



A GUIDANCE SYSTEM FOR CHOOSING ANALYTICAL CONTAMINANT  
TRANSPORT MODELS

A Dissertation

Presented to

the Faculty of the Interdisciplinary Graduate Program

in Environmental Engineering

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In Partial Fulfillment

of the Requirements for the Degree

Doctor of Philosophy

in Environmental Engineering

by

Lu-chia Chuang

August, 1998

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## **ABSTRACT**

This research proposes a new approach to solve two main problems that users often face in contaminant transport modeling: where to find models quickly and how to choose an appropriate model? The approach in this study differs from other efforts in that a groundwater contaminant transport model is a result of a decision process rather than an object for manipulating. The fundamental assumption of the approach is that any given groundwater contaminant transport model can be represented as a set of properties. By matching a contaminant transport problem to a list of model property sets, an appropriate model for the given problem can be found.

The approach is demonstrated through the design and implementation of the ANalytical contaminant Transport modeling guidance System, or ANTS. The basic function of the system is to assist a user in choosing an appropriate analytical solution model to solve a groundwater contaminant transport problem via the Internet. The system offers: an Internet-based graphical user interface, a flexible model search capability, a large collection of analytical solution models, a hierarchical modular system structure, and referable reusability, as well as a database of model characteristics.

In this research, properties of more than 100 analytical solutions of groundwater contaminant transport models were studied, characterized, and stored in a database. A user survey was conducted to understand the domain knowledge and computer skill of

the potential users. Different match strategies were developed to meet the needs of the potential users.

A preliminary evaluation was conducted to verify and validate the system. The results indicate that the system does match the author's expectation in finding appropriate models for groundwater contaminant transport cases. The test subjects were able to find appropriate models for most (74.7%) test problems.

The results demonstrate that the approach worked very well for this research and may be applicable to other areas of natural resources modeling. The system could be used as a quick screening tool to enhance the decision making capabilities in managing subsurface pollution problems.



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# CHAPTER 1 PROBLEM EXPOSITION

## 1.1 Difficulties in Contaminant Transport Modeling

The purpose of groundwater contaminant transport modeling is twofold. First the models are intended to help gain a better understanding of changes occurring in the movement of groundwater pollutants. Second, models can provide planners and managers with estimates of the relative changes in groundwater quality resulting from alternative management policies. However, groundwater contaminant transport modeling requires a considerable amount of human expertise and other resources. In a research institute where human expertise and time are usually not critical factors, modeling a groundwater contaminant transport case may not pose a problem. However, in the decision making environment, such as government regulatory agencies or industrial settings, these resources, especially human expertise and time, can be scarce. There are three main problems that users often face in contaminant transport modeling.

### ***1.1.1 Where to Look for Models?***

Over the past few decades, numerous contaminant transport models have been developed and implemented, available as mathematical equations or coded computer programs. However, most users do not have extensive knowledge about the currently available models and do not know where to look for models. A practice to reduce this problem is to build an analytical solution library that contains many models. There are

two publications that fit into this category. One is a technical report by van Genuchten and Alves (1982) that has 44 analytical solutions of one-dimensional single chemical constituent in a unidirectional groundwater flow field models. The other is a U. S. Geological Survey open file report by Wexler (1989) that has 11 analytical solutions of single chemical constituent in a unidirectional groundwater flow field models. One drawback of these two reports is that they only contain models of single chemical constituent in a unidirectional groundwater flow field. The other drawback is that users usually can not obtain these models in a short period of time. If the users can not obtain the models in time, the models are useless to the users.

### ***1.1.2 How to Choose a Model?***

Another problem is how to choose the most appropriate model from the set of the already existing models for the case of interest? A solution library can not overcome this problem alone because a user may not have sufficient knowledge to choose a model in the library. One solution is to incorporate a guidance module into the model library. The guidance module can guide users to select the most appropriate model. The guidance module can be a decision-support system or a knowledge-based system. An example of such a system is FRAME by Calori et al. (1994). FRAME is a knowledge-based tool for choosing the appropriate air pollution model for a particular scenario. So far, there is no guidance system for choosing a groundwater contaminant transport model.

### **1.1.3 How to Set up the Chosen Model?**

Once a model is chosen, the user of the model needs to assign parameters' values to the model. The user, however, may not have sufficient knowledge to set up a model. Several parameter assistant modules have been developed to address this problem. A parameter assistant module can help users choose reasonable parameter values for contaminant transport problems. An example is EXPAR by McClymont and Schwartz (1991).

A model library that contains an extensive collection of analytical models does not currently exist; a computerized guidance module that can guide users to select appropriate analytical groundwater contaminant transport models is also not available; and there is no computer system that integrates the functions of a model library and a guidance module. These problems suggest the need for a modeling guidance system that would help planners or managers to make a decision to choose appropriate models from a contaminant transport model library.

## **1.2 Background**

This research was funded by the Gulf Coast Hazardous Substance Research Center, GCHSRC. The purpose of the project was to develop a software library of analytical fate and transport models with a selection algorithm to guide the user to the most appropriate model for a particular case. The system can operate stand alone or in concert with general purpose spreadsheet programs. The first part of the project was spent in developing a spreadsheet based prototype, ExcelDSS, and a Visual Basic based prototype, VBAnts.

Since 1996, the focus of the project has been changed in part due to the growing popularity of the Internet. The purpose of the project was to develop a software library of analytical contaminant transport models with selection guidance modules that can be accessed by any user from any where in the world at any time. Such a system could be a very useful tool for the environmental engineering community.

### **1.3 Objectives and Scope of the Research**

The focus of this research is on introducing a new approach to model groundwater contaminant transport problems, with potential applicability to other areas of natural resources modeling. The approach in this research differs from other approaches in that a model is a result of a decision process rather than an object for manipulating. In this process, a user makes a series of decisions through a provided guidance module to find an appropriate model. The system could be used as a screening tool to enhance the decision making capabilities in managing subsurface pollution problems.

The objectives and scope of this research are as follows:

1. to study characteristics of analytical solutions of groundwater contaminant transport models and characterize the models,
1. to understand the computer skill and domain knowledge of the potential users by conducting a user survey.
1. to build an analytical groundwater contaminant transport model library and to design and implement a modeling guidance system, ANalytical contaminant Transport modeling guidance System (or ANTS), for predicting contaminant

transport in groundwater from the knowledge gathered from the study of analytical groundwater contaminant transport models and the potential users. The system will serve the following purposes:

- The system will serve as a model library that contains an extensive collection of analytical solutions of contaminant transport models.
  - The system should function as a user-friendly guidance tool for selecting an appropriate analytical contaminant transport model from a model library to predict the outcome of a contaminant transport problem.
  - The system will be accessible by any user via the Internet.
  - The system will be an easily maintained system.
1. to validate the system by conducting a preliminary evaluation to know how successful the developed system is in meeting the set objectives.

The system will not support the following functions:

1. The system will not be an expert. The system should be more a decision-support system than an expert system, because its decision process is controlled by the user not by the system. In other words, the ANTS system will not be a computerized expert; it will be a computerized assistant for the user.
1. The system is not meant to replace three-dimensional multicomponent FEM/FDM numerical models (such as MOFAT). The system should be considered as a screening tool.
1. The system will not address the problem of difficulties in setting up model parameters, because many efforts have been done in dealing with this problem (such as McClymont and Schwartz, 1991).



## **1.4 Organization of the Dissertation**

Chapter 2 reviews some of the popular and most widely used analytical solution models for predicting the extent of subsurface contamination, general concepts of expert systems and decision-support systems and environmental related expert systems and decision-support systems, and concepts of the Internet and Internet programming and available Internet-based resource related to contaminant transport modeling on the Internet. The conceptual framework of the proposed approach is introduced in Chapter 3. Chapter 4 describes two earlier groundwater modeling decision-support system prototypes. Development of the Internet-based modeling guidance system is presented in Chapter 5. Validation of the model codes is presented in the Chapter 6. In the Chapter 7, the results of testing and evaluating in regard to its functionality and the ability to predict changes in contaminant transport are presented. The summary, research conclusion, and possible future works are presented in Chapter 8.

Appendix A, the glossary, presents definitions for key terms used throughout the text. Appendix B describes the results of the user classification survey. Groundwater contaminant transport models, their authors, and properties of the models are listed in Appendix C.

## **CHAPTER 2 LITERATURE REVIEW**

### **2.1 A Review of Analytical Groundwater Contaminant**

#### **Transport Models**

This section reviews and organizes some of the popular and most widely used analytical solution models for predicting the extent of subsurface contamination. Descriptions of abstracts, characteristics, and properties of analytical solutions are presented in this section.

##### **2.1.1 Introduction**

###### **Background**

The chemical and biological constituents of groundwater depend on two factors: the natural environment of groundwater storage and movement, and human activities. Precipitation, infiltration, and surface water percolation are the natural sources of groundwater. Human contamination activities usually are results of mismanagement of waste materials that are stored or disposed of on or beneath the land surface. These waste materials are potentially hazardous to groundwater. In many instances, human activities have altered natural processes and caused groundwater to contain organisms, hydrocarbons, heavy metals and other harmful matter.

The groundwater resource is limited. Optimal use of limited resources and achievement of maximum economic benefits can only be attained through scientific management and rational use. An incorrect management decision not only causes economic waste, but also brings serious consequences, such as the depletion of water, the deterioration of water quality, and the subsidence of land.

Many mathematical models have been used for simulating groundwater contaminant transport problems. A mathematical model consists of a set of differential equations known to describe the transport of groundwater contaminants. The reliability of predictions from a contaminant transport model depends on how well the model approximates the field situation. Mathematical models are usually classified according to the two techniques available for solution: analytical and numerical solutions.

### **Analytical Solutions vs. Numerical Solutions**

Simplifying assumptions must always be made in order to construct a model because the field situations are too complicated to be simulated exactly. Usually the assumptions necessary to solve a mathematical model analytically are fairly restrictive. For example, many analytical solutions require that the transport medium be homogeneous and isotropic. To deal with more realistic situations, it is usually necessary to solve the mathematical model approximately using numerical techniques. However, analytical solutions are often much easier to use than numerical solutions generated by finite difference methods or finite element methods (FDM/FEM). Analytical solutions to contaminant transport models can be a very useful screening tool for groundwater specialists to quickly predict the outcome of a groundwater contamination case. Another reason to use analytical solutions is that numerical

solutions require verification, and an analytical solution can serve as a second opinion to a numerical solution. Analytical solutions are often ideally suited to the interpretation of experimental results obtained under controlled laboratory conditions.

### An Analytical Solution Example

The governing equation of contaminant transport for a three-dimensional single chemical constituent in a unidirectional groundwater flow field is (van Genuchten and Alves, 1982)

$$R \frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - V_x \frac{\partial C}{\partial x} - \mu C + \gamma, \quad (2-1)$$

where  $R$  is the retardation factor,  $D_i$  is dispersivity in  $i$  direction ( $i$  can be the  $x$ ,  $y$ , or  $z$  direction),  $C$  is volumetric concentration,  $V_x$  is average fluid velocity,  $\mu$  is a first-order chemical decay rate coefficient, and  $\gamma$  is a zero-order chemical production rate coefficient.

Although the literature uses different governing equations for contaminant transport, most are very similar in form to Equation (2-1). There are various initial conditions and boundary conditions which can apply to this equation.

In this research, we define a model as a combination of one particular governing equation, a set of initial conditions and a set of boundary conditions. Analytical models with different sets of initial and boundary conditions usually yield different solutions.

The following section provides a solution of a contaminant transport model (van Genuchten and Alves, 1982). The model is a one-dimensional contaminant transport model with a governing equation defined as

$$R \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - V \frac{\partial C}{\partial x} - \mu C + \gamma. \quad (2-2)$$

The initial and boundary conditions are

$$C(x,0) = C_i, \quad C(0,t) = C_a + C_b e^{-\lambda t}, \quad \text{and} \quad (2-3)$$

$$\frac{\partial C}{\partial x}(\infty, t) = 0. \quad (2-4)$$

The analytical solution can be represented in the form,

$$C(x,t) = \frac{\gamma}{\mu} + (C_i - \frac{\gamma}{\mu})A(x,t) + (C_a - \frac{\gamma}{\mu})B(x,t) + C_b E(x,t), \quad (2-5)$$

where

$$A(x,t) = \exp\left(\frac{\mu t}{R}\right) \left\{ 1 - \frac{1}{2} \operatorname{erfc}\left[\frac{Rx - Vt}{2(DRt)^{1/2}}\right] - \frac{1}{2} \exp\left(\frac{Vx}{D}\right) \operatorname{erfc}\left[\frac{Rx + Vt}{2(DRt)^{1/2}}\right] \right\}, \quad (2-6)$$

$$B(x,t) = \frac{1}{2} \exp\left[\frac{(V-U)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx - Ut}{2(DRT)^{1/2}}\right] + \frac{1}{2} \exp\left[\frac{(V+U)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx + Ut}{2(DRT)^{1/2}}\right], \quad (2-7)$$

$$E(x,t) = e^{-\lambda t} \left\{ \frac{1}{2} \exp\left[\frac{(V-W)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx - Wt}{2(DRT)^{1/2}}\right] + \frac{1}{2} \exp\left[\frac{(V+W)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx + Wt}{2(DRT)^{1/2}}\right] \right\}, \quad (2-8)$$

$$U = V \left( 1 + \frac{4\mu D}{V^2} \right)^{1/2}, \quad \text{and} \quad (2-9)$$

$$W = V \left( 1 + \frac{4D}{V^2} (\mu - \lambda R) \right)^{1/2}, \quad (2-10)$$

where *erfc* represents the complementary error function.

