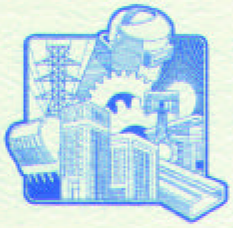
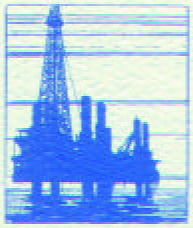
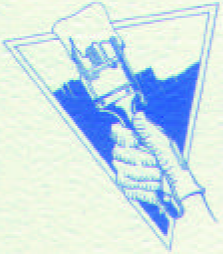
TECHNICAL &
PROFESSIONAL
TRAINING

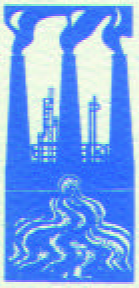
Training in the Performance, Use,
and Application of ASTM Standards







RBCA
FATE and TRANSPORT MODELS: COMPENDIUM and SELECTION GUIDANCE



This document has been funded wholly by the United States Environmental Protection Agency under assistance agreement # X 825708-01 to the American Society for Testing and Materials. The information contained herein may not necessarily reflect the views of the Agency and no official endorsement should be inferred.

ASTM • 100 Barr Harbor Drive • West Conshohocken, PA 19428-2959
610-832-9686 • FAX: 610-832-9668 • http://www.astm.org

TECHNICAL & PROFESSIONAL
TRAINING

RBCA
FATE and TRANSPORT MODELS: COMPENDIUM and SELECTION GUIDANCE

This document has been funded wholly by the United States Environmental Protection Agency under assistance agreement # X 825708-01 to the American Society for Testing and Materials. The information contained herein may not necessarily reflect the views of the Agency and no official endorsement should be inferred.

ADDITIONAL INFORMATION

Do you want additional copies of this Document?

You can write, fax, or phone your request to:

ASTM
Attn: Technical & Professional Training Dept.
100 Barr Harbor Drive
West Conshohocken, PA 19428
Tel: 610-832-9685
Fax: 610-832-9668

An electronic copy of this document can be downloaded at the web site:

http://www.epa.gov/oust/rbdm

Do you want more information about ASTM or its voluntary consensus standards on Risk-Based Corrective Action?

You can contact us via our web site at:

http://www.astm.org

Do you want more information on the U.S. EPA's Underground Storage Tank (UST) Program or Risk-Based Decision making?

Visit the U.S. Environmental Protection Agency's UST program web site at:

http://www.epa.gov/oust

Or you can call EPA's RCRA/Superfund Hotline, Monday through Friday, 8:30 a.m. to 7:30 p.m. EST. The toll-free number is 800-424-9346.

This document is not a standard and has not been approved by the ASTM consensus system.

ACKNOWLEDGMENTS

The American Society for Testing and Materials (ASTM) would like to acknowledge the many individuals who contributed to this document. The guidance was developed by Foster Wheeler Environmental Corporation by Dr. James Kennedy, principal author, with contributions from Dr. Ronald Marnicio, Ms. Monica Caravati and Dr. Emily Kennedy. Mr. Scott Murphy was the ASTM project manger. The guidance was funded under an assistance agreement # X825708-01 by the U.S. EPA (USEPA) Office of Underground Storage Tanks (OUST). Mr. Richard Mattick was the USEPA OUST project officer and coordinated the technical review of the document.

This document received extensive peer review from State programs, USEPA and the National Partnership in RBCA Implementation (PIRI). ASTM and USEPA would like to thank those who commented and participated in the review process. These comments helped to significantly shape this Guidance into a product that has targeted “real world” modeling issues of State corrective action programs for leaking underground storage tanks. These reviewers include Gilberto Alvarez (USEPA), Michael R. Anderson (Oregon Department of Environmental Quality), David Ariail (USEPA), Steven Bainbridge (Alaska Department of Environmental Quality), Phil Bartholomae (BP Oil Company), Paul Bauer (New Jersey Department of Environmental Protection), Dave Brailey (OilRisk Consultants), Chet Clarke (Texas Natural Resource Conservation Commission), Tom Conrardy (Florida Department of Environmental Protection), Scott Ellinger (USEPA), Geoff Gilman (Amoco Corporation), Annette Guiseppi-Elie (Exxon Biomedical Sciences Inc.), John Gustafson (Equilon Enterprises LLC), Merlyn Hough (Oregon Department of Environmental Quality), Steve Howe (Unocal Corp.), Walter Huff (Mississippi Department of Environmental Quality), Jack Hwang (USEPA), Robin Jenkins (Utah Department of Environmental Quality), Karen Lyons (Equilon Enterprises LLC), Mark Malander (Mobil Oil Corp.), Donna Miller (Chevron), Norm Novick (Mobil Oil Corp.), Richard Oppel (Oklahoma Corp. Comm.), Roger Przybysz (Michigan Department of Environmental Quality), Jim Rocco (BP Exploration and Oil Co.), Matthew Small (USEPA), Ken Springer (Shell Oil Co.), Sandra Stavnes (USEPA), John Stephenson (Pennsylvania Department of Environmental Protection), Karen Synoweic (Chevron Research and Technology Co.), Michael Trombetta (Montana Department of Environmental Quality), James Weaver (USEPA), and Joe Williams (USEPA).

RBCA Fate and Transport Models:
Compendium and Selection Guidance

Prepared for

ASTM

Prepared by

Foster Wheeler Environmental Corporation

302 Research Drive, Norcross GA

NOVEMBER 1998

TABLE OF CONTENTS

Forward

This Guidance document catalogs and describes non-proprietary fate and transport models that are readily available and in common use for risk-based corrective action (RBCA) at the time of publication. It is meant to function as a compendium and resource guide, assisting the user in the model selection process. It is not intended to be a comprehensive review of every available fate and transport model nor a comprehensive guidance on the use of any single model. The Guidance does not endorse models listed nor attempts to rank them or evaluate their performance or accuracy. Models other than those included in this Guidance may be appropriate choices for fate and transport modeling at any site. It is the responsibility of the experienced fate and transport modeler to select the appropriate model. The Guidance does not, at this time, include complex multi-phase, multi-component models for simulating movement of nonaqueous phase liquid; models for constituent movement through fractured media; nor does it include proprietary models.

Regulatory agencies may have certain technical preferences or requirements regarding the selection or use of fate and transport models. For example, certain agencies may require the use of models that are peer reviewed and within the public domain (i.e., readily available, widely distributed, and generally accepted). These preferences or requirements should be considered when selecting a fate and transport model. Determination of the degree of model calibration (or the determination on whether or not a model can be calibrated) should also involve consultation with the appropriate regulatory agencies.

Fate and transport modeling is only one of the many tools needed to successfully implement the Risk-Based Corrective Action (RBCA) process. The purpose of this Guidance is to assist in selection of models that can be used to implement the RBCA process, and not to be a substitute for sound professional judgment. The Guidance does not advocate modeling over the collection and interpretation of quality media-specific site data.

• 1.0 INTRODUCTION

· *1.1 Purpose*

The purpose of this Guidance Document on Fate and Transport Modeling (Guidance) is to provide a compendium of commonly used fate and transport models and pertinent information to aid users in the selection of an appropriate model to be used in the Risk-Based Corrective Action (RBCA) process. Various formulations of fate and transport models have been used for more than twenty years to assess and predict movement and behavior of chemicals in the environment. Over time, more sophisticated fate and transport models have been developed to take advantage of advances in computer hardware and software technologies, and of improved understanding of fate and transport processes. There are now many models ranging from very simple to very complex.

Fate and transport models may utilize simple equations that require minimal data input, or complex equations that require detailed site-specific information. The RBCA process advocates a gradual process of using models, starting from simple approaches that will produce conservative results (i.e., over-prediction of likely constituent concentrations) and moving, as needed, to complex approaches requiring more data and time. Objectives of modeling should be defined before model selection begins for it is possible that a simple model will be adequate to provide the desired information. The complexity of selected models should balance the quantity and quality of available input data (or of data which can be obtained easily) with the desired model output.

Fate and transport models are most often used to simulate or predict the distribution of constituent concentrations in environmental media. In some situations, the collection and interpretation of good quality data on constituent concentrations in soil and groundwater can defer the need for modeling. Also, situations may arise where fate and transport models cannot be adequately calibrated or validated, in which case it may be best to use field data rather than modeling results in the RBCA process. An application of the RBCA process should consider both data collection and modeling options for meeting information needs.

This Guidance is presented in a way that information can be used by audiences with varying levels of experience in fate and transport modeling. It addresses a multitude of chemical fate and transport pathways, including vapor migration, soil leaching, and groundwater transport pathways. The Guidance contains information on specific types of models, describes governing equations and model applicability, lists key input parameters for each model, describes model output formats and limitations, and presents procedures for sensitivity testing of input parameters and for validating individual model simulations and predictions.

· *1.2 Methods*

The sources of information used to describe the models included in this document are listed in the Bibliography section of the document. The survey of publications focused on those aspects of models noted in the Introduction. The survey did not focus on the history of development of each model, or on literature critiques of the use of a model, except where such critiques provide insight on the applicability or limitations of a model. Models in the Guidance are applicable to movement of constituents in porous media; none of the models specifically address movement in fractured media. This Guidance addresses models which are, for the most part, referenced in the American

Society for Testing and Materials (ASTM) *Standard Guide for Risk-Based Corrective Action Applied at Petroleum Release Sites* (E 1739-95), or in documents cited by the *Guide.*

This Guidance describes readily-available and published models that were in common use at the time of writing. Models include those in the public and private domain. For the purpose of this Guidance, public domain models are considered to be those which can be obtained without cost from government agencies, such as the U.S. EPA Center for Subsurface Modeling Support at the Robert S. Kerr Environmental Research Center (http://www.epa.gov/ada/models/html) and the U.S. Geological Survey (http://water.usgs.gov/software/ground_water.html), where models can be downloaded from the Internet. Private domain models are considered to be those that can be obtained at cost from trade associations, university research associations, and commercial vendors. Specific sources of models, including URL addresses, are included on the model summaries in an appendix to this Guidance. The models listed in the Guidance have been through various degrees of peer review. The user should be aware of peer review or other model use or selection policy requirements of a specific RBCA program and the implementing regulatory agency.

· *1.3 Organization*

This Guidance is presented as five components:

- Text
- Bibliography
- Matrices
- Figures
- Model Summaries-Appendix A

Information in each of the matrices is grouped by fate and transport pathway. Matrix 1 presents a summary of key information for various models, including:

- Model/algorithm name;
- Description of model processes and simulations;
- Type of model code/algorithm;
- Model outputs;
- Model features, characteristics, use conditions, and limitations;
- Computer needs; and
- Sources of additional information.

The matrix provides a snap-shot of commonly-used models allowing a user of the Guidance to, for example, quickly identify which models:

- Are applicable to which fate and transport pathway;
- Use analytical methods, and may be relatively simple:
- Are more complex, using numerical methods; and
- Can be run using standard spreadsheet applications.

Matrix 2 correlates specific models with generic site conditions. The matrix allows a user of the Guidance to, for example, distinguish those soil-to-ambient-air models applicable to infinite source depth from those applicable to finite sources. Distinctions are also made on the basis of soil or aquifer homogeneity and isotropy, steady-state versus transient conditions, and incorporation of biodegradation and transformation, among other site conditions. Matrix 3 identifies key input parameters for models and comments on sensitivity of model output to the input parameter. Input parameters are those commonly needed for fate and transport modeling, grouped by fate and transport pathway. Sensitive input parameters are highlighted in Matrix 3.

Figures 1, 2, and 3 illustrate the process of selecting a fate and transport model. Figure 1 addresses the decision process for selecting analytical versus numerical models. The figure is in the form of a decision diagram considering questions on regulatory requirements for modeling, model calibration, site complexity, and availability of input parameter values. Figure 2 illustrates the process for selecting analytical fate and transport models for the pathways:

- Soil-to-ambient air;
- Soil-to-indoor-air;
- Soil-to-groundwater;
- Groundwater-to-ambient-air;
- Groundwater-to-indoor-air; and
- Groundwater-transport.

Figure 3 illustrates the process for selecting numerical fate and transport models for the pathways:

- Soil-to-groundwater; and
- Groundwater-transport.

Both Figures 1 and 2 present information on input data requirements and model output that correlate with information in the matrices.

Each of the fate and transport models included in the matrices and figures are summarized in the appendix to this Guidance. The summaries include information on model operation, key and sensitive input parameters, applicability of the model, and sources of additional information on the model. The distinction is made between models for which computer programs are available from common sources, and models that are in the form of equations typically executed in a spreadsheet environment. Where available, URL locations of model information are included in the summaries. The summaries are intended to allow further screening of fate and transport models selected using information in the matrices and figures.

The text of the Guidance intentionally does not refer to specific fate and transport models so that selection of a model can be made using information in the matrices, figures, and appendix. Instead, the text provides general information on fate and transport process and types of fate and transport models. It describes site conditions for model application, provides information on model input parameters, and describes model selection criteria relative to RBCA-process tier levels. The text describes packages incorporating models for a variety of fate and transport pathways, and describes the process of model calibration and validation. The Guidance includes a Bibliography with references on fate and transport processes, specific fate and transport models, measurement of model input parameters, and model packages.

2.0 DESCRIPTIVE MODEL INFORMATION

2.1 Fate and Transport Processes

A principal purpose of fate and transport modeling is to predict and quantify migration of constituents in the environment that are subject to one or more transport mechanisms. For example, within ASTM and state RBCA programs, fate and transport modeling is one of the tools used to establish exposure point concentrations and their corresponding risk-based screening and cleanup levels.

Fate and transport models are used to predict the migration of chemical constituents through soil, groundwater and air (or a combination thereof) over time, with most models focusing on specific fate and transport processes. Fate (i.e., chemical) processes address persistence of a constituent along the migration pathway while transport (i.e., physical) processes address mobility of the constituent along the migration pathway. The processes incorporated into fate and transport models include:

- Advection, the movement of dissolved constituents caused by the bulk movement of fluid (liquids and gasses);
- Dispersion, the three-dimensional spreading of dissolved constituents as fluid migrates through environmental media;
- Diffusion, the spreading of a mass of constituents as a result of concentration gradients;
- Equilibrium partitioning of constituent mass between solid and fluid (i.e., liquid and gas) portions of the environmental medium as a result of sorption, solubility, and equilibrium chemical reactions;
- Biodegradation of constituents by indigenous microorganisms along the migration pathway; and
- Phase separation of immiscible liquids.

Fate and transport models developed for constituent migration analyses have been cited in numerous guidance documents. Models incorporate, to varying degrees, one or more of the fate and transport processes highlighted above. For example, a model of vapor migration from soil to ambient air may incorporate the processes of diffusion and advection for vapor movement to the ground surface, and atmospheric dispersion of vapors emanating from the ground surface.

Information in this Guidance is grouped into the following fate and transport pathways:

- Vapor migration from soil with dispersion in ambient air;
- Vapor migration from soil to enclosed spaces and indoor air;
- Vapor migration from groundwater to ambient air;
- Vapor migration from groundwater to indoor air;
- Transfer of constituents from soil to groundwater;
- Groundwater transport of dissolved constituents.

Following are brief descriptions of the principal processes incorporated into most fate and transport models or modeling approaches.

• 2.1.1 Advection

Advective transport processes are modeled to quantify movement of fluids. Advection is the dominant mass transport process in groundwater flow systems (Domenico and Schwartz, 1990). Within a groundwater flow system, for example, advective movement of water occurs through pores and fractures within soil or rock (often referred to as the “water bearing medium” or “aquifer”). Equations for advective movement of groundwater therefore require information on material properties of the soil or rock (e.g., hydraulic conductivity, effective porosity) and a quantitation of the potential gradient driving groundwater movement (hydraulic gradient).

Conservative constituents do not partition to the environmental media and therefore move at the same velocity as groundwater. Other constituents move at a velocity less than that of the bulk groundwater movement due to partitioning between solid and fluid portions of the water-bearing medium. The retardation equation generates a ratio of the groundwater and dissolved constituent movement velocities called the retardation factor.

Calculation of the retardation factor for organic constituents requires information on soil bulk density and effective porosity, fraction of organic carbon in the water-bearing medium, and the organic carbon partitioning coefficient of the constituent. For inorganic constituents, the fraction of organic carbon and organic carbon partitioning coefficient are replaced with analogous coefficients and parameters such as the selectivity coefficient, cation exchange capacity, and total competing cation concentration in solution (Domenico and Schwartz, 1990), and information may be needed on geochemical properties such as pH or Eh. It must be noted that the retardation equation incorporates assumptions on equilibrium partitioning (discussed in a following paragraph) and may not be representative of all situations.

Advective transport is an important process for vapor movement in the vadose zone. Advective movement of vapors can be caused by both temperature and pressure gradients. Temperature gradients can be caused by seasonal or diurnal heating of shallow soil, and pressure gradients can be caused by wetting fronts of groundwater recharge that trap and compress soil vapors. Pressure differentials can also be caused by building ventilation systems, or by winds blowing over a structure, which can result in advective movement of vapors from soil to interior spaces. Impermeable geologic strata and man-made structures such as pavements can redirect advective movement of vapors and must be considered in fate and transport modeling.

• 2.1.2 Dispersion

Dispersion is characterized by the tortuous movement of fluid through an environmental medium and results in spreading of constituent mass beyond the region that would be occupied due solely to advective movement of fluid (Domenico and Schwartz, 1990). In the modeling of groundwater flow systems, coefficients of hydrodynamic dispersion are calculated using a characteristic of the solid medium referred to as dispersivity and the advective velocity of groundwater movement. Dispersivity, which is a quantitation of the mechanical mixing that occurs as a consequence of local variations in flow velocity around the mean velocity, can be measured or estimated statistically. Dispersivity is often calculated in a fate and transport model as a scale- and direction-dependent coefficient of the downgradient distance of groundwater movement. Dispersivity is multiplied by the advective velocity to yield the dispersion coefficient. The dependence of dispersion on advection is captured in the advection-dispersion equation, which is the principal differential equation describing mass transport of dissolved constituents in groundwater flow systems.

Subsurface vapors emanating to ambient air are dispersed by wind and other atmospheric phenomena. Atmospheric dispersion is the process of growth of the volume of ambient air in which a given amount of emanated vapor is spread or mixed. The growth of the imaginary "balloon" containing the emanated vapor arises from a combination of distortion, stretching and convolution whereby a compact "blob" or "puff" of released vapor is distributed in an irregular way over a volume which is larger owing to the effective capturing and enclosure of "clean" air (Pasquill, 1974). Unlike dispersion in groundwater flow systems, atmospheric dispersion incorporates turbulent movement of the fluid medium. Equations for calculation of atmospheric dispersion require information on emission rates or fluxes of vapors or surface particles, wind speed and direction, lateral and vertical dispersion factors, ground-surface characteristics, and mixing heights.

• 2.1.3 Diffusion

The process of diffusion occurs as a result of concentration gradients. Constituent molecules in an environmental medium will move toward media characterized by lower constituent concentrations. Unlike dispersion, diffusion can occur both in the absence or presence of advective flow. The diffusive flux of vapors is characterized by an effective vapor phase diffusion coefficient which is affected by the porosity and moisture content of the environmental medium, and by the size and structure of constituent molecules.

In groundwater flow systems, the process of diffusion is quantified using the diffusion coefficient of the constituent and the concentration gradient of the constituent in groundwater. In the advection-dispersion equation, a coefficient of molecular diffusion can be included in the coefficient of hydrodynamic dispersion. The coefficient of molecular diffusion is often negligible compared to the dispersivity term and is typically ignored, except when groundwater is not moving or the velocity of movement is very small.

Diffusion of soil vapors also occurs as a result of concentration gradients. Depending on the soil porosity, diffusion may be the major component of vapor movement. However, as pore spaces decrease in size or become filled with liquids, vapor diffusion decreases. Soil moisture content and water-filled porosity are therefore important considerations in modeling of fate and transport of soil vapors.

• 2.1.4 Equilibrium Partitioning

When groundwater containing constituent contamination is mixed with a solid medium, the constituent mass begins to partition between the solution, the solid, and any gas present in the medium (Domenico and Schwartz, 1990). A partitioning coefficient is used to relate the constituent concentrations in the liquid and solid portions of the medium. The sorption process is very complex and influenced by physical and mineralogical properties of the solid media, chemistry of the groundwater, temperature, and pressure. The retardation equation cited in the preceding description of the advective transport process is a means of quantifying the sorption process.

Equilibrium partitioning of constituents in environmental media dictates that the total mass of constituent is equal to the sum of the masses of constituent in the dissolved and vapor phases, and the mass of constituent sorbed to solid media. When free-phase of the constituent is present, the total mass of constituent is equal to the sum of the masses in the dissolved, vapor, sorbed, and free phases. The presence of free phase must be considered so that contaminant mass is not inappropriately allocated to the other three phases.

The amount of constituent in the vapor and sorbed phases is related to the amount in the dissolved phase by equations involving Henry’s Law constant for vapor phases and partition coefficients for sorbed phases. Estimating constituent concentration under equilibrium partitioning conditions requires information on dissolved constituent concentration, water content and bulk density of the solid medium, distribution coefficient between dissolved and sorbed phases, Henry’s Law constant, and vapor content of the medium.

• 2.1.5 Biodegradation/Transformation

Biodegradation and transformation are processes that reduce constituent concentrations by changing the form in which the individual chemical components exist. The most significant rates of biodegradation/transformation occur by means of aerobic reactions where constituents act as an electron donor, energy source, and source of carbon for growth of microorganisms (e.g., biodegradation of petroleum hydrocarbon constituents). Oxygen acts as the electron receptor for aerobic processes and is reduced to water, causing a decrease in dissolved oxygen concentrations (Wiedemeier, et al, 1995). Availability of oxygen and the rate of oxygen transport are the factors that most significantly control aerobic processes in subsurface environments. Nitrate, sulfate, ferric iron, and carbon dioxide can be electron receptors in anaerobic processes, which tend to have slower reaction rates than aerobic processes.

In some of the less-complex fate and transport models, biodegradation and transformation reactions can be incorporated as first-order reactions where the decay rate is proportional to the constituent concentration. Reductions in constituent concentrations (or mass) are calculated using rate constants and incorporate the concept of half-life, defined as the time it takes for constituent concentration to be decreased by one-half due to biological degradation or transformation processes. More complex models can utilize more fundamental approaches for incorporating the processes. If rates of biodegradation or transformation are unknown, or not considered appropriate by regulatory agencies or others (e.g., if a conservative over-estimation of constituent concentrations is desired), the effect of these processes can be eliminated from most fate and transport models.

• 2.1.6 Separate Phase Flow

Movement of immiscible liquids can result in migration of liquids under gravitational forces. Within a groundwater system, light nonaqueous phase liquids (LNAPL) such as petroleum hydrocarbons that are released at or near the ground surface will move vertically downward to the water table. The buoyant volume of immiscible liquid will then move horizontally to flatten out. The LNAPL layer may concurrently move hydraulically downgradient with groundwater. Dense nonaqueous phase liquids (DNAPL) will move vertically downward, penetrate the water table, and continue to move vertically downward until gravitational movement is restrained by physical barriers (e.g., an impermeable geologic stratum) or until the DNAPL volume has been depleted by residual containment in the zone through which the DNAPL is descending (Domenico and Schwartz, 1990). Both LNAPLs and DNAPLs are identified as secondary sources and transport mechanisms in the ASTM *Standard Guide for Risk-Based Corrective Action Applied at Petroleum Release Sites* (E 1739-95).

2.2 Types of Fate and Transport Models

A model is any device or construct used to represent or approximate a field situation (Anderson and Woessner, 1992). They are an assembly of concepts in the form of mathematical equations that represent some understanding of natural phenomena. Models can be conceptual representations, physical representations, or mathematical representations (i.e., an equation or series of equations representing the governing physical processes and boundary conditions).

Modeling is an iterative series of questions and decisions, the first question being the purpose of the model. Once the purpose is established, a conceptual model is developed. This is often a pictorial representation of the site to be studied that distills the available field data and descriptive site information into a simplified representation of the study area. This simplified representation of natural processes and settings can be more easily represented by a mathematical model. Typically, simplifying assumptions are made to allow the fate and transport processes to be represented in mathematical terms.

An equation or computer code is then selected that can both satisfy the modeling purpose(s) and represent the conceptual model. The model is constructed using field, laboratory, and literature data, and can be calibrated to observed conditions. Following the completion of the model run, output data are checked against the simplifying assumptions to confirm that none of the assumptions were violated, and if so, to what degree.

Fate and transport models can be applied in a forward-calculation mode where constituent concentrations are predicted based on source area concentrations. Some of the less complex (typically analytical) models can also be applied in a back-calculation mode where one or more models are combined to determine the source-area constituent concentration corresponding to an acceptable concentration at the point of interest (ASTM, 1995). Calculations in either mode require information on the physical and chemical properties of the constituent; mechanism of releases of constituents to environmental media; physical, chemical and biological properties of the media through which migration occurs; and interactions between the constituent and medium along the migration pathway. Models focusing on specific processes vary in complexity and information requirements depending on assumptions made during model development and use.

