube sources of different sizes. For a constant mass loading, a source with a volume of 10 m³ (Figure 10b) will produce a similar plume as a 100-m³ source (Figure 10c). The concentration in the heart of the plume from the source of

Parameter File Editor for SSGPlume

Current File: EXAM1.PAR

Run Title:

test site

<p>SITE DESCRIPTION:</p> <table border="0"> <tr><td>X minimum point (m)</td><td>0</td></tr> <tr><td>X maximum point (m)</td><td>50</td></tr> <tr><td>X resolution (number of points)</td><td>100</td></tr> <tr><td>Y minimum point (m)</td><td>0</td></tr> <tr><td>Y maximum point (m)</td><td>4</td></tr> <tr><td>Y resolution (number of points)</td><td>100</td></tr> <tr><td>Width of facility (m)</td><td>4</td></tr> <tr><td>Area of facility (m²)</td><td>10</td></tr> <tr><td>10-meter wind velocity (m/s)</td><td>1</td></tr> <tr><td>Water infiltration rate (m/d)</td><td>0.05</td></tr> </table> <p>VADOSE ZONE CHARACTERISTICS:</p> <table border="0"> <tr><td>Vadose zone thickness (m)</td><td>10</td></tr> <tr><td>Contaminated zone thickness (m)</td><td>2</td></tr> <tr><td>First-order decay rate (1/d)</td><td>0.01</td></tr> </table>	X minimum point (m)	0	X maximum point (m)	50	X resolution (number of points)	100	Y minimum point (m)	0	Y maximum point (m)	4	Y resolution (number of points)	100	Width of facility (m)	4	Area of facility (m ²)	10	10-meter wind velocity (m/s)	1	Water infiltration rate (m/d)	0.05	Vadose zone thickness (m)	10	Contaminated zone thickness (m)	2	First-order decay rate (1/d)	0.01	<p>CONTAMINANT CHARACTERISTICS:</p> <table border="0"> <tr><td>Loading rate (g/m²-d)</td><td>1</td></tr> <tr><td>Water bulk partition coefficient</td><td>0.1</td></tr> <tr><td>Henry's Law constant (no dim)</td><td>0.01</td></tr> <tr><td>Schmidt number</td><td>1</td></tr> <tr><td colspan="2">(Range 0.2 to 5.0; 1.0 typical)</td></tr> </table> <p>AQUIFER CHARACTERISTICS:</p> <table border="0"> <tr><td>Seepage velocity along X (m/d)</td><td>1</td></tr> <tr><td>Dispersivity in X (m)</td><td>0.5</td></tr> <tr><td>Dispersivity in Y (m)</td><td>0.1</td></tr> <tr><td>Retardation factor (no dim)</td><td>2</td></tr> <tr><td>First-order decay rate (1/d)</td><td>0.01</td></tr> <tr><td>Regional infiltration rate (m/d)</td><td>0.005</td></tr> <tr><td>Saturated thickness (m)</td><td>20</td></tr> <tr><td>Porosity</td><td>0.3</td></tr> </table>	Loading rate (g/m ² -d)	1	Water bulk partition coefficient	0.1	Henry's Law constant (no dim)	0.01	Schmidt number	1	(Range 0.2 to 5.0; 1.0 typical)		Seepage velocity along X (m/d)	1	Dispersivity in X (m)	0.5	Dispersivity in Y (m)	0.1	Retardation factor (no dim)	2	First-order decay rate (1/d)	0.01	Regional infiltration rate (m/d)	0.005	Saturated thickness (m)	20	Porosity	0.3
X minimum point (m)	0																																																				
X maximum point (m)	50																																																				
X resolution (number of points)	100																																																				
Y minimum point (m)	0																																																				
Y maximum point (m)	4																																																				
Y resolution (number of points)	100																																																				
Width of facility (m)	4																																																				
Area of facility (m ²)	10																																																				
10-meter wind velocity (m/s)	1																																																				
Water infiltration rate (m/d)	0.05																																																				
Vadose zone thickness (m)	10																																																				
Contaminated zone thickness (m)	2																																																				
First-order decay rate (1/d)	0.01																																																				
Loading rate (g/m ² -d)	1																																																				
Water bulk partition coefficient	0.1																																																				
Henry's Law constant (no dim)	0.01																																																				
Schmidt number	1																																																				
(Range 0.2 to 5.0; 1.0 typical)																																																					
Seepage velocity along X (m/d)	1																																																				
Dispersivity in X (m)	0.5																																																				
Dispersivity in Y (m)	0.1																																																				
Retardation factor (no dim)	2																																																				
First-order decay rate (1/d)	0.01																																																				
Regional infiltration rate (m/d)	0.005																																																				
Saturated thickness (m)	20																																																				
Porosity	0.3																																																				

Figure 8a. Input data for a test simulation with SSGPLUME with solute attenuation in the vadose zone and retardation and degradation in the saturated zone.