The solution shown here is not as complicated as it appears. In fact, if the boundary conditions given in Equation (2-4), which represents the semi-infinite domain, is changed to

$$\frac{\partial C}{\partial x}(L, t) = 0 \text{ for finite domain,} \quad (2-11)$$

the solution of the new model contains at least twice as many terms as given in Equations (2-5) through (2-10).

The purpose of this example is to illustrate the complexity of analytical solutions to contaminant transport models (though analytical solutions are easier to program than numerical FEM/FDM solutions). It is obvious that a library of ready-to-use models could be a very useful tool for groundwater specialists.

### **2.1.2 Analytical Solution Models**

In this section, some of the popular and most widely used analytical solution models for predicting the extent of subsurface contamination are discussed. The models presented range from simple one-dimensional, single chemical constituent analytical models to complex three-dimensional, multichemical constituent analytical models.

#### **The Standard Model Set**

Van Genuchten (1981) presented models of the movement of a chemical in a porous medium as influenced by linear equilibrium adsorption, zero-order production, and first-order decay.

Van Genuchten and Alves (1982) reorganized van Genuchten's models (1981) and published a U.S.D.A. technical bulletin that contains mathematical models and

associated computer programs for solving of the one-dimensional convective dispersive solute transport equations. The governing transport equations include terms accounting for convection, diffusion and dispersion, and linear equilibrium adsorption. In some cases, the effects of zero-order production and first-order decay have also been taken into account. There are 44 models listed in the report. The authors divided 44 models listed in the book into three cases based on their governing equations. This reference is one of the earliest and most useful model libraries. The models in this reference come with analytical solution equations and FORTRAN source codes. These models were chosen as the standard model set in this project. Properties of the standard model set, such as governing equations, boundary conditions, and source types, are listed in Table 2-1. The reason to choose their models as the standard model set rests in their usefulness for most laboratory column experiments.

**Table 2-1 Properties of the standard model set**

<b>Governing Equation</b>	$R \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - V \frac{\partial C}{\partial x},$ $R \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - V \frac{\partial C}{\partial x} + \gamma, \text{ or}$ $R \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - V \frac{\partial C}{\partial x} - \mu C + \gamma$
<b>Inflow Boundary</b>	First type or third type
<b>Outflow Boundary</b>	Semi-infinite or finite length
<b>Source Type</b>	instantaneous, step, finite pulse, decaying source, or continuous injection

## A Chronicle of Analytical Solution Models

Hoopes and Harleman (1967) presented an approximate solution of a model that has dispersion in radial flow from a recharging well. Radial flow and radial dispersion are the characteristics that distinguish them from the standard model set.

Eldor and Dagan (1972) presented an approximate analytical method that solves problems involving hydrodynamic dispersion in porous media with radioactive decay and/or adsorption of the tracer. The method is applied to four examples of hydrologic interest: radial flow from a recharging well, a recharging well in a uniform flow field, two wells, and soil leaching by uniform recharge. The models are different from the standard model set in their characteristics of radial flow and radioactive decay source.

Van Genuchten and Wierenga (1976) presented an analytical model for the movement of chemicals through a sorbing porous medium with lateral or intra aggregate diffusion. The liquid phase of the model is divided into mobile and immobile regions. Diffusional transfer between the two liquid regions is assumed to be proportional to the concentration difference between the mobile and immobile liquids. Sorption processes in both the dynamic and stagnant regions of the medium are assumed to be instantaneous and the adsorption isotherm is assumed to be linear. The solution is used to model unsaturated, aggregated sorbing medium.

Cleary and Unger (1978) developed analytical solutions of two-dimensional dispersion models that simulate one-dimensional principal and arbitrary directional flow fields and exponential decaying source terms.

Hunt (1978) developed analytical solutions for an instantaneous and a continuous point contaminant source and then for an instantaneous source of finite size.



Domenico and Palciauskas (1982) presented a model for maximum concentration predictions is developed for one-dimensional steady flow and dispersion in directions perpendicular to the flow path. This model is reasonably operational with a minimum of data. The model avoids chemical reaction and the inherent fitted parameter known as longitudinal dispersion. The model employs the actual measured concentration at the solid waste boundary as a boundary condition. This model provides a conservative estimate of whether or not minimum performance standards will be achieved at an alternative boundary.

Mironenko and Pachevsky (1984) presented an analytical solution to the set of equations describing chemical transport in soils which account for dispersion, the presence of a stagnant liquid phase, and sorption in which the solute is involved in biological or chemical transformations. The model is used for describing nitrate transport and denitrification in a soil column.

Chen (1985) presented analytical and approximate solutions for radial dispersion in aquifers with simultaneous diffusion into adjacent strata. Contaminants from the injection well are transported within the main aquifer by advection and mechanical dispersion, assuming a steady state and radially diverging groundwater flow field. The leakage of contaminants from the main aquifer to the aquitards is accounted for by molecular diffusion. The solutions can be applied to study radial dispersion in granular aquifers bounded by relatively low permeability aquitards, or in planar fractures contained in porous formations.

Domenico and Robbins (1985) presented analytical expressions for contaminant transport from a finite pulse source and a continuous source in a continuous flow

regime. The difference between their models and the standard model set is that their models include one, two, and three-dimensional dispersion models.

Van Genuchten (1985) presented an analytical solution of sequential first-order decay reactions. Applications of this model include radionuclide transport and nitrification.

Gureghian and Jansen (1985) presented one-dimensional analytical solutions for the migration of a three-member radionuclide decay chain in a multilayered geologic medium. The practical use of the solutions in a two-dimensional domain is illustrated by a scenario of radionuclide migration from a high level waste repository located in a saturated multilayered aquifer.

Booker and Rowe (1987) presented two analytical solutions of one-dimensional advective dispersive transport into a deep layer having a variable surface concentration. These solutions take account of changes in surface concentration with time as mass is transported into the soil. The first solution is developed for the case of rapid landfill construction. The second solution considers a time-dependent mass input to the landfill.

Chen (1987) presented analytical solutions for radial dispersion with a Cauchy boundary at an injection well. This Cauchy boundary condition includes effects of radial advection and longitudinal dispersion but molecular diffusion is neglected in the problem. Analytical solutions related to a continuous and a pulse injection are determined for the radial dispersion problem concerning such a Cauchy boundary condition. These solutions give resident concentrations in the radial flow system. Results of the continuous injection solution and of that related to a Dirichlet boundary condition (the first type) are different for short injection periods but converged for long

injection periods. The deviation caused by using two different boundary conditions is further studied with appropriate asymptotic solutions valid only for short injection periods. It is found that significant concentration gradients may exist across the well aquifer interface for short injection periods.

Domenico and Robbins (1987) presented analytical solutions for multidimensional contaminant transport from an exponential decaying source in a continuous flow regime. The exponential decaying source is the only difference between these models and the Domenico and Robbins 1985 models.

Galya (1987) presented a model to simulate three-dimensional contaminant transport from a horizontal plane source (HPS). This model incorporates retardation and decay, and can simulate varying source emission rates. The HPS model should provide more accurate results than the point source solution, particularly near the source.

Guvanasen and Guvanasen (1987) presented an approximate semianalytical solution for tracer injection tests in a confined aquifer with a radially converging flow field and finite volume of tracer and chase fluid. The solution is divided into two phases: injection and transport. During the injection phase, an injection of chase fluid immediately following the tracer is allowed. Hydrodynamic dispersion effects are assumed to be negligible during this phase. The geometry of the tracer plume is determined by a particle tracking technique. During the plume transport phase, the tracer plume is approximated by a series of contiguous pulses. An approximate analytical solution for each pulse has been derived through linearization of the transport equation.

Chen (1989) presented a mathematical model amenable to analytical solution techniques for the investigation of contaminant transport from an injection well into a leaky aquifer system, which comprises a pumped and an unpumped aquifer connected to each other by an aquitard. The model assumes that contaminants are transmitted in the pumped aquifer by radial advection, and in the aquitard by vertical one-dimensional advection and longitudinal dispersion.

Dillon (1989) presented an analytical two-dimensional model of solute transport along a vertical cross section of an aquifer. The model extends analytical methods to two-dimensional dispersive solute transport in a two-dimensional flow field which until now has been the exclusive province of numerical models. The model is intended for preliminary evaluation of groundwater quality on a regional scale in areas subject to diffuse sources of contamination.

Wexler (1989) presented eleven analytical solutions of one-, two-, and three-dimensional analytical models. Wexler's solutions were compiled from available literature or derived by the author for a variety of boundary condition types and solute source configurations with uniform groundwater flow. This is another popular model library.

Brown and McWhorter (1990) presented an analytical solution for the case of isothermal, transient, one-dimensional sorption of water with constant liquid content boundaries. A relation is also obtained for the evaporation and condensation within flow field.

Yates (1990) presented an analytical solution for one-dimensional transport in heterogeneous porous media with a distance-dependent dispersion relationship. The

solution can be used to characterize differences in the transport process relative to the classical convection dispersion equation that assumes that the hydrodynamic dispersion in the porous medium remains constant.

Leij, Skaggs, and van Genuchten (1991) presented analytical solutions for solute transport in three-dimensional semi-infinite porous media.

Bosma and van der Zee (1992) presented an analytical approximation solution for nonlinear adsorbing solute transport in layered soils. They consider reactive solute transport in a soil consisting of two layers that have different biochemical properties. Assuming adsorption is adequately described with the Freundlich equation, the degree of adsorption nonlinearity differs. Using simple corrections the fronts are approximated analytically for case 1, where that the top layer adsorbs nonlinearly whereas the subsoil layer adsorbs linearly, and for case 2 where the layering order is reversed. By comparison with numerical calculations, Bosma and van der Zee show the adequacy of the analytical approximations as well as the effect of layering order on the subsoil front shapes. For the case of a layered soil with nonlinear adsorption and first-order decay, analytical approximations appear to describe the numerically found fronts well.

Neville (1992) presented an analytical solution for one-dimensional subsurface transport of organic contaminants with multiprocess nonequilibrium. The model is a combination of the two-site and two-region conceptualizations. The mobile and immobile regions are each subdivided into three compartments. The first compartment in each region is the dissolved phase and the second and third compartments constitute the sorbed phase. In the second compartment, sorption occurs instantaneously, while in the third it is rate limited. The first-order mass transfer approach is used to model

transport between the mobile and immobile regions. The analytical solution can represent domains of both finite and semi-infinite extent and accommodates non zero initial concentrations.

Serrano (1992) described field scale solute transport parameters in terms of regional hydrologic and aquifer hydraulic properties, such as recharge rate, transmissivity, hydraulic gradient, aquifer thickness and soil porosity. A dispersion equation in an aquifer subject to recharge and variable groundwater velocity is one with coefficients given as variable functions of distance. An analytical solution of this equation is presented along with numerical comparisons with the classical convection dispersion equation and sensitivity tests on the effect of hydrologic hydraulic variables on the contaminant evolution. It was found that the recharge rate substantially affects the contaminant distribution and may partially explain the scale dependence of dispersion parameters. Transmissivity and hydraulic gradient values also determine the velocity distribution and therefore the rate of migration.

Yates (1992) presented an analytical solution describing the transport of dissolved substances in heterogeneous porous media with an asymptotic distance-dependent dispersion relationship. The solution has a dispersion function that is linear near the origin and approaches an asymptotic value as the travel distance becomes infinite. This solution can be used to characterize differences in the transport process relative to both the classical convection dispersion equation that assumes that the hydrodynamic dispersion in the porous medium remains constant and a dispersion solution that has a strictly linear dispersion function. The model may provide an

alternate means for obtaining a description of the transport of solutes in heterogeneous porous media.

Angelakis et al. (1993) presented an analytical solution for transient soil gas diffusion coupled to two convective dispersive solute transport equations. First-order kinetic transformations, linear equilibrium distribution coefficient for both solutes, and equilibrium gas solubility for the gaseous product were assumed. The solution was verified by comparison to a numerical solution using an explicit finite difference scheme. The analytical solution shows that the soil gas distributions were highly affected by the gas solubility and by the distribution coefficient and the transformation rate constants of both solutes. The gas distributions were not significantly affected by the dispersion coefficient of either solute. The gas distributions are slightly affected by changes in the gas diffusivity over the range expected for different gas species at a single value of air filled porosity. Changes in soil water content and the corresponding change in air filled porosity would result in large changes in the gas concentration profiles.

Basha and El-Habel (1993) presented an analytical model that provides an approximate description of scale dependent transport. The model is based on the advection dispersion equation but with the dispersion coefficient dependent on the travel time of the solute from a single input source. The time dependence of the dispersion coefficient can assume arbitrary functional forms. Eight particular solutions for various dispersion functions and mass injection scenarios are presented. These include linear, exponential, and asymptotic variation of the dispersion functions and instantaneous as well as continuous mass injection. The analytical solutions could

model the transport of solute in a hydrogeologic system characterized by a dispersion coefficient that varies as a function of travel time from the input source. It could provide a modeling solution to solute transport problems in heterogeneous media and be used as a suitable model for the inversion problem, especially since more than one fitting parameter is available to fit the field tracer data that exhibit a scale effect.