Models are categorized as analytical, numerical, or a hybrid of the two. Some models are analytical, in which the governing equation is solved directly or by means of a simplified solution to the governing equation. Numerical models use techniques such as finite difference or finite element methods to solve the governing equation. Different types of models may be used in different phases of the RBCA process. Analytical models are typically used in simplistic screening-level fate and transport analyses while more complex numerical models may be used for:

- Analyses for which more detailed output are needed or desired;
- Analyses where analytical models do not or cannot yield acceptable output due to conditions such as heterogeneity of environmental media; or
- Analyses for which applicable analytical approaches are not available.

Limits on available data and the resulting need for simplifying assumptions can result in complex models reducing to the more simplistic models. Unless superseded by one of the above or other considerations, analytical models are typically used in RBCA Tier 1 and Tier 2 analyses while numerical models, if used at all, are limited to Tier 3 analyses.

Models can be described further as either steady-state or transient. Steady-state models do not include a time domain and do not project variations over time. An example of a time-independent input value is constant source-area concentrations of constituents. Transient models incorporate a time domain, and model input and output values can vary over time. Transient models can incorporate time-dependent input such as varying source-area concentrations and groundwater recharge rates. Using the specific example of source-area concentrations, a steady-state model incorporating constant concentrations may over-estimate constituent concentrations at some times or locations in the model domain when compared to output from an analogous transient model incorporating source-area concentrations that are decreasing due to migration of the constituent mass or biodegradation/transformation.

• 2.2.1 Analytical Models

Analytical models use mathematical solutions to governing equations that are continuous in space and time and applicable to the mass flow and constituent transport processes. They are generally based on assumptions of uniform properties and regular geometry. Most analytical models have a simple mathematical form and are based on multiple limiting assumptions rather than on actual phenomena. A major advantage of analytical models is that such models are relatively quick to setup and use (ASTM, 1995). Other advantages include:

- Analytical models are easy to apply;
- Analytical models can be solved for a set of input parameters and used to validate other numerical codes;
- Analytical models can accommodate some anisotropic medium properties;
- Analytical models are numerically stable; and
- Analytical models can be used as quick, conservative screening tools before using more complex models.

Analytical models also can be used to quickly develop insight on how model output is affected by ranges of values for input parameters. A limitation of analytical models is that, in many cases, such models are so simplistic that important aspects of the environmental system may be neglected (ASTM, 1995). Other limitations include:

- Analytical models cannot accommodate heterogeneous medium properties (i.e., medium properties must be constant or uniform in space or time);
- Analytical models may not be able to accommodate multiple sources contributing to a single plume; and
- Analytical models may not be able to accommodate irregular site boundaries.

In the matrices presented later in this Guidance, analytical model dimensions are described as one-dimensional (1D), two-dimensional (2D), or three dimensional (3D) depending on the number of directions in which model parameters can vary and for which output can be generated. Forms of the governing equation are described as linear ($Y = A + B \text{ x } X$), geometric ($Y = A + B \text{ x } X^{n}$), exponential ($Y = A + B \text{ x } e^{X}$ or $Y = A + B \text{ x } \ln X$) or a transformation (e.g., $Y = A + B \text{ x } \operatorname{erf} X$ where "erf" is the error function transformation, which is a mathematical technique for linearizing the governing equation describing a free-surface boundary condition such as a water table).

2.2.2 Numerical Models

Compared to analytical models, numerical models can accommodate more complex heterogeneous systems with distributed, non-uniform properties and irregular geometry. Advantages of numerical models include the ability to:

- Simulate more complex physical systems;
- Simulate multi-dimensional systems;
- Incorporate complex boundary conditions;
- Accommodate spatial variability of input parameters;
- Accommodate both steady-state and transient conditions; and
- Simulate both spatial and temporal distributions of model output.

Numerical models are, in comparison to analytical models, better suited to simulating multiple combinations of spatially variable input parameters and boundary conditions for the purpose of calibrating model output to measured site conditions.

Common limitations of numerical models include the:

- Requirement of more development time compared to an analytical model of the same transport process;
- Requirement of greater amounts of input information; and
- Possibility of numerical instability, which may cause the numerical model to become difficult to implement without major modifications to the geometric layout of the model domain.

Numerical models of constituent transport processes are solved using either finite difference or finite element methods. In each method, the area to be modeled (the model domain) is divided into sub-areas (i.e., discretized) and the governing differential equation is replaced by a difference equation (Freeze and Cherry, 1979). In finite difference models, the model domain is discretized into a finite number of blocks using an orthogonal grid and each block is assigned its own properties. In the finite element method, the model domain is discretized using an irregular triangular or quadrilateral mesh. This can result in a smaller nodal grid to model the area of interest while accommodating irregular boundaries.

The properties can be different within each block (within limits) which allows for numerical models to accommodate heterogeneous conditions. The difference equation is formulated with increments of Δx, Δy, and Δz for the spatial coordinates, and Δt for time. A solution is obtained by solving the sets of difference equations for nodes along the rows or columns of the grid. A model domain may comprise several hundred or thousands of nodes so that a large number of equations must be solved simultaneously to obtain the output value at each block center (Fetter, 1980). Model output is calculated for the center of each block. Finite difference models can be limited by their low accuracy for solving some fate and transport problems, and by the requirement for a regular gridding of the model domain.

2.3 Specific Model Information

This Guidance is a compendium of available, published fate and transport models that address multiple pathways. Matrix 1 presents information regarding various fate and transport models so key algorithms and parameters can be readily identified and directly compared. Matrix 1 includes the following information:

- Fate and Transport Pathway;
- Name of Model/Algorithm;
- Model Description/Process Simulation;
- Type of Code/Algorithm;
- Model Outputs;
- Features/Characteristics;
- Computer Needs;
- Use Conditions/Technical Support;
- References to Model Use; and
- Sources to obtain the Model/Algorithm.

Additional information on operation, input parameters, applicability, and sources of additional information for the models are presented in an appendix to this Guidance.

3.0 INFORMATION REQUIRED FOR SELECTION OF MODELS

3.1 Site Conditions for Model Application

Different fate and transport models are applicable under different conditions relating to:

- Properties of environmental media;
- Sources and distributions of constituents in environmental media;
- Physical pathways available for constituent migration;
- Geometric constraints on constituent migration;
- Temporal variance of fluid movement (i.e., steady-state or transient flow conditions); and
- Attenuation of constituents, or lack thereof, during transport.

Matrix 2 summarizes generic site conditions for application of various fate and transport models. For each fate and transport pathway, candidate models are identified for specific site conditions.

3.2 Input Parameters

Input parameters commonly needed for fate and transport modeling are summarized in Matrix 3. The matrix indicates the typical parameter symbol and units, and comments on the sensitivity of model output to the input parameter. Model output does not have the same degree of sensitivity to each input parameter. Variation in certain input parameters will have a greater affect on model output than other input parameters, depending on the fate and transport process being modeled, assumptions incorporated into the conceptual development of the model, and the equation or computer code used to implement the model. Input parameters are grouped by fate and transport pathway in Matrix 3 and the generally more sensitive input parameters are highlighted. Sensitivity of specific models to input parameters is indicated on the model summaries in the appendix to this Guidance. The purpose of the matrix is to highlight sensitive input parameters and not to provide a comprehensive compilation of every required input parameter for the fate and transport model under consideration.

3.2.1 Sources of Input Parameter Values

Values for input parameters may be measured or obtained from published literature. Published parameter values are generally based on direct measurements or on calculations made using direct measurements. Repeating measurements for site or chemical-specific parameters is often beyond the scope of the effort with which the modeling is associated, or is unjustified given the defined modeling objectives. This can be the situation for chemical and physical properties of constituents, and for some properties of the environmental media. Published values of such input parameters can be evaluated for use at a particular site in lieu of data generated from site-specific measurements (evaluation of the sensitivity of model output to values of input parameters is discussed in a later section of this Guidance).

Data input requirements may be fulfilled using default or site-specific values that can be obtained from published literature or established through measurement. Default values may be selected from the model itself, the governing regulatory agency, or literature values. Literature values for many input parameters are often presented as broad ranges, which can confound the selection of a specific value (e.g., values of hydraulic conductivity are generally given in order-of-magnitude ranges). The candidate fate and transport model may be sensitive to the value given the input parameter in which case data from direct measurements should be considered for use with the model. Use of a complex model to simulate site-specific conditions can increase the need for direct measurement of input parameter values. Often, numerical fate and transport models cannot be adequately calibrated for their intended use without data from direct measurements.

• 3.2.2 Techniques for Measuring Input Parameters

When the need for fate and transport modeling is anticipated, consideration should be given to the techniques and methods for measuring the physical and chemical properties of environmental media that may be required as model inputs. Values for input parameters can be obtained from laboratory measurements made on samples collected from the site, or from direct measurements made at the site. The input parameters listed in Matrix 3 include those that can be measured in either the field or the laboratory. By identifying required, sensitive, or influential input parameters, and planning for their measurement during the assessment of the nature and extent of constituents, the efficiency of site-specific data collection efforts can be increased and costs associated with multiple data-collection efforts can be minimized or eliminated.

Methods typically used for collection of soil samples for chemical analyses are generally not adequate for obtaining samples for geotechnical analyses. The former samples are usually disturbed during collection while geotechnical samples should be undisturbed to produce representative values of parameters such as bulk density, total porosity, and natural moisture content. Undisturbed samples can be collected using thin-walled sampling devices (i.e., Shelby tubes) advanced using standard subsurface drilling and soil sampling equipment, or from bulk undisturbed samples collected from excavations. Undisturbed samples should be preserved in the field to retain their structural integrity and moisture content (e.g., by sealing the sample in wax) and later submitted to a geotechnical laboratory for analyses.

Grain size distribution can be measured using either undisturbed or disturbed samples (e.g., split-spoon samples). Sieve analyses of samples will define the distribution of gravels and sands, and will indicate the total percentage of silts and clays (i.e., percent passing the #200 sieve), and hydrometer analyses of samples can be used to determine the distribution of silts and clays. Grain size distribution curves can be used as an indicator for many other input parameters, which cannot otherwise be, measured easily (e.g., intrinsic permeability, and thickness of capillary fringe).

The fraction of organic carbon (f_{oc}) in soil is an important input parameter for fate and transport modeling organic constituents, as it is needed to calculate the soil sorption coefficient. Fraction of organic carbon can be measured on samples collected specifically for this purpose, or on samples collected for analysis of constituent concentrations or geotechnical properties. Measurements can be made on samples collected from contaminated areas of a site or from areas where constituents are absent. Where possible, it is best to make measurements on samples collected from the lithologic zone(s) incorporated in the model. There are many procedures available for measurement of f_{oc} in soil. Users of fate and transport models should assure that f_{oc} measurements are expressed in the form (i.e., units) required for the model being used.

It is best to obtain site-specific data for some of the input parameters in Matrix 3. These parameters may include:

- Soil properties such as grain size distribution, bulk density, total porosity, and natural moisture content (for calculation of volumetric water- and air-content);
- Infiltration rate for the soil-to-groundwater pathway, which can be measured using lysimeters or double-ring infiltrometers;
- Saturated hydraulic conductivity for the soil-to-groundwater and groundwater transport pathways, which can be measured using single-well slug tests, pumping tests of single wells, or aquifer tests incorporating pumping and observation wells; and
- Hydraulic gradient for the soil-to-groundwater and groundwater transport pathways, which can be measured from contours of groundwater elevations (i.e., potentiometric surface contours) generated from concurrent water level measurements in a distributed set of wells and piezometers.

Chemical-specific properties such as carbon-water sorption coefficient (K_{oc}, also called the organic carbon partition coefficient) and biodegradation rates can be determined from laboratory experiments conducted on site-specific samples. However, values for these input parameters are often obtained from literature. The modeling objectives and sensitivity of model output may, however, justify the cost of such laboratory measurements. Similarly, dispersivity values can be obtained from in-field tracer testing of water-bearing units, but such testing is also often beyond the scope of the modeling effort. Values of diffusivity used in modeling of vapor migration are typically default values based on soil type.

Care must be taken when adopting literature values for use alone, or in combination with site-specific measured values, as model input parameters. The usefulness of many input parameters may depend on site characteristics not well documented in the literature, which can make it difficult to evaluate the appropriateness of the parameter value for use in the chosen fate and transport model. Measurement of certain indicator parameters (e.g., grain size distribution) can be performed to provide a basis for selection of appropriate literature values for input parameters that would be impractical or expensive to measure directly.

Many input parameters to fate and transport models are related to spatial and geometric factors such as source width, area of enclosed building, area of floor cracks, thickness of affected soil zone, thickness of vadose zone, saturated thickness of water-bearing unit, and distance along a flow-path from the downgradient edge of a plume. Values for these case-specific geometric input parameters can be estimated based on local or regional maps and cross-sections available prior to collection of site-specific data, from measurements made by on-site personnel, or from maps and cross-sections generated as part of data collection efforts.

Data quality and quantity requirements should be linked to modeling objectives, the complexity of the selected model, and the RBCA tier-level requirements. In Tier 1 and Tier 2 analyses, for example, conservative default values can be used to characterize a range of potential site conditions. As conservative default values are replaced by measured values in higher tier analyses, more site-specific data may be required to produce the desired quality of model output, particularly if model output is sensitive to input parameter values. Design of sampling programs to collect site-specific data should balance modeling objectives and model output sensitivity to the cost of data collection.

This Guidance is not intended to provide detailed information on measurement of input parameters. Such information is available in the broad-based published literature. However, key references from this literature on the measurement of input parameters are cited together in a separate section of the Bibliography of the Guidance.

• 3.2.3 Sensitivity of Model Output to Input Parameters

Sensitivity testing is the process of determining the degree to which output of a fate and transport model changes as values of input parameters are changed. Sensitivity testing can:

- Identify the fate and transport process(es) with the greatest influence on model output;
- Quantify change in the model output caused by uncertainty and variability in the values of input parameters; and
- Identify the input parameters that have the most influence on model output and overall model behavior (ASTM, 1995).

A model is considered to be sensitive to an input parameter if model output changes notably when the value of the input parameter is changed only slightly. Sensitivity of a fate and transport model to input parameter values depends on the governing equation of the model, the form of the solution to the governing equation and simplifications made in the model to allow solution of the governing equation.

Many input parameters used in fate and transport models are best characterized as ranges of reasonable values. Published values of input parameters are often given as ranges, and field measurements often produce a range of reasonable values. A procedure for using sensitivity analyses to determine how model output varies as the range of parameter values are used is:

- Identify input parameters for which a range of reasonable values exists.
- Conduct model runs varying the value of the target input parameter while holding other values of other input parameters constant.
- The number of model runs needed to determine sensitivity of an input parameter will depend on how the parameter is incorporated into the solution of the governing equation. Fewer model runs are needed if the input parameter is used in a linear form than if it is used as an exponent, raised to a power, used as a logarithm, or incorporated into a functional transformation.
- Compare model runs incorporating uncertainty and variability of the various input parameters and identify the most and least sensitive input parameters for the model algorithm.

If model output is not or only slightly sensitive to the range of reasonable values used for an input parameter, there is generally little or no need for additional effort to better define the value. On the other hand, if model output is highly sensitive to an input parameter for which an assumed or default value has been used, consideration should be given to:

- Using a model which is less sensitive to the input parameter;
- Using a model that has greater flexibility (and therefore is probably more complex) and thereby allows manipulation of boundary conditions or other input parameters to compensate for sensitivity to the input parameter;
- Obtaining more relevant values of the input parameter from literature; or
- Making field or laboratory measurements of the input parameter.

Analyses of model sensitivity to values of input parameters can sometimes be used to select parameter values. This process is sometimes referred to as parametric analysis. A determination of the sensitivity of model output to a reasonable range of input parameter values is derived. If model output is not sensitive to the input parameter value (or if model output falls within a reasonably expected range), a value for the input parameter can be selected from the range of values used in the sensitivity analysis. For example, if constituent concentration at a downgradient location is not sensitive to a reasonable range of decay constants, but is sensitive to a reasonable range of aquifer hydraulic conductivities, a value for decay constant can be selected from the tested range while additional measurements or analyses may be needed to select an appropriate hydraulic conductivity value. Sensitivity analysis operates on the assumption that input parameters are mutually independent. However, some parameter are correlated to some degree (e.g., effective porosity and hydraulic conductivity) Therefore care must be taken when conducting parametric analyses to assure that the model has been calibrated and validated by means of comparisons to input parameters other than the one(s) for which parametric analyses are being conducted.

4.0 MODEL SELECTION

4.1 Model Selection Criteria

Criteria for selection of an appropriate fate and transport model include:

- Type of information required from the model (e.g., screening versus detailed evaluation);
- The fate and transport pathway to be modeled;
- Complexity of available models;
- Required input parameters;
- Availability of data on input parameter values;
- Model output requirements;
- Limitations on model use and output; and
- The user's and target audiences' familiarity and comfort with the model.

Criteria for selecting a fate and transport model are illustrated in the process diagrams presented as Figures 1, 2, and 3. The issue of model complexity is addressed in Figure 1 where the selection of analytical versus numerical models is illustrated. Figure 2 illustrates the criteria for selecting an analytical model for a particular fate and transport pathway, given input data and model output requirements. In a similar manner, Figure 3 illustrates criteria for selecting a numerical model. Information on the principal limitations of each model is presented in Matrix 1 and in the model summaries in the appendix to this Guidance. Regulatory agencies often prefer particular models based on familiarity, output formats, and ease of use. These preferences should be considered when selecting a fate and transport model.

Selection of an appropriate model can be an iterative process, involving use of more than one model to achieve the desired results. For example, previous modeling results may support switching to another model to satisfy needs for more detailed output or output which is less sensitive to input parameters. In some cases, site-specific values for key input parameters may not be available, forcing the user to rely on default values for the input parameters. The default values for a particular model may not be a good match for the site or constituents, which may cause modeling results to be less representative than desired for making necessary decisions.

4.2 Selection of Models for Tier 2 and Tier 3 RBCA Evaluations

4.2.1 Tier 2 Usage

Migration and/or transformation of constituents in Tier 2 usage of the RBCA process is typically predicted using one or a combination of relatively simple analytical fate and transport models. Use of analytical models requires the acceptance of simplifying assumptions regarding material properties and migration processes. The models attempt to capture the operative physical and chemical phenomena relevant to the fate and transport process. Unlike the Look-Up Tables generated for Tier 1 usage in the RBCA process, analytical models used in Tier 2 can be tailored to reflect site-specific conditions. The ability to simulate fate and transport processes in a cost-effective manner makes analytical modeling a good middle-ground between the Tier 1 Look-Up Tables and the complex numerical modeling typically conducted for Tier 3 usage.

The decision for tier upgrade, or for the use of complex rather than simple models, can be predicated on several factors, including:

- How well the site conditions are accommodated by the conceptual basis of the selected model;
- The potential differences between the current-tier cleanup targets and the cleanup targets likely to be associated with the higher-tier analyses;
- The cost for collection of additional site-specific data; and
- The acceptability and reasonableness of corrective action alternatives suggested by lower-tier analyses.

Use of analytical models can result in predicted constituent concentrations that are greater than those that will actually occur. This over-estimation of constituent concentrations (i.e., conservative predictions of constituent migration) is an important consideration in the selection of fate and transport models in the RBCA process (ASTM, 1995). Evaluations based on conservative predictions can preclude the need to collect additional site-specific data in situations where conservatively predicted constituent concentrations do not exceed acceptable levels. This may not be true, however, for all situations and model applications, and the model selection process should consider this possibility.

Data collection for fate and transport models in Tier 2 usage is typically limited to economically or easily obtained site-specific data, or to easily estimated quantities. Most of the data collected for Tier 2 usage are related to geometric descriptions of the model area, physical properties of the environmental media through which migration is occurring, potential gradients causing advective movement of fluids, and constituent concentrations in source areas. When selecting a fate and transport model for Tier 2 usage, availability of values for key and sensitive input parameters should be considered. In general, the fewer the measured data available for input parameters, the simpler should be the fate and transport model selected for Tier 2 usage. By the same token, if the scope of the effort associated with the fate and transport modeling is limited to collection of only limited data for input parameters, simpler models should be selected for Tier 2 usage.

Input parameters for which measurement data have not been generated are given assumed or default values in Tier 2 usage of fate and transport models. Default values are typically used for chemical and physical properties of constituents and some properties of the environmental medium. Assumed values can usually be based on reasonable application of published data, or can be obtained from regulatory agencies. Fate and transport models selected for Tier 2 usage should incorporate assumed and default values which are reasonably appropriate to the site to be modeled, and which are consistent with regulatory requirements for modeling (if any). Default values determined to be unrepresentative can be measured.

Uncertainties associated with Tier 2 usage of fate and transport models result from:

- Simplification of site geometry;
- Simplification of physical properties of environmental media through which migration occurs (e.g., homogeneity);
- Inaccurate definition of site geology and hydrogeology;
- Simplification of potential gradients causing fluid movement;

- Inability to incorporate time-dependent values of input parameters such as source-area constituent concentrations;
- Potential inability to predict time-dependent constituent concentrations;
- Use of assumed or default values for many input parameters; and
- Use of simplified representations of some of the fate and transport mechanisms incorporated in the model.

The conservative nature of many fate and transport models associated with Tier 2 usage compensates to varying degrees for uncertainties in the modeling process. However, care must be taken to select fate and transport models that will, in fact, result in conservative predictions of constituent concentrations given the availability of data on input parameters.

• 4.2.2 Tier 3 Usage

Fate and transport modeling in Tier 3 usage may involve use of numerical models which can accommodate time-dependent constituent migration under conditions of spatially-varying properties of the environmental media through which migration is occurring. Tier 3 usage does not always involve use of numerical models. To meet modeling objectives, a higher-tier analysis may only require use of more sophisticated analytical models or use of the lower-tier models with additional site-specific values for input parameters. However, numerical models are not commonly used for Tier 1 or Tier 2 analysis.

Tier 3 evaluations commonly involve collection of additional site information and completion of more extensive fate and transport model development and verification than for Tier 2 usage. In certain situations, successful use of complex fate and transport models in Tier 3 usage may require field and laboratory measurement of many of the default input parameters, or of input parameters for which values are assumed in the simpler Tier 2 analytical models.

Data collection objectives for numerical fate and transport models in Tier 3 usage include the data required for Tier 2 usage of analytical models plus additional information on boundary and initial conditions. Data collected for Tier 3 usage include geometric descriptions of the model domain and physical properties of the environmental media through which constituent migration is occurring. The models will generate potential gradients driving advective movement of fluids. Data objectives for Tier 3 solute transport models include source-area concentrations of constituents, the initial distribution of dissolved constituents throughout the model domain, and constituent loading to environmental media in the source area. Data objectives for Tier 3 usage of fate and transport models should include measurement of constituent concentrations for use in model calibration.

Fate and transport models for Tier 3 usage can incorporate the same assumptions and defaults used in Tier 2 usage. However, the value and usefulness of simulations generated using the complex numerical models typical of Tier 3 usage can be eroded if many assumed and default values are used as input parameters. However, as with Tier 2 usage, assumed and default values are still typically used for input parameters associated with chemical and physical properties of constituents.

Uncertainties associated with Tier 3 usage of fate and transport models can be the same as those associated with Tier 2 usage of models. The degree of uncertainty depends on the complexity of the numerical model grid and the assumptions and default values used for input parameters.

The complex methods used to solve governing differential equations in Tier 3 usage, and the ability to adjust boundary and initial conditions, provides a greater ability to calibrate models to measured site conditions than models typical of Tier 2 usage, thus reducing some of the uncertainty associated with model output.

· 4.3 Model Packages

Packages of fate and transport models have been developed to incorporate models for a variety of different pathways and to link model outputs and inputs. References to specific model packages are cited in a separate portion of the Bibliography section of this Guidance. Use of a modeling package can decrease the time and cost of performing a model evaluation, assure a uniform approach to modeling fate and transport processes at a variety of sites, and standardize data input and model output formats to simplify training on model usage and review of model output.

Important technical considerations in selection of a model package(s) are:

- The algorithm(s) used to model each fate and transport pathway, and the inherent limitations on applicability of each model;
- Degree of documentation, validation, and general acceptance of algorithms incorporated in the package;
- Ability to access and modify data fields for input parameters (i.e., are input values "hard-wired" from databases of default values or can individual input parameters be tailored to site-specific conditions);
- How the model results or output from individual fate and transport models are reported and linked to other model components; and
- Familiarity of the user with various risk assessment components (i.e., model packages are not intended to be expert systems for use by those with little or no risk assessment expertise).

Each model package will have some level of documentation describing fate and transport algorithms, required formats for data input, model output options, hardware and supporting software requirements (e.g., spreadsheet software external to the model package), installation instructions, and troubleshooting aids. Model packages can embed fate and transport models to estimate cross-media transfer or migration of constituents (i.e., transport of constituents from one environmental medium to another, such as from soil-to-ambient air or soil-to-groundwater) and to calculate target cleanup levels for the various media.

Packages may allow both "forward" calculations (i.e., calculations to assess potential adverse impacts associated with user-specified constituent concentrations) and "backward" calculations (i.e., calculations of cleanup levels corresponding to acceptable risk targets for limiting potential adverse impacts), incorporate Monte Carlo simulation capabilities to quantify uncertainties in input parameters, a chemical database, tools for statistical analyses of site data, and an option to consider additive risk due to multiple pathways and constituents.