100 m³, however, is almost 50% higher than in the plume from a source of 10 m³. As no degradation is in effect, dilution is the only process responsible for reducing the concentration. The difference is due to faster dilution of the small source compared to the dilution of the large one, even when the solute mass in the sources is equal. In a large source, the original concentrations will be maintained longer because of the greater distance the solute must travel from the core of the source to its boundary than in a small source.

5.3 Comparison of a Point, a Plane, and a Cube Source

The AT123D model has been used to generate plumes evolving from a point source, a vertical plane source that is perpendicular to the groundwater flow, and a cube source. The input used for the cube source scenario is shown in Figure 11a. The inputs for the plane source and the point source are similar to those in Figure 11a, except that the length of the source is zero for a plane source, and the length, width, and depths of the source are zero for a point source. All three source configurations are assumed to be present for a duration of ten years in an aquifer for which the characteristics are kept the same. These characteristics correspond to a silty sand aquifer with solute retardation $R = 2$, typical for persistent hydrocarbons. The three sources are assumed to have the same constant solute concentration of 1000 mg/L during the active life (10 years) of the source.

Figure 8b. Output generated with data from Figure 8a. The screens were stretched to obtain the same scales on the concentration axes of the X- and Y- Transects. Also, the vertical and horizontal scales on the Contour Map are approximately the same.

Figure 11b shows three concentration distributions along the center lines of the plumes, predicted to be in the aquifer at an observation time of 20 years, that is, ten years after the respective sources have been removed. The concentration predicted for the point source is 7.5% above the one predicted by the cube source, even after twenty years of solute residence in the subsurface. Also, the distance traveled by the solute does not exceed 100 meters for the point and plane source, while the cube source does indicate the possibility of solutes at distances greater than 100 meters from the source. These differences may be significant enough to play a critical role in the screening of sites with solute migration.

Parameter File Editor for AT123D Horizontal Plane Source			
Run Title: <input type="text" value="test file 31"/>		File Name: AT123D.PRM	
Contaminant Setting:		Contaminant Movement Parameters:	
Source length in X (m)	<input type="text" value="2.5"/>	Groundwater seepage velocity in the X or flow direction (m/yr)	<input type="text" value="109.5"/>
Source width in Y (m)	<input type="text" value="4"/>	Dispersivity in X (m)	<input type="text" value="0.5"/>
Aquifer thickness (m) (0= ∞)	<input type="text" value="20"/>	Dispersivity in Y (m)	<input type="text" value="0.1"/>
Aquifer width (m) (0= ∞)	<input type="text" value="0"/>	Dispersivity in Z (m)	<input type="text" value="0.05"/>
Viewing Window Area Definition:		Contaminant Behavior Parameters:	
Offset in X dimension (m)	<input type="text" value="0"/>	Retardation factor (no dim)	<input type="text" value="2"/>
Start X value for viewing (m) ..	<input type="text" value="0"/>	First-order decay rate (1/yr)	<input type="text" value="3.65"/>
End X value for viewing (m) ..	<input type="text" value="50"/>		
Contamination Release Timing:			
Duration waste release (yr) ...	<input type="text" value="2"/>		
Source flux (kg/yr)	<input type="text" value="0.073"/>		
Time of observation (yr)	<input type="text" value="2"/>		
		<input type="button" value="OK"/> <input type="button" value="Cancel"/> <input type="button" value="Help"/>	

Figure 9a. Input data for a test simulation of AT123D with a horizontal plane source. Same input is chosen as in the steady-state simulation in Figure 8.

Figure 9b. Transects generated by data from Figure 9a. After two years, the transects resemble the steady-state output from Figure 9b. Additional distribution of solute with depth is shown in the Z-Transect.

Figure 9c. Contours generated by data from Figure 9a. The X-Y Contours represent a plane view; the X-Z Contours represent a profile view in the flow direction; and the Y-Z Contours represent a "head-on" view of the plume.