Ellsworth and Butters (1993) presented three-dimensional analytical solutions to the advection dispersion equation in arbitrary Cartesian coordinates. Using the method of Green's functions, a generalized analytical solution of the three-dimensional advection dispersion equation set in an arbitrary Cartesian coordinate system is given for the solute resident concentration in a semi-infinite porous medium with an arbitrary initial condition, surface boundary condition, and sink/source terms. Two particular solutions for a rectangular surface flux boundary condition and a buried parallelepiped, respectively, are derived from the general solution. The corresponding frequency domain solutions, analytical expressions without numerical integration, are given which provide a more efficient method of computation for generating two and three-dimensional fast Fourier transform algorithm.

Fry and Istok (1993) presented an analytical solution to the solute transport equation with rate limited desorption and decay. This solution is derived for the advection dispersion equation with rate limited desorption and first-order decay, using an eigen-function integral equation method. The model equations represent one-dimensional solute transport in a homogeneous isotropic porous medium where the porous medium is saturated with the aqueous solution. The flow field is uniform. Rate



limited desorption is described as a first-order process where the rate is proportional to the difference in concentration between the sorbed phase and the aqueous phase.

Leij et al. (1993) presented analytical solutions for nonequilibrium solute transport in three-dimensional porous media during steady unidirectional flow. The solutions can be used to model transport in porous media where the liquid phase consists of a mobile and an immobile region (physical nonequilibrium) or where solute sorption is governed by either an equilibrium or a first-order rate process (chemical nonequilibrium). The transport equation incorporates terms for advection, dispersion, zero-order production, and first-order decay. General solutions were derived for the boundary, initial, and production value problems using Laplace and Fourier transforms. A comprehensive set of specific solutions is presented using Dirac functions for the input and initial distribution, and/or Heaviside or exponential functions for the input, initial, and production profiles. A rectangular or circular inflow area was specified for the boundary value problem while for the initial and production value problems the respective initial and production profiles were located in parallelepipedal, cylindrical, or spherical regions of the soil. Solutions are given for both the volume averaged or resident concentration as well as the flux averaged or flowing concentration.

Lerner and Papatolios (1993) presented an analytical expression that predicts how solute concentrations evolve with time in a pumped well. The basic expression represents uniform recharge and uniform concentration of a conservative solute in the recharge. It shows that pumped concentrations are independent of pumping rates. The expression can be developed to allow for more complex patterns of recharge and solute

loading, and an example is given with three zones of recharge and concentrations, induced river recharge, and a cross boundary inflow.

Wallach (1993) presented an approximate analytical solution for soil chemical transfer to runoff with a modified boundary condition. Two mass balance equations were used to model the transfer of dissolved chemicals from the soil solution to the surface runoff water and the transport of these chemicals to the field outlet. One mass balance equation was written for chemicals dissolved in the overland water, the other for chemicals within the soil profile. Chemical input into the surface water was expressed as a rate limited convective mass transfer, depending on both soil surface the runoff concentrations.

Zaidel and Russo (1993) presented analytical models of steady state organic species transport in the vadose zone with kinetically controlled volatilization and dissolution. Kinetically controlled volatilization and dissolution of nonaqueous phase liquids (NAPLs) may play an important role in the transport of volatile compounds in the unsaturated (vadose) zone. In this study, one- and two-dimensional steady state transport problems are solved analytically. The one-dimensional case is pertinent to pollution by a relatively long, mainly horizontally spread leak of NAPL. The two-dimensional case corresponds to situations in which the pollution spreads primarily vertically, originating at the ground surface and migrating to the top of the capillary fringe, and in which the solution domain may be represented by a cross sectional model. Solutions of the steady state transport problems are used to investigate effects of several parameters, characterizing the advective dispersive and purely diffusive transport

regimes, on the NAPL concentration distribution for the one and two-dimensional cases, respectively.

Illangasekare et al. (1994) presented a quasi-analytical technique for the solution of governing equations of steady groundwater flow and advective transport in aquifers. This technique is based on integral transforms and does not require any spatial discretization of the solution domain. It produces a continuous and differentiable solution to the groundwater flow equation, thus making it possible to obtain conveniently a continuous velocity field in three-dimensional physical domains without any spatial discretization. This velocity field, in conjunction with a method of characteristics particle tracking scheme is used to solve the advection component of the transport equation. A three-dimensional transport model based on this technique was developed and analyzed for effectiveness as a modeling tool. The model was used to study the effect of complex three-dimensional flow on two-dimensional apparent macrodispersion.

Kool et al. (1994) presented a composite modeling approach for simulating the three-dimensional subsurface transport of dissolved contaminants with transformation products. The approach is based on vertical infiltration and contaminant transport in the unsaturated zone and three-dimensional groundwater flow and contaminant migration in the saturated zone. Moisture movement and groundwater flow are considered to be steady, but contaminant transport is treated as transient. The model allows for advection, dispersion, linear or nonlinear equilibrium sorption, and first-order biochemical transformation of either a single contaminant species, or a multispecies, straight or branched, decay chain. The model contains fully three-dimensional solutions

for flow and transport in the saturated zone, as well as two-dimensional solutions for vertical cross sectional and areal scenarios.

Leij and Bradford (1994) presented analytical solutions for selected cases of three-dimensional solute transport during steady unidirectional water flow in porous media with uniform transport and flow properties. The transient solutions are evaluated for five different transport scenarios in either a Cartesian or cylindrical coordinate system. The steady state solutions are also provided for three initial value problems.

Zaidel and Russo (1994) presented a one-dimensional vertical model of kinetically controlled diffusive transport of organic vapors pertinent to pollution caused by a relatively long, ground surface originating, mainly horizontally spread leak of NAPL, the volatile compound of which undergoes sorption and degradation in the soil. Analytical solutions of this model are applicable to homogeneous soils with ground surface fully open to the atmosphere.

Yuan's solutions (1995) were established through the extension of Domenico and Robbins' model to simulate one-, two-, and three-dimensional contaminant transport from an exponentially decaying source of finite size. The models incorporate one-dimensional groundwater velocity, longitudinal and transverse dispersion.

### Characteristics of References

The references reviewed in this study have characteristics that are distinguish them from the standard model set. Characteristics of the references are listed in Table 2-2.

**Table 2-2 Characteristics of models**

<b>References</b>	<b>Distinguished Characteristics</b>
Hoopes and Harleman (1967)	radial flow and radial dispersion
Eldor and Dagan (1972)	radial flow and radioactive decay source
Van Genuchten and Wierenga (1976)	unsaturated, two liquid regions (mobile and immobile) flow, and aggregated sorbing medium
Cleary and Ungs (1978)	one-dimensional principal and arbitrary flow fields, two-dimensional dispersion, and decay source type
Domenico and Palciauskas (1982)	minimum data requirement, maximum concentration level prediction
Mironenko and Pachepsky (1984)	stagnant liquid phase
Chen (1985)	radial dispersion with simultaneous diffusion into adjacent strata, radial dispersion from an injection well into a planar fracture contained in a porous formation
Domenico and Robbins (1985)	multidimensional dispersion, pulse source term (instantaneous and continuous source)
Van Genuchten (1985)	sequential first-order decay reactions
Gureghian and Jansen (1985)	multilayered geologic medium, three member radionuclide decay chain migration from a high level waste repository located in a saturated multilayered aquifer
Booker and Rowe (1987)	deep layer with a variable surface concentration, time dependent mass input to the landfill, lumped diffusion coefficient
Chen (1987)	radial flow, radial dispersion, resident and flux concentration distributions with a continuous or a pulse injection
Domenico and Robbins (1987)	multidimensional dispersion, exponential decay source
Galya (1987)	horizontal plane source
Guvanasean and Guvanasean (1987)	radially converging flow field, finite volume of tracer
Chen (1989)	contaminant transport from an injection well into a leaky aquifer
Dillon (1989)	vertical cross section, two-dimensional dispersion with two-dimensional flow
Wexler (1989)	eleven multidimensional dispersion models
Brown and McWhorter (1990)	combined liquid and vapor multiple phase transport by a volatile solvent
Yates (1990)	heterogeneous porous media, distance dependent dispersion
Leij et al. (1991)	three-dimensional semi-infinite porous media

**Table 2-2 Characteristics of models (continued)**

Bosma and van der Zee (1992)	a dual porosity medium with nonlinear sorption in the immobile region and linear sorption in the mobile region
Neville (1992)	multiprocess nonequilibrium
Serrano (1992)	field scale solute transport subject to recharge rate, transmissivity, hydraulic gradient
Yates (1992)	heterogeneous porous media, exponential dispersion function, a linear dispersion model solution
Angelakis et al. (1993)	transient soil gas diffusion, three species of two solutes and a gaseous product in soil
Basha and El-Habel (1993)	heterogeneous media, time dependent dispersion
Ellsworth and Butters (1993)	three-dimensional ADE, three-dimensional dispersion, arbitrary Cartesian coordinates
Fry and Istok (1993)	rate limited desorption and decay
Leij et al. (1993)	three-dimensional dispersion, two side chemical nonequilibrium, two-region physical nonequilibrium
Lerner and Papatolios (1993)	predicting nitrate concentrations in pumped groundwater with zones of different recharge rates
Wallach (1993)	chemical input into the surface water
Zaidel and Russo (1993)	homogeneous unsaturated flow/transport domains
Illangasekare et al. (1994)	three-dimensional flow on two-dimensional apparent macrodispersion
Kool et al. (1994)	steady state solution, infiltration through the unsaturated zone
Leij and Bradford (1994)	three-dimensional dispersion in either a Cartesian or cylindrical coordinate system
Zaidel and Russo (1994)	homogeneous unsaturated medium with ground surface fully open to the atmosphere
Yuan (1995)	multidimensional dispersion, exponentially decay source

## Summary

Analytical solution models from 38 references were reviewed in this study. Analytical solutions to many groundwater contaminant transport areas were developed according to the review. The references cover a great deal of groundwater contaminant

transport areas as shown in Table 2-2. The author is not aware of the availability of analytical solutions of the following groundwater contaminant transport models:

1. models with characteristics of saturated zone, homogeneous medium, multichemical, and multidimensional dispersion,
1. models with characteristics of saturated zone, heterogeneous medium, multichemical, and multidimensional dispersion,
1. models with characteristics of one-dimensional arbitrary flow, multidimensional dispersion, and heterogeneous medium, and
1. models with characteristics of multidimensional flow.

## **2.2 A Review of the Developments in Environmental Modeling Systems**

This section describes general concepts of expert systems and decision-support systems. Reviews of environmental related expert systems and decision-support systems are included in the section. The purpose of the review is to present the recent developments of the contaminant transport modeling on expert systems and decision-support systems and to allow one to compare the approach used in this research with other recently developed approaches.

### **2.2.1 Introduction**

Loucks et al. (1985) evaluated the constraints to the widespread use of environmental modeling and suggested that technical problems, such as poor scientific representations of natural processes, were not as significant as institutional constraints,

such as difficulties people have in interacting with the model itself. They suggested that decision-support systems can increase the use of environmental modeling and enhance technical communication. Hushon (1990) also had the similar conclusion about environmental expert systems. She stated that the environmental expert systems can be expected to increase rapidly for at least several years since there are many problems for which expert systems can provide superior solutions to those available from traditional computer programs. The purpose of this section is to introduce expert systems and decision-support systems for developing environmental modeling systems. Reviews of some environmental modeling computer systems are also shown in this section.

## Expert Systems

The term “Expert Systems” is often used as a synonym for “Knowledge-based Systems”. Expert systems are generally considered to be a branch of artificial intelligence. Expert systems have been defined as “man and machine systems with specialized problem solving expertise.” An expert system relies on a database of knowledge about a particular subject area, an understanding the problems addressed within that subject area, and skill at solving these problems. Expert System development began in the late 1960s. These systems generally sought to solve problems in narrowly defined areas that were well understood by a few experts. The earliest and most published system is MYCIN that was developed at Stanford University to help diagnose and identify drug therapies for treating pulmonary bacterial blood infections.

Hushon (1990) described several ways in which expert systems can be distinguished from traditional data processing systems:

1. perform difficult tasks at expert performance levels,



1. emphasize problem solving strategies,
1. employ a certain amount of self knowledge to evaluate their own inference mechanisms and justify their conclusions,
1. deal with both symbolic and numeric logic,
1. provide for the consideration of incomplete or uncertain data sets, and
1. also follow the human consultation paradigm.

### Decision-Support Systems

The term “Decision-support System” was first used in the business and management world to describe a new class of software for supporting executive decision making instead of computing solutions to everyday operational problems. Gorry and Scott-Morton (1971) developed a framework for contrasting conventional software programs with decision-support systems. Conventional software was characterized by the authors as automation for repetitive, highly structured problems, such as payroll and inventory where there is a well defined procedure for processing information. A decision-support system on the other hand, was defined as software for increasing the effectiveness of a decision maker while he or she performs less structured tasks, typically managerial or planning. These problems are nonroutine and nonrepetitive, and the decision maker usually does not have an established approach to solving the problem. A decision-support system supports, but does not replace, the decision making process of the person solving the problem.

Sprague and Carlson (1982) gave a description of decision-support systems:

1. They tend to be aimed at the less well structured underspecified problems that upper level managers and professionals typically face.

1. They try to combine the use of models or analytical techniques with traditional data access and retrieval functions.
1. They specifically focus on features that make them easy to use by noncomputer people in an interactive mode.
1. They stress flexibility and adaptability to fit changes in the situation and decision making approach of the user.

### Expert Systems vs. Decision-Support Systems

What are the differences between decision-support systems and expert systems?