Model packages can include relatively simple analytical fate and transport models for predicting constituent concentrations incorporated into a spreadsheet workbook. Spreadsheet frameworks may consist of a group of spreadsheets integrated by a macro interface. The spreadsheets can be used to calculate baseline risks and soil and groundwater cleanup standards (i.e., "forward" and "backward" calculations, respectively) for each constituent of concern. Input parameters and calculated results generated by the package can be contained within linked worksheets that can be saved, viewed on-screen, or selectively printed.

Model packages can generate pathway-specific attenuation factors corresponding to either cross-media (migration of constituents from one environmental medium to another) or lateral migration of constituents. Examples of cross-media attenuation factors are:

- Surface Volatilization Factor
- Particulate Emission Factor
- Subsurface Volatilization Factor
- Soil-to-Enclosed Space Volatilization Factor
- Groundwater Volatilization Factor
- Groundwater-to-Enclosed Space Volatilization Factor
- Soil-to-Leachate Partition Factor
- Leachate-Groundwater Dilution Factor

Lateral transport factors apply to constituent migration within air or groundwater where concentrations are diminished due to mixing and attenuation effects. Examples of such attenuation factors are:

- Lateral Air Dispersion Factor
- Lateral Groundwater Dilution-Attenuation Factor

Model packages can include modules linked in an integrated exposure/risk assessment framework. The modules can include:

- Development of a conceptual model of the site;
- Fate and transport models to simulate movement of constituents from sources to receptors;
- A module which uses internally-calculated exposure-point concentrations or user-entered concentrations to estimate chemical intake; and
- Presentation of estimated chemical intake, carcinogenic risk, and hazard indices in tabular and graphical formats.

4.4 Model Calibration and Validation

4.4.1 Calibration

Model calibration is the process of adjusting the model geometry or input parameter values so that the model output matches observed conditions at a site. In developing a strategy for model calibration, decisions are needed on whether calibration is to be steady-state, transient, or both; what data are to be matched to achieve calibration; and what input parameter value(s) or boundary condition(s) are be adjusted to achieve calibration. Examples of model calibration include:

- Adjustment of source area constituent concentrations or average linear velocity of groundwater movement so that predicted concentrations at locations downgradient of the source area better match measured concentrations.

- Adjustment of volumetric water and air contents in vadose zone soil so that predicted migration of vapors from subsurface soil to ambient air better matches measurements of constituent concentrations in air at the ground surface above the source area.
- Adjustment of hydraulic head or flow at boundaries of a numerical groundwater flow model so that the hydraulic heads simulated by the model better match potentiometric surface contours generated from groundwater elevations calculated from well measurements.

Model calibration is typically accomplished through trial-and-error adjustment of the input parameter values. Calibration of a model is most often evaluated through analysis of residuals, which are the differences between the predictive model output and measurements of actual conditions (ASTM, 1995). Knowledge of the model algorithm used to solve the governing equation and knowledge of model sensitivity to various input parameters can reduce the amount of trial-and-error adjustments needed to calibrate a model. The calibration process should continue until the degree of correspondence between model output and actual conditions is consistent with objectives of the modeling effort (ASTM, 1995).

The degree of model calibration required can depend on how model output will be used in the overall RBCA process. If, for example, fate and transport modeling is being used to predict constituent concentrations at a critical water supply or in indoor air of an occupied building, a greater degree of calibration may be needed than if the model is used to predict downgradient movement of dissolved constituents in groundwater not used for potable supplies or to predict vapor migration to ambient air at an unoccupied site. However, even conservative models may require some type of calibration for certain applications. Determination of the degree of model calibration should consider stakeholder concerns and should involve consultation with over-seeing regulatory agencies. The degree of model calibration can be determined during development of the conceptual site model.

Calibration of a model to a single set of field measurements does not guarantee a unique solution of the model algorithm (ASTM, 1995). Uniqueness of model solutions can be tested by running the model using different input parameter values or boundary conditions than those used to generate the desired output and comparing the model output to a separate set of independent calculations or field measurements. If the initial model runs can be calibrated, but output from subsequent model runs does not adequately match the corresponding calculations or measurements, additional model calibration or definition of input parameter values may be warranted.

• 4.4.2 Validation

Validation is the process of determining how well the fate and transport model describes actual system behavior (ASTM, 1995). Validation of the model can be achieved by matching model output to measurements (Wang and Anderson, 1982). It involves the process of using a set of input parameter values and boundary conditions for a calibrated model to approximate, within an acceptable range, an independent set of measurements made under conditions similar to the model conditions (ASTM, 1995). A calibrated but unverified model may be used to model fate and transport of constituents if sensitivity analyses indicate that model output is not sensitive to variability in the portions of the model which cannot be verified (ASTM, 1995).

An analytical model run using a computer spreadsheet can be validated by comparing model output to independent calculations (e.g., calculations generated using a different “reference” model or by “pencil-and-paper” calculations) of the output values. Numerical models used to predict spatial and temporal changes in dissolved constituent concentrations can be validated by determining concentrations of dissolved constituents at locations where initial concentrations are not known, and by time-series sampling at locations where initial conditions are known.

Care must be taken to ensure that the number of independent calculations or field measurements is sufficient to effectively validate the model. The number and extent of calculations and measurements needed to validate a model can increase as the complexity of the model algorithm increases. If an analytical model is composed of a combination of independent equations, several independent calculations may be needed to validate a single model output. The Domenico (1987) model incorporates an average linear velocity of groundwater movement calculated from hydraulic conductivity, hydraulic gradient and effective porosity. Validation of output from a Domenico model can therefore require independent calculation of both the groundwater velocity, using the appropriate linear equation, and calculation of the downgradient constituent concentration using the error function transformation of the advection-dispersion equation.

• 4.4.3 Modeling versus Field Data

There is always the possibility that a model cannot be calibrated to field measurements. For example, assigning source area concentrations that match present conditions, but do not match previous conditions, may result in the inability to calibrate a modeled groundwater plume of dissolved constituents that formed under past constituent loading conditions. This may occur in a model that does not allow for time-variation of source area concentrations, and may limit the predictive capabilities of the model. If a model process and algorithm are not representative of site conditions, it may not be possible to calibrate the model even when measured values for input parameters are use. This could occur when a steady-state model is used to simulate transient fate and transport processes, or when a model used to simulate fate and transport of degradable constituents does not incorporate biodegradation or transformation.

When a selected model can not be calibrated sufficiently to meet modeling objectives, consideration should be given to using field data in lieu of modeling. Overseeing regulatory agencies often prefer field data to simulations generated using models that cannot be adequately calibrated. Collecting field data on constituent concentrations may, in fact, be less expensive than collecting the data on sensitive input parameters needed to calibrate a model, or than using a more complex model requiring greater user skill and operation time. Where field information is adequate, such as where spatial measurements define the full extent of contamination and time-series measurements indicate decreasing constituent concentrations, fate and transport modeling of any sort, whether or not it can be calibrated, may not be necessary to implement the RBCA process.

• 5.0 DEFINITION OF TERMS

Anisotropic Conditions: Exhibiting properties with different values when measured along axes in all directions; opposite of isotropic.

Boundary Conditions: The physical or chemical conditions at the boundary of the area to be modeled. Boundary conditions must be defined, but are often assumed, to allow for mathematical solution of governing differential equations.

Capillary Zone: Region in a solid environmental medium in which water is held by capillary tension at pressure heads less than one atmosphere. The zone may be saturated and referred to as the tension-saturated zone.

Computer or Source Code: The computer program or software used to run a fate and transport model.

Deterministic Risk Characterization: The process of determining risk by use of established, single-valued exposure parameters and direct calculation of constituent concentrations at point(s) of exposure to human or environmental receptors.

Dispersivity: Characteristic property of a porous environmental medium quantifying the process of dispersion.

Effective Porosity: The porosity of the environmental medium through which groundwater movement occurs (i.e., does not include porosity containing water which does not move with groundwater flow).

Environmental Media: Soil, soil vapor, soil pore water, groundwater, leachate, surface water, indoor air, or the ambient atmosphere which may be a source of constituents, or which may be a pathway(s) for migration of constituents from the source to the point of exposure to human or environmental receptors.

Evapotranspiration: A combination of evaporation from open bodies of water, evaporation from soil surfaces, and transpiration from the soil by plants.

Heterogeneous Conditions: Properties are not the same at each location in an environmental medium; opposite of homogenous.

Homogenous Conditions: Properties are the same at each location in an environmental medium; opposite of heterogeneous.

Hydraulic Conductivity: A physical property measuring the ability of groundwater to move through an environmental medium under a unit hydraulic head.

Hydraulic Gradient: The maximum slope of the water table or potentiometric surface.

Immiscible Liquids: Liquids which to not readily mix at standard temperature and pressure.

Isoconcentration Contours: Contours of equal concentrations of constituents in environmental media (analogous to topographic elevation contours).

Isotropic Conditions: Exhibiting properties with the same values when measured along axes in all directions; opposite of anisotropic.

Leaching: The process whereby constituents in soil are transferred to water infiltrating through the vadose zone.

Model Algorithm: A procedure for solving a mathematical problem (e.g., an equation) in a fate and transport model.

Model Domain: The area to be modeled.

Natural Attenuation: The combination of naturally occurring physical and chemical processes causing concentrations of constituents in environmental media to decrease over time.

Organic Carbon Partitioning Coefficient: A chemical-specific property related to the distribution of constituents between solid and liquid environmental media under equilibrium conditions.

Orthogonal Model Coordinates: Coordinate axes each of which are perpendicular to the other axes (e.g., *X*, *Y*, and *Z* axes of Cartesian coordinates).

Probabilistic Risk Characterization: The process of characterizing risk by statistical evaluation, using Monte Carlo or similar analyses, of exposure parameters and constituent concentrations at the points of exposure to human and environmental receptors.

Risk Assessment: Risk assessment is the systematic, scientific characterization of potential adverse effects of exposure of human or environmental receptors to hazardous agents or activities.

Risk-Based Corrective Action: Risk-based corrective action (RBCA) is incorporation of risk-based decision making into the underground storage tank corrective action process. It is typically a tiered decision-making process for the assessment and response to a release of constituents, based on the protection of human health and the environment.

Risk-Based Decision Making: A process that utilizes risk and exposure methodology to help implementing agencies make determinations about the extent and urgency of corrective action and about the scope and intensity of their oversight of corrective action by UST owner/operators. The process is flexible to allow for varying implementation concerns of the implementing program.

Steady-State Conditions: Conditions when the magnitude and direction of groundwater movement at any point in a flow field are constant with time.

Transient Conditions: Conditions when the magnitude and direction of groundwater movement at any point in a flow field change with time.

Vadose Zone: The zone of unsaturated soil above the water table.

Water Table: The level to which groundwater will rise in a well open to the atmosphere.

• 6.0 BIBLIOGRAPHY

1. American Petroleum Institute (API), 1994: *Transport and Fate of non-BTEX Petroleum Chemicals in Soil and Groundwater*, API Publication No. 4593, Washington DC.
2. American Petroleum Institute (API), 1996: *Estimation of Infiltration and Recharge for Environmental Site Assessments,* API Publication No. 4643, Washington DC.
3. American Society of Civil Engineers (ASCE), 1995: *Groundwater Quality: Guideline for Selection of Commonly Used Groundwater Models,* New York, NY.
4. American Society for Testing and Materials (ASTM), 1993: *Guide for Application of Groundwater Flow Models to a Site Specific Problem,* West Conshohocken PA.
5. American Society for Testing and Materials (ASTM), 1995: *Standard Guide for Risk-Based Corrective Action Applied at Petroleum Release Sites,* E 1739-95, West Conshohocken PA.
6. Anderson, M.P., and W.W. Woessner, 1992: *Applied Groundwater Modeling,* Academic Press, Inc., San Diego CA.
7. Association of American Railroads, 1996: *Risk-Based Management of Diesel-Contaminated Soil,* Publication No. R-897, Washington DC.
8. Bauer, P., 1998: *Disperse: Advection/Dispersion Model for MTBE and TBA*, New Jersey Department of Environmental Protection.
9. Bear, J., 1972: *Dynamics of Fluids in Porous Media,* Dover Publications, Inc., Mineola NY.
10. Bedient, P.B., et al., 1995: *Groundwater Contamination Transport and Remediation,* Prentice-Hall, Inc., Englewood Cliffs NJ.
11. Bonazountas, M., and J.M. Wagner, 1984: *SESOIL: A Seasonal Soil Compartment Model*; prepared for the US EPA. Arthur D. Little, Inc., Cambridge MA.
12. Campbell, G.S., 1974: "A Simple Method for Determining Unsaturated Hydraulic Conductivity from Moisture Retention Data", *Soil Science,* Vol. 117, pp. 311-314.
13. Clapp, R.B., and G.M. Hornbeyer, 1978: "Empirical Equations for Some Hydraulic Properties", *Water Resources Research,* Vol. 14, pp. 601-604.
14. Cline, P.V., et al., 1991: "Partitioning of Aromatic Constituents Into Water from Gasoline and other Complex Solvent and Mixtures", *Environmental Science and Technology,* Vol. 25, pp. 914-917.
15. Connor, J.A., et al., 1996: *Soil Attenuation Model for Derivation of Risk-Based Soil Remediation Standards,* Groundwater Services, Inc., Houston TX.
16. Crum, J.A., 1997: *Generic Groundwater and Soil Volatilization to Indoor Air Inhalation Criteria: Technical Support Document,* Michigan Department of Environmental Quality, Environmental Response Division.
17. Domenico, P.A., 1972: *Concepts and Models in Groundwater Hydrology,* McGraw-Hill, New York NY.
18. Domenico, P.A., 1987: "An Analytical Model for Multidimensional Transport of a Decaying Contaminant Species", *Journal of Hydrology,* Vol. 9, pp. 49-58.

19. Domenico, P.A. and F.W. Schwartz, 1990: *Physical and Chemical Hydrogeology*, John Wiley & Sons, New York NY.

20. Eagleson, P.S., 1978: “Climate, Soil and Vegetation”, *Water Resources Research,* Vol. 14, pp. 705-776.

21. Electric Power Research Institute (EPRI), 1995*: Mineral Insulating Oil Characterization Report*, prepared by CH_2M Hill and META Environmental.

22. EPA, 1991: *MOFAT: A Two-Dimensional Finite Element Program for Multiphase Flow and Multicomponent Transport*, U.S. EPA Robert S. Kerr Environmental Research Laboratory, Ada OK, EPA/600/2-91/020, PB91-191692.

23. EPA, 1993: *MULTIMED: The Multimedia Exposure Assessment Model for Evaluating the Land Disposal of Wastes--Model Theory: Project Summary,* U.S. EPA Environmental Research Laboratory, Athens GA, EP1.89/2:600/SR-93/081, PB93-1048-M.

24. EPA, 1989: *Risk Assessment Guidance for Superfund, Vol. 1: Human Health Evaluation Manual, Part A*, EPA/540/1-89/002.

25. EPA, 1994: *Assessment Framework for Ground-Water Model Applications,* Office of Emergency and Remedial Response, Washington DC, EPA 500-B-94-003.

26. EPA, 1994: *Ground-Water Modeling Compendium-Second Edition,* Office of Emergency and Remedial Response, Washington DC, EPA 500-B-94-004.

27. EPA, 1996: *Soil Screening Guidance: Technical Background Document,* Office of Emergency and Remedial Response, Washington DC, EPA/540/R-95/128, PB96-963502.

28. EPA, 1996: *Soil Screening Guidance: Users Guide,* Office of Emergency and Remedial Response, Washington DC, EPA/540/R-96/018, PB96-963505.

29. EPA, 1995: *SCREEN3 Model User’s Guide,* Office of Air Quality Planning and Standards, Emissions, Monitoring, and Analysis Division, Research Triangle Park NC, EP4.8: SCR2/2, PB97-0383-M.

30. EPA, 1998: *Superfund Exposure Assessment Manual,* Office of Emergency and Remedial Response, Washington DC, OSWER Directive 9285.5-1.

31. EPA, 1992: *User’s Guide for the Industrial Source Complex (ISC2) Dispersion Models,* Office of Air Quality Planning and Standards, Technical Support Division, Research Triangle Park NC, EP4.8: IN2/V.2, PB93-0858-M.

32. Farmer, W.J., et al., 1980: “Hexachlorobenzene: Its Vapor Pressure and Vapor Phase Diffusion in Soil”, *Soil Science Society of America Journal,* Vol. 44, pp. 445-450.

33. Fetter, C.W., 1988: *Applied Hydrogeology,* 2nd Edition, Merrill Publishing, Columbus, OH.

34. Freeze, A. R. and J.A. Cherry, 1979: *Groundwater,* Prentice-Hall, Inc., Englewood Cliffs NJ.

35. Groundwater Services, Inc., *Tier 2 RBCA Guidance Manual for Risk-Based Corrective Action,* Houston TX.

36. Gustafson, J., et al., 1996: “Selection of Representative TPH Fractions Based on Fate and Transport Considerations”, Total Petroleum Hydrocarbon Criteria Working Group, Volume 3.

37. Hayden, A.J., et al., 1992: “Prediction of Leachate Concentrations in Petroleum-Contaminated Soils”*, Journal of Soil Contamination,* Vol. 1, pp. 81-93.

38. Hemond, H.F., and E.J. Fechner, 1994: *Chemical Fate and Transport in the Environment,*

Academic Press, New York NY.

39. Howard, P.H., et al, 1991: *Handbook of Environmental Degradation Rates,* Lewis Publishers Inc., Chelsea MI.
40. Johnson, P. C. and R.A. Ettinger, 1991: “Heuristic Model for Predicting the Intrusion Rate of Contaminant Vapors into Buildings”, *Environmental Science and Technology,* Vol. 25, No.8, pp. 1445-1452.
41. Jury, W.A., et al., 1990: “Evaluation of Volatilization by Organic Chemicals Residing Below the Soil Surface”, *Water Resource Research,* Vol. 26, pp. 13-20.
42. Konikow, L.F., et al., 1994: *User’s Guide to Revised Method-of-Characteristics Solute-Transport Model (MOC-Version 3.1),* U.S. Geological Survey Earth Science Information Center, Denver CO.
43. Liptak, J.F. and G. Lombard, 1996: “The Development of Chemical-Specific, Risk-Based Soil Cleanup Guidelines Results in Timely and Cost-Effective Remediation”, *Journal of Soil Contamination,* Vol. 5, pp. 83-94.
44. Lyman, W.J., et al., 1982: *Handbook of Chemical Property Estimation Methods*, McGraw Hill, New York NY.
45. Lyman, W.J. et al., “Organic Contaminants in Subsurface Environments*”, Mobility and Degradation of Organic Contaminants in Subsurface Environments*, Camp Dresser and McKee, Inc., Chelsea MI.
46. Mercer, J.W. and R.M. Cohen, 1990: “A Review of Immiscible Fluids in the Subsurface: Properties, Models, Characterization and Remediation,” *Journal of Contaminant Hydrogeology,* Vol. 6, 1990, pp. 107-163.
47. Nevin, J.P., 1997: “FATE5: A Natural Attenuation Calibration Tool for Groundwater Fate and Transport Modeling”, *1996 Petroleum Hydrocarbons and Organic Chemicals in Ground Water: Prevention, Detection, and Remediation Conference,* National Ground Water Association Catalog #T539.
48. Odencrantz, J.E., et al, 1990: “Transport Model Sensitivity for Soil Cleanup Level Determination Using SESOIL and AT 123D in the Context of the California Leaking Underground Fuel Tank Field Manual*”, Proceedings Fifth Annual Conference on Hydrocarbon Contaminated Soils,* Amherst MA.
49. Odencrantz, J.E., et al., 1991: “A Better Approach to Soil Cleanup Level Determination”, *Sixth Annual Conference on Hydrocarbon Contaminated Soils,* Amherst MA.
50. Pasquill, R., 1974: *Atmospheric Diffusion,* John Wiley & Sons, New York NY.
51. Penman, H.L., 1963: “Vegetation and Hydrogeology”, *Technical Comment No 53,* Commonwealth Bureau of Soils, Harpenden, England.
52. Pollock, D., 1989: *A Graphical Kernel System (gks) Version of Computer Program Modpath-Pilot for Displaying Pathlines Generated from the U.S. Geological Survey Modular Three-dimensional Ground-water Flow Model,* U.S. Geological Survey.
53. Prickett, T.A. and C. G. Lonquist, 1971: *Selected Digital Computer techniques for Groundwater Resource Evaluation*, Illinois State Water Survey, Bulletin 55.

54. Ravi, V., and J.A. Johnson, 1997: *VLEACH: A One-Dimensional Finite Difference Vadose Zone Leaching Model,* U.S. EPA Robert S. Kerr Environmental Research Laboratory, Ada OK.

55. Rawls, W.J., et al., 1985: "Prediction of Soil Water Properties for Hydrologic Modeling Proceedings", *Watershed Management in the Eighties,* American Society of Civil Engineers, New York NY.

56. Reynolds, B., 1984: "A Simple Method for the Extraction of Soil Solution by High Speed Centrifugation" *Plant and Soil,* Vol. 78, pp. 437-440.

57. Sanders, P.F., and A.H. Stern, 1994: "Calculation of Soil Cleanup Criteria for Carcinogenic Volatile Organic Compounds as Controlled by the Soil-to-Indoor Air Exposure Pathway", *Environmental Toxicology and Chemistry*, Vol. 13, pp.1367-1374.

58. Schroeder, P.R., et al., 1994: *The Hydrologic Evaluation of Landfill Performance (HELP) Model, Version 3.* Risk Reduction Engineering Laboratory, Cincinnati OH, EPA/GOV/R-94/168b.

59. Shiozawa, S. and G.S. Campbell, 1991: "On the Calculation for Mean Particle Diameter and Standard Deviation for Sand, Silt and Clay Fractions", *Soil Science,* Vol. 152, pp. 427-431.

60. Schulz, E.F., 1976: *Problems in Applied Hydrology*., Water Resources Publications, Ft. Collins CO.

61. Thibodeaux, L.J. and S.T. Hwang, 1982: "Landfarming of Petroleum Wastes - Modeling the air emissions Problem", *Environmental Progress*, Vol. 1, No. 1, pp. 44-46.

62. Tomich-Kent, L.J., 1998: *Guidance for Fate and Transport Modeling,* Alaska Department of Environmental Conservation, Division of Spill Prevention and Response, Contaminated Sites Remediation Program, Guidance No. CSRP-98-001.

63. Ungs, J.U., 1997: "IBM-PC Applications in Risk Assessment, Remediation and Modeling", *National Groundwater Education Foundations Short Course*, Orlando FL, January 8-12.

64. Voss, C.I., 1984: *A Finite-Element Simulation Model for Saturated-Unsaturated, Fluid Density-Dependent Ground. Water Flow with Energy Transport or Chemically-Reactive Single-Species Transport*", U.S. Geological Survey Report No. 84-4369.

65. Walton, W.C., 1985: *Practical Aspects of Groundwater Modeling*, Second Edition, national Water Well Association.

66. Wang, H.F. and M.P. Anderson, 1982: *Introduction to Groundwater Modeling,* W.H. Freeman and Company, San Francisco CA.

67. Weidemeier, T.H., et al., 1995: *Technical Protocol for Implementing Intrinsic Remediation with Long-Term Monitoring for Natural Attenuation of Fuel Contamination Dissolved in Groundwater,* Air Force Center for Environmental Excellence.

68. Yeh, G.T., 1981; *AT123D: Analytical Transient One-, Two-, and Three-Dimensional Simulation of Waste Transport in the Aquifer System*, Oak Ridge National Laboratory Publication No. 1439.

69. Zheng, C., 1990: *A Modular Three-Dimensional Transport Model for Simulation of Advection, Dispersion and Chemical Reactions of Contaminants in Groundwater Systems,* S.S. Papadopulos & Associates, Inc.

70. Zheng C., and G.D. Bennett, 1995: *Applied Contaminant Transport Modeling*, Van Nostrand Reinhold, New York NY.

Bibliography on Measurement of Input Parameters:

71. Clapp, R.B. and G.M. Hornberger, 1978: “Empirical Equations for Some Soil Hydraulic Properties”, *Water Resources Research*, Vol. 14, No. 4.
72. Connor, J.A., et al., 1997: “Parameter estimation Guidelines for Risk-Based Corrective Action (RBCA) Modeling”, *1996 Petroleum Hydrocarbons and Organic Chemicals in Ground Water: Prevention, Detection, and Remediation Conference*, National Ground Water Association Catalog #T539.
73. EPA, 1991: *Characterizing Soils for Hazardous waste Site Assessments,* Office of Research and Development, EPA/540/4-91/003.
74. EPA, 1991: *Compendium of ERT Soil Sampling and Surface Geophysics Procedures,* OSWER Publication 9360.4-02, EPA/540/P-91/006, PB91-921273.
75. EPA, 1991: *Compendium of ERT Surface Water and Sediment Sampling Procedures,* OSWER Publication 9360.4-03, EPA/540/P-91/005, PB91-921274.
76. EPA, 1992: *Compendium of ERT Air Sampling Procedures*, OSWER Publication 9360.4-05, PB92-963406.
77. EPA, 1991: *Compendium of ERT Ground Water Sampling Procedures,* OSWER Publication 9360.4-06, EPA/540/P-91/007, PB91-921273.
78. EPA, 1998: *Estimation of Infiltration Rate in the Vadose Zone: Application of Selected Mathematical Models,* Office of Research and Development, EPA/600/R-97/128a and 128b.
79. EPA, 1993: *Subsurface Characterization and Monitoring Techniques: A Desk Reference Guide,* Center for Environmental Research Information, Environmental Monitoring Systems Laboratory, EPA/625/R-93/003a.
80. Rawls, W.J., et al., 1983: “Green-Ampt Infiltration Parameters from Soils Data”, *Journal of Hydraulic Engineering*, Vol. 109, No. 1.
81. Rawls, W.J. and D.L. Brakensick, 1989: *Estimation of Soil water Retention and Hydraulic Properties; Unsaturated Flow in Hydrologic Modeling,* Kluwer Academic Publishers, 1989.