Parameter File Editor for 3DADE Cube Source	
Run Title: <input type="text" value="spill 10 m³"/>	File Name: EXAM3.PFL
<div>Contaminant Setting:</div> <div>Contaminant Movement Parameters:</div>	
Source length in X (m) <input type="text" value="2.154"/>	Groundwater seepage velocity in the X or flow direction (m/yr)..... <input type="text" value="50"/>
Source width in Y (m) <input type="text" value="2.154"/>	Dispersivity in X (m)..... <input type="text" value="20"/>
Source depth in Z (m) <input type="text" value="2.154"/>	Dispersivity in Y (m)..... <input type="text" value="2.5"/>
Viewing Window Area Definition:	Dispersivity in Z (m)..... <input type="text" value="0.125"/>
Offset in X dimension (m) <input type="text" value="0"/>	Contaminant Behavior Parameters:
Start X value for viewing (m) <input type="text" value="0"/>	Retardation factor (no dim) <input type="text" value="1"/>
End X value for viewing (m) <input type="text" value="130"/>	First-order decay rate (1/yr)..... <input type="text" value="0"/>
Contamination Release Timing:	
Duration waste release (yr) .. <input type="text" value="20"/>	
Source flux (kg/yr) <input type="text" value="100"/>	
Time of observation (yr) <input type="text" value=".5"/>	
<input type="button" value="OK"/>	<input type="button" value="Cancel"/> <input type="button" value="Help"/>

Figure 10a. Input data for a test simulation of 3DADE with an initial cube source of 10 m³.

Figure 10b. Contour map and X-Transect for a 10-m^3 source based on input data from Figure 10a. The contouring values are, from inside out, 8.8, 6.8, 4.9, 2.9, and 1.0 mg/L, respectively.

Figure 10c. Same graphs as in Figure 10b for a source of 100 m³ and other parameters unchanged. Note that the shape of the plume is similar, but the contouring values are, from inside out, 12.9, 10.0, 7.1, 4.3, and 1.4 mg/L, respectively.

Parameter File Editor for AT123D Cube Source			
Run Title: CUBE		File Name: CUBE.PRM	
Contaminant Setting:		Contaminant Movement Parameters:	
Source length in X (m)	10	Groundwater seepage velocity in the X or flow direction (m/yr)	5
Source width in Y (m)	10	Dispersivity in X (m)	2
Source depth in Z (m)	3	Dispersivity in Y (m)	1
Aquifer thickness (m) (0=∞)	0	Dispersivity in Z (m)	0.5
Aquifer width (m) (0=∞)	0		
Viewing Window Area Definition:		Contaminant Behavior Parameters:	
Offset in X dimension (m)	0	Retardation factor (no dim)	2
Start X value for viewing (m)	0	First-order decay rate (1/yr)	0
End X value for viewing (m)	100		
Contamination Release Timing:			
Duration waste release (yr)	10		
Source concentration (mg/L)	1000		
Time of observation (yr)	20		
OK Cancel Help			

Figure 11a. Input data used in the AT123D cube source model to generate concentration profiles shown in Figure 11b.

Figure 11b. Concentration profiles along the center line of a plume originating from different landfill representations. The profiles correspond to approximations of the geometry by a point, a plane (10×3 meter cross-section), and a cube ($10 \times 10 \times 3$ meters), respectively.

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APPENDIX A

GLOSSARY

GLOSSARY

Adsorption Adherence of molecules or ions to the surfaces of solids with which they come in contact.

Aquifer A geologic formation, part of a formation, or a group of formations saturated with water that will yield water to wells and springs.

Concentration Chemical concentration refers here only to mass of a contaminant that is dissolved in water. The units of concentration for the solute or dissolved phase are mg/L.

Contour Plots Contour plots are graphs in which the concentration is mapped against two orthogonal dimensions (x-y, x-z, or y-z). When a concentration is mapped in the x and y dimensions, the typical "contour map" is obtained.

Cube Source An approximation of a three-dimensional source with a rectangular parallelepiped (cube) that is described by three dimensions. At least one side of the cube coincides with the water table.

Darcy's Law A derived formula for the laminar flow of water or other fluids through porous media. Groundwater discharge is equal to a coefficient times the cross-sectional area times the head difference (or loss in head) divided by the length of the flow path.

Darcy Velocity The average velocity of a groundwater front, which equals the seepage velocity times porosity.

Deterministic Model A deterministic model will, for the same input, always produce the same output. The relationship between input and output is uniquely related through process parameters that all have a physical meaning, for example, seepage velocity. This is opposed to a stochastic model that generates a statistical output.

Diffusion Mass spreading due to molecular motion in response to concentration gradients.

Dispersion A solute will spread through a porous medium as a result of variations in path lengths, as well as by molecular diffusion of the solute in the liquid phase. The expression for dispersion lumps the porous matrix configuration, flow velocity, and molecular diffusion into one term.