Newell (1990) made a comparison:

“An expert system is usually applied to narrow and very specific problems. The knowledge an expert has about a particular topic is enormous, and developers of expert systems must stay within a very small area to limit the amount of knowledge that is needed to answer the problem. Expert systems are usually system driven; the computer dictates what the next step is, usually by asking the user a question. Because expert systems are expensive to develop, they usually deal with operational problems that need to be answered frequently by users. In summary, an expert system is an attempt to impose structure on a semistructured problem by trying to extract rules from an expert that have never been recorded or expressed. Decision-support systems are more like a collection of tools and data that are used to solve problems. The problems are often very broad; the user can play with the tools and experiment to find a solution. The decision process is controlled by the user when he or she decides how to apply the different types of tools and data that are available. Generally, decision-support systems are best suited to solving management and

planning domain, instead of routine operational problems. The decision-support systems are not a computerized expert; they are a computerized assistant for the user.”

Grenney (1994) suggested that different practical applications require different subsystem emphasis and characteristics:

“For example, Kraszewski and Soncini-Sessa (1985) refer to their interactive water quality simulation model (WODA) as a “modeling support system” (MSS) although it exhibits attributes similar to models that have been labeled decision-support systems by others. Complex simulation models are being enhanced by the application of rule-based pre and post processors. For example, software to expedite calibration of the widely used storm water management model (SWMM) relies heavily on rule base subsystems to assist the user in selecting parameter values for the main simulation model (Liong, 1991).”

Loucks (1995) suggested that an expert system can be a component in a decision-support system:

“The analysis tools included within a decision-support system will depend on the problems being addressed, on the spatial and temporal resolutions required, and on the skills and judgments of their developers. The tools can include descriptive or proscriptive models of natural, physical, economic, and social processes, geographical information systems, expert systems (knowledge-based or intelligent decision systems that exploit artificial intelligence techniques), executive information (data bases, analysis tools, and interfaces that address the needs of top

managers), and group negotiation support systems (that support teams of cooperative and uncooperative decision makers).”

The viewpoint in this dissertation is similar to Loucks’ viewpoint. Many of knowledge representation methods, problem solving approaches, and software tools of expert systems can be applied in building a decision-support system.

### Components of Decision-support Systems

Davis (1988) suggests that the a decision-support system can be structured into five major components as follows: the database, database management facilities, quantitative modeling component, report generator, and the human interface. The descriptions follow:

1. The database contains the reservoir of information that describes all of the pertinent conditions and characteristics of the problem in question.
1. The data base management component is responsible for getting information to and from the database. The data base management component acts as both a conductor and controller in directing and funneling the flow of information between the database and other parts of the system.
1. The quantitative modeling component provides a mathematical representation of the complex structure and relationship between the various parts of the problem. Quantitative models are necessary in order that a physical system can be depicted and analyzed by a computer. The mathematical formulation embedded within the model provides a descriptive mechanism through which information can be manipulated repeatedly and the decision maker can emulate what will actually take place.

1. The function of the report generator is to consolidate, arrange, sort, and display data in a concise and easily understandable format. The effective report generator allows each user to prescribe what range of information is to be examined and how it will be displayed.
1. The user interface component is responsible for providing all interaction and communication between the computer and the manager. In the ideal decision-support system, the interface component hides the technical complexities and internal mechanism necessary to automate the process.

Loucks (1995) suggests decision-support systems can include the following:

1. optimization and simulation models that find values of decision variables or system performance indicators given inputs and constraints,
1. geographic information systems that permit analyses and displays of spatial data,
1. genetic algorithms that can help in the calibration of physical and chemical process models as well as determine parameter values of system design and operating policies,
1. neural networks that can learn to reproduce results of complex processes and hence serve as “black boxes” for those processes,
1. expert or knowledge-based systems that can process rules and symbols to draw conclusions principally through logical or plausible inference sequences and that can provide users with an explanation of how those conclusions were reached, and
1. statistical and graphical packages for data analyses and display.

This dissertation adopts the viewpoint of Grenney et al. (1994) that components of decision-support systems depend on the problem being solved, on the size of the

problems being addressed, on the preference of developers, and on the resources available to and the requirements of the end users. The author expects that decision-support systems' input and output data can be in a wide variety of forms, ranging from tables to text to static and dynamic time or space series graphs, to static and dynamic pictures and displays on maps to sound and video, and even to multidimensional virtual reality. The researcher also believes that decision-support systems must be able to run on personal computers, workstations, and any other computer platforms.

### **2.2.2 Environmental Modeling Systems**

#### **Reviews**

Newell et al. (1990) developed OASIS that integrates four groundwater contaminant transport models, a database, and Macintosh HyperCard graphical user interface. The system was targeted at two groups of users: current modelers who need more efficient interfaces and data management tools, and people who are not using models now because the modeling process is too involved and requires specialized knowledge. The OASIS system is the first groundwater contaminant transport modeling system that has a user-friendly graphical user interface.

McClymont and Schwartz (1991) developed the Expert ROKEY system that is a combination of a contaminant transport model (ROKEY), a knowledge-based system (EXPAR), and three other utility programs. EXPAR, the focus of this work, is partitioned into two levels. The top level is a preprocessor with a built in database for ROKEY. This level consists of a program control unit, a global database, and a set of computer forms. The bottom level consists of elaboration programs and assistance

programs. Elaboration programs provide supporting information for each parameter and brief tutorials for the mass transport processes included in the model. Assistance programs are individual knowledge-based systems that provide help to determine parameter values. One evaluation was conducted to test the usefulness of EXPAR. The exercise tested the ability of 18 participants to simulate the distribution of three organic compounds at a hazardous waste site near Ottawa, Canada. From the results, the embedded knowledge in the EXPAR system appeared to provide valuable assistance in modeling, and the system itself met the authors' expectations in terms of the user friendliness and robustness. The ROKEY system is one of the first environmental modeling systems that provides a parameter assistant program to help users in solving a contaminant transport problem.

Rozenblit and Jankowski (1991) proposed an approach to simulation modeling of natural systems in the context of water quality modeling in streams affected by point source pollution. In the approach presented in their work, a stream or its section is viewed as a collection of components, i.e., stream segments. The structure of a stream is its segments and their couplings. For each stream segment, a single constituent model describing processes affecting the segment's water quality is defined. Models are coupled in a hierarchical manner. The hierarchical, modular model specification results in a stream model comprised of a finite number of subsegment models. Fundamental theoretical concepts supporting such a specification are described. A prototype simulation modeling environment to support prediction of water quality in streams has been implemented and tested. The approach differs from other natural systems

modeling frameworks in its modular model specification facilities, high degree of model reusability and support for model selection and coupling.

Booty et al. (1994) presented RAISON, Regional Analysis by Intelligent Systems ON a microcomputer, system that is a multimedia environmental data analysis tool kit that contains a fully integrated database management system, spreadsheet, geographical information system (GIS) graphics, statistics, modeling, expert system modules and a programming language that allows the user to create specialized applications. Authors provided a special application of the system for carrying out environmental impact assessments for point source discharges, with an example of assessment of acid mine drainage in Ontario, Canada.

Burde et al. (1994) introduced an expert system SAFRAN that has been developed to derive decision related conclusions from a tuple of attributes assigned to each area of a digital map. The user interface, designed to fit the needs of environmental planners, allows to enter rules defining relationships among the attributes. All of the needed data are managed by a GIS, to which SAFRAN has an interface. The expert system SAFRAN was used to evaluate the impact of atmospheric acid formers on soil and groundwater quality in forestal ecosystems.

Calori et al. (1994) presented a prototype of a knowledge-based tool, FRAME, to support the user in choosing the appropriate air pollution model for his particular scenario. The system integrates a relational database for the management of all classes of information and a rule-based expert system for the explication and help phases. In order to assemble the knowledge base of the system and to give the most complete picture of the current state of the art, an extensive literature review has been performed,



followed by a conceptual classification of the set of possible scenarios. The end user can access the information about the models in different ways, depending on his expertise about the application domain.

Crowe and Mutch (1994) presented EXPRES, EXpert system for Pesticide Regulatory Evaluations and simulations, that has been developed to assist those who are knowledgeable, but not proficient, in the theory of pesticide transport in the subsurface or in the use of pesticide assessment models with a means of assessing the potential for pesticides to contaminate groundwater. The EXPRES system is intended to be used as a screening tool by nonexperts who need to evaluate the potential for pesticides to contaminate groundwater. EXPRES combines a knowledge-based system, a graphically based user system interface, extensive geographical and pesticide data bases, and three existing pesticide assessment models (LP/LI, PRZM, and LEACHM). Based on the user's available data, objectives of the assessment and time constraints, EXPRES selects the most appropriate model, assists the user in the construction of an input data set, initiates an assessment, and aids in the interpretation of the results of an assessment model. Specific assistance in the Construction of the input data set includes providing pertinent data for characterizing a site or a pesticide from its data bases, assisting the user to respond to a prompt from EXPRES, aiding the user in estimating missing values for pesticide or site parameters, and ensuring the integrity of the input data set.

### Comparisons of Contaminant Transport Modeling Systems

OASIS is a decision-support system to guide a user setup a contaminant transport problem that comes with several analytical solution models and a numerical solution model. OASIS is only available on Apple Macintosh platform.

ROKEY/EXPAR is a decision-support system to guide a user in setting up a contaminant transport problem. The system contains one numerical model. ROKEY/EXPAR is a Microsoft DOS platform program. Both OASIS and POKEY/EXPAR systems do not provide guidance in choosing an appropriate groundwater contaminant transport model. Neither system is easy for users to maintain and upgrade.

EXPRES selects the most appropriate model, assists the user in the construction of an input data set, initiates an assessment, and aids in the interpretation of the results of an assessment model. EXPRES contains three pesticide assessment models (LP/LI, PRZM, and LEACHM). EXPRES's purpose is to solve a specific pesticide contaminant problem rather than to choose a best model for solving general contaminant transport problems.

FRAME is a knowledge-based tool for choosing the appropriate air pollution model for a particular scenario only. FRAME is a UNIX platform application.

None of the systems can be used as a guidance tool to choose appropriate groundwater contaminant transport models for a particular scenario, although the FRAME system is conceptually close. None of the systems can be used via the Internet.

## Summary

Table 2-3 is a summary of the systems reviewed in this section.

**Table 2-3 A list of environmental modeling systems**

<b>System</b>	<b>Authors</b>	<b>Description</b>
OASIS	Newell et al. (1990, 1991)	OASIS : a graphical decision-support system for groundwater contaminant modeling
ROKEY/ EXPAR	McClymont and Schwartz (1991)	Embedded knowledge in software: a system for contaminant transport modeling
DEVS-Scheme	Rozenblit and Jankowski (1991)	An integrated framework for knowledge-based modeling and simulation of natural systems
FRAME	Calori et al. (1994)	FRAME, a knowledge-based tool, in choosing the appropriate air pollution model for a particular scenario
EXPRES	Crowe and Mutch (1990, 1994)	Expert system for assessing the migration and transformation of pesticides in the subsurface
SPEC	Grenney et al. (1994)	Knowledge-based system for evaluating in stream habitat
RAISON	Booty et al. (1994)	Expert system for point source water quality modelling
SAFRaN	Burde et al. (1994)	S A F Ra N : environmental impact assessment for regional planning

## **2.3 A Review of Related Resources on the Internet**

This section describes the concept of the Internet and Internet programming and available Internet-based resource related to contaminant transport modeling on the Internet.

### **2.3.1 Introduction**

The purpose of this section is to introduce the concepts of using the Internet as the development platform for the modeling guidance system. Brief descriptions of some groundwater and environmental related resources on the Internet are presented in this section.

## The Internet and the World Wide Web

The Internet is the catch-all word used to describe the numerically huge world wide network of computers. The word "Internet" literally means "network of networks". The Internet started with the Advanced Research Projects Agency Network (ARPANET), but now includes such networks as National Science Foundation Network (NSFNET), and thousands of others. On any given day it connects roughly 15 million users in over 50 countries. The World Wide Web, Web or WWW, is mostly used on the Internet; they do not mean the same thing. The Web refers to a body of information, an abstract space of knowledge, while the Internet refers to the physical side of the global network, a giant mass of cables and computers (Malkin and Marine, 1991). NSFNET statistics (Hughes, 1993) shows that from January to August 1993, the amount of network traffic (in bytes) across the NSF's North American network attributed to web use multiplied by 414 times. The Web can be thought as the graphical Internet service that provides a network of interactive documents and the software to access them. It is based on documents called pages that combine text, pictures, forms, sound, animation, and hypertext links called hyperlinks. To navigate the Web, users move from one page to another by pointing and clicking on hyperlinks in text or graphics. The Web has been used as a helpdesk, marketplace, art gallery, library, community center, school, publishing house, and many other uses (Microsoft, 1997).

### A Hypothetical Case

A hypothetical example is shown in the following paragraph to show how useful the Internet could be in groundwater contaminant transport modeling.

John is a hydrogeologist working on a construction project for a small village. The construction damages an underground storage tank that contains organic liquids at 10 AM this morning. John has reasons to believe that the contaminant plume is moving toward a 10-acre shrimp pond that is located 100 feet east of the leaking underground tank. John needs to find out how long will this plume reach the pond and kill all shrimp. The only tool he can find is a Web TV in a local Radio Shack. John heard about a web site that contains many analytical solutions for groundwater contaminant transport modeling. So he uses the Web TV to connect to the web site in no time. John inputs requests via a user interface of the web site. His requests are analyzed by a guidance engine. The guidance engine queries the database on the web site, finds an appropriate model, activates the model, gets results from the model, and returns the results to the interface. So John gets information what he is looking for - shrimp in the pond will surely die in 4 hours.