Bibliography on Fate and Transport Model Packages:

82. Spence, L.R. and T. Walden, 1997: *Risk-Integrated Software for Clean-Ups: User’s Manual Version 3.0,* BP Oil.
83. Connor, J.A., et al., 1995: *Tier 2 Guidance Manual for Risk-Based Corrective Action,* Groundwater Services, Inc., Houston TX.
84. American Petroleum Institute (API), *Exposure and Risk Assessment Decision Support System (DSS) Software: Version 1* (find at http:///www.api.org/ehs/software.htm).

MATRICES

MATRIX 1
Key Model Information

Fate & Transport Pathway	Name of Model/Algorithm	Model Description/ Process Simulations	Type of Code/ Algorithm	Model Outputs	Features/Characteristics/ Use Conditions/Limitations	Computer Needs	References/ Sources
Soil to Ambient Air	Jury - Infinite Source	Vapor Migration from the surficial soils to ambient air.	1D Analytical Geometric	Average flux at surface	Assumes soils are impacted from the surface to an infinite depth, no leaching or evaporation, no soil-air boundary layers, and soil concentration is in the dissolved phase only (no residuals). Appropriate for thick zones of impacted soil or short exposure time. Assumes the effective diffusion coefficient is constant in isotropic/homogeneously mixed soil	Standard spreadsheet application	Jury et al., 1983; ASTM Risk-Based Corrective Action (RBCA) Guidance, Soil Screening Guidance (SSG)
	Jury - Finite Source	Vapor Migration from the surficial soil to ambient air.	1D Analytical Geometric-Exponential	Flux to ambient air over time	Assumes characteristics of the infinite model except soils are impacted from the surface to a finite depth. Appropriate for defined zones of impacted soil.	Standard spreadsheet application	Jury et al., 1990; SSG, EMSOFT
	Farmer	Vapor Migration from subsurface soils to ambient air.	1D Analytical - Linear	Instantaneous flux at surface	Assumes the location and source concentration remain constant and that there is a discrete layer of unimpacted soil between the atmosphere and the impacted zone. Simplest model, since the concentration remains constant, the surface flux term does not change with time.	Standard spreadsheet application	Farmer et al., 1980; ASTM RBCA, SSG
	Thibodeaux-Hwang	Vapor Migration from subsurface soils to ambient air.	1D Analytical - Geometric	Average flux at surface	Assumes that concentrations near the surface and surface flux decrease with time. Developed for land-farming processes. Biodegradation is not easily incorporated into the model. Most representative for low biodegradable petroleum compounds.	Standard spreadsheet application	Thibodeaux and Hwang, 1982; ASTM RBCA, SSG
	Box	Dispersion of Vapors in Ambient Air, no biodegradation	1D Analytical - Linear	Breathing zone concentration	Assumes complete and total mixing, constant wind velocity, no degradation. The mixing zone is rectangular with one side parallel to the wind direction. Assumes simple vapor dispersion from constant soil emissions. In common use and readily available.	Standard spreadsheet application	SEAM, 1988; ASTM RBCA, SSG
Soil to Ambient Air (continued)	SCREEN 3	Dispersion of vapors in ambient air. Can be configured to model worst-case atmospheric conditions and multiple sources	1D Analytical - Exponential	1 hour average concentration above the ground	Allows input of mixing zone and down-wind distance to exposure point. Does not incorporate the effects of terrain. Appropriate for area, volume and point (stack) sources. Also appropriate for one rectangular source and a limited number of receptors. Requires dimensions of source, emission rate, and downwind receptor distance. Does not consider particle settling, deposition, or wind direction. Commonly used, easy model with extensive testing.	Intel 80286, DOS 3.0 or higher, 640 Kb RAM, 500 Kb free disk space, math coprocessor	SCREEN3 User's Guide, EPA, 1995; SSG

MATRIX 1
Key Model Information
(continued)

Fate & Transport Pathway	Name of Model/Algorithm	Model Description/ Process Simulations	Type of Code/ Algorithm	Model Outputs	Features/Characteristics/ Use Conditions/Limitations	Computer Needs	References/ Sources
	ISCST 3	Dispersion of Vapors in Ambient Air - Can adequately model complex geometrical configurations of the source(s) and receptors. Revised to perform a double integration of the Gaussian plume kernel for area sources	1D Gaussian plume model	"N"-day average concentration or total deposition calculated at each receptor for any desired source combinations	Appropriate for multiple sources, numerous receptors, and where the source and receptor are separated by some distance. Will predict deposition rates. Considers terrain and hourly meteorological data. Chemical half-life transformations possible. Requires dimensions and emissions rate for each source, hourly meteorological data, and receptor locations. Can consider particle settling, depositions rates, and rudimentary chemical reactions. Commonly used model with extensive testing.	486/Pentium with 8 MB RAM running Windows® 3.1, Windows® 95 or Windows® NT	Superfund Exposure Assessment Manual (SEAM), 1988; EPA, 1992; Scientific Software Group, National Technical Information Service (NTIS)
Soil to Indoor Air	Farmer	Vapor diffusion from soil through floor or foundation	1D Analytical - Linear	Instantaneous flux at surface	Assumes that the floor provides resistance to diffusion. Models indoor air mixing based on a box model with air exchange rate and dimensions of the enclosed space as input.	Standard spreadsheet application	Jury, Farmer, 1983; SSG
	Farmer (modified)	Vapor diffusion from soil through floor or foundation , considers advection.	1D Analytical - Linear	Instantaneous flux at surface	Assumes that the floor provides resistance to diffusion. Considers advection and the permeability of site soils. Not a conservative model when sites have highly permeable soils.	Standard spreadsheet application	Jury, Farmer, 1983; SSG
Soil to Indoor Air (continued)	Johnson and Ettinger	Vapor migration from subsurface soil through a cracked foundation. Includes diffusion and advection processes but no biodegradation.	1D Analytical - Exponential	Average flux at surface and indoor air concentration	Similar to Farmer model but adds set of terms to account for flow resistance due to a floor or foundation. Assumes constant soil concentration, no biodegradation, no leaching, and all soil vapors will enter building, primarily through cracks and openings in the basement wall or foundation. Assumes advective air flow from the soil into the enclosed space. Assumes all chemical vapors below the basement will enter and will have a well-mixed dispersion in air once in the building.	Standard spreadsheet application	Johnson and Ettinger, 1991; ASTM RBCA, SSG
Soil to Groundwater	LEACH	Calculates soil leaching partitioning factor and an attenuation factor for mixing with groundwater specifically developed for use with hydrocarbon fractions. Has linear equilibrium partitioning, no biodegradation and well-mixed dispersion in groundwater.	1D Analytical - Linear	Leaching factor	Assumes constant concentration in subsurface soils, linear equilibrium partitioning, steady-state leaching from the soil to groundwater, no biodegradation, and well-mixed dispersion of leachate in groundwater. Relatively simple and very conservative. Commonly used for Tier 1.	386/486 with math coprocessor, 4 MB RAM, 2.5 MB free disk space, and DOS 3.0 or higher	ASTM,1995; ASTM RBCA, SSG

MATRIX 1
Key Model Information
(continued)

Fate & Transport Pathway	Name of Model/Algorithm	Model Description/ Process Simulations	Type of Code/ Algorithm	Model Outputs	Features/Characteristics/ Use Conditions/Limitations	Computer Needs	References/ Sources
	SAM	A modification of the LEACH model to provide a more rigorous characterization of soil to groundwater process with dilution, evapotranspiration, sorption, biodegradation time average factor.	1D Analytical - Exponential	Leaching factor with biodegradation/ time-average factor	Augments the LEACH model to characterize critical input parameters and more accurately simulate rainfall infiltration and leachate migration. Applicable to analysis of porous media soils impacted by either organic and inorganic constituents in the absence of NAPLs. Can predict groundwater concentration given affected soil value or calculate a SSTL given a groundwater exposure limit	386/486 with math coprocessor, 4 MB RAM, 2.5 MB free disk space, and DOS 3.0 or higher	J. A. Connor et al, 1996; TNRCC
	VADSAT	Contaminant transport through unsaturated soil using compartmental approach with different models to describe source zone, vadose zone above the source, and vadose zone between source and groundwater.	1D Analytical - Exponential	Contaminant transfer to groundwater, volatilization losses	Homogenous/uniform soil conditions below source, hydraulic conductivity calculated as a function of constant moisture content, assumes source has uniform concentration, does not consider water table fluctuations. Considers finite-mass source zone, pseudo steady-state volatilization , diffusive vapor transport from source to ground surface, leaching from source zone	IBM 486 or compatible, 10 MB RAM, 8 MB free disk space, Windows® 3.1	Scientific Software Group
Soil to Groundwater (continued)	Jury-Unsaturated	Designed to simulate chemical flux in vadose zone. Can predict concentration in the aqueous phase and estimate mass loading to groundwater over time.	1D Analytical	Concentration with depth, flux to ambient air, flu to groundwater	Accounts for capillarity, advection, diffusion, infiltration, recharge, absorption, degradation. Uses a multiphase partitioning equation to relate concentration between media. Assumes uniform and steady infiltration. Most appropriate for time-varying volatile flux simulations. Assumes homogeneous soils with uniform chemical distribution within the source layer. The hydrology model is very simple. Commonly used for Tiers 2 and 3.	Intel 80i86, DOS 3.0 or higher, 640 Kb RAM, 3MB free disk space, and math coprocessor	W. A. Jury, D. Russo, G. Streile, H. El Abd, 1990; SSG
	SESOIL	Flow and Transport. Describes chemical fate and transport in the vadose zone with dissolution, diffusion, absorption, dispersion, biodegradation, and volatilization.	1D - Hybrid analytical - numerical	Concentration with depth, flux to ambient air, flux to groundwater	Assumes a finite source. The most sensitive parameters are biodegradation rate, soil organic carbon content, annual precipitation, and depth to groundwater. Combines 3 modules: a hydrologic module simulating the water balance, a pollutant transport module simulating chemical fate and transport, and a sediment erosion module. Does not address contaminant movement in saturated zone. Widely used, readily available, and commonly used for Tiers 2 and 3.	Intel 80i86, DOS 5.0 or higher, 2MB RAM, 2 MB free disk space, and math coprocessor	Bonazountas and Wagner, 1984; Scientific Software Group, International Ground Water Modeling Center (IGWMC)

MATRIX 1
Key Model Information
(continued)

Fate & Transport Pathway	Name of Model/Algorithm	Model Description/ Process Simulations	Type of Code/ Algorithm	Model Outputs	Features/Characteristics/ Use Conditions/Limitations	Computer Needs	References/ Sources
	HELP	Simulates the water balance in unsaturated and variably-saturated soils. Developed for landfills and solid waste containment facilities as a tool to evaluate impacts of design alternatives.	Quasi 2D Deterministic	Infiltration rate	Considers effects of vegetation, topography, engineered covers and liners, and differential soil layers on runoff and interception of precipitation. Includes a large database for weather data for different cities. Can calculate unsaturated hydraulic conductivity and soil particle size distribution from input data. Does not address transport processes. User-friendly and commonly used over several tiers.	Written in Basic Language for use under DOS 3.1 or higher in IBM-PC or compatible computers with 3 MB free disk space	Payton, R. and P. Schroeder, 1994; IGWMC
Soil to Groundwater (continued)	VLEACH	Describes movement of organic constituents within and between three phases: solute dissolved in groundwater, gas in the vapor phase, adsorbed compound in the solid phase. Leaching is simulated in a number of distinct, user-defined polygons vertically divided into a series of user-defined cells.	1D Numerical Finite Difference	Equilibrium distribution of constituent mass between liquid, gas, and sorbed phases. Area-weighted groundwater impact for modeled area.	Assumes vadose zone is in a steady-state condition with respect to water movement. Assumes moisture profile within vadose zone is constant. Assumes homogenous soil conditions within polygon. Does not incorporate biodegradation. Does not account for nonaqueous phase liquids.	Intel 8086, 80286, 80386, 80486, 256Kb RAM, DOS 2.0 or higher, CGA board, math coprocessor	Ravi, V. and J.A. Johnson, 1997; Center for Subsurface Modeling Support (CSMoS); Scientific Software Group
	SUTRA	Steady-state or transient flow, saturated and unsaturated conditions, simulates flow under variable density conditions with transport of energy or dissolved substances.	2D Numerical Hybrid Finite-difference and Finite-element	Pressure heads, concentration distribution over time	Accounts for capillarity, convection, dispersion, diffusion, absorption. Allows sources, sinks, and boundary conditions to be time-dependent.. Links both unsaturated leaching and saturated groundwater flow. Relatively complex site-specific model commonly used for Tier 3. Requires experienced user and reviewer.	Intel 80i86, DOS 3.0 or higher, 640 Kb RAM, 3MB free disk space, and math coprocessor	C.I. Voss, 1984; IGWMC, Scientific Software Group, U.S. Geological Survey (USGS)
	MOFAT	Flow and transport of three fluid phases. Includes advection, dispersion, diffusion, sorption, decay, and mass transfer. Handles cases in which gas and/or NAPL phases are absent in part or all of the domain.	2D Numerical Finite Element	Distribution of constituent concentration	Accounts for advection, dispersion, diffusion, absorption, decay, mass transfer. Can represent the transport of up to 5 chemicals in four phases (water, air, soil, and oil) while allowing up to 10 layers of differing soil layers. Difficult to use and does not have the same regulatory acceptance as SESOIL. Commonly used for Tier 3.	386/486 with math coprocessor, 4 MB RAM, 2.5 MB free disk space, and DOS 3.0 or higher	ESTI, 1991; EPA 1991; CSMoS, Scientific Software Group
	VS2DT	Simulates contaminant transport in the vadose zone, simulating variably saturated soils.	2D Numerical Finite Difference	Time history, spatial profiles of pressure and total head, volumetric moisture content, saturation, velocities, solute concentration	Accounts for evaporation, infiltration, plant uptake. Considers non-linear storage, conductance, and sink terms and boundary conditions. It is widely used, has a high degree of credibility and peer review, and is highly sophisticated. Most commonly used for higher tier analyses.	386/486 with math coprocessor, 4 MB RAM, 2.5 MB free disk space, and DOS 3.0 or higher	Healy, R. 1988, IGWMC, Scientific Software Group, USGS.

MATRIX 1
Key Model Information
(continued)

Fate & Transport Pathway	Name of Model/Algorithm	Model Description/ Process Simulations	Type of Code/ Algorithm	Model Outputs	Features/Characteristics/ Use Conditions/Limitations	Computer Needs	References/ Sources
Groundwater to Ambient Air	Farmer	Simulates vapor diffusion from groundwater through soil and vapor dispersion in air assuming an infinite source.	1D Analytical - Linear	Contaminant flux at surface	Assumes the flux term is constant, the water in the capillary fringe is clean, has high moisture content, and has low air-filled porosity. The thickness of the capillary zone affects the resistance to diffusion. A thin fringe can reduce the rate of vapor diffusion	Standard spreadsheet application	Farmer, 1980, ASTM RBCA
Groundwater to Indoor Air	Farmer	Simulates vapor diffusion from groundwater through soil and vapor dispersion in air.	1D Analytical - Linear	Contaminant flux at surface	Can calculate flux with or without advection through a modified equation. The effects of a capillary fringe are included through a modified diffusion coefficient	Standard spreadsheet application	Farmer, 1980; ASTM RBCA
	Johnson and Ettinger (modified)	Vapor migration from groundwater through a cracked foundation. Includes diffusion and advection processes but no biodegradation.	1D Analytical - Exponential	Average flux at surface and indoor air concentration	Modification of the Johnson and Ettinger (1991) model. Assumes constant soil concentration, no biodegradation, no leaching, and all soil vapors will enter building, primarily through cracks and openings in the basement wall or foundation. Assumes advective air flow from the soil into the enclosed space. Assumes all chemical vapors below the basement will enter and will have a well-mixed dispersion in air once in the building.	Standard spreadsheet application	Crum, J.A., 1997
Groundwater Transport	Disperse	Calculates conservative estimates for the size and duration of a MTBE or TBA plume using finite mass advection/dispersion equation.	2D Analytical	Distribution of constituent concentration	Assumes horizontal, homogenous aquifer; constant velocity; constant dispersion coefficient proportional to velocity. To be used for slug release of constituents.	Standard spreadsheet application	Bauer, P., 1998
	SOLUTE	A set of five programs based on analytical solutions of the advection-dispersion equation for a non-conservative tracer solute.	1D, 2D, 3D, and Radialsymetric Analytical	Distribution of constituent concentration	1D and radialsymetric models simulate effects of a single source; 2D and 3D models support multiple point sources using superposition to calculate accumulated effects or to represent line or areal sources.	Intel 80i86, DOS 3.1or higher, 640 Kb RAM, VGA graphics, math coprocessor	IGWMC
	AT123D	Mass Transport, uniform stationary regional flow, 3D dispersion, first order decay, retardation	3D Hybrid analytical - numerical	Distribution of constituent concentration	Assumes stationary flow field parallel to the source. Source release may be instantaneous, continuous, or finite step-wise duration and is equally distributed over the source area or volume. Water table does not fluctuate, flow direction is uniform and 1D. Simulates mass transport of dissolved phase, radionuclides, or heat.	DOS 2.1 or higher, 640 Kb RAM, 1 MB free disk space and a math coprocessor	Yeh, G. T., 1981; IGWMC, Scientific Software Group

MATRIX 1
Key Model Information
(continued)

Fate & Transport Pathway	Name of Model/Algorithm	Model Description/ Process Simulations	Type of Code/ Algorithm	Model Outputs	Features/Characteristics/ Use Conditions/Limitations	Computer Needs	References/ Sources
Groundwater Transport (continued)	Domenico	Dispersion in three dimensions over time.	3D Analytical - Exponential, Error Function Transformation (1D flow, 3D transport)	Normalized concentration at specified location	Transport is 1D along the centerline, between the source and receptor, the transport is 3D due to dispersion, and accounts for transport across the site over time. Requires input on advective flow velocity, dispersivity, source concentration and geometry. Can accommodate biodegradation. Commonly used to conduct a Tier 2 evaluation.	Standard spreadsheet application	Domenico, 1987; ASTM RBCA, SSG
	FATE5	Determine site-specific natural attenuation rates for organic constituents dissolved in groundwater (enhancement to Domenico analytical model)	3D Analytical - Exponential, Error Function Transformation (1D flow, 3D transport)	Normalized concentration at specified location	Same as Domenico. Includes optimization routine to match model results to measured site concentrations, database of chemical property data, calculation of time needed for a plume to reach steady-state conditions.	Standard spreadsheet application	Nevin, J.P., 1997; Groundwater Services, Inc.
	MULTIMED	1D unsaturated dispersion with volatilization, biodegradation, and decay. Saturated transport with 3D dispersion, linear absorption, 1st order decay, steady state or transient flow, single aquifer and dilution due to recharge.	3D Semi-Analytical - Linear	Leachate flux	Assumes constant source concentration, homogeneous and isotropic environment. Developed for landfills. Simulates precipitation, runoff, infiltration, evapotranspiration, barrier layers, and lateral drainage. Uses a finite thickness saturated zone and finite infiltration rate. Must specify vertical dispersivity and disposal facility parallel to flow. Not actively updated, functionally duplicated by other current software.	DOS-based, 640 Kb RAM with math coprocessor	Salhotra, 1990; SSG, Scientific Software Group
	Summers	Simulates non-dispersive mass transport in a single layer of soil from an infinite source. Steady-state flow conditions and equilibrium between absorbed and dissolved phase.	1D Analytical - Linear (mixing equation)	Constituent concentration in groundwater downgradient of source	Assumes complete mixing of the water-bearing zone. Developed as screening model to conservatively estimate concentrations in groundwater directly beneath vadose-zone source. Does not consider biodegradation, first-order decay or volatilization. Very conservative and appropriate for screening level.	Standard spreadsheet application	Summers, 1982; IGWMC
	BIOSCREEN	Dispersion in two dimensions, retardation, and biodegradation	2D Analytical - Exponential, Error Function Transformation (1D flow, 2D transport)	Constituent concentration in groundwater downgradient of source	Can run in a deterministic mode to compute concentration versus time at a given location or in the Monte Carlo mode to compute probability for occurrence of a concentration. Includes databases for soil and chemical properties and their variability. Requires planar groundwater flow field.	Intel 80486, DOS 3.1 or higher, 2MB RAM, graphics adapter	CSMoS; American Petroleum Institute (API)

MATRIX 1
Key Model Information
(continued)

Fate & Transport Pathway	Name of Model/Algorithm	Model Description/ Process Simulations	Type of Code/ Algorithm	Model Outputs	Features/Characteristics/ Use Conditions/Limitations	Computer Needs	References/ Sources
Groundwater Transport (continued)	VADSAT	Chemical movement from a source in the unsaturated zone or below the water table, considering evaporation of VOCs, leaching of constituents, planar groundwater flow field, dispersion, adsorption, first-order decay.	3-D Analytical	Peak constituent concentration in groundwater at receptor, time to reach peak concentration, time for source depletion	Ability to simulate advection, dispersion, adsorption, aerobic and anaerobic decay. Do not apply where pumping systems create a complicated flow system. Assumes unidirectional groundwater movement, constant flow rate. Easy screening tool.	Intel 80286, DOS 3.0 or higher, 640 Kb RAM, 500 Kb free disk space, math coprocessor	CSMoS; Scientific Software Group
	MODFLOW	Saturated, steady-state or transient flow for single or multiple aquifers, commonly used for Tiers 2 or 3.	2D or 3D Numerical Finite Difference	Hydraulic head	Assumes saturated zone can be heterogeneous and anisotropic, confined or unconfined aquifer system. Limited to groundwater flow. Commonly used for Tiers 2 or 3.	Intel 80286, DOS 3.0 or higher, 640 Kb RAM, 500 Kb free disk space, math coprocessor	McDonald, M. and Harbaugh, A., 1988; IGWMC, USGS
	PLASM	Saturated, steady-state or transient flow for single or multiple aquifers.	2D or 3D Numerical Finite Difference	Hydraulic head	Assumes saturated zone can be heterogeneous and anisotropic, confined or unconfined aquifer system. Limited to groundwater flow. Does not consider advection, diffusion, or dispersion. Commonly used for Tiers 2 or 3.	Intel 80i86, DOS 2.1or higher, 640 Kb RAM, 1.5 MB free disk space, math coprocessor	Prickett, T. and Lonnquist, C., 1971; IGWMC
	MOC	Groundwater flow and mass transport model, steady state or transient flow for a single aquifer. Considers advection, dispersion, and diffusion.	2D Numerical - Finite Difference	Distribution of constituent concentration	Assumes saturated zone can be heterogeneous and anisotropic, confined aquifer system. Commonly used for Tiers 2 or 3.	386/486 processor with math coprocessor, 4 MB RAM, DOS 5.0 or higher, at least 2 MB free disk space	Konikow, L. and Bredehoeft, J., 1994; IGWMC, USGS
	BIOPLUME	Contaminant transport under influence of oxygen limited biodegradation; Version III incorporates influence of oxygen, nitrate, iron, sulfate, and methanogenic biodegradation.	2D Numerical - Finite Difference (based on MOC)	Distribution of constituent concentration, velocity vectors, time history plots at user-defined observation points	Simulates processes of advection, dispersion, sorption, aerobic and anaerobic biodegradation, and reaeration. Version III includes biodegradation through instantaneous, first, or zero order decay; or Monod kinetics. Hydrocarbon source and each active electron acceptor are simulated as separate plumes.	386/486 processor with math coprocessor, 4 MB RAM, DOS 5.0 or higher, at least 2 MB free disk space; Windows 95® for Version III	CSMoS; Scientific Software Group
	Random Walk	Groundwater flow and mass transport model, steady state or transient flow heterogeneous aquifers. Considers convection, dispersion, first-order decay, and retardation.	2D Numerical - Finite Difference	Hydraulic head, distribution of constituent concentration	Assumes saturated zone can be heterogeneous, isotropic or anisotropic, confined or unconfined aquifer system. Commonly used for Tiers 2 or 3.	Intel 80i86, DOS 3.0 higher, 640 Kb RAM, 2.0 MB free disk space, math coprocessor	Prickett, T.; Naymik, T.; Lonnquist, C., 1981; IGWMC, Scientific Software Group
Groundwater Transport (continued)	MT3D	Mass Transport in the saturated zone, steady-state or transient flow for single or multiple aquifers.	3D Numerical - Finite Difference	Simulates changes in concentration	Assumes saturated zone can be heterogeneous and anisotropic, confined or unconfined aquifer system Handles a variety of discretization schemes and boundary conditions. Commonly used for Tiers 2 or 3.	386/486 with math coprocessor, 2 MB RAM, DOS 3.0 or higher	Zheng, C., 1990; IGWMC, Scientific Software Group

MATRIX 1
Key Model Information
(continued)