Dispersivity An anisotropic coefficient of dispersion that relates this process to flow velocity.

Flux Flux is the rate of solute mass passing through a unit area. For consistent units it can be expressed as concentration times the seepage velocity.

Gaussian Source A source configuration where the solute concentration is distributed according to the Gaussian, or normal (bell-shaped), curve. There is one maximum in this distribution, which is in the center of the source.

Homogeneous Aquifer The flow properties, such as permeability and dispersivity, of the aquifer are the same at all points.

Isotropic A property, such as permeability, that is independent of flow direction.

Laminar Flow Water flow in which the fluid particles move along smooth paths in layers and the direction of flow at every point remains unchanged with time.

Longitudinal In the direction of groundwater flow. Note that groundwater flow is assumed to be horizontal in the x-direction.

Oil-Water Partitioning Coefficient The ratio of the equilibrium concentration of a chemical residing in oil (hydrocarbon) matrix to the equilibrium concentration of the same chemical dissolved in pore water.

Orthogonal In an orthogonal coordinate system, the axes defining a three-dimensional space are mutually perpendicular.

Phase Physical condition of a substance. In single-solute models, the chemical is assumed to be in equilibrium between the dissolved, adsorbed, and vapor phases in the unsaturated zone and between the dissolved and adsorbed phases in the saturated zone.

Point Source A mathematical representation of a source at the water table (upper aquifer boundary) from which all solutes enter the aquifer through a single location.

Plane Source An approximation of an areal source with a rectangle that is described by two dimensions. At least one side of the plane coincides with the water table.

Pore An opening or space in soils or rocks that is not occupied by solid matter, but may be occupied by air, water, or other gases or liquids.

Porosity Fraction of the total volume of the material that is occupied by pores or voids.

Regional Infiltration Rate The rate at which infiltrating water from precipitation travels through the unsaturated soil zone and reaches the groundwater. This infiltration rate may be different from the (local) water infiltration rate.

Retardation Factor Retardation represents the adsorption of a chemical to the aquifer material. The adsorption is assumed to be linear and reversible. The retardation factor can be multiplied by the average seepage velocity to determine the rate of movement of dissolved chemicals.

Saturated Zone The soil zone below the water table where all pores are filled with water. This is commonly referred to as the groundwater zone or aquifer.

Seepage Velocity The velocity of water moving through individual pores of an aquifer. Seepage velocity is calculated as the average velocity of the groundwater (or Darcy velocity) divided by the porosity.

Single Solute Transport The behavior of the contaminant is controlled only by its chemical characteristics and the groundwater. Presence of other chemicals is not expected to affect the fate and transport of the contaminant.

Soil Bulk Density The density of the total soil or aquifer material, including solids and voids, after the sample has been dried.

Soil-Water Partitioning Coefficient The ratio of the equilibrium concentration of a chemical adsorbed to the soil matrix to the equilibrium concentration of the same chemical dissolved in pore water.

Steady-State Flow A flow at which the magnitude and direction are constant in time.

Transient Transport Propagation of solutes from a source that has been interrupted in the past. Solute transport continues under different conditions than while the source was active.

Transversal A horizontal direction that is perpendicular to groundwater flow. Note that groundwater flow is assumed to be horizontal in the x-direction.

Unsaturated Zone The soil zone from the ground surface to the water table. Water and air fill the soil pores, and infiltrating rain drives the movement of the contaminant downward to the groundwater.

Vadose Zone Thickness The average thickness of the unsaturated (vadose) zone layer in units of length.

Volumetric Water Content The ratio of water volume in a sample to the total sample volume.

Volumetric Gas Content The ratio of gas volume in a sample to the total sample volume.

Volumetric Oil Content The ratio of oil, or hydrocarbon, volume in a sample to the total sample volume.

Water Infiltration Rate The amount of water entering a unit surface area of the contaminant source per day. This is the local infiltration, defining the rate of water that carries solutes from the source to the water table.

Water Table The surface of a groundwater body that has a pressure equal to atmospheric pressure. It is the surface that separates the unsaturated and saturated zones. It is defined by the level that water will stand in a well completed in an unconfined aquifer.

X-Transect The concentration profile directly downstream from the source. The x-transect shows solute concentration plotted against the distance along the x-, or flow, direction.

Y-Transects The concentration profiles at given distances along the x-axis. The solute concentration is plotted against the y-axis at different values of x.

Z-Transects The concentration profiles at given distances along the x-axis. The solute concentration is plotted against the z-axis at different values of x.