### Advantages of the Internet-based System

Advantages of the Internet-based modeling guidance system described in this hypothetical case are as follows:

1. Location transparency. A web page on a web server may be accessed by any client machine running a web browser, anywhere in the world.
1. Client-platform independence. Because only the browser resides on the client side, the Internet-based system may be accessed from any client machine with an Internet ready browser.
1. Instantaneous deployment of system upgrades. Under non-Internet modeling guidance systems, software upgrades must be “pushed” to each user’s machine,

usually at considerable expense in terms of time and money. Under the Internet-based system, all database, guidance facilities, and models are located on the server. Software upgrades only involve the server computer.

### **2.3.2 Concepts of HTML, CGI and Java**

This section explains basic concepts of HTML, CGI, and Java that are heavily used in the system.

#### **HyperText Markup Language (HTML)**

The basic element of the Web is a page. Pages are written in an evolving language called HyperText Markup Language, or HTML. HTML documents are composed of plain text and special text, called tags. Tags are instructions to the web browser to do special functions with the associated plain text. The major advantages of using HTML are its universal appearance under different platforms and its plain text format:

1. Universal appearance. The appearance of a web page under Netscape Navigator 3.0 for Macintosh looks similar to the appearance of the web page under Microsoft Internet Explorer for Windows 95 or other browsers. A web developer does not have to consider different constraints for different platforms.
1. Plain text format. A HTML web page is stored in a plain text format (ASCII). It is very easy for a web developer to edit or modify a web page using any text editor.

#### **Common Gateway Interface (CGI)**

HTML has a built-in gateway, Common Gateway Interface (CGI), that allows HTML programmers to call a program written in any language they want to use. A

gateway is a connection to the external operating system. CGI gives programmers a way for HTML web pages to call external programs and get back the results. The following list explains the process Behind CGI. Several things must occur for a CGI program to execute successfully:

1. The user calls a CGI program by clicking on a link or by pushing a button.
1. The web browser contacts the web server asking for permission to run the CGI program.
1. The web server checks the configuration and accesses files to make sure the requester is allowed access to the CGI program.
1. The web server checks to make sure the CGI program exists.
1. If it exists, the CGI program is executed.
1. Any output produced by the CGI program is returned to the web browser.
1. The web browser displays the CGI output.

CGI can be used for manipulating a web server's database from a client computer. A popular combination of CGI tools is by using Structured Query Language (SQL) via Microsoft ODBC to access a Microsoft Access database file. In this method, ODBC and database are located in the server computer. SQL programs can be either predefined by programmers or created by end users. The major advantage of this method is that end users can manipulate the database in the way they want.

## Java

Java is a language developed by Sun Microsystems that allows World Wide Web pages to contain code that is executed on the browser. It is a general purpose

concurrent class based object oriented programming language, specifically designed to have as few implementation dependencies as possible.

The major advantage of Java over other programming tools (such as Microsoft ActiveX, Visual C++, Visual Basic) is that Java is platform independent. Java allows a single application to run on multiple platforms. In contrast, ActiveX allows routines written in multiple languages (C, C++, Basic, and so on) to coexist within a single application on a single platform (Microsoft Windows running on an Intel CPU). Java allows application developers to write a program once and then be able to run it everywhere on the Internet. Unlike a CGI program, a Java applet runs on the user's (client's) machine.

### Building a Decision-Support System in HTML, CGI, and Java

As mentioned in the previous section, components of a decision-support system depend on the problem being solved (Grenney et al., 1994). The components of an Internet-based decision-support system could include a graphical user interface, database, database management facilities, and quantitative modeling component. All components except the database can be created by using HTML, CGI, and Java. The database component can be generated by using Microsoft Access or other database programs. The combination of HTML, CGI, and Java is a capable development toolkit to develop a decision-support system on the Internet.

### **2.3.3 Reviews of Internet Resources**

Sharing of computation resources over the Internet is becoming common in groundwater contaminant transport modeling. There are many web sites that contain



useful information regarding groundwater contaminant transport modeling. In this section, these web sites were classified to four categories: informative web sites, commercial web sites, FTP sites, and interactive groundwater modeling web sites.

### Informative Web Sites

Informative web sites contain information regarding groundwater research projects or/and useful links to other Internet groundwater resources. The following are some examples:

1. Dr. Alexander H. D. Cheng's WaterEcoNet web site at <http://www.ce.udel.edu/faculty/cheng/wenet/program.html> contains information regarding some public domain groundwater contaminant transport software programs and their specifications.
1. Groundwater.Com at <http://www.groundwater.com> is the Internet domain of Bannister Research and Consulting. It contains several online resources relating to groundwater.
1. International Ground Water Modeling Center, IGWMC, that is an internationally oriented information education and research center for groundwater modeling has a web sit at <http://www.mines.edu/igwmc>. IGWMC supports and advances the appropriate use of quality assured models in groundwater resources protection and management.
1. Pacific Northwest National Laboratory's Environmental Technology Division's Hydrology web site at <http://terrassa.pnl.gov:2080/hydrology/software.html> contains information regarding hydrology software and computer modeling programs.

## Commercial Web Sites

Commercial web sites contain commercial Internet-based groundwater related modeling software. Two examples are shown as follows:

1. Environmental HydroSystems web site at <http://hydrosystems.com> is maintained by Environmental HydroSystems, Inc. (EHI) that specializes in the open analysis of hydrologic and hydraulic systems and in the open development and application of scientific software and hardware systems to support such analysis. One of their products is an Internet-based groundwater and porous media modeling and environmental software server. This server is provided to promote the dissemination of public domain and proprietary porous media and environmental software and supporting information.
1. Horizontal Technologies, Inc. web site at <http://www.horizontal.com> is maintained by Horizontal Technologies, Incorporated (HTI) that is a provider of trenched horizontal systems in the U.S. This web site has a online Java-powered horizontal well design system.

## FTP Web Sites

FTP web sites contain non-Internet based software that can be downloaded by users via the Internet. An example is the GWRP web site that is basically an FTP site decorated with HTML pages. There are many of these web sites on the Internet. The following nine web sites are typical:

1. USEPA CSMOS web site at <http://www.epa.gov/ada/csmos.html> is maintained by Center for Subsurface Modeling Support (CSMOS) that provides a

source for publicly available groundwater and vadose zone modeling software and services.

1. U.S. Geological Survey Water Resources Applications Software Page at [http://water.usgs.gov/software/ground\\_water.html](http://water.usgs.gov/software/ground_water.html) contains many public domain groundwater software and source codes.
1. GWRP web site at <http://gw2.cciw.ca/gwrp> is maintained by the Groundwater Remediation Project of the National Water Research Institute of Environment Canada, and is located at the Canada Centre for Inland Waters in Burlington, Ontario. This web site has a collection of groundwater modeling and analysis software for download.
1. Waterloo Hydrogeologic at <http://www.golden.net/~whs/index.html> is maintained by Waterloo Hydrogeologic that is a company in developing and distributing applications of numerical and analytical modeling techniques for groundwater flow and contaminant transport interpretation. This web site has a few collections of groundwater modeling software for sell.
1. Center for Computational Sciences at Oak Ridge National Laboratory (ORNL) has a web site <http://www.ccs.ornl.gov/HomePage.html> that contains information regarding environmental modeling and remediation. There is a Groundwater Contaminant Transport (GCT) code that is a fully three-dimensional parallel code for groundwater contaminant transport. This site also has two groundwater transport movies that demonstrates how contaminant flow moves in subsurface.

1. United States Salinity Laboratory (USSL) that is a National Laboratory for basic research on the chemistry, physics, and biology of salt affected soil plant water systems has a web site at <http://www.usssl.ars.usda.gov>. This site has some models and database available for download.
1. Computer Oriented Geologic Society (COGS) has a web site at <ftp://ftp.csn.org/COGS/Hydrology/00-index.txt> that contains several public domain hydrogeology software.
1. University of Manitoba Groundwater Shareware Database and FTP site at [http://www.umanitoba.ca/geo\\_eng/Groundwater](http://www.umanitoba.ca/geo_eng/Groundwater) that has several groundwater software and database.
1. Intera Inc.'s software FTP site at <http://www.intera.com/link/lnksoft.html> has several groundwater models and well test analysis programs.

### Interactive Groundwater Model Web Sites

Interactive groundwater model web sites contain groundwater contaminant transport Java model applets. Users can use Java model applets via the Internet. So far, the ANTS web site is the only web site that the author is aware of with this capability. The URL address of ANTS is <http://cleveland1.cive.uh.edu/index.html>.

## CHAPTER 3 CONCEPTUAL FRAMEWORK

### 3.1 Introduction

This dissertation presents a new approach to model groundwater contaminant transport problems with potential applicability to other areas of natural resources modeling. The approach in this research differs from conventional approaches in that a model is a result of a decision making process rather than an object for manipulating. In this approach, a user makes a series of decisions through a guidance module to find an appropriate model.

The fundamental assumption in this study is that any given groundwater contaminant transport model can be represented as a set of property keywords. By matching a contaminant transport problem to model keywords, an appropriate model for the given problem can be found.

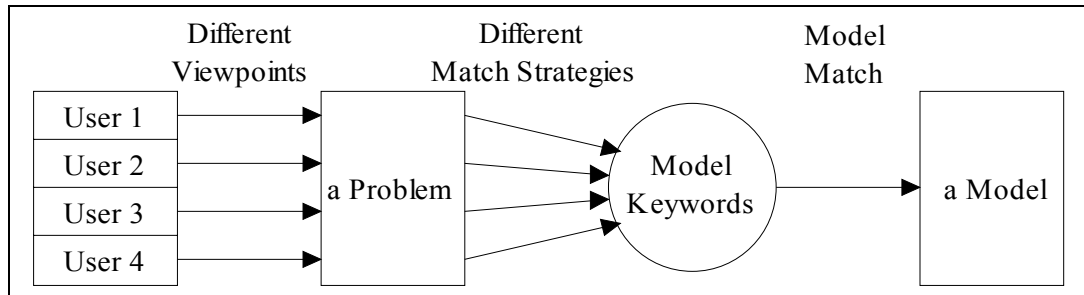
The assumption begs two questions: How to characterize a model as a keyword set? How to match a given problem to model keywords? To answer these two questions, a three-step approach was used.

1. Potential user classification: The degree of knowledgeableability of domain experience can affect the design of the system, where the word “domain” represents the field of groundwater contaminant transport modeling in this study. An expert of the domain field approaches a contaminant transport problem differently than a domain novice does. The way the expert user matches a problem to a model is usually superior to

the way the novice does. It is difficult to design a single model search module to meet the needs of all potential users. It is necessary to identify and classify the potential users of the system.

1. Model characterization: The link between a scenario and a model is a set of model keywords. Model keywords for each model can be generated by classification.
1. Match strategy development: Once the potential users of the system are classified into different user groups, appropriate match strategies can be applied to meet the needs of different user groups.

Figure 3-1 depicts users of different groups having different viewpoints on a problem. They would likely use different approaches to find appropriate model keywords that can represent the problem. Once appropriate keywords are chosen, the system will try to select an appropriate model for the problem.



**Figure 3-1 System concepts**

The potential user classification is described in the second section of the chapter. The concept of model characterization is described in the third part of this chapter. Match strategy development is presented in the last section of this chapter.

## **3.2 Potential Users Classification**

### **3.2.1 Contaminant Transport Modeling Survey**

#### Survey Overview

A survey was conducted on December 1, 1997. The purpose of this survey was to understand the computer skills and groundwater contaminant transport modeling knowledge of the potential users. A questionnaire was designed and intended for the general public and expert users who have been interacting with groundwater contaminant transport problems (industrial pollution cases, laboratory experiments, class work, etc.). The questionnaire was completed by a group of environmental engineering professors and graduate students at the University of Houston.

#### Results of the Survey

The questionnaire consisted of four categories with total of 45 questions. The four categories are general demographics, technology demographics, domain knowledge, and a question specified for the ANTS project. There were 17 respondents to this survey. Some respondents did not answer all questions. A copy of the questionnaire and the statistics of the survey are attached in Appendix B. The results of the survey are presented in the following:

1. General Information: A majority of the respondents were environmental engineering full time graduate students in the University of Houston. Most respondents obtained their knowledge of groundwater contaminant transport from classrooms rather than

from their work experience. All respondents had less than three years study or work experience in the domain field.

1. Computer Related: The largest percentage (41.2%) of the respondents used the computer 10 to 20 hours per week with 29.4% using it more frequently and 29.4% less frequently. A majority of respondents used PCs and the Microsoft Windows operating system with some using Macintosh computers and Mac OS. Most users had ability to use Microsoft Excel as a computation tool and had experience in writing computer programs. Most respondents frequently connected to the Internet. Netscape Navigator was the most used browser (76.5%) in this group with Microsoft Internet Explorer used by 17.6% of the respondents. Many (41.2%) users did not know if their browser was Java-enabled or not. A majority (76.5%) of the respondents used Internet search engines. Most respondents believed that they were above average in using computers, the Internet, and spreadsheet programs. Most users were not comfortable in coding computer programs, using database, and writing SQL programs.
1. Contaminant Transport Modeling: About one-half of (46.7%) the respondents believed that they had no problem in describing a model's governing equation, initial conditions, boundary conditions and source conditions. Most respondents had solved a groundwater contaminant transport problem by using analytical solutions or approximate solutions. About two-thirds of the respondents had not solved a groundwater contaminant transport problem by using numerical solutions (such as FDM/FEM). More than one-half of the respondents had solved a groundwater contaminant transport problem without knowing what method had been applied.