Fate & Transport Pathway	Name of Model/Algorithm	Model Description/ Process Simulations	Type of Code/ Algorithm	Model Outputs	Features/Characteristics/ Use Conditions/Limitations	Computer Needs	References/ Sources
	MODPATH	Semi-analytical Particle Tracking Scheme for steady-state flow, single or multiple aquifers	3D Numerical Finite Difference	Computes 3D path lines	Assumes saturated zone can be heterogeneous and anisotropic confined or unconfined aquifer system. Can handle multiple release times for particles and can draw true cross-section grids displaying spatial data. Superimposes particle tracks on flow field typically generated using another model.	Requires 386/486 with math coprocessor, 4MB RAM 5MB free disk space, DOS 3.0 or higher	Pollock, D. W. 1989; IGWMC, Scientific Software Group, USGS

MATRIX 2
Generic Site Conditions for Model Application

Site Condition for Model Application	Candidate Models									
Soil to Ambient Air	**Jury Infinite Source**	**Jury Finite Source**	**Farmer**	**Thibodeaux /Hwang**	**Box**	**SCREEN 3**	**ICST 3**			
Homogenous/isotropic soil	•	•	•	•						
Infinite source depth	•									
Finite source depth		•								
Constant source			•		•					
Dissolved-phase constituents	•	•								
Depth to source increases				•						
Unimpacted soil above source			•							
Constant diffusion coefficient	•	•	•							
Dispersion w/complete mixing					•	•				
Constant wind speed					•					
Downwind receptor						•	•			
Dispersion w/ multiple sources							•			
Dispersion considers terrain							•			
Particle settling							•			
Biodegradation/transformation							•			
Soil to Indoor Air	**Farmer**	**Farmer (modified)**	**Johnson Ettinger**							
Floor provides resistance	•	•	•							
Mixing of indoor air	•	•	•							
Considers advection		•	•							
Considers soil permeability		•	•							
Constant soil concentrations	•	•	•							
All soil vapors enter building			•							
Soil to Groundwater	**LEACH**	**SAM**	**VADSAT**	**SESOIL**	**HELP**	**VLEACH**	**SUTRA**	**Jury Un-saturated**	**MOFAT**	**VS2DT**
Homogenous soil conditions	•		•			•		•		
Layered soil conditions		•		•	•		•		•	•
Finite source				•		•				
Constant source concentration	•	•				•				
Constant moisture content			•			•				
Linear equilibrium partitioning	•	•								
Steady-state vadose zone cond.	•	•	•			•		•		
Transient vadose zone cond.				•			•			•
Biodegradation/transformation		•	•	•					•	
Well-mixed leachate dispersion	•	•	•							
Considers vegetation/topo.					•					•
Rainfall infiltration		•		•	•			•		•
Analytical model	•	•	•	•				•		
Numerical model				•		•	•		•	•

MATRIX 2
Generic Site Conditions for Model Application
(continued)

Site Condition for Model Application	**Candidate Models**															
Engineered covers/liners					•											
Accounts for capillarity							•									
Uniform, steady infiltration	•	•	•			•		•								
Includes evaporation				•	•											
Considers multiple sources							•			•						
Handles non-aqueous phase			•	•					•							
Considers sinks							•			•						
Groundwater to Ambient Air	**Farmer**															
Constant flux term	•															
Clean capillary water in fringe	•															
High soil moisture content	•															
Low air-filled porosity	•															
Groundwater to Indoor Air	**Farmer**	**Johnson Ettinger**														
Constant flux term	•	•														
Clean capillary water in fringe	•	•														
High soil moisture content	•															
Low air-filled porosity	•															
Groundwater Transport	**Disperse**	**SOLUTE**	**AT123D**	**Domenico**	**FATE 5**	**MULTI-MED**	**Summers**	**BIO-SCREEN**	**VADSAT**	**MOD-FLOW**	**PLASM**	**MOC**	**BIO-PLUME**	**Random Walk**	**MT3D**	**MOD-PATH**
One dimensional		•					•	•								
Multi-dimensional	•	•	•	•	•	•			•	•	•	•	•	•	•	•
Steady-state conditions				•	•	•				•	•	•		•	•	
Transient conditions										•	•	•		•	•	
Finite difference form										•	•	•	•	•	•	•
Analytical model	•	•		•	•	•	•	•					•	•		
Hybrid analytical/numerical			•													
Unconfined aquifers				•	•					•	•			•	•	•
Confined aquifers				•	•					•	•	•		•	•	•
Homogenous/isotropic aquifer	•	•		•	•	•	•	•	•				•	•		
Horizontal water-bearing units	•	•		•	•	•	•						•	•		
Heterogeneous aquifer										•	•	•		•	•	•
Constant groundwater velocity	•	•		•	•	•	•									
Calculates velocity													•			
Calculates constituent conc.	•	•	•	•	•		•	•	•			•	•	•	•	
Calculates hydraulic head										•	•		•	•		
Groundwater flow paths																•
Considers dispersion	•	•		•	•	•		•				•	•	•		
Adsorption/retardation		•	•			•	•	•					•	•		
Continuous source		•	•	•	•		•						•			

MATRIX 2
Generic Site Conditions for Model Application
(continued)

Site Condition for Model Application	**Candidate Models**															
Instantaneous/finite source	●	●	●										●			
Variable source concentrations		●	●										●			●
Uniform flow direction	●	●	●	●	●											
Biodegradation/transformation		●	●	●	●			●					●	●		
Mass transport		●	●			●	●	●				●	●	●	●	
Mixing of water-bearing zone			●				●									
Run in probabilistic mode									●							
Chemical property database					●											

MATRIX 3
Key Input Parameters

Fate and Transport Pathway	Input Parameter	Parameter Symbol (typ.)	Parameter Units (typ.)	Comment on Sensitivity to Input Parameter
Soil to Ambient Air	***Source area concentration***	C_S	mg/Kg	Site-specific; ***sensitive parameter***
	Volumetric air content in vadose zone soil	Θ_{as}	cm^3/cm^3	Variation effects water content; ***sensitive parameter***
	Volumetric water content in vadose zone soil	Θ_{ws}	cm^3/cm^3	Variation effects air content; ***sensitive parameter***
	Total soil porosity	Θ_T	cm^3/cm^3	Correlated with volumetric air/water contents; ***sensitive parameter***
	Depth to soil contamination	L_s	cm, ft.	Highly variable, site-specific; ***sensitive parameter***
	Thickness of soil contamination	L	cm, ft.	Highly variable, site-specific; ***sensitive parameter***
	Diffusion coefficient in air	D_{air}	cm^2/sec.	Chemical-specific; limited sensitivity
	Fraction of organic carbon	f_{oc}	g-C/g-Soil	Not a sensitive parameter for this pathway
	Henry's Law constant	H	cm^3-H_2O/cm^3-air	Chemical-specific; limited sensitivity
	Carbon-water sorption coefficient	K_{oc}	cm^3-H_2O/g-C	Chemical specific; moderate sensitivity
	Soil-water sorption coefficient	K_s	cm^3-H_2O/g-soil	f_{oc} x K_{oc}; moderate sensitivity
	Soil bulk density	ρ_s	g/cm^3	Varies little for common soil types; limited sensitivity
	Wind speed above ground surface	U_{air}	cm/sec., mi./hr.	Not a sensitive parameter for this pathway
	Ambient air mixing zone height	δ_{air}	cm	Not a sensitive parameter for this pathway
	Source width parallel to wind	W	cm	Highly variable, site-specific; moderate sensitivity
Soil to Indoor Air (in addition to input parameters for soil to ambient air)	***Enclosed-space volume/infiltration area ratio***	L_B	cm	Relates to volume of air in enclosed space; ***sensitive parameter***
	Enclosed space air exchange rate	ER	L/sec., L/hr.	Causes advective flow of vapors to building; ***sensitive parameter***
	Thickness of foundation/floor	L_{crack}	cm, in.	Not a sensitive parameter for this pathway
	Areal fraction of cracks in foundation/walls	η	cm^2-cracks/cm^2	Not a sensitive parameter for this pathway
	Volumetric water content in cracks	Θ_{wcrack}	cm^3-H_2O/cm^3	Not a sensitive parameter for this pathway
	Volumetric air content in cracks	Θ_{acrack}	cm^3-air/cm^3	Not a sensitive parameter for this pathway
	Effective diffusion coefficient through crack	D_{crack}	cm^2/sec.	Chemical-specific; limited sensitivity
	Floor/wall seam perimeter	X_{crack}	cm, in.	Not a sensitive parameter for this pathway
	Depth of crack below ground surface	Z_{crack}	cm, in.	Not a sensitive parameter for this pathway
	Effective radius of crack	r_{crack}	cm, in.	Not a sensitive parameter for this pathway
Soil to Groundwater	***Source area concentration***	C_S	mg/Kg	Site-specific; ***sensitive parameter***
	Total soil porosity	Θ_T	cm^3/cm^3	Correlated with volumetric air/water contents; ***sensitive parameter***
	Fraction of organic carbon	f_{oc}	g-C/g-Soil	Highly variable, site-specific; ***sensitive parameter***
	Carbon-water sorption coefficient	K_{oc}	cm^3-H_2O/g-C	Chemical specific; ***sensitive parameter***
	Soil-water sorption coefficient	K_s	cm^3-H_2O/g-soil	f_{oc} x K_{oc}; ***sensitive parameter***
	Width of source area parallel to groundwater flow	W	cm	Highly variable, site-specific; moderate sensitivity
	Soil bulk density	ρ_s	g/cm^3	Varies little for common soil types; limited sensitivity

MATRIX 3
Key Input Parameters
(continued)

Fate and Transport Pathway	Input Parameter	Parameter Symbol (typ.)	Parameter Units (typ.)	Comment on Sensitivity to Input Parameter
	Volumetric air content in vadose zone soil	Θ_{as}	cm^3/cm^3	Not a sensitive parameter for this pathway
	Volumetric water content in vadose zone soil	Θ_{ws}	cm^3/cm^3	Not a sensitive parameter for this pathway
	Infiltration rate of water through soil	I	cm/yr., in./yr.	Highly variable, site-specific; moderate sensitivity
	Groundwater mixing zone thickness	δ_{gw}	cm	Depends on soil type and does not very greatly; limited sensitivity
	Groundwater Darcy velocity	U_{gw}	cm/yr., ft./day	Volume flux, U_{gw}/area = K_s x i ; moderate sensitivity
	Degradation rate in vadose zone	λ	$yr.^{-1}$	Chemical specific, affected by site conditions; moderate sensitivity
	Depth to subsurface soil sources	L_S	cm, ft.	Highly variable, site-specific; moderate sensitivity
	Thickness of vadose zone	h_v	cm, ft.	Highly variable, site-specific; moderate sensitivity
	Pure constituent solubility in water	S	mg/L	Chemical specific; moderate sensitivity
Groundwater to Ambient Air	***Source area concentration***	C_W	ug/L	Site-specific; ***sensitive parameter***
	Thickness of capillary fringe	h_{cap}	cm, in.	Serves as barrier to vapor transport; ***sensitive parameter***
	Volumetric air content in vadose zone soil	Θ_{as}	cm^3/cm^3	Variation effects water content; ***sensitive parameter***
	Volumetric water content in vadose zone soil	Θ_{ws}	cm^3/cm^3	Variation effects air content; ***sensitive parameter***
	Total soil porosity	Θ_T	cm^3/cm^3	Correlated with volumetric air/water contents; ***sensitive parameter***
	Depth to Groundwater	L_{GW}	cm, ft.	Highly variable, site-specific; ***sensitive parameter***
	Diffusion coefficient in air	D_{air}	cm^2/sec.	Chemical-specific; limited sensitivity
	Diffusion coefficient in water	D_{water}	cm^2/sec.	Chemical-specific; limited sensitivity
	Volumetric water content in capillary fringe	Θ_{wcap}	cm^3-H_2O/cm^3-soil	Correlated with thickness of capillary fringe; moderate sensitivity
	Volumetric air content in capillary fringe	Θ_{acap}	cm^3-air/cm^3-soil	Correlated with thickness of capillary fringe; moderate sensitivity
	Fraction of organic carbon	f_{oc}	g-C/g-Soil	Not a sensitive parameter for this pathway
	Henry's Law constant	H	cm^3-H_2O/cm^3-air	Chemical-specific; limited sensitivity
	Carbon-water sorption coefficient	K_{oc}	cm^3-H_2O/g-C	Chemical specific; moderate sensitivity
	Soil-water sorption coefficient	K_s	cm^3-H_2O/g-soil	f_{oc} x K_{oc}; moderate sensitivity
	Soil bulk density	ρ_s	g/cm^3	Varies little for common soil types; limited sensitivity
	Wind speed above ground surface	U_{air}	cm/sec., mi./hr.	Not a sensitive parameter for this pathway
	Ambient air mixing zone height	δ_{air}	cm	Not a sensitive parameter for this pathway
	Source width parallel to wind	W	cm	Highly variable, site-specific; moderate sensitivity
Groundwater to Indoor Air (in addition to input parameters for ground-water to ambient air)	***Enclosed-space volume/infiltration area ratio***	L_B	cm	Relates to volume of air in enclosed space; ***sensitive parameter***
	Enclosed space air exchange rate	ER	L/sec., L/hr.	Causes advective flow of vapors to building; ***sensitive parameter***
	Thickness of foundation/floor	L_{crack}	cm, in.	Not a sensitive parameter for this pathway
	Areal fraction of cracks in foundation/walls	η	cm^2-cracks/cm^2	Not a sensitive parameter for this pathway
	Volumetric water content in cracks	Θ_{wcrack}	cm^3-H_2O/cm^3	Not a sensitive parameter for this pathway

MATRIX 3
Key Input Parameters
(continued)

Fate and Transport Pathway	Input Parameter	Parameter Symbol (typ.)	Parameter Units (typ.)	Comment on Sensitivity to Input Parameter
	Volumetric air content in cracks	Θ_{acrack}	cm^3-air/cm^3	Not a sensitive parameter for this pathway
	Effective diffusion coefficient through crack	D_{crack}	cm^2/sec.	Chemical-specific; limited sensitivity
	Floor/wall seam perimeter	X_{crack}	cm, in.	Not a sensitive parameter for this pathway
	Depth of crack below ground surface	Z_{crack}	cm, in.	Not a sensitive parameter for this pathway
	Effective radius of crack	r_{crack}	cm, in.	Not a sensitive parameter for this pathway
Groundwater Transport	***Source area concentration***	C_S	ug/L	Site-specific; ***sensitive parameter***
	Fraction of organic carbon	f_{oc}	g-C/g-Soil	Highly variable, site-specific; ***sensitive parameter***
	Carbon-water sorption coefficient	K_{oc}	cm^3-H_2O/g-C	Chemical specific; ***sensitive parameter***
	Soil-water sorption coefficient	K_s	cm^3-H_2O/g-soil	f_{oc} x K_{oc}; ***sensitive parameter***
	Downgradient distance to nearest receptor	x	cm, ft.	Highly variable, site-specific; ***sensitive parameter***
	Saturated hydraulic conductivity	K_S	cm/sec., ft./min.	Highly variable, site-specific; ***sensitive parameter***
	Hydraulic gradient	i	ft./ft.	Highly variable, site-specific; ***sensitive parameter***
	Average linear velocity	ν	ft./day, ft./yr.	$\nu = K_S \times i / \Theta_T$, site-specific; ***sensitive parameter***
	Width of source area parallel to groundwater flow	W	cm	Highly variable, site-specific; moderate sensitivity
	Total soil porosity	Θ_T	cm^3/cm^3	Affects velocity and retardation factor; moderate sensitivity
	Soil bulk density	ρ_s	g/cm^3	Varies little for common soil types; limited sensitivity
	Saturated thickness	b	cm/ ft.	Site-specific; moderate sensitivity in numerical models
	Storativity (storage coefficient)	S	unitless	Depends on confined/ unconfined aquifer; limited sensitivity
	Infiltration rate of water through soil (recharge)	I	cm/yr., in./yr.	Highly variable, site-specific; limited sensitivity
	Longitudinal dispersivity	a_x	cm	Varies little for common soil types; limited sensitivity
	Transverse dispersivity	a_y	cm	Varies little for common soil types; limited sensitivity
	Vertical dispersivity	a_z	cm	Varies little for common soil types; limited sensitivity
	Degradation rate	λ	yr.$^{-1}$	Chemical specific, affected by site conditions; moderate sensitivity
	Time since release	t	days, yr.	Highly variable, site-specific; moderate sensitivity

Note: The purpose of Matrix 3 is to highlight sensitive input parameters and not to provide a comprehensive compilation of all input parameters for every possible fate and transport model. Sensitive input parameters are highlighted in ***bold italics***. Input parameters are those commonly needed for fate and transport modeling, grouped by fate and transport pathway. Sensitivity of specific models to input parameters is indicated in the model summaries in Appendix A.

FIGURES

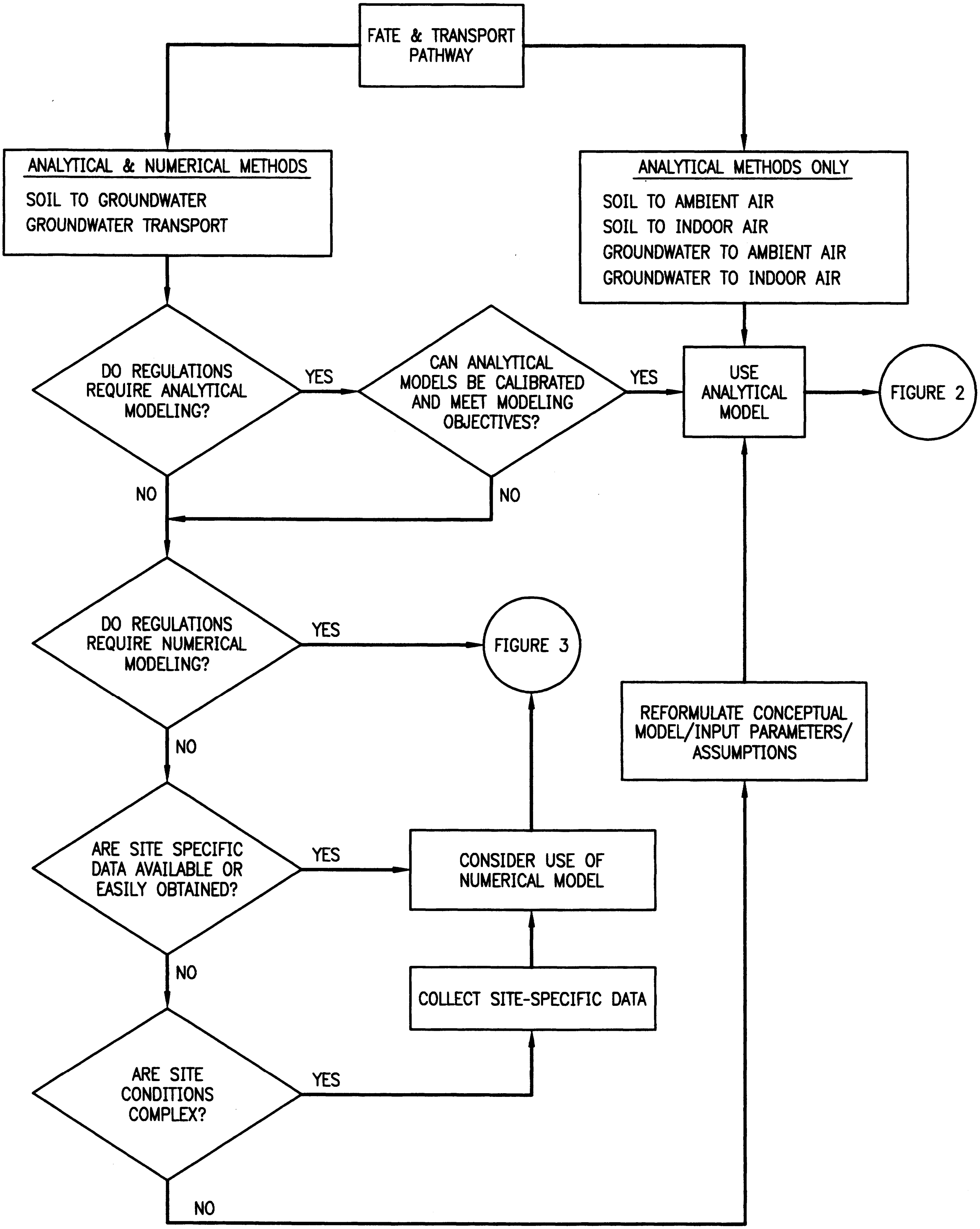
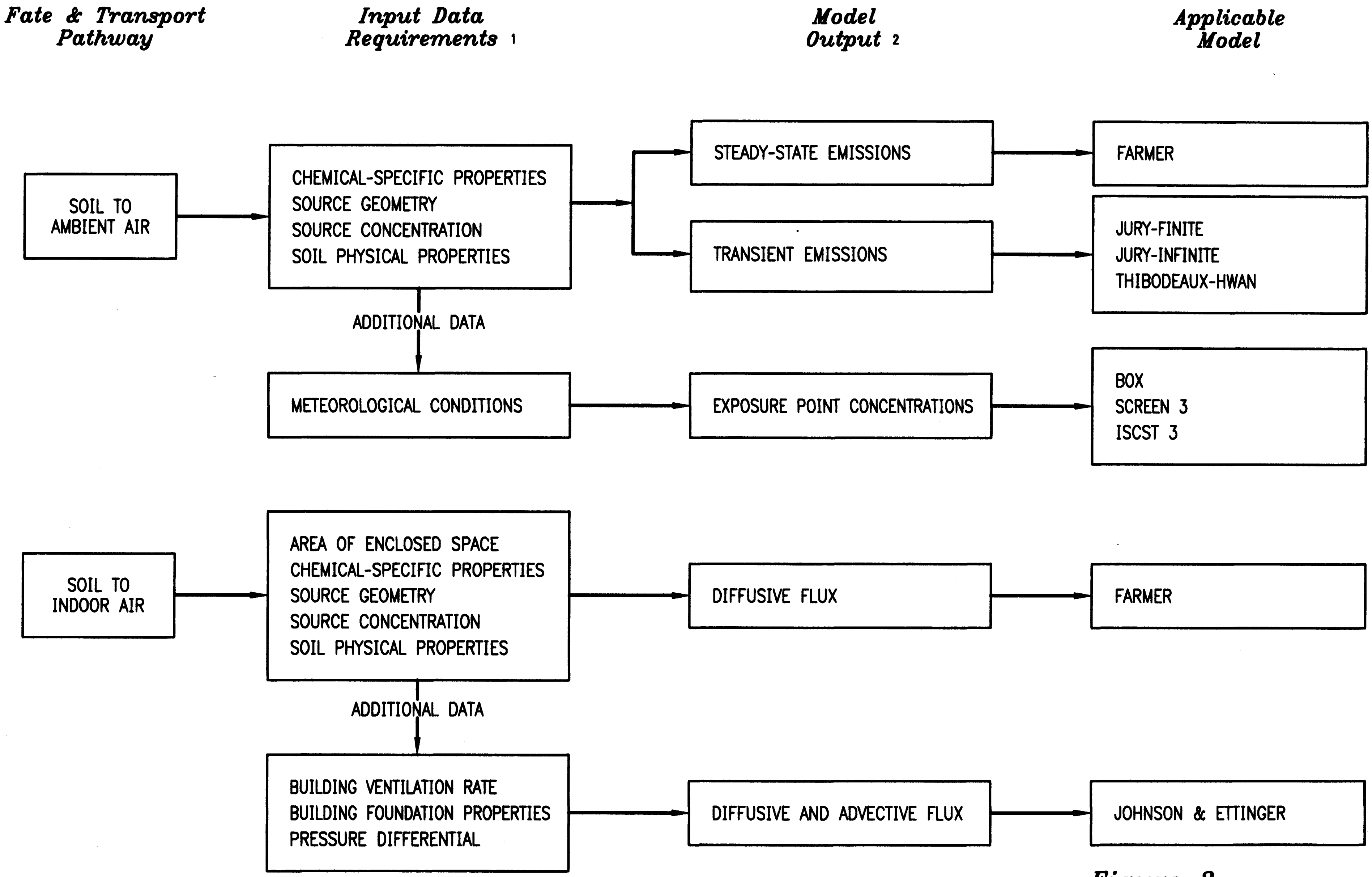