Most respondents believed that they had no problem identifying a model flow, dispersion, and source conditions. Only one person was able to identify the difference between the Dirichlet (the first type) and Cauchy (the third type) inflow boundary conditions. Most respondents were not familiar with several popular groundwater and contaminant transport modeling programs. One-half of the respondents had difficulties solving a two-dimensional dispersion, unidirectional flow groundwater contaminant transport model that has a decaying source. One-third of the respondents did not know if a contaminant transport model could produce a reasonable result or not. More than one-half of the respondents believed that their domain knowledge was above average.

1. ANTS Related: More than one-half of the respondents (52.9%) thought an Internet-based contaminant transport modeling system would be useful. The rest of the respondents did not know if the system would be useful or not.

## Summary and Result Analysis

The summary of the survey is shown in the following list:

1. A majority of the users had good computer skills and Internet browsing experience, but not good in writing their own computer programs.
1. A majority of the users in the survey population learned their domain knowledge from school.
1. A majority of the users had experience in using analytical contaminant transport models, but not numerical models. They had difficulty in solving complicated problems.

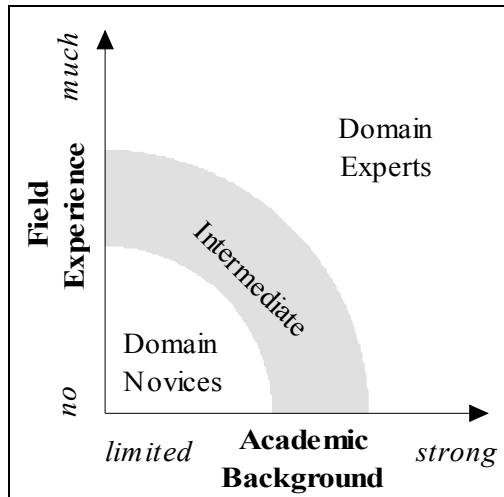
1. Most users thought the ANTS system was useful in solving groundwater contaminant transport problems.

Item 1 suggests that even the frequent computer users did not like to create their own programs. Items 2 and 3 suggest that a majority of the respondents were relatively inexperienced in the field of groundwater contaminant transport modeling. Item 4 suggests that an Internet-based modeling guidance system should be useful in the field of groundwater contaminant transport modeling. From the results of the survey, the author was confident that the concept of the ANTS system would be useful in the field of groundwater contaminant transport modeling.

### **3.2.2 Classification**

The potential users of the system are mainly civil engineers, environmental engineers, hydrogeologists, government environmental agents, local environmental regulators, researchers, and students. The potential users range from being domain novices and computer novices all the way to domain experts and computer experts.

The potential users can be classified into three domain knowledge groups as follows: domain experts, domain intermediate users, and domain novices, as shown in Figure 3-2.



**Figure 3-2 Domain knowledge classification**

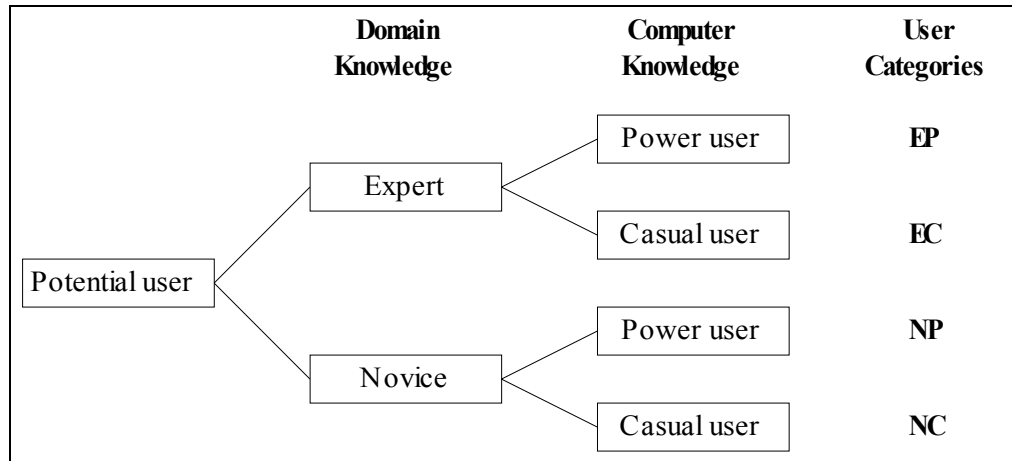
To simplify the design of the system, only two domain user groups were considered in this research:

1. The expert users have academic background and much field experience in groundwater contaminant hydrology.
1. The novice users have limited academic background and limited or no field experience in groundwater contaminant hydrology.

The potential users can be divided into two computer skill groups as follows:

1. The casual users have basic knowledge of computer operating systems (such as Microsoft Windows) and web browsers.
1. The power users have experience in computer programming (such as HTML, Java, FORTRAN, or BASIC) or macro programming (such as the Excel macro).

To explore the needs of the potential users, the users were categorized to four categories as shown in Figure 3-3:



**Figure 3-3 The user classification**

1. Category EP: The EP users are both experienced engineers and power computer users. They are likely to know how to apply an appropriate model to a groundwater contaminant transport problem. They can solve a problem using any computer tool (such as Microsoft Excel). They can even use a scientific calculator to predict the result of a groundwater contaminant problem. A popular Hewlett Packard 48 series calculator is probably good enough for them to solve the problem.
1. Category EC: The EC users are both experienced engineers and casual computer users. They are likely to know how to apply an appropriate model to solve a groundwater contaminant transport problem. They may have problems using an unfamiliar computer program.
1. Category NP: The NP users are both novice engineers and power computer users. They usually do not know how to apply an appropriate model to a groundwater contaminant transport problem. They have no problem in using an unfamiliar computer program.

1. Category NC: The NC users are both novice engineers and casual computer users. They usually do not know how to apply an appropriate model to a groundwater contaminant transport problem. They have problems to use an unfamiliar computer tool.

From the results of the user survey, a majority of the potential users belong to the NC users that are both novice engineers and casual computer users.

### **3.3 Model Characterization**

#### **3.3.1 Introduction**

A contaminant transport model can be described by its properties, such as medium type, flow type, dispersion type, initial conditions, boundary conditions, source type, and other properties. The combination of medium type, flow type, initial conditions, boundary conditions, and other properties can be considered as a model's signature, or a model property keyword set. As an example, the 1DWX030 model (Wexler, 1989) that has a semi-infinite aquifer with the Dirichlet type inflow boundary condition can be described as a property set shown in Table 3-1. Similarly, the 1DVG05B model (van Genuchten and Alves, 1982) can be described as a property set in Table 3-1.

**Table 3-1 A comparison of the properties between two models**

<b>Property</b>	<b>1DWX030</b>	<b>1DVG05B</b>
Flow	one-dimensional principal directional	one-dimensional principal directional
Medium	homogeneous	homogeneous
Zone	saturated	saturated
Dispersion	one-dimensional constant	one-dimensional constant
<i>Inflow boundary</i>	<i>Dirichlet</i>	<i>the first type</i>
Outflow boundary	semi-infinite	semi-infinite
Initial condition	constant distribution	constant distribution
<i>Source type</i>	<i>pulse</i>	<i>continuous constant</i>

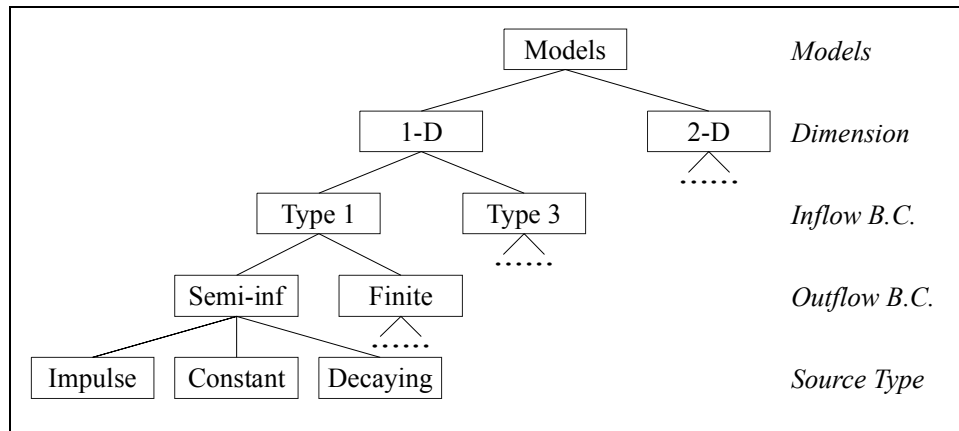
By comparing two model property sets shown in Table 3-1, one may conclude that these two models are different because of the differences in their inflow boundary conditions and source types. However, the *Dirichlet* inflow boundary is the same as the *first type* inflow boundary. The *Pulse* source in the 1DVG05B model can be used as a *continuous constant* source. In other words, the layout of the 1DWX030 model is the same as the 1DVG05B model layout. Both models were designed to solve a similar problem. They can be considered functionally the same model. Some other confusing property keywords are as follows: the terms *outflow boundary* and *lower boundary* have the same meaning; the terms *decay* and *production* are different only in their signs. The confusion of similar keywords could be a problem in identifying a set of property keywords to a model. To overcome this problem, a model has to pass through a classification process before being added to the model library.

### **3.3.2 Model Classification**

The task of finding a keyword set for a particular model can be considered as a classification problem. Classification is a problem common to many domains, such as

botany and zoology. The result of a classification usually is a hierarchical organization (a hierarchical tree), in which subclasses possess the discriminating features of their superclasses, and classes which are ‘siblings’ in the hierarchy are mutually exclusive with respect to the presence or absence of some set of features (Jackson, 1990).

A sample of a model hierarchical tree is shown in Figure 3-4. There are five property classes in the sample hierarchical tree: *Models*, *Dimension*, *Inflow B. C.*, *Outflow B. C.*, and *Source Type*. Each property class usually has more than one element. For examples, the *Dimension* class has two elements: one-dimensional and two-dimensional dispersions. In this sample tree, the *Models* class is the superclass of the *Dimension* class. The *Dimension* class is the subclass of the *Models* class.



**Figure 3-4 A sample hierarchical tree**

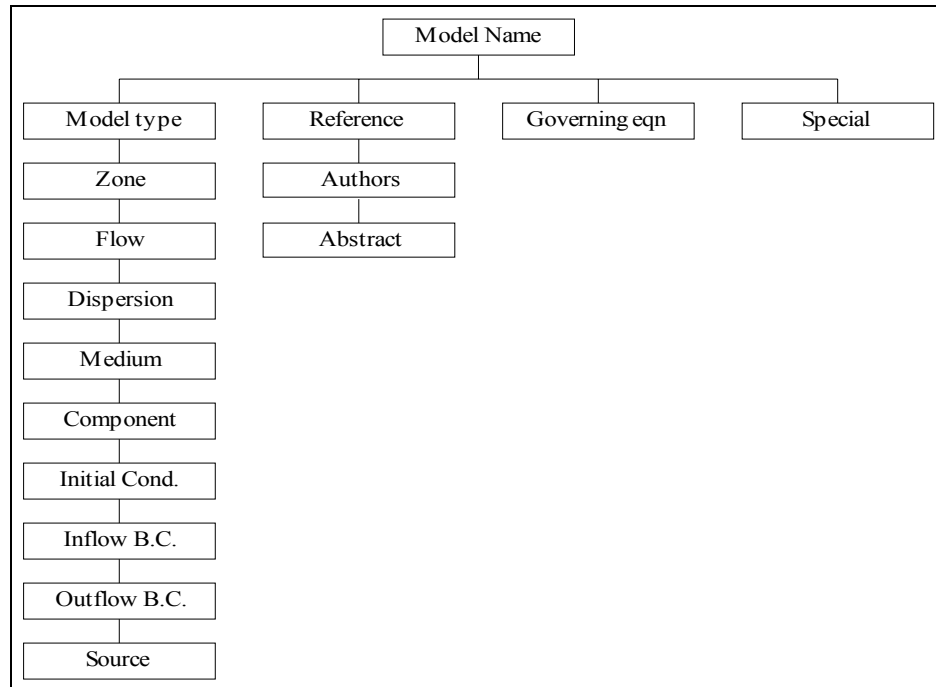
Every model has its own property keyword set that contains 16 elements. Each element belongs to a particular property class. Descriptions of the classification property classes are shown in Table 3-2.

**Table 3-2 The classification property classes**

<b>Property Class</b>	<b>Description</b>
Model Name	name of a model in the model library
Reference	reference of the model
Authors	authors of a model
Abstract	abstract from the model reference
Governing equations	governing equations of a model
Special	special characteristics of a model
Models	type of model
Zone	type of flow zone
Flow	type of groundwater flow field
Dispersion	dispersion dimension
Media	homogeneous or heterogeneous medium
Component	single component or multicomponents
Initial condition	initial concentration distribution
Inflow boundary condition	boundary conditions in the inflow (upper) end
Outflow boundary condition	boundary conditions in the outflow (lower) end
Source type	contaminant source type

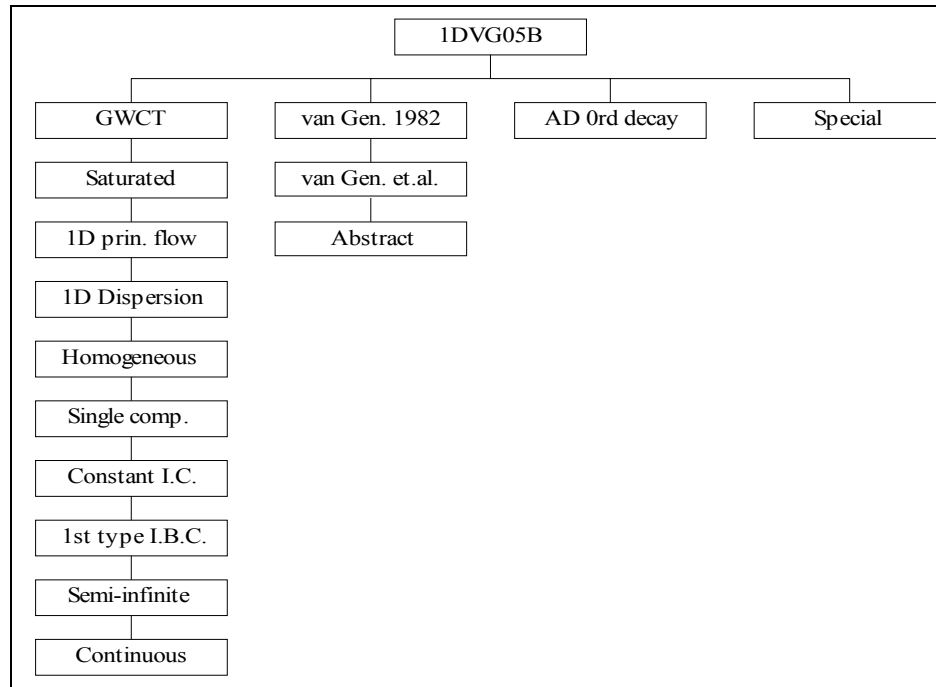
The data structure of the property classes is shown in Figure 3-5. The *Model Name* class is the root class that has four subclasses: *Model type*, *Reference*, *Governing Equations*, and *Special*. The *Reference* class has a *Authors* subclass that has a *Abstract* subclass. The *Governing equations* and *Special* classes do not have any subclass. The *Model* class type has nine layers of subclasses. The maximum depth of the data structure is 11.





**Figure 3-5 The data structure of the property classes**

All models in the system were classified using the property classes given in Figure 3-5. To avoid the confusion problem, similar keywords were identified at this step. There are more than 100 model property sets stored in the ANTS model database. Figure 3-6 is the property keyword set of the 1DVG05B model.



**Figure 3-6 The property keyword set of the 1DVG05B model**

## 3.4 Match Strategies

### 3.4.1 Overview

Hypertext, database, and scenario match strategies were developed in the system to satisfy the needs of the potential users. The concepts of the match strategies are shown in this section. The detailed designs of the match modules are described in Chapter 5.

The hypertext strategy uses the link feature of the hypertext. A hypertext is basically the same as a regular text that can be stored, read, searched, or edited with an important exception: a hypertext contains links within the text to other documents. The

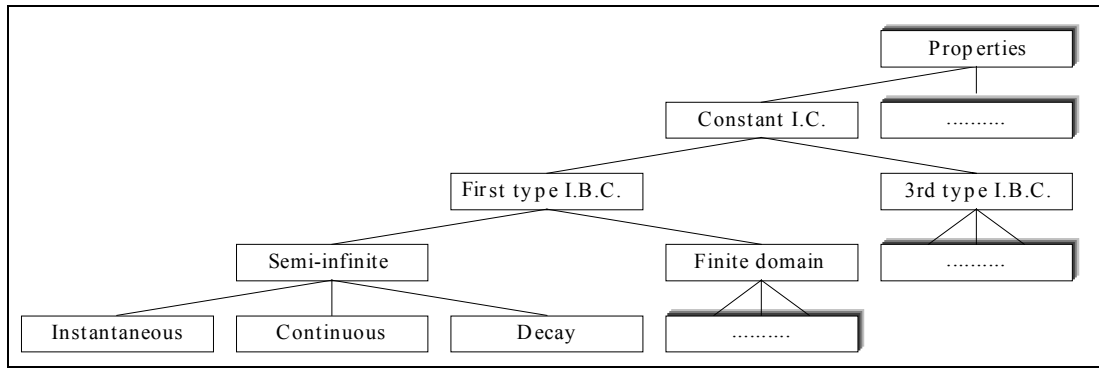
link feature of the hypertext can be used as a two-way pointer to connect a models and its properties. The hypertext strategy was applied on the hierarchy module.

The database strategy uses SQL as an indirect tool to manipulate a model database to get results. This strategy was applied on the ranking module and the querying module.

In the scenario strategy, a user can generate a scenario of the problem from a number of scenario parts. Once a scenario is created, the system will find a model to match the scenario. The strategy was applied to the scenario module.

### **3.4.2 Hypertext Strategy**

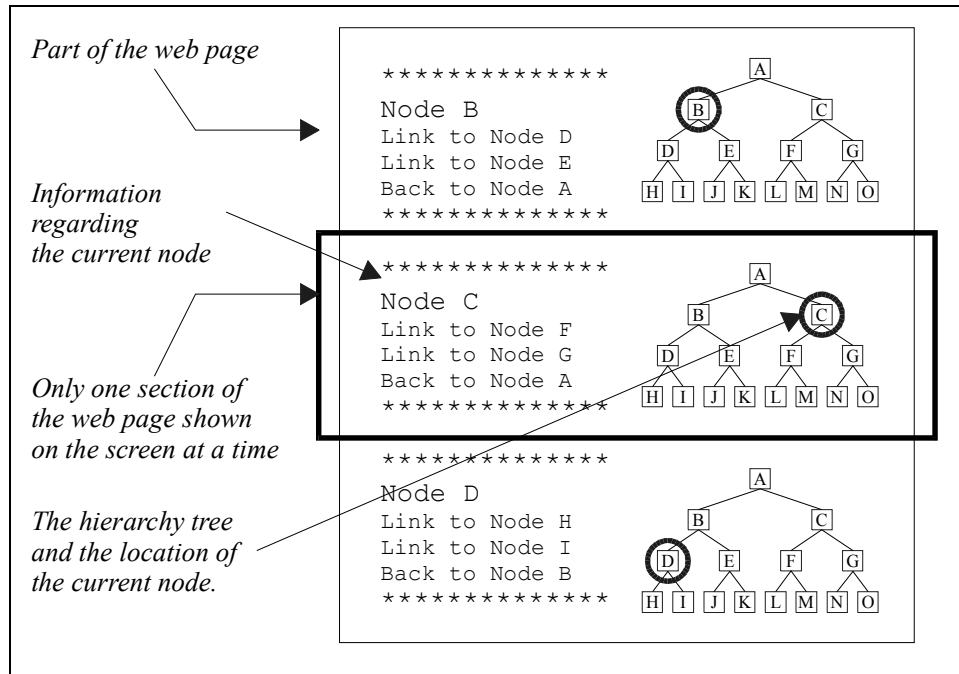
A hierarchy module is a combination of a hierarchical tree and its elements. The basic idea is that a model is located in the deepest level of the tree. In a hierarchy module, a user travels from the top of the tree to the bottom of the tree. The user has to make a decision to advance to the next layer. The final result of the decision-making process is a model. Figure 3-7 is a fraction of a hierarchy module. In order to find a model, a user has to make three decisions in this example. By choosing *First type I. B. C.*, *Semi-infinite*, and *Continuous*, the user should find a model that meets these three conditions.



**Figure 3-7 A fraction of a hierarchy module**

The hierarchy modules are more useful to experienced hydrogeologists than to inexperienced engineers. The experienced hydrogeologists usually have clear ideas in analyzing a case, so they are more likely to make the right decisions to find an appropriate model.

If users are not well versed in the domain, they may have trouble seeing the *big picture* of what the system contains and addresses. To solve this problem, a parallel hierarchy scheme aids in building a hierarchy module. As shown in Figure 3-8, a web page has many sections. Each section includes information regarding a particular node (model) and a synchronized hierarchical tree. Only one section is shown on the screen at a time. The relative location of this section (node or model) to the hierarchy scheme can be found in the synchronized hierarchical tree.



**Figure 3-8 An illustration of a parallel hierarchy web page**

There is one drawback in a hierarchy module. The problem is the travel length problem. As shown in Figure 3-9(a), the path of the binary tree from the H node to the O node is

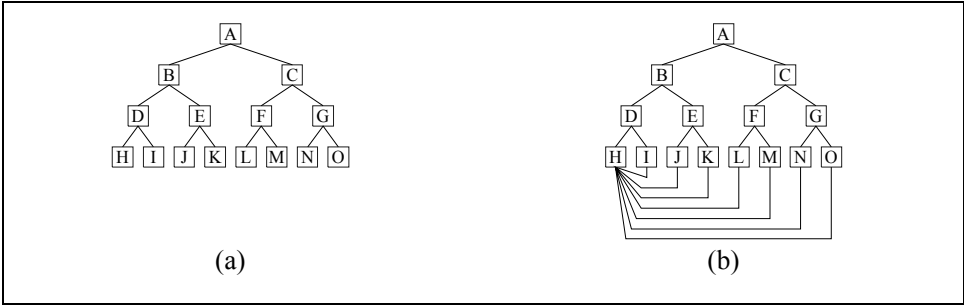
$$[ H \rightarrow D \rightarrow B \rightarrow A \rightarrow C \rightarrow G \rightarrow O ]. \quad (3-1)$$

The length from the H node to the O node is 6. Let's say a user is at the H node and want to go to the O node. Under a hierarchy module, the user has to travel six lengths to reach the O node. In a binary hierarchical tree that contains N nodes in the deepest level, the travel length between two nodes could be as long as

$$[ 2 \times \text{LOG}_2(N) ]. \quad (3-2)$$

A user may be lost in the system even with the present of a synchronized hierarchical tree. This problem can be solved by constructing the hierarchy module as a wrapped

hierarchical tree. In a wrapped hierarchical tree, all nodes in the deepest level are linked. In this case, there will be a direct link between the H node and the O node. So the length from node H to node O will be reduced to 1. Figure 3-9(b) is an illustration of an incomplete wrapped binary tree.



**Figure 3-9 An illustration of two binary trees**

**3.4.3 Database Strategy**

**Ranking module**

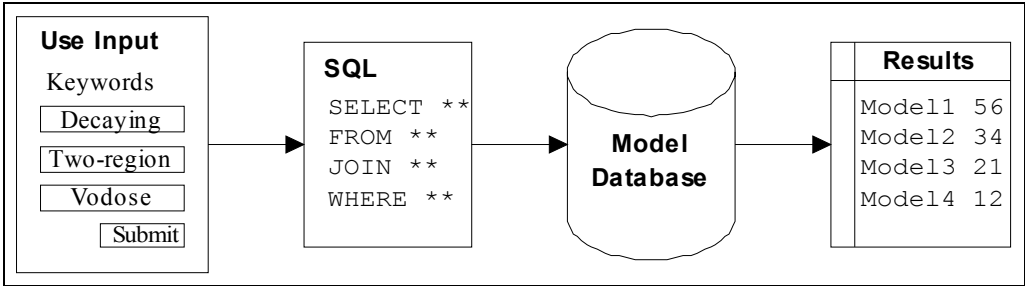
The ranking module ranks all models based on a user’s requests. The system has a multikeyword search capability. In the ranking module, a built-in SQL program is overlaid by the web page. To use the module, a user enters requests through the web page and clicks the *OK* button. The system will pass the user’s requests to a built-in SQL program. The SQL program will query the relational database and provide a result back to the user. The decision process of the ranking module can be described as a Pascal procedure shown in Figure 3-10. Figure 3-11 is a flowchart of the process.

```

/* Keyword : user's requests */
do j = 1 to number_of_keywords
begin
  do i = 1 to number_of_models;
  begin
    if (Model_Characteristics[i] = Keyword[j])
    then final_rank = final_rank + Weight[j];
  end
end
end;

```

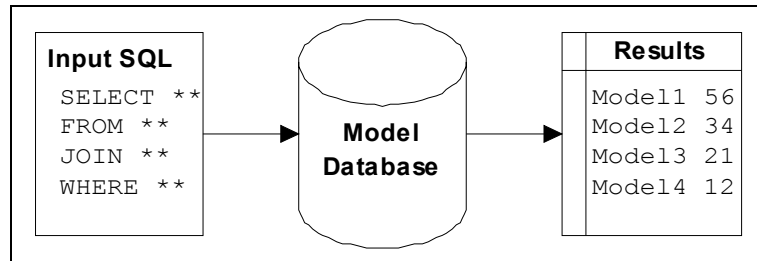
**Figure 3-10 The decision process of the ranking module**



**Figure 3-11 A flowchart of the ranking module**

Querying module

The querying module is designed for the users that know how to write SQL programs. In this scheme, a user has to write an SQL program to manipulate the model database. The database will return a list of possible models that match the user's requests. Figure 3-12 is an illustration of the process.