Figure 1

DECISION DIAGRAM



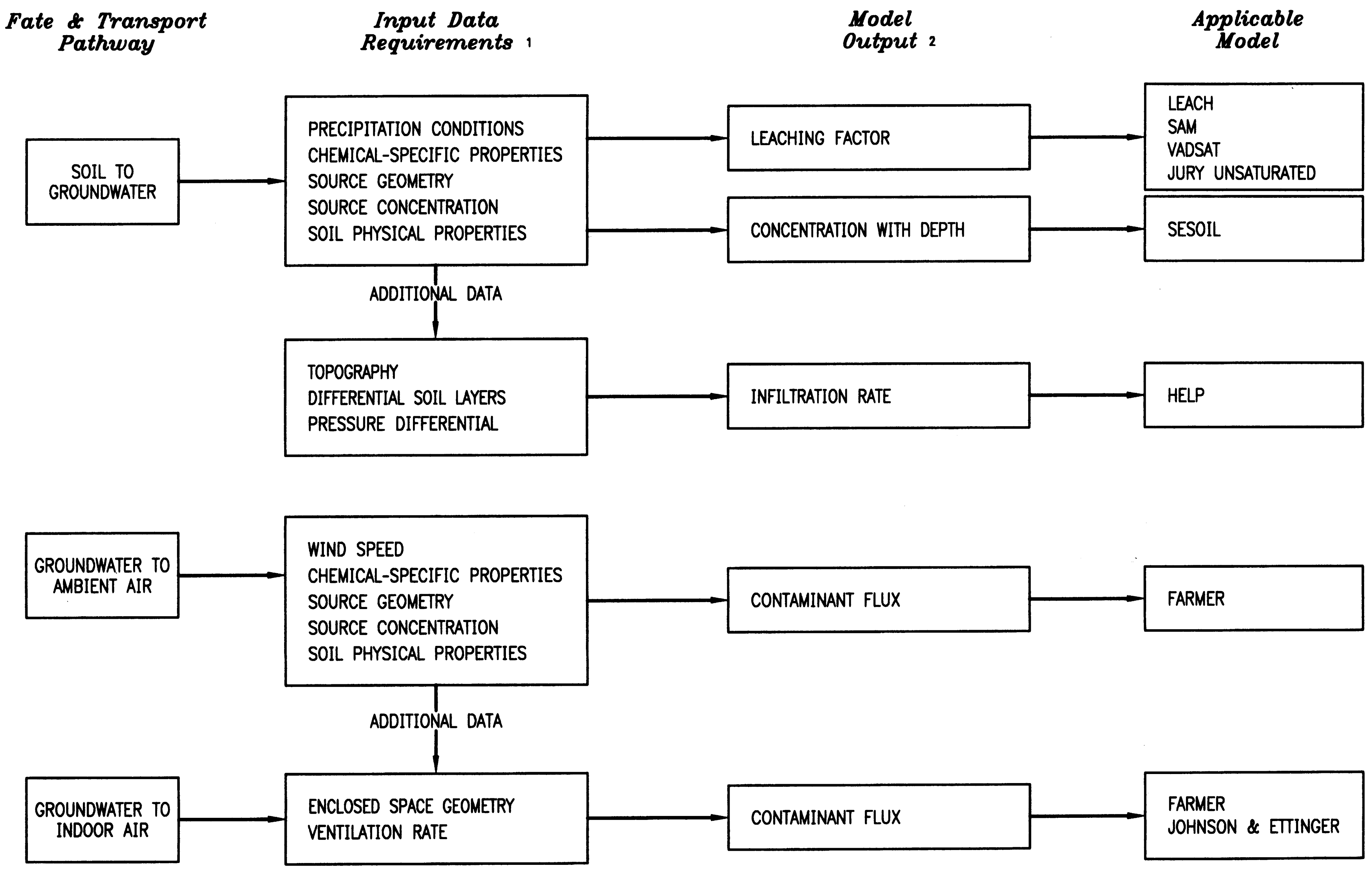
NOTES

1) CAN BE DEFAULT OR SITE-SPECIFIC VALUES
2) REFER TO MATRICES

Figure 2

ANALYTICAL MODEL SELECTION PROCESS DIAGRAM

SHEET 1 OF 3



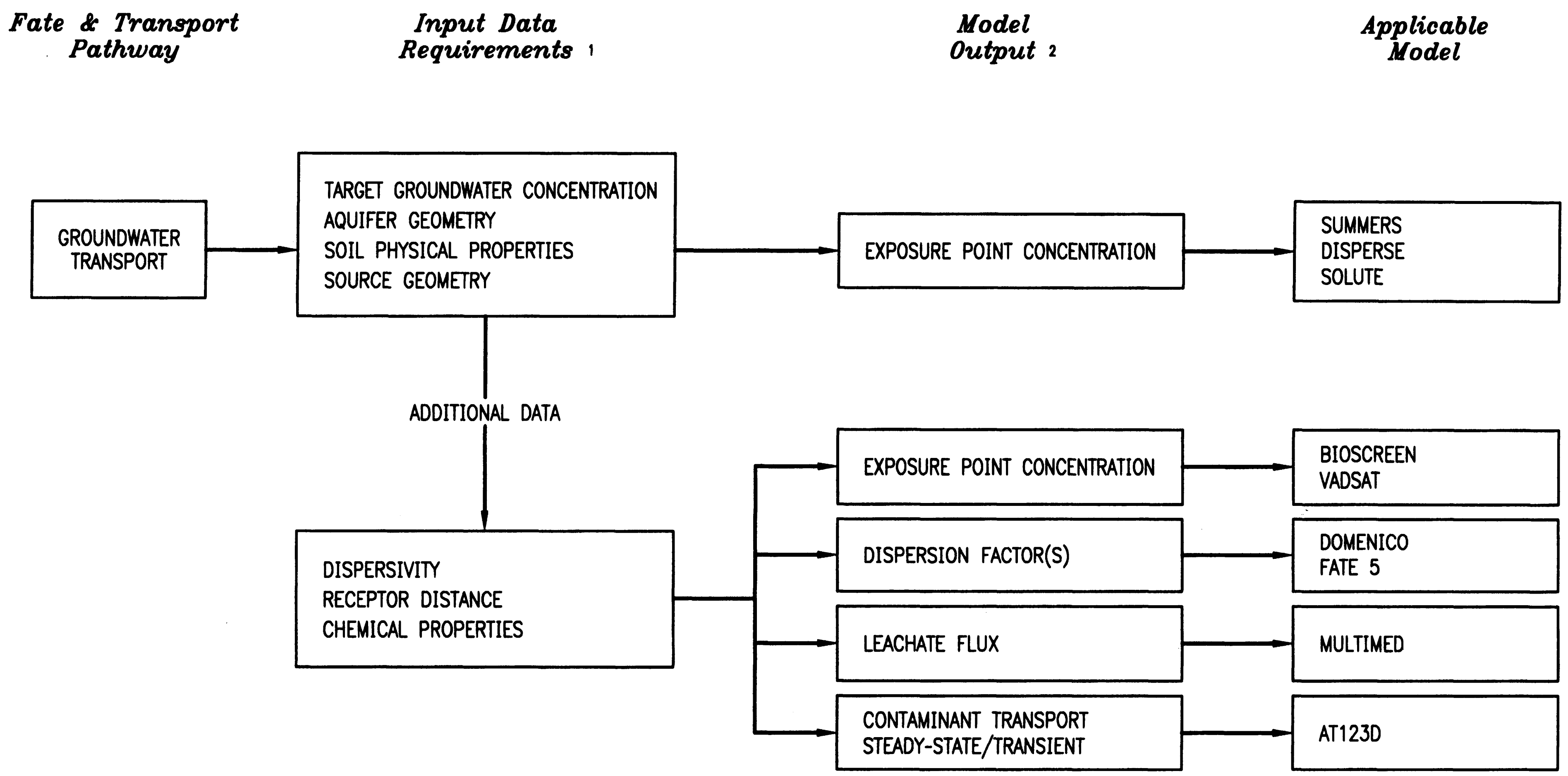
NOTES

1) CAN BE DEFAULT OR SITE-SPECIFIC VALUES
2) REFER TO MATRICES

Figure 2

ANALYTICAL MODEL
SELECTION PROCESS DIAGRAM

SHEET 2 OF 3



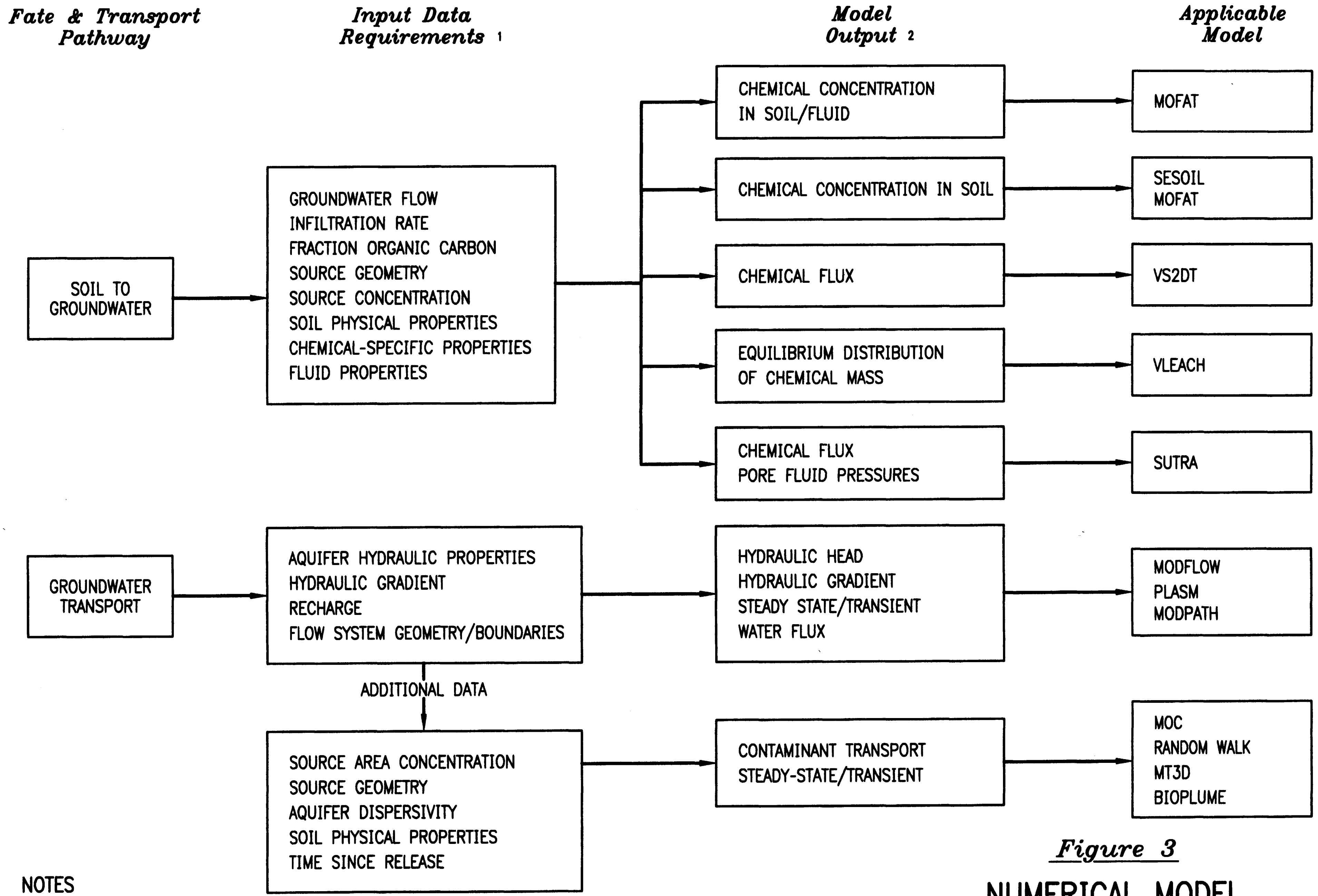
NOTES

1) CAN BE DEFAULT OR SITE-SPECIFIC VALUES
2) REFER TO MATRICES

Figure 2

ANALYTICAL MODEL
SELECTION PROCESS DIAGRAM

SHEET 3 OF 3



NOTES

1) CAN BE DEFAULT OR SITE-SPECIFIC VALUES
2) REFER TO MATRICES

Figure 3

NUMERICAL MODEL
SELECTION PROCESS DIAGRAM

APPENDIX A

SOIL TO AMBIENT AIR

JURY INFINITE SOURCE

MODEL OPERATION

This model assumes an infinite source for migration of volatiles from soils to ambient air and enclosed spaces. The model assumes that the soils are initially contaminated from the ground surface to an infinite depth. As the petroleum constituents diffuse to the ground surface, the concentration in the shallow soil decreases. The flux or rate of vapor migration to the ground surface decreases with time as the shallow soils become less contaminated. Because the flux changes with time, an average flux is used in the volatilization factor. Model assumes:

- No biological degradation
- One-dimensional flow field (no horizontal dispersion)
- Contaminated soil extends from the surface to an infinite depth
- Diffusion in both the liquid and vapor phases
- Equilibrium partitioning between sorbed, dissolved, and vapor phases
- Reversible mass transfer between sorbed, dissolved, and vapor phases

KEY INPUT PARAMETERS

Soil bulk density
Diffusion coefficient in air
Diffusion coefficient in water
Fraction of organic carbon
Henry's Law constant
Carbon-water sorption coefficient
Soil-water sorption coefficient
Averaging time for fluxes
Wind speed above ground surface
Soil intrinsic permeability
Source width parallel to wind
Ambient air mixing zone height

SENSITIVE INPUT PARAMETERS

Source area concentration
Depth to soil contamination
Volumetric air content in vadose zone soil
Total soil porosity
Volumetric water content in vadose zone soil

Note : The parameter D_A combines variables that relate to soil porosity and moisture content, diffusion coefficients in the vapor and aqueous phases, and partitioning coefficients that describe relationships between concentrations in the solid, aqueous, and vapor phases. These variables are combined together in the D_A parameter to make the equations more concise and readable.

APPLICABILITY

Focus of multiple studies, the model is highly used and tested.

ADDITIONAL INFORMATION

EPA Soil Screening Guidance (find at http://www.ntis.gov/search.htm)

SOURCES

Model is in the form of equations that are typically executed in a spreadsheet environment.

Computer programs for the model are currently not available from common sources.

THE JURY FINITE SOURCE

MODEL OPERATION

The Jury Finite Source Model is an alternative for the infinite source model for migration from surficial soils to ambient air and enclosed spaces. This model assumes that the contaminated soil has a finite depth. The equation used for the finite source model requires that values be averaged over a short period of time. Model assumes:

- Biological degradation can be included
- One-dimensional vertical transport model, dispersion considered in vertical direction only
- Contaminated soil has a finite depth
- Diffusion in both the liquid and vapor phases
- Equilibrium partitioning between sorbed, dissolved, and vapor phases
- Reversible mass transfer between sorbed, dissolved, and vapor phases

KEY INPUT PARAMETERS

Soil bulk density
Diffusion coefficient in air
Diffusion coefficient in water
Fraction of organic carbon
Henry's Law constant
Carbon-water sorption coefficient
Averaging time for fluxes
Wind speed above ground surface
Ambient air mixing zone height
Source width parallel to wind

SENSITIVE INPUT PARAMETERS

Source area concentration
Volumetric air content in vadose zone soil
Total soil porosity
Depth to soil contamination
Thickness of soil contamination
Volumetric water content in vadose zone soil

APPLICABILITY

Very simple and easy to use.

ADDITIONAL INFORMATION

ASTM 1739-95 Risk-based Corrective Action Guidance

EPA Soil Screening Guidance (find at http://www.ntis.gov/search.htm)

API DSS manual

SOURCES

Model is in the form of equations that are typically executed in a spreadsheet environment.

Computer programs for the model are currently not available from common sources.

FARMER MODEL

MODEL OPERATION

The Farmer model estimates the migration of vapors from soil to ambient air. The model assumes that the concentration in the contaminated soils and the depth to the contaminated soils do not change with time. This is equivalent to assuming that the soils represent an infinite source for contamination. Farmer is a soil emission model, air dispersion is modeled separately. The Model assumes:

- No biological degradation
- One-dimensional flow field (no horizontal dispersion)
- Constant source composition and concentrations
- Diffusion in both the liquid and vapor phases
- Equilibrium partitioning between sorbed, dissolved, and vapor phases
- Reversible mass transfer between sorbed, dissolved, and vapor phases

KEY INPUT PARAMETERS

Diffusion coefficient in air
Diffusion coefficient in water
Fraction of organic carbon
Henry's Law constant
Carbon-water sorption coefficient
Soil-water sorption coefficient
Soil bulk density
Averaging time for fluxes
Soil intrinsic permeability

SENSITIVE INPUT PARAMETERS

Source area concentration
Total soil porosity
Volumetric air content in vadose zone soil
Depth to soil contamination
Thickness of soil contamination
Volumetric water content in vadose zone soil

APPLICABILITY

Simplest of the soil to ambient air models and highly used.

ADDITIONAL INFORMATION

EPA Soil Screening Guidance (find at http://www.ntis.gov/search.htm)

SOURCES

Model is in the form of equations that are typically executed in a spreadsheet environment.

Computer programs for the model are currently not available from common sources

THIBODEAUX-HWANG MODEL

MODEL OPERATION

The Thibodeaux-Hwang model assumes that the concentration in the soil remains constant however the distance to the top of the contaminated layer increases as contaminants are volatilized. The model is only slightly more complicated to use than the Farmer model, yet provides significantly more realism. For petroleum compounds not readily biodegradable, the Thibodeaux-Hwang model should be used.

The Thibodeaux-Hwang model is an alternative for the Farmer model in that it assumes the near-surface soil concentrations decrease with time. The Thibodeaux-Hwang equation provides an estimate of the average flux over the time period, which produces a more realistic long-term estimate of vapor flux than the instantaneous flux model. The effects of biological degradation can be incorporated into the soil to ambient air models if the assumption is made that biological degradation follows a first-order decay equation.

KEY INPUT PARAMETERS

Diffusion coefficient in air
Diffusion coefficient in water
Fraction of organic carbon
Henry's Law constant
Carbon-water sorption coefficient
Soil-water sorption coefficient
Soil bulk density
Averaging time for fluxes
Soil intrinsic permeability

SENSITIVE INPUT PARAMETERS

Source area concentration
Total soil porosity
Depth to soil contamination
Thickness of soil contamination
Volumetric air content in vadose zone soil
Volumetric water content in vadose zone soil

APPLICABILITY

Highly tested and used when there is a finite source.

ADDITIONAL INFORMATION

ASTM 1739-95 Risk-based Corrective Action Guidance

EPA Soil Screening Guidance (find at http://www.ntis.gov/search.htm)

SOURCES

Model is in the form of equations that are typically executed in a spreadsheet environment.

Computer programs for the model are currently not available from common sources.

BOX MODEL

MODEL OPERATION

ASTM uses a simple box model approach. A “box” model assumes the contaminant vapors from the soil are mixed with clean air within some box-shaped breathing zone near the ground surface. This breathing zone, which is assumed to be located immediately above the contaminated soil, is dependent upon the width of the contaminated soil parallel to the wind and a mixing height that is generally assumed to be 2 meters. The amount of mixing that occurs within this breathing zone is determined by the average wind speed in the breathing zone. The assumptions used to develop fixed-box models are: the mixing zone is a rectangle with one side parallel to the wind direction; atmospheric turbulence produces complete and total mixing of the contaminants up to some mixing height, H, and no mixing above this height; the turbulence is strong enough in the upwind direction that the contaminant concentration is uniform throughout the mixing zone and not higher at the downwind side than the upwind side; the velocity of the wind is independent of time, location, or elevation above the ground surface; the concentration of the contaminant in the air entering the mixing zone is zero; the contaminant emission rate from the soil is constant and uniform over the base of the mixing zone; no contaminant enters or leaves through the top of the mixing zone nor through the sides that are parallel to the wind direction; and the contaminant does not degrade in the atmosphere.

KEY INPUT PARAMETERS

Length of the mixing zone in the direction of the wind
Wind speed above the ground surface
The ambient air mixing zone height
The width of the source parallel to wind
Contaminant flux into the box (soil emissions rate)

APPLICABILITY

Useful model for screening purposes due to its conservative assumptions.

ADDITIONAL INFORMATION

ASTM 1739-95 Risk-based Corrective Action Guidance

SOURCES

Model is in the form of equations that are typically executed in a spreadsheet environment.

Computer programs for the model are currently not available from common sources.

SCREEN 3

MODEL OPERATION

SCREEN 3 uses a Gaussian plume model that incorporates source-related factors and meteorological factors to estimate pollutant concentration from continuous sources. It is assumed that the pollutant does not undergo any chemical reactions and that no other removal processes, such as wet or dry deposition, act on the plume during its transport from the source. It models the plume impacts from point sources, flare release, and volume releases in SCREEN. The SCREEN model uses a numerical integration algorithm for modeling impacts from area sources. The area source is assumed to be a rectangular shape, and the model can be used to estimate concentrations within the area.

KEY INPUT PARAMETERS

Background air concentration
Stack height wind speed
Vertical dispersion parameter
Plume centerline height
Emission rate
Lateral dispersion parameter
Receptor height above ground
Mixing height

APPLICABILITY

Commonly used, easy model with extensive testing.

ADDITIONAL INFORMATION

The Gaussian model equations and the interactions of the source-related and meteorological factors are described in Volume II of the ISC User's Guide (EPA, 1995b), and in the Workbook of Atmospheric Dispersion Estimates (Turner, 1970).

SOURCES

Scientific Software Group
P.O. Box 23041
Washington, D.C. 20026-3041
Phone: (703) 620-9214
Fax: (703) 620-6793
www.scisoftware.com

ISCST3

MODEL OPERATION

The ISCST3 model may be used to model primary pollutants and continuous releases of toxic and hazardous waste pollutants. It can handle multiple sources including point, volume, area, and open pit source types. Line sources may also be modeled as a string of volume sources or as elongated area sources. Source emission rates can be treated as constant or may be varied by month, season, hour-of-day, or other optional periods of variation. These variable emission rate factors may be specified for a single source or for a group of sources. The model can account for the effects of aerodynamic down wash due to nearby buildings on point source emissions. The model contains algorithms for modeling the effects of settling and removal (through dry deposition) or large particulates and for modeling the effects of precipitation scavenging for gases or particulates. Receptor locations can be specified as gridded and/or discrete receptors in a Cartesian or polar coordinates. The model uses real-time meteorological data to account for the atmospheric conditions that affect the distribution of air pollution impacts on the modeling area.

KEY INPUT PARAMETERS

Location of the source
Physical stack height
Source elevation
Building dimensions
Stack gas exit velocity
Emission rate
Variable emission rates
Particle size distributions

APPLICABILITY

Commonly used model and widely tested.

ADDITIONAL INFORMATION

Scientific Software Group

SOURCES

Scientific Software Group
P.O. Box 23041
Washington, D.C. 20026-3041
Phone: (703) 620-9214
Fax: (703) 620-6793
www.scisoftware.com

SOIL TO INDOOR AIR

FARMER MODEL

MODEL OPERATION

The same model used to estimate emissions to ambient air can be adapted to model emissions to enclosed spaces or indoor air. The Farmer model assumes that the concentration in the contaminated soils and the depth to the contaminated soils do not change with time. This is equivalent to assuming that the soils represent an infinite source for contamination. For petroleum fractions that are biodegradable, a modified Farmer model can be used. Model assumes:

- No biological degradation
- One-dimensional flow field (no horizontal dispersion)
- Constant source composition and concentrations
- Diffusion in both the liquid and vapor phases
- Equilibrium partitioning between sorbed, dissolved, and vapor phases
- Reversible mass transfer between sorbed, dissolved, and vapor phases

KEY INPUT PARAMETERS

Source area concentration
Fraction of organic carbon
Henry's Law constant
Carbon-water sorption coefficient
Soil-water sorption coefficient
Volumetric air content in vadose zone soil
Total soil porosity
Soil bulk density
Area of cracks through which vapor enter the enclosed space or building
Thickness of the foundation or floor of the enclosed space or building
Effective diffusion coefficient through the crack
Effective radius of crack
Depth to soil contamination
Thickness of soil contamination

Averaging time for fluxes
Soil intrinsic permeability
Building under pressure
Diffusion coefficient in air
Diffusion coefficient in water
Floor/wall seam perimeter
Viscosity of gas
Depth of crack below ground surface

SENSITIVE INPUT PARAMETERS

Enclosed space volume/infiltration area ratio
Ventilation rate for the enclosed space or building

APPLICABILITY

Simplest of the soil to ambient air models and highly used.

ADDITIONAL INFORMATION

EPA Soil Screening Guidance (find at http://www.ntis.gov/search.htm)

SOURCES

Model is in the form of equations that are typically executed in a spreadsheet environment. Computer programs for the model are currently not available from common sources.

JOHNSON AND ETTINGER MODEL

MODEL OPERATION

The Johnson/Ettinger Model includes advective flux and is recommended for high permeability sites. For low permeability sites, these effects are less important. The effects of advective flow may be important for higher permeability sites. Neglecting advection may result in non-conservative cleanup levels.

The flux term for the Johnson and Ettinger model is based on the same model used to simulate migration from subsurface soils to ambient air (i.e., the Farmer model). An additional set of terms has been added to the contaminant flux term to account for the resistance to flow that is provided by the floor or foundation of the enclosed space. This resistance is quantified using parameters that describe the number and widths of cracks in the foundation floor. The importance of advection from the soil into enclosed spaces will depend upon the magnitude of the sub-atmospheric pressures in the enclosed space, on the number and size of cracks in the floor or basement of the enclosed space, and on the permeability of the soil. The effects of soil permeability are especially significant. The effects of biological degradation can be incorporated into the soil to enclosed space models if the assumption is made that biological degradation follows a first-order decay equation.

KEY INPUT PARAMETERS

Effective diffusion coefficient through the crack
Building under pressure
Soil permeability
Floor/wall seam perimeter
Viscosity of gas
Depth of crack below ground surface
Effective radius of crack
Area of cracks through which vapor enter the enclosed space or building
Thickness of the foundation or floor of the enclosed space or building

SENSITIVE INPUT PARAMETERS

Enclosed space volume/infiltration area ratio
Ventilation rate for the enclosed space or building

APPLICABILITY

This model is widely tested and used especially for screening purposes due to its conservative assumptions.

ADDITIONAL INFORMATION

ASTM 1739-95 Risk-based Corrective Action Guidance

BP Oil RISC model

SOURCES

Groundwater Services, Inc.
2211 Norfolk, Suite 1000
Houston, Texas 77098-4044

Phone: (713) 522-6300
Fax: (713) 522-8010

SOIL TO GROUNDWATER

LEACH

MODEL OPERATION

The model, developed for ASTM (1995), calculates a soil leaching partitioning factor and an attenuation factor for mixing with groundwater. Dissolution of contaminants into infiltrating precipitation is estimated using equilibrium partitioning (which can be capped at the effective solubility), and dilution into groundwater is estimated using a relatively simple box model.

Calculation of the leaching factor is based on the following assumptions: A constant chemical concentration in subsurface soils; linear equilibrium partitioning within the soil matrix between sorbed, dissolved, and vapor phases, where the partitioning is a function of constant chemical- and soil-specific parameters; steady-state leaching from the vadose zone to groundwater resulting from the constant leaching rate I [cm/s]; no loss of chemical as it leaches toward groundwater (that is, no biodegradation); and steady well-mixed dispersion of the leachate within a groundwater mixing zone.

LEACH assumes that no attenuation of the compounds or fractions occurs from the source area to the groundwater. Thus, the concentrations entering the groundwater are identical to those in the pore water leaving the impacted source area.

KEY INPUT PARAMETERS

Thickness of affected soil zone
Bulk density
Volumetric water content
Soil-water sorption coefficient
Henry's Law Constant
Volumetric air content
Dilution factor
Darcy groundwater velocity
Mixing zone depth
Infiltration rate
Source width parallel to the groundwater flow

SENSITIVE INPUT PARAMETERS

Source area concentration
Soil-water sorption coefficient
Total soil porosity
Organic carbon content
Carbon-water sorption coefficient

APPLICABILITY

Relatively simple and very conservative.

ADDITIONAL REFERENCES

ASTM 1739-95 Risk-based Corrective Action Guidance

EPA Soil Screening Guidance (find at http://www.ntis.gov/search.htm)

SOURCES

Model is in the form of equations that are typically executed in a spreadsheet environment. Computer programs for the model are currently not available from common sources.

SAM

MODEL OPERATION

A modification of LEACH is known as the Soil Attenuation Model or SAM. The soil-to-groundwater leachate process is characterized as a three-step procedure, beginning with 1) equilibrium partitioning of soil contaminants from a finite source mass to infiltrating rainwater, followed by 2) sorptive redistribution of contaminants from the leachate onto underlying clean soils, and 3) subsequent leachate dilution within the receiving groundwater flow system.

KEY INPUT PARAMETERS

Thickness of affected soil zone
Biodecay rate of COC in vadose zone
Bulk water partitioning coefficient
Time averaging factor
Net infiltration
Distance from top of affected soil zone to top of water-bearing unit
Distance from top of affected soil zone to top of water-bearing unit

SENSITIVE INPUT PARAMETERS

Source area concentration
Soil-water sorption coefficient
Total soil porosity
Organic carbon content
Carbon-water sorption coefficient

APPLICABILITY

The SAM model has undergone peer review and has recently been adopted by the state of Texas for use in deriving risk-based screening levels.

ADDITIONAL INFORMATION

Texas Natural Resource Conservation Commission

SOURCES

Model is in the form of equations that are typically executed in a spreadsheet environment. Computer programs for the model are currently not available from common sources.

SESOIL

MODEL OPERATION

SESOIL (the Seasonal SOIL Component Model) is a one-dimensional model developed by Bonazountas and Wagner (1984) to describe pollutant fate and transport in the unsaturated zone. Transformations through biodegradation, hydrolysis and cation exchange can also be simulated.

The model allows input of up to four soil layers, the hydrology calculations use only a depth-weighted average value. This component of the model limits its applicability to site-specific assessments.

The model uses a mass balance approach, continuously calculating the mass input and removal from each layer or sublayer and the masses in each of three phases: solid, liquid (non-aqueous phase), dissolved liquid (soil moisture), and soil gas. Communication between layers is through advection and diffusion. Importantly, SESOIL assumes all phases are in equilibrium at all times, using partitioning equations such as Henry’s law, and Freundlich adsorption isotherms to calculate concentrations in different phases. The model does not include surface ponding, or plant uptake (unless the user specifically inputs an evapotranspiration rate to account for this mechanism). SESOIL can be used to calculate time until a plume reaches groundwater, as well as the peak concentrations reaching groundwater.

KEY INPUT PARAMETERS

First-order decay, biodegradation rate
Hydrolysis rate
Soil disconnectedness index
Cation exchange
Depth to groundwater
Precipitation by month
Albedo
Relative humidity
Number of storms per month
Average storm duration
Temperature
Evapotranspiration
Effective solubility
Intrinsic permeability
Diffusion coefficients

SENSITIVE INPUT PARAMETERS

Source area concentration
Soil-water sorption coefficient
Total soil porosity
Organic carbon content
Carbon-water sorption coefficient

APPLICABILITY

Has been widely adopted for its ease and scientific credibility.

ADDITIONAL INFORMATION

American Petroleum Institute’s Decision Support System

EPA’s Graphical Exposure Modeling System

California Leaking Underground Fuel Tank Program

SOURCES

Scientific Software Group
P.O. Box 23041
Washington, D.C. 20026-3041
Phone: (703) 620-9214
Fax: (703) 620-6793
www.scisoftware.com

International Groundwater Modeling Center
Colorado School of Mines
Golden, Colorado 80401-1887
Phone: (303) 273-3103
Fax: (303) 384-2037
www.mines.edu/igwmc/

HELP

MODEL OPERATION

The HELP (Hydrogeologic Evaluation of Landfill Performance) model (Schroeder et al., 1994) is a quasi-two-dimensional, deterministic water-routing model for evaluating the water balance at sites. It was developed for landfills and solid waste containment facilities, as a tool for evaluating the impacts of various design alternatives. It is therefore very applicable to evaluating hydrocarbon leaching at contaminated sites, including the assessment of the impacts of different remedial design alternatives on leaching potential.

HELP is very user-friendly, and is written in the Basic language for use under DOS in IBM-PC or compatible computers. The program includes a large database for weather data for different cities, or more site-specific weather data can be input. It also includes default values for the hydrogeological characteristics of different soil types, waste materials and geosynthetic materials (such as liners), or again empirical data can be substituted if known. Subsurface layers can be accommodated, and seasonal differences in weather patterns are also included. In fact, the model simulates daily water movement into, through and out of the impacted soils. The model includes changes in infiltration capacity when frozen conditions are predicted, and changes in the energy balance caused by the presence of snow at the surface, and snow melting with and without rain on a surface snow layer. The HELP model also calculates changes in evapotranspiration due to the presence and health of vegetation at the site surface, and accounts for such factors as topography and vegetation on runoff and interception of precipitation.

KEY INPUT PARAMETERS

Thickness of affected soil zone
Cap thickness
Weather data
Soil data
 Permeability
Snow melt
Leakage
Soil storage
Evapotranspiration
Runoff
Leachate recirculation
Unsaturated vertical flow

SENSITIVE INPUT PARAMETERS

Source area concentration
Soil-water sorption coefficient
Total soil porosity
Organic carbon content
Carbon-water sorption coefficient

APPLICABILITY

The HELP model is easy to use and adaptable to a range of site-specific parameters. It has a long history of field validation, ease of use, and broad acceptance of the approach and results.

ADDITIONAL INFORMATION

International Groundwater Modeling Center

USACE - Waterways Experiment Station, Vicksburg, Mississippi

SOURCES

Scientific Software Group
P.O. Box 23041
Washington, D.C. 20026-3041
Phone: (703) 620-9214
Fax: (703) 620-6793
www.scisoftware.com

International Groundwater Modeling Center
Colorado School of Mines
Golden, Colorado 80401-1887
Phone: (303) 273-3103
Fax: (303) 384-2037
www.mines.edu/igwmc

VLEACH

MODEL OPERATION

VLEACH is a one-dimensional finite difference vadose zone-leaching model. The model estimates impact to groundwater due to the mobilization and migration of organic contaminates in the vadose zone. The model describes the movement of an organic contaminant within and between three phases: liquid (dissolved phase), vapor, and absorbed (solid phase). VLEACH employs a number of simplifying assumptions:

- Instantaneous equilibrium occurs between the three phases in each vertical cell.
- The moisture content profile within the vadose zone is constant.
- Liquid phase dispersion is not considered.
- No degradation or in situ production occurs.
- Homogeneous soil conditions are assumed.
- Volatilization is either completely unimpeded or completely restricted.
- Non-aqueous phase liquid or variable density flow is not considered.

KEY INPUT PARAMETERS

Solubility in water
Recharge rate
Henry’s law constant
Air diffusion coefficient
Dry bulk density
Number of model cells
Upper boundary conditions for vapor
Volumetric water content
Time step
Lower boundary conditions for vapor

SENSITIVE INPUT PARAMETERS

Organic carbon distribution coefficient
Effective porosity
Soil organic carbon content
Initial contaminant concentration

APPLICABILITY

VLEACH can be used as a screening model due to conservative assumptions.

ADDITIONAL INFORMATION

EPA Soil Screening Guidance (find at http://www.ntis.gov/search.htm), Technical Background Document

SOURCES

Scientific Software Group
P.O. Box 23041
Washington, D.C. 20026-3041
Phone: (703) 620-9214
Fax: (703) 620-6793
www.scisoftware.com

Robert S Kerr Environmental Research Center
Center for Subsurface Modeling Support
P.O. Box 1198
Ada, Oklahoma 74821-1198
Phone: (580) 436-8586
Fax: (580) 436-8718
www.epa.gov/ada/models.html

SUTRA

MODEL OPERATION

SUTRA is a two-dimensional model simulating flow and transport (of energy or dissolved substances) in the subsurface (Voss, 1984). It was developed by the U.S. Geological Survey, and is available in the public domain. It operates under the DOS environment on IBM-PC or compatible computers.

SUTRA uses hybrid finite-difference and finite-element methods to simulate flow and transport in the subsurface, under both saturated and unsaturated conditions. The model allows sources, sinks and boundary conditions to be time-dependent, which is a more realistic approach than simpler models. It also allows simulation of the complete subsurface environment (i.e., it links both unsaturated leaching and saturated ground water flow). SUTRA also calculates fluid pressures over time and distance, and is one of the few public-domain programs capable of simulating flow under variable-density conditions.

KEY INPUT PARAMETERS

Thickness of affected soil zone
Hydraulic conductivity
Specific yield
Pumping wells
Bulk density
Volumetric water content
Volumetric air content
Henry's Law Constant
Transmissivity
Boundary conditions
Recharge from precipitation, rivers, drains
Dilution factor
Darcy groundwater velocity
Mixing zone depth
Infiltration rate
Source width parallel to the groundwater flow

SENSITIVE INPUT PARAMETERS

Source area concentration
Soil-water sorption coefficient
Total soil porosity
Organic carbon content
Carbon-water sorption coefficient

APPLICABILITY

Relatively complex site-specific model. Requires experienced user and reviewer.

ADDITIONAL INFORMATION

International Groundwater Modeling Center

Scientific Software Group

SOURCES

Scientific Software Group
P.O. Box 23041
Washington, D.C. 20026-3041
Phone: (703) 620-9214
Fax: (703) 620-6793
www.scisoftware.com

International Groundwater Modeling Center
Colorado School of Mines
Golden, Colorado 80401-1887
Phone: (303) 273-3103
Fax: (303) 384-2037
www.mines.edu/igwmc

U.S. Geological Survey
water.usgs.gov/software

JURY - UNSATURATED

MODEL OPERATION

Although designed for estimating chemical flux volatilizing from the soil to air, the Jury model also predicts concentrations within the aqueous phase and can be used to estimate contaminant mass loading through the unsaturated, or vadose, zone to groundwater over time. The hydrology portion of the model is very simple to use and uniform and steady infiltration is assumed.

Other assumptions to consider include the assumption of homogeneous and isotropic soil (without depth variation), uniform chemical distribution within the source area, and compositional equilibrium between all phases at all times. These assumptions limit the model's usefulness. The model is most appropriate for simulating time-varying volatile flux from soil but it may also be used for initial-tier evaluations of mass loading to groundwater. In such cases, the infiltration rate is a sensitive parameter and the results should be compared to other screening-level model predictions.

KEY INPUT PARAMETERS

Effective solubility
Retardation factor
Unsaturated hydraulic conductivity
First order decay rate
Volumetric air content in vadose zone soil
Soil bulk density
Volumetric water content in vadose zone soil
Henry's law constant
Dilution factor
Mixing zone depth
Source width parallel to groundwater movement

SENSITIVE INPUT PARAMETERS

Total soil porosity
Source area concentration
Soil-water sorption coefficient
Fraction of organic carbon
Carbon-water sorption coefficient

APPLICABILITY

Tested model that is very simple to operate.

ADDITIONAL INFORMATION

EPA Soil Screening Guidance (find at http://www.ntis.gov/search.htm)

SOURCES

Model is in the form of equations that are typically executed in a spreadsheet environment. Computer programs for the model are currently not available from common sources.

MOFAT

MODEL OPERATION

Features are:

- Simulate multiphase transport of up to five non-inert chemical species.
- Model flow of light or dense organic liquids in three fluid phase systems.
- Handles cases in which gas and/or NAPL phase are absent in part or the entire domain at any given time.
- Solve flow equations for phases exhibiting transient behavior using the ASD method.
- Simulate dynamic or passive gas as a full three-phase flow problem.
- Use a three-phase van Genuchten model for saturation-pressure-permeability relations.
- Handle flux type, specified head, specified concentration or mixed type boundary conditions.
- Consider hysteresis in oil permeability due to fluid entrapment.
- Model water flow, transport, coupled oil-water flow, or water-oil-gas flow.

KEY INPUT PARAMETERS

Fluid properties
Boundary condition data
Porous media dispersivities
Diffusion coefficients
Mass transfer coefficients
Time integration parameters
Mesh geometry
Initial water phase concentrations
Component densities
First-order decay coefficients

SENSITIVE INPUT PARAMETERS

Initial contaminant concentrations
Equilibrium partition coefficients
Soil hydraulic properties

APPLICABILITY

Applicable for multi-phase flow and transport of three fluid phases. Written in DOS.

ADDITIONAL INFORMATION MODEL OPERATION

Scientific Software Group

SOURCES

Scientific Software Group
P.O. Box 23041
Washington, D.C. 20026-3041
Phone: (703) 620-9214
Fax: (703) 620-6793
www.scisoftware.com

Robert S Kerr Environmental Research Center
Center for Subsurface Modeling Support
P.O. Box 1198
Ada, Oklahoma 74821-1198
Phone: (580) 436-8586
Fax: (580) 436-8718
www.epa.gov/ada/models.html

VS2DT

MODEL OPERATION

VS2DT is a U.S.G.S. program for flow and solute transport in variably saturated, single-phase flow in porous media. A finite-difference approximation is used to solve the advection-dispersion equation. Simulated regions include one-dimensional columns, two-dimensional vertical cross-sections, and axially symmetric, three-dimensional cylinders. Program options include backward or centered approximations for both space and time derivatives, first-order decay, equilibrium adsorption (Freundlich or Langmuir) isotherms, and ion exchange. Nonlinear storage terms are linearized by an implicit Newton-Raphson method. Relative hydraulic conductivity is evaluated at cell boundaries using full upstream weighting, arithmetic mean or geometric mean. Saturated hydraulic conductivities are evaluated at cell boundaries using distance-weighted harmonic means.

KEY INPUT PARAMETERS

Thickness of affected soil zone
Dispersivities
Hydraulic conductivity
First-order decay rate

SENSITIVE INPUT PARAMETERS

Source area concentration
Soil-water sorption coefficient
Total soil porosity
Organic carbon content
Carbon-water sorption coefficient

APPLICABILITY

This model was developed and tested by the U.S.G.S., not widely used.

ADDITIONAL INFORMATION MODEL OPERATION

Scientific Software Group

SOURCES

Scientific Software Group
P.O. Box 23041
Washington, D.C. 20026-3041
Phone: (703) 620-9214
Fax: (703) 620-6793
www.scisoftware.com

International Groundwater Modeling Center
Colorado School of Mines
Golden, Colorado 80401-1887
Phone: (303) 273-3103
Fax: (303) 384-2037
www.mines.edu/igwmc

U.S. Geological Survey
water.usgs.gov/software

American Petroleum Institute
www.api.org/ehs

GROUNDWATER TO AMBIENT AIR

FARMER

MODEL OPERATION

The model that is used in the ASTM approach to estimate the contaminant flux term from groundwater to ambient air is the Farmer model. It assumes that that the contaminated groundwater is located at some depth beneath the ground surface. The model also assumes that the concentration in the groundwater and the depth to the groundwater do not change with time. This is equivalent to assuming that the groundwater represents an infinite source for contamination. The model assumes that the water in the capillary fringe is “clean.” The capillary fringe is assumed to have a relatively high moisture content and a relatively low air-filled porosity. The effect of this capillary fringe is to reduce the diffusion coefficient. It can be seen that a relatively thin capillary fringe can significantly reduce the rate of vapor diffusion to the ground surface.

KEY INPUT PARAMETERS

Source area concentration
Diffusion coefficient in air
Diffusion coefficient in water
Fraction of organic carbon
Henry's Law constant
Carbon-water sorption coefficient
Soil-water sorption coefficient
Total soil porosity
Soil bulk density
Depth to groundwater contamination
Thickness of groundwater contamination
Averaging time for fluxes
Soil intrinsic permeability
Volumetric water content in vadose zone soil
Volumetric air content in vadose zone soil

APPLICABILITY

This model is highly tested and used especially for screening purposes dues to its conservative assumptions.

ADDITIONAL INFORMATION

ASTM 1739-95 Risk-based Corrective Action Guidance

SOURCES

Model is in the form of equations that are typically executed in a spreadsheet environment. Computer programs for the model are currently not available from common sources.

GROUNDWATER TO INDOOR AIR

FARMER

MODEL OPERATION

The contaminant flux term for migration from groundwater to an enclosed space is based on the same model that is used to simulate migration from groundwater to ambient air (i.e., the Farmer model). The equations for estimating the flux from groundwater to enclosed spaces include the effects of degradation.

The flux is an average over time. The effects of a capillary fringe are also included through the modified diffusion coefficient, D_{ws}^{eff}.

KEY INPUT PARAMETERS

Source area concentration
Fraction of organic carbon
Henry's Law constant
Thickness of groundwater contamination
Soil-water sorption coefficient
Volumetric air content in vadose zone soil
Effective diffusion coefficient through the crack
Effective radius of crack
Thickness of the foundation or floor of the enclosed space or building
Area of cracks through which vapor enter the enclosed space or building
Soil bulk density
Depth to groundwater contamination
Carbon-water sorption coefficient
Averaging time for fluxes
Soil intrinsic permeability
Floor/wall seam perimeter
Viscosity of gas
Total soil porosity
Building under pressure
Depth of crack below ground surface
Diffusion coefficient in air
Diffusion coefficient in water

SENSITIVE INPUT PARAMETERS

Enclosed space volume/infiltration area ratio
Ventilation rate for the enclosed space or building

APPLICABILITY

This model is used especially for screening purposes dues to its conservative assumptions.

ADDITIONAL INFORMATION

ASTM 1739-95 Risk-based Corrective Action Guidance

SOURCES

Model is in the form of equations that are typically executed in a spreadsheet environment. Computer programs for the model are currently not available from common sources.

JOHNSON/ETTINGER (modified)

MODEL OPERATION

The Johnson/Ettinger Model is modified to include migration of contaminants from groundwater sources. The model consists of five fundamental steps:

1. Calculation of the ratio of the soil vapor phase concentration to total concentration at the source.
2. Calculation of the effective diffusion coefficient.
3. Calculation of the infiltration rate of contaminant vapors into the building.
4. Calculation of the building vapor concentration to groundwater vapor source concentration ratio.
5. Back-calculation of the generic groundwater to indoor air inhalation criteria.

The model incorporates the following assumptions:

- Soil is homogenous such that the effective diffusion coefficient is constant.
- Contaminant loss from leaching downward does not occur.
- Source degradation and transformation is not considered.
- Concentration at the soil particle surface/soil pore air space interface is zero.
- Convective vapor flow near the building foundation is uniform.
- Contaminant vapors enter the building through openings in the walls and foundation at or below grade.
- Convective vapor flow rates decrease with increasing contaminant source-building distance.
- All contaminant vapors directly below the building will enter the building, unless the floor and walls are perfect vapor barriers.
- The building contains no other contaminant sources or sinks; well mixed air volume.

KEY INPUT PARAMETERS

Effective diffusion coefficient through the crack
Effective diffusion coefficient through capillary fringe
Effective diffusion coefficient through vadose zone
Thickness of vadose zone below enclosed space floor
Thickness of capillary fringe
Building foundation thickness
Crack depth below grade to bottom of enclosed floor space
Crack radius
Depth below grade to bottom of enclosed space floor
Building floor length/width/height

SENSITIVE INPUT PARAMETERS

Ventilation rate for the enclosed space or building
Vapor flow rate into the building

Source-building separation distance for groundwater

APPLICABILITY

This model is widely tested and used especially for screening purposes due to its conservative assumptions.

ADDITIONAL INFORMATION

Michigan department of Environmental Quality

SOURCES

Model is in the form of equations that are typically executed in a spreadsheet environment. Computer programs for the model are currently not available from common sources.

GROUNDWATER TRANSPORT

DOMENICO

MODEL OPERATION

The Domenico Model is a mathematical solution of the advection-dispersion equation using many simplifying assumptions. Several of the simplifying assumptions are:

- groundwater transport is one-dimensional along the centerline, between the source and the receptor
- dispersion is quantified in three-dimensions
- the solution includes error functions that provide approximate solutions for groundwater transport equations across the site, over time
- source area concentrations are constant
- aquifer is initially clean.

The Domenico equation error functions are used to approximate the integration of the groundwater transport differential equation. In order to solve this equation, an integration scheme such as the Gauss-Legendre quadrature method could be used (Ungs, 1997).

KEY INPUT PARAMETERS	SENSITIVE INPUT PARAMETERS
Source width	Source concentration
Source depth	Retardation coefficient
First order decay rate	Enclosed space volume/infiltration area ratio
Longitudinal dispersivity	Distance to receptor
Transverse-horizontal dispersivity	
Transverse-horizontal dispersivity	

APPLICABILITY

The Domenico Model is a straightforward mathematical solution of the advection-dispersion equation using many simplifying assumptions. The models AT123D and VADSAT also satisfy the conditions of one direction uniform advection, three-dimensional dispersion, and first-order decay.

ADDITIONAL INFORMATION

International Groundwater Modeling Center

ASTM RBCA guidance

GSI Tier 2 Tool Kit

SOURCES

Groundwater Services, Inc.
2211 Norfolk, Suite 1000
Houston, Texas 77098-4044
Phone: (713) 522-6300
Fax: (713) 522-8010

FATE 5

MODEL OPERATION

FATE 5 is a modification of the Domenico analytical groundwater transport model. The model allows calibration to site conditions and both prediction of down gradient concentration and back calculation of SSTLs. Key assumptions of the model are;

- The aquifer and flow field are homogeneous and isotropic.
- Groundwater flow is fast enough that molecular diffusion can be ignored.
- Adsorption is a linear, reversible process.
- Assumes simple groundwater flow conditions.
- Based on steady-state formulation of the Domenico model.
- Not applicable where vertical gradients affect contaminant transport.
- Assumes simple first-order decay.

KEY INPUT PARAMETERS

Source width
Source depth
First order decay rate
Longitudinal dispersivity
Transverse-horizontal dispersivity
Transverse-horizontal dispersivity

SENSITIVE INPUT PARAMETERS

Source concentration
Retardation coefficient
Enclosed space volume/infiltration area ratio
Distance to receptor

APPLICABILITY

FATE 5 is designed to predict the extent of contaminant plumes in the absence of further source control and to determine the site-specific steady-state rate of chemical decay.

ADDITIONAL INFORMATION

Groundwater Services, Inc.

SOURCES

Groundwater Services, Inc.
2211 Norfolk, Suite 1000
Houston, Texas 77098-4044
Phone: (713) 522-6300
Fax: (713) 522-8010

DISPERSE

MODEL OPERATION

Disperse is an advection/dispersion model developed to predict the size and duration of methyl tertiary butyl ether (MTBE) and tertiary butyl alcohol (TBA) plumes. The model is conservative and represents the potential worst case scenario. The model assumes:

- Finite source, contaminate introduced as a slug
- Contaminant does not degrade
- Contaminant does not absorb to soil
- Aquifer is horizontal and homogenous
- Velocity is constant
- Dispersion coefficients are constant and proportional to velocity

KEY INPUT PARAMETERS

Rate of discharge
Period of discharge
Mass discharge
Longitudinal dispersivity
Transverse dispersivity
Time
Distance to exposure point perpendicular to direction of flow

SENSITIVE INPUT PARAMETERS

Distance to exposure point parallel to direction of flow
Initial concentration
Groundwater velocity

APPLICABILITY

The model provides an analytical solution of the classic dispersion equation for bi-dimensional flow in a horizontal aquifer.

ADDITIONAL INFORMATION

New Jersey Department of Environmental Protection

SOURCES

Software available from New Jersey Department of Environmental Protection.

SOLUTE

MODEL OPERATION

SOLUTE is a set of five programs based on analytical solutions of the advective-dispersive transport equation for solutes. All SOLUTE programs facilitate menu-driven, interactive data entry and editing, and results are given tabular and graphic form, including contour plots and line graphs.

The five programs include one dimensional and radial symmetric models to simulate the effects of a single source of contaminants, and two- and three-dimensional models that support multiple point sources using the principal of superposition to calculate the accumulated effects of various sources or to represent line (strip) or areal (patch) sources. These multiple sources may have a different starting time and may be of limited duration. All models support advection and dispersion, and the one-, two-, and three-dimensional models support retardation and decay. The radial symmetric models handle only retardation. The programs use either consistent metric units or a system of English units. The individual programs are:

- ONED-1: One-dimensional solute transport in a semi-infinite area with constant concentration as inlet boundary condition.
- ONED-2: Same as ONED-1 with decaying source as inlet boundary condition.
- ONED-3: Same as ONED-1 with concentration-dependent mass flux as inlet boundary condition.
- PLUME-2D: Two-dimensional areal or cross-sectional transport of a plume from one or more limited duration point sources in a uniform groundwater flow field.
- PLUME-3D: Same as PLUME -2D for three-dimensional transport
- SLUG-2D: Two-dimensional areal or cross-sectional transport of a slug caused by one or more instantaneous point sources in a uniform groundwater flow field.
- SLUG-3D: Same as SLUG-2D for three-dimensional transport.
- RADIAL: Solute transport in a plane radial flow field.
- LTIRD: Same as RADIAL but no retardation.

KEY INPUT PARAMETERS

Longitudinal, transverse, and vertical dispersivity
Aquifer thickness

SENSITIVE INPUT PARAMETERS

Groundwater seepage velocity
Contaminant concentration at the source
Duration of solute pulse
First-order decay rate
Retardation factor

APPLICABILITY

The model has been thoroughly tested with accurate results.

ADDITIONAL INFORMATION

EPA Soil Screening Guidance (find at http://www.ntis.gov/search.htm)
Scientific Software Group

SOURCES

International Groundwater Modeling Center
Colorado School of Mines
Golden, Colorado 80401-1887
Phone: (303) 273-3103
Fax: (303) 384-2037
www.mines.edu/igwmc

MULTIMED

MODEL OPERATION

MULTIMED, Multimedia Assessment Model, is a user-friendly model that simulates the fate and transport of contaminants leaching from a waste disposal facility into the multimedia environment. Release to either air or soil, including the unsaturated and saturated zone, and possible interception of the subsurface contaminant plume by a surface stream are included in the model. The model includes two options for simulating leachate flux. Either the infiltration rate to the unsaturated or saturated zone can be specified directly or a landfill module can be used to estimate the infiltration rate. The landfill module is one-dimensional and steady state, and simulates the effect of precipitation, runoff, infiltration, evapotranspiration, barrier layers (which can include flexible membrane liners), and lateral drainage.

A steady state, one-dimensional, semi-analytical module simulates flow in the unsaturated zone. The output from this module, water saturation as a function of depth, is used as input to the unsaturated zone transport module. The latter simulates transient, one-dimensional (vertical) transport in the unsaturated zone and includes the effects of longitudinal dispersion, linear adsorption, and first-order decay. Output from the unsaturated zone modules is used to couple the unsaturated zone transport module with the steady state or transient, semi-analytical saturated zone transport module. The latter includes one-dimensional uniform flow, three-dimensional dispersion, linear adsorption, first-order decay, and dilution due to direct infiltration into the groundwater plume. Contaminant of a surface stream due to the complete interception of a steady-state saturated zone plume is simulated by the surface water module. The air emissions and the atmosphere dispersion modules simulate the movement of chemicals into the air.

KEY INPUT PARAMETERS

Porosity
Depth of unsaturated zone
Residual water content
Biological decay rate
Soil bulk density
Recharge rate
Area of waste unit
Infiltration rate
Duration of pulse
Source decay rate
Number and thickness of each layer
Dispersivities

SENSITIVE INPUT PARAMETERS

Saturated hydraulic conductivity
Hydraulic gradient
Sorption coefficients
Initial concentration
Well distance from the site
Organic carbon content

APPLICABILITY

The model has been thoroughly tested with accurate results.

ADDITIONAL INFORMATION

EPA Soil Screening Guidance (find at http://www.ntis.gov/search.htm)
Scientific Software Group

SOURCES

Groundwater Services, Inc.
2211 Norfolk, Suite 1000
Houston, Texas 77098-4044
Phone: (713) 522-6300
Fax: (713) 522-8010

SUMMERS

MODEL OPERATION

SUMMERS is a screening level interactive computer program for estimating soil cleanup levels. The model assumes that a percentage of rainfall at a polluted site will infiltrate and desorb contaminants from the soil based on equilibrium soil-water partitioning. Using a mass balance approach and assuming equilibrated, complete mixing in the aquifer, the soil cleanup level is calculated from the original soil concentration, the concentration of the infiltrating water, and an equilibrium coefficient.

The public domain SUMMERS model was developed to estimate when contaminant concentrations in the soil will produce aquifer contaminant concentrations above acceptable levels. The resulting soil concentrations can then be used as guidelines in estimating boundaries or extent of soil contamination by applying the derived maximum soil contaminant concentration level to the observed concentration in the soil at the site.

KEY INPUT PARAMETERS

Target concentration in groundwater
Downward porewater velocity
Void fraction
Width of spill perpendicular to flow
Equilibrium partition coefficient
Volumetric infiltration rate into aquifer
Horizontal area of spill
Darcy velocity in aquifer
Volumetric groundwater flow rate

SENSITIVE INPUT PARAMETERS

Initial concentration
Groundwater seepage velocity

APPLICABILITY

Highly used and simple model for screening purposes.

ADDITIONAL INFORMATION

International Groundwater Modeling Center

SOURCES

International Groundwater Modeling Center
Colorado School of Mines
Golden, Colorado 80401-1887
Phone: (303) 273-3103
Fax: (303) 384-2037
www.mines.edu/igwmc

BIOSCREEN

MODEL OPERATION

BIOSCREEN is an easy-to-use-screening model that simulates remediation through natural attenuation (RNA) of dissolved hydrocarbons at petroleum fuel release sites. The software, programmed in the Microsoft® Excel spreadsheet environment and based on the Domenico analytical solute transport model, has the ability to simulate advection, dispersion, adsorption, and aerobic decay, as well as anaerobic reactions that have been shown to be the dominant biodegradation processes at many petroleum release sites. BIOSCREEN includes three different model types: 1) solute transport without decay; 2) solute transport with biodegradation modeled as a first order decay process (simple, lumped-parameter approach), and 3) solute transport with biodegradation modeled as an “instantaneous” biodegradation reaction (approach used by BIOPLUME models). The model is designed to simulate biodegradation by both aerobic and anaerobic reactions. It was developed for the Air Force Center for Environmental Excellence (AFCEE) Technology Transfer Division at Brooks Air Force Base by Groundwater Services, Inc., Houston, Texas.

KEY INPUT PARAMETERS

Depth below water table
Lateral distance from center line of plume
Specific discharge
Porosity
Dissolved oxygen
Saturated thickness
Transmissivity
Leakance, between aquifer layers, vertical conductivity
Storativity, storage coefficient
Recharge
Longitudinal dispersivity
Transverse dispersivity
Vertical dispersivity
Anions/cations
First-order degradation constant

SENSITIVE INPUT PARAMETERS

Source area contaminant concentrations

Saturated hydraulic conductivity
Distance along the center line from downgradient edge of dissolved plume source zone

APPLICABILITY

Easy screening tool, can be used for natural attenuation simulations.

ADDITIONAL INFORMATION

EPA Soil Screening Guidance (find at http://www.ntis.gov/search.htm)

SOURCES

Robert S Kerr Environmental Research Center
Center for Subsurface Modeling Support
P.O. Box 1198
Ada, Oklahoma 74821-1198
Phone: (580) 436-8586
Fax: (580) 436-8718
www.epa.gov/ada/models.html

VADSAT

MODEL OPERATION

The VADSAT model is a 3-D transport model that simulates contaminant leaching and volatilization in the vadose zone and advective/dispersive transport in the saturated zone. The model considers:

- A well-mixed finite-mass source zone
- Pseudo steady-state volatilization and diffusive transport from the source to ground surface
- Leaching from the source zone to groundwater
- Dissolved-phase advection and dispersion in groundwater
- Adsorption
- First-order decay in the leachate
- Van Genucten’s algorithm to estimate moisture content
- Simulate transport of individual contaminants that are part of a mixture
- Presence of residual level hydrocarbons
- Ability to make both deterministic and Monte Carlo simulations

KEY INPUT PARAMETERS

Porosity
Van Genucten’s n parameter
Soil bulk density
Molecular weight of chemical and TPH mixture
Organic carbon partition coefficient for chemical
Henry’s Law constant
Irreducible water content
Fraction organic carbon
Diffusion coefficients in air and water
Degradation rate

SENSITIVE INPUT PARAMETERS

Hydraulic conductivity

APPLICABILITY

Tested model that is very simple to operate.

ADDITIONAL INFORMATION

API’s VADSAT Manual

BP RISC Manual , as incorporated in RISC has the extended capability to consider a lens between the source and ground surface with difference soil properties.

SOURCES

Scientific Software Group
P.O. Box 23041
Washington, D.C. 20026-3041
Phone: (703) 620-9214
Fax: (703) 620-6793
www.scisoftware.com

Environmental Systems & Technologies, Inc.
2608 Sheffield Drive
Blacksburg, VA 24060
Phone: (540) 552-0685
Fax: (540) 951-5307
www.esnt.com

American Petroleum Institute
www.api.org/ehs

MODFLOW

MODEL OPERATION

MODFLOW is the name that has been given the USGS Modular Three-Dimensional Flow Model. Because of its ability to simulate a wide variety of systems, its extensive publicly available documentation, and its rigorous USGS peer review, MODFLOW has become the worldwide standard ground-water flow model. It is a flow model only with no mass transport component. It is used to simulate systems for water supply, containment remediation and mine dewatering. When properly applied, it is the recognized standard model used by courts, regulatory agencies, universities, consultants and industry.

The main objectives in designing MODFLOW were to produce a program that can be readily modified, is simple to use and maintain, can be executed on a variety of computers with minimal changes, and has the ability to manage the large data sets required when running large problems.

Ground-water flow within the aquifer is simulated using a block-centered finite-difference approach. Layers can be simulated as confined, unconfined, or a combination of both. Flows from external stresses such as flow to wells, areal recharge, evapotranspiration, flow to drains, and flow through riverbeds can also be simulated. MODFLOW is most appropriate in those situations where a relatively precise understanding of the flow system is needed to make a decision. MODFLOW was developed using the finite-difference method. The finite-difference method permits physical explanation of the concepts used in construction of the model. Therefore, MODFLOW is easily learned and modified to represent more complex features of the flow system.

To use MODFLOW, the region to be simulated must be divided into cells with a rectilinear grid resulting in layers, rows and columns. Files must then be prepared that contain:

KEY INPUT PARAMETERS

Specific yield
Pumping wells
Initial groundwater heads
Transmissivity
Boundary conditions
Recharge from precipitation, rivers, drains

SENSITIVE INPUT PARAMETERS

Hydraulic conductivity

APPLICABILITY

The most widely used groundwater flow model in the world.

ADDITIONAL INFORMATION

International Groundwater Modeling Center.

SOURCES

International Groundwater Modeling Center
Colorado School of Mines
Golden, Colorado 80401-1887
Phone: (303) 273-3103
Fax: (303) 384-2037
www.mines.edu/igwmc

Robert S Kerr Environmental Research Center
Center for Subsurface Modeling Support
P.O. Box 1198
Ada, Oklahoma 74821-1198
Phone: (580) 436-8586
Fax: (580) 436-8718
www.epa.gov/ada/models.html

PLASM

MODEL OPERATION

PLASM, Prickett Lonnquist Aquifer Simulation Model (PLASM) was first published in 1971 by the Illinois State Water Survey. It consists of three finite-difference simulation programs and a preprocessor. The programs simulate two-dimensional nonsteady flow of ground water in heterogeneous anisotropic aquifers under water table, nonleaky, and leaky confined conditions. Included are options for time-varying pumpage from wells, induced infiltration from streams or shallow aquifers, and water-table-depth-dependent evapotranspiration. The finite-difference equations are solved using a modified alternating direction method.

KEY INPUT PARAMETERS

Volumetric water content in saturated zone
Depth below water table
Lateral distance from center line of plume
Specific discharge
Saturated hydraulic conductivity
Porosity
Saturated thickness
Transmissivity
Storativity, storage coefficient
Leakance, between aquifer layers, vertical conductivity
Recharge
Longitudinal dispersivity
Transverse dispersivity
Vertical dispersivity
First-order degradation constant
Time since release
Source width
Source depth

SENSITIVE INPUT PARAMETERS

Source area concentration

Hydraulic gradient
Distance along the center line from downgradient edge of dissolved plume source zone

APPLICABILITY

Tested and validated but not as widely used due to development of more advanced numerical models like MODFLOW.

ADDITIONAL INFORMATION

International Groundwater Modeling Center

SOURCES

International Groundwater Modeling Center
Colorado School of Mines
Golden, Colorado 80401-1887
Phone: (303) 273-3103
Fax: (303) 384-2037
www.mines.edu/igwmc

MOC

MODEL OPERATION

This model simulates solute transport in flowing ground water. The model is both general and flexible in that it can be applied to a wide range of problem types. It is applicable for one- or two-dimensional problem involving steady state or transient flow. The model computes changes in concentration over time caused by the processes of convective transport, hydrodynamic dispersion, and mixing (or dilution) from fluid sources. The model assumes that gradients of fluid density, viscosity and temperature do not affect the velocity distribution. However, the aquifer may be heterogeneous and/or anisotropic. The model is based on a rectangular, block-centered, finite-difference grid. It allows the specification of injection or withdrawal wells and of spatially varying diffuse recharge or discharge, saturated thickness, transmissivity, boundary conditions and initial heads and concentrations. MOC incorporates: first-order irreversible rate-reaction; reversible equilibrium controlled sorption with linear, Freundlich, or Langmuir isotherms; and reversible equilibrium-controlled ion exchange for monovalent or divalent ions.

The model couples the ground-water flow equation with the solute-transport equation. The program uses an alternating-direction implicit procedure to solve a finite-difference approximation to the ground-water flow equation, and it uses the method of characteristics to solve the solute-transport equation. The latter uses a particle tracking procedure to represent convective transport and a two-step explicit procedure to solve a finite-difference equation that describes the effects of hydrodynamic dispersion, fluid sources and sinks, and divergence of velocity. This explicit procedure has several stability criteria, but the consequent time-step limitations are automatically determined by the program.

KEY INPUT PARAMETERS

Specification of injection or withdrawal wells
Saturated thickness
Boundary conditions
Specification varying diffuse recharge or discharge
Transmissivity

SENSITIVE INPUT PARAMETERS

Initial concentrations
Initial heads

APPLICABILITY

Limited application and cumbersome to use. However, verified and tested by U.S.G.S.

ADDITIONAL INFORMATION

International Groundwater Modeling Center

Scientific Software Group
P.O. Box 23041
Washington, D.C. 20026-3041
Phone: (703) 620-9214
Fax: (703) 620-6793
www.scisoftware.com

International Groundwater Modeling Center
Colorado School of Mines
Golden, Colorado 80401-1887
Phone: (303) 273-3103
Fax: (303) 384-2037
www.mines.edu/igwmc

U.S. Geological Survey
water.usgs.gov/software

BIOPLUME II/III

MODEL OPERATION

BIOPLUME II is a two-dimensional model that simulates the transport of contaminants in groundwater under conditions of oxygen limited biodegradation. The model provides for convective transport, dispersion, fluid source or sinks, chemical (nitrate, iron, sulfate) and physical reactions (first order decay), and three potential sources of oxygen. BIOPLUME III simulates the biodegradation of organic contaminants using a number of aerobic and anaerobic electron acceptors: oxygen, nitrate, iron (III), sulfate, and carbon dioxide. The model solves the transport equation six times to determine the fate and transport of the hydrocarbons and the electron acceptors/reaction by-products. For the case where iron (II) is used as an electron acceptor, the model simulates the production and transport of iron (II). BIOPLUME III runs in a Windows 95® environment whereas BIOPLUME II was mainly developed in a DOS environment.

KEY INPUT PARAMETERS

Oxygen concentration
Contaminant utilization rate
Contaminant half saturation constant
First order decay rate
Microbial concentration
Microbial yield coefficient
Ratio of oxygen to contaminant consumed
Oxygen half saturation constant
Microbial decay rate

SENSITIVE INPUT PARAMETERS

Groundwater velocity
Contaminant concentration
Contaminant retardation factor
Natural organic carbon concentration

APPLICABILITY

An extremely versatile model which allows the simulation of hydrocarbon plumes undergoing biodegradation.

ADDITIONAL INFORMATION

CSMoS

SOURCES

Scientific Software Group
P.O. Box 23041
Washington, D.C. 20026-3041
Phone: (703) 620-9214
Fax: (703) 620-6793
www.scisoftware.com

Robert S Kerr Environmental Research Center
Center for Subsurface Modeling Support
P.O. Box 1198
Ada, Oklahoma 74821-1198
Phone: (580) 436-8586
Fax: (580) 436-8718
www.epa.gov/ada/models.html

International Groundwater Modeling Center
Colorado School of Mines
Golden, Colorado 80401-1887
Phone: (303) 273-3103
Fax: (303) 384-2037
www.mines.edu/igwmc

RANDOM WALK

MODEL OPERATION

RANDOM Walk is a generalized FORTRAN computer code for simulation of two-dimensional ground-water flow and solute transport, written by T.A. Prickett, et.al. and released in 1981 by the Illinois State Water Survey (ISWS). Ground-water flow is simulated using either analytical solutions or a two-dimensional version of the PLASM finite difference model. The solute transport portion of the code is based on a particle-in-a-cell technique for the convective mechanisms and a random-walk technique for the dispersion effects. The model also handles first-order decay, linear equilibrium sorption (retardation), and zero-order production.

RANDOM WALK is a DOS-based program that can simulate two-dimensional nonsteady/steady flow problems in heterogeneous aquifers under water table and/or artesian or leaky artesian conditions. Furthermore, the program covers time-varying pumpage or injection by wells, natural or artificial recharge, the flow relationships between surface water and ground water, evapotranspiration, conversion of storage coefficients from artisan to water table conditions, and flow from springs. The program allows injection of solute by wells, leachate entering the aquifer from landfills or surface spills, location of a vertically averaged solute front representing salt water intrusion, leakage of water from overlying source beds with different water quality than the aquifer, and specification of concentrations along surface water boundaries to reflect their water quality.

KEY INPUT PARAMETERS

Volumetric water content in saturated zone
Depth below water table
Lateral distance from center line of plume
Specific discharge
Porosity
Saturated thickness
Transmissivity
Storativity, storage coefficient
Leakance, between aquifer layers, vertical conductivity
First-order degradation constant
Time since release
Source width
Source depth
Recharge
Longitudinal dispersivity
Transverse dispersivity
Vertical dispersivity

SENSITIVE INPUT PARAMETERS

Source area concentration
Saturated hydraulic conductivity
Hydraulic gradient
Distance along the center line from downgradient edge of dissolved plume source zone

APPLICABILITY

Tested and validated but not as widely used due to development of more advanced numerical models like MT3D.

ADDITIONAL INFORMATION

International Groundwater Modeling Center

SOURCES

International Groundwater Modeling Center
Colorado School of Mines

Phone: (303) 273-3103
Fax: (303) 384-2037
www.mines.edu/igwmc

Golden, Colorado 80401-1887

MT3D

MODEL OPERATION

The most current version of MT3D^{96} is a numerical simulation code that models the fate and transport of dissolved, single-species contaminants in saturated ground-water systems. MT3D^{96} calculates concentration distributions, concentration histories at selected receptor points and hydraulic sinks (for example, extraction wells), and the mass of contaminants in the ground-water system. The code can simulate three-dimensional transport in complex steady state and transient flow fields and can represent anisotropic dispersion, source-sink mixing processes, first-order transformation reactions and linear and nonlinear sorption.

KEY INPUT PARAMETERS

Depth below water table
Lateral distance from center line of plume
Specific discharge
Saturated thickness
Transmissivity
Leakance, between aquifer layers, vertical conductivity
Storativity, storage coefficient
Recharge
First-order degradation constant
Longitudinal dispersivity
Transverse dispersivity
Vertical dispersivity

SENSITIVE INPUT PARAMETERS

Source area concentration
Saturated hydraulic conductivity
Porosity
Distance along the center line from downgradient edge of dissolved plume source zone

APPLICABILITY

MT3D^{96} is widely accepted by regulators and the ground-water consulting and research communities and has been used to model thousands of sites.

ADDITIONAL INFORMATION

Scientific Software Group

SOURCES

Scientific Software Group
P.O. Box 23041
Washington, D.C. 20026-3041
Phone: (703) 620-9214
Fax: (703) 620-6793
www.scisoftware.com

Robert S Kerr Environmental Research Center
Center for Subsurface Modeling Support
P.O. Box 1198
Ada, Oklahoma 74821-1198
Phone: (580) 436-8586
Fax: (580) 436-8718
www.epa.gov/ada/models.html

International Groundwater Modeling Center
Colorado School of Mines
Golden, Colorado 80401-1887
Phone: (303) 273-3103
Fax: (303) 384-2037
www.mines.edu/igwmc

AT123D

MODEL OPERATION

AT123D, analytical, transient One-, Two-, and Three-Dimensional Model, is an analytical ground-water transport model. AT123D computes the spatial-temporal concentration distribution of wastes in the aquifer system and predicts the transient spread of a contaminant plume through a ground-water aquifer. The fate and transport processes accounted for are advection, dispersion, adsorption, and decay. AT123D estimates all the above components at a user defined time interval for up to 99 years of simulation time.

AT123D can be used as an assessment tool to help the user estimate the dissolved concentration of a chemical in three-dimensions in ground water resulting from a mass release over a source area. AT123D can handle: two kinds of source releases-instantaneous, continuous with a constant loading or time-varying releases; three types of waste-radioactive, chemicals, heat; four types of source configurations-a point source, a line source parallel to the x-, y-, z-axis, and area source perpendicular to the z-axis, a volume source; four variations of the aquifer dimensions-finite depth and finite width, finite depth and infinite width, infinite depth and finite width, infinite depth and infinite width.

KEY INPUT PARAMETERS

Bulk density
Dispersivities in x, y, and z directions
First-order decay rate
Molecular diffusion coefficient
Heat exchange

SENSITIVE INPUT PARAMETERS

Hydraulic conductivity
Porosity
Hydraulic gradient
Sorption coefficients
Distance to receptor

APPLICABILITY

Widely used and U.S.G.S. approved.

ADDITIONAL INFORMATION

International Groundwater Modeling Center

Scientific Software Group

SOURCES

Scientific Software Group
P.O. Box 23041
Washington, D.C. 20026-3041
Phone: (703) 620-9214
Fax: (703) 620-6793
www.scisoftware.com

International Groundwater Modeling Center
Colorado School of Mines
Golden, Colorado 80401-1887
Phone: (303) 273-3103
Fax: (303) 384-2037
www.mines.edu/igwmc

MODPATH

MODEL OPERATION

MODPATH is a particle tracking post-processing package that was developed to compute three-dimensional flowpaths using output from steady state or transient ground-water flow simulations by MODFLOW. MODPATH uses a semi-analytic particle-tracking scheme that allows an analytical expression of the particle's flow to be obtained within each finite-difference grid cell. Particle paths are computed by tracking particles from one cell to the next until the particle reaches a boundary, an internal sink/source, or satisfies some other termination criterion. Data input for MODPATH is a combination of data files and interactive keyboard input.

Output from steady state or transient MODFLOW simulations is used in MODPATH to compute paths for imaginary "particles" of water moving through the simulated ground-water system. In addition to computing particle paths, MODPATH keeps track of the time of travel for particles moving through the system. By carefully defining the starting locations of particles, it is possible to perform a wide range of analyses such as delineating capture and recharge areas or drawing flow nets.

KEY INPUT PARAMETERS

Lateral distance from center line of plume
Specific discharge
Transmissivity
Leakance, between aquifer layers, vertical conductivity
Depth below water table
Saturated thickness
Storativity, storage coefficient
Longitudinal dispersivity
Transverse dispersivity
Vertical dispersivity
Recharge
First-order degradation constant

SENSITIVE INPUT PARAMETERS

Source area concentration
Saturated hydraulic conductivity
Porosity
Distance along the center line from downgradient edge of dissolved plume source zone

APPLICABILITY

Tested and validated by U.S.G.S.

ADDITIONAL INFORMATION

Scientific Software Group

International Groundwater Modeling Center

SOURCES

Scientific Software Group
P.O. Box 23041
Washington, D.C. 20026-3041
Phone: (703) 620-9214
Fax: (703) 620-6793
www.scisoftware.com

International Groundwater Modeling Center
Colorado School of Mines
Golden, Colorado 80401-1887
Phone: (303) 273-3103
Fax: (303) 384-2037
www.mines.edu/igwmc