**Figure 3-12 A flowchart of the querying module**

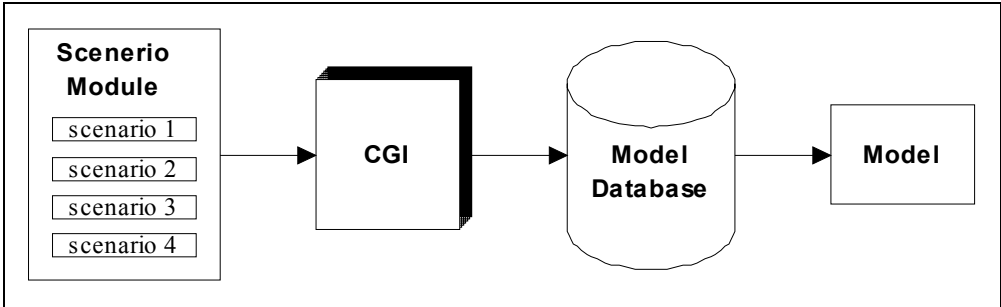
### **3.4.4 Scenario Strategy**

The basic idea of the scenario module is that a scenario can be assembled from a number of characteristics. Rather than choose between two models with different characteristics, a user can create a scenario that is a conceptual model of the problem he (she) is facing. The system will find an appropriate model for the scenario. The scenario module includes a model database that contains the properties of the ANTS models. The scenario module uses CGI to manipulate the model databases. A series of questions were predesigned. A user answers these questions. The system will analyze the user's answers and suggest a model to use. The decision process of the scenario module can be described as a Pascal procedure shown in Figure 3-13. Figure 3-14 is a flowchart of the process.



```
/* n : number of user's input */
do j = 1 to number_of_models
begin
    if ((Model_class[j][1] = User_input[1]) and
        Model_class[j][2] = User_input[2]) and
        . . . . .
        Model_class[j][n] = User_input[n]))
    then Appropriate_model = Model[j];
end;
```

**Figure 3-13 The decision process of the scenario module**



**Figure 3-14 A flowchart of the scenario module**

### 3.5 Summary

The developments of the potential user classification, the model characterization, and the match strategies were described in this chapter. The system was built on the three-step approach.

# **CHAPTER 4 DEVELOPMENT TOOLKITS AND PROTOTYPES**

## **4.1 Overview**

This chapter introduces three development toolkits. Two of the original groundwater modeling guidance prototypes are described in this chapter. Demonstration sessions of the prototypes are also shown in the chapter to illustrate how one works with the prototypes from a user's perspective. The last section sums up the advantages and disadvantages of the prototypes.

## **4.2 Choices of Development Tools**

### **4.2.1 Introduction**

A search was conducted to identify appropriate development tools to meet the objectives of the system.

One issue that was taken into account is what operating systems and graphical user interfaces were available for the system development, what the interface should look like, and what elements needed to be implemented into the system to make it useful. Microsoft Windows was chosen as being best suited for this project for a number of reasons. First, this operating system would run on much of the currently available hardware. Second, the application programming interface (API),

programmers' tools (Borland C++, Visual C++, Visual Basic), interface maturity, and multimedia extensions currently available to Microsoft Windows were not available in other operating environments. A prototype could be up and running in reasonably short order using Microsoft Windows. This prototype would include all the graphical user interface features available to Microsoft Windows.

The other issue is Internet accessibility. Until quite recently, computer programs were platform-dependent, that is, programs developed on one computer platform can not be easily used on the other computer platform. This situation has been changed since the popularity of the Internet. An Internet-based system can be used on almost any computer platform. The modeling guidance system should take advantages of the Internet-based development tools (such as HTML, CGI, and Java) that have become one of the most powerful and convenient tools. So the users of the system may use the system from anywhere in the world via the Internet.

#### ***4.2.2 Comparisons of Three Development Toolkits***

Three development toolkits were used to develop system prototypes:

1. The spreadsheet-based toolkit includes Microsoft Excel.
1. The Visual Basic based (VB-based) development toolkit includes Microsoft Visual Basic (VB), Microsoft Access, and Microsoft FORTRAN 5.1.
1. The Internet-based development toolkit consists of three components that are HTML, CGI, and Java.

The following factors were used to grade a toolkit: platform dependence, query and search capability, speed, design environment, and cost. Here is a brief description of the advantages and the disadvantages of these development toolkits. The advantages

of the Internet-based development toolkit are low cost, platform independence, and sufficient computing power. The disadvantage is its inferior computational performance as compared to FORTRAN programs. The VB-based development toolkit has a good interface design environment, fast application performance, a powerful SQL capability search engine, stand alone applications, and lots of third party applications that can be used to improve its capability. Its disadvantages are relatively high cost, only available on the Microsoft Windows platform, and not available on the Internet. The Microsoft Excel spreadsheet toolkit suffers from its slow performance. It also needs Microsoft Excel to run a worksheet model, and it is only available on the Microsoft Windows and Apple Macintosh platforms. It lacks ability to do any query, sort, or search request. However, it is relatively easy to program and use. The details of the advantages and the disadvantages of the three development toolkits are listed in Tables 4-1, 4-2, 4-3, and 4-4.

**Table 4-1 Comparisons of the toolkits - the user interfaces**

<b>Factors</b>	<b>Visual Basic</b>	<b>HTML/CGI/Java</b>	<b>Excel 97</b>
<b>Which platform can it run?</b>	Microsoft Windows	Almost any computer platform	Microsoft Windows, Apple Macintosh
<b>How easy is it to design an interface?</b>	Very Easy	Easy	Easy
<b>What is the requirement to use an interface?</b>	Stand alone application	Need a web browser	Need a Microsoft Excel to run a worksheet
<b>How flexible is it to design an interface?</b>	Very flexible	Very flexible	Not flexible
<b>How fast is it to run a program?</b>	Fast	Depend on the speed of the network	Slow
<b>Price<sup>1</sup></b>	\$ 444.95	Free	\$ 299.95

**Table 4-2 Comparisons of the toolkits - the guidance modules**

<b>Factors</b>	<b>Access 97 / VB</b>	<b>HTML/CGI/Java</b>	<b>Excel 97</b>
<b>Which platform can it run?</b>	Microsoft Windows	Almost any computer platform	Microsoft Windows, Apple Macintosh
<b>Does this tool have query or search capability?</b>	Built-in Microsoft JET database engine	Java, CGI+ODBC <sup>2</sup> , Microsoft Access 97 <sup>3</sup>	Possible but difficult (Excel Macro language)
<b>Can this tool use SQL?</b>	Yes	Possible	No
<b>How fast is it to do a query?</b>	Fast	Depend on the speed of the network	Not applicable
<b>Price<sup>1</sup></b>	\$ 744.90	Free	\$ 299.95

**Table 4-3 Comparisons of toolkits - the database**

<b>Factor</b>	<b>Access 97</b>	<b>HTML/CGI/Java</b>	<b>Excel 97</b>
<b>Which platform can it run?</b>	Microsoft Access database can be converted to other relational database format.	Almost any computer platform	Microsoft Windows
<b>What kind of database is used in this tool?</b>	Relational database	HTML hypertext or any database program	Microsoft Excel file
<b>How can a user update a database?</b>	Microsoft Access	Any text editor or particular database program	Microsoft Excel
<b>What is the requirement to use the database?</b>	Microsoft Access	Any web browser	Microsoft Excel
<b>Price<sup>1</sup></b>	\$ 299.95	Free	\$ 299.95

**Table 4-4 Comparisons of toolkits - the models**

<b>Factor</b>	<b>FORTRAN 5.1</b>	<b>Java Developers Kit</b>	<b>Excel 97</b>
<b>Which platform can it run?</b>	Microsoft Windows and DOS	Almost any computer platform	Microsoft Windows and Apple Macintosh
<b>How easy is it to code a model?</b>	Easy for a FORTRAN programmer	Easy for a C++ programmer. Not as easy for a FORTRAN programmer	Very easy
<b>How fast is it to run a program?</b>	Fast	Depend on the speed of the network	Slow
<b>What is the requirement to use a model?</b>	Stand alone application	Any web browser with Java capability	Microsoft Excel
<b>Price<sup>1</sup></b>	\$99.95 <sup>4</sup>	Free	\$101.95

<sup>1</sup> Price from PC Connection, (August 1998)

<sup>2</sup> Database file can be accessed by combining CGI and ODBC only on Microsoft Windows 95/NT platform.

<sup>3</sup> Microsoft Access 97 creates database file that can be accessed via the Internet only on Microsoft Windows 95/NT platform.

<sup>4</sup> Microsoft has stopped producing Microsoft FORTRAN 5.1.

### **4.2.3 Other Development Tools**

It is worth mentioning that a good alternative tool in developing a guidance system is the Microsoft Help Compiler (MSHC). Using the MSHC, a developer can create a help facility for a model library.

Mathematica is a software product that can be used to create contaminant transport models. Mathematica is a very powerful tool for quantitative analysis, symbolic calculations and manipulations, and visualization of functions or data. Mathematica is an interpreted language that reads an expression, evaluates the expression, and then prints the results of the evaluation. Being interactive makes it easier to use than a compiled language such as C, FORTRAN, or Pascal. However, the slow computation speed is its major weakness.

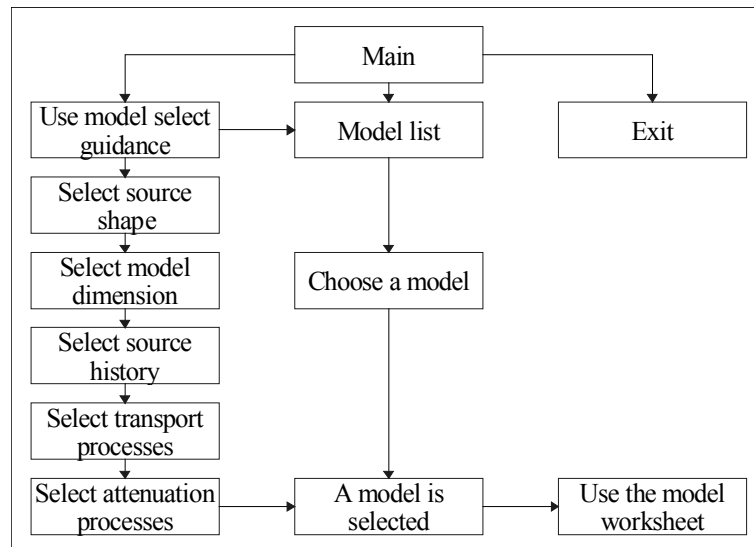
The other tool that can be used to develop analytical models is Reverse Polish Language, RPL. RPL is a programming language only common on HP 48 series calculators. (RPL-based applications could be used on Microsoft DOS, Microsoft Windows 95 and some Unix-based workstations with specific software and hardware selections.) The advantage of RPL is that it is used on an HP 48 series calculator. To many engineers, an HP 48 series calculator is probably the most portable and useful device. The disadvantages of the RPL-based applications are as follows:

1. The RPL-based applications can not be accessed via the Internet.
1. RPL is not easy to learn and program.

## 4.3 Spreadsheet Based Prototype - ExcelDSS

### 4.3.1 Introduction

The ExcelDSS prototype is a collection of Microsoft Excel worksheets that includes a main worksheet, a model select worksheet, a model list worksheet, macro worksheets, and 22 model worksheets. Each model worksheet consists of a one-dimensional groundwater contaminant transport model and a chart that plots the concentration profile or the concentration history of the model. This system is relatively easy to program and use. Its results can be plotted into a Microsoft Excel chart. Figure 4-1 shows the flowchart of the ExcelDSS prototype.



**Figure 4-1 The flowchart of the ExcelDSS prototype**



### **4.3.2 Hardware and Software Requirements**

The hardware and software requirements of the ExcelDSS prototype are as follows:

1. Intel 80486 CPU or better,
1. 8 MB RAM,
1. 5 MB hard disk storage space,
1. Microsoft DOS 5.0 and Microsoft Windows 3.1 or better, and
1. Microsoft Excel for Windows Version 4.0 or better.

### **4.3.3 ExcelDSS User Interface**

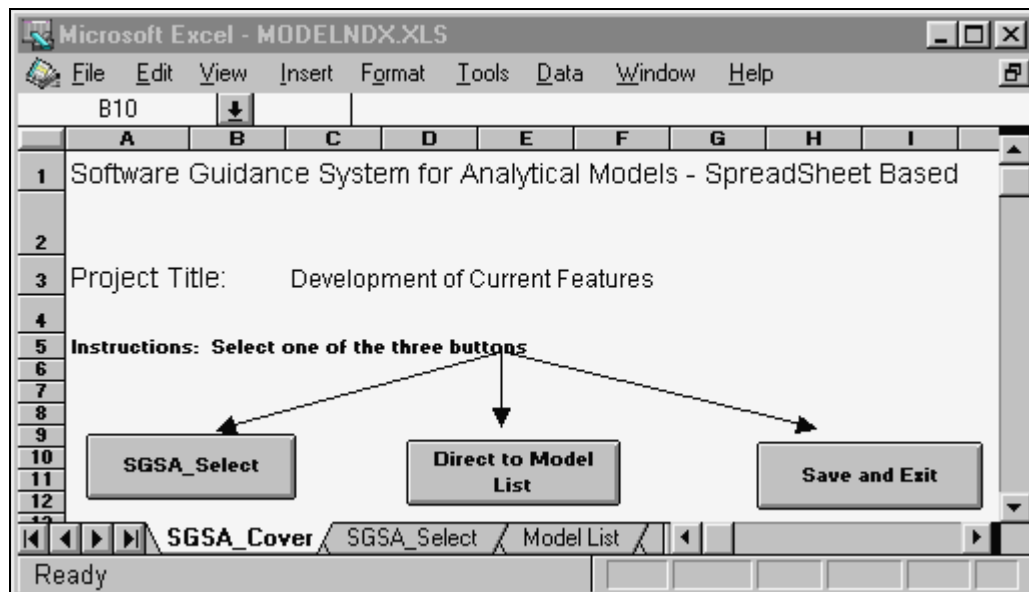
The user interface components of the ExcelDSS prototype are worksheets, buttons and graphics. The prototype use worksheets to store the models. The prototype uses graphics and buttons to guide a user in choosing an appropriate model.

### **4.3.4 ExcelDSS Demonstration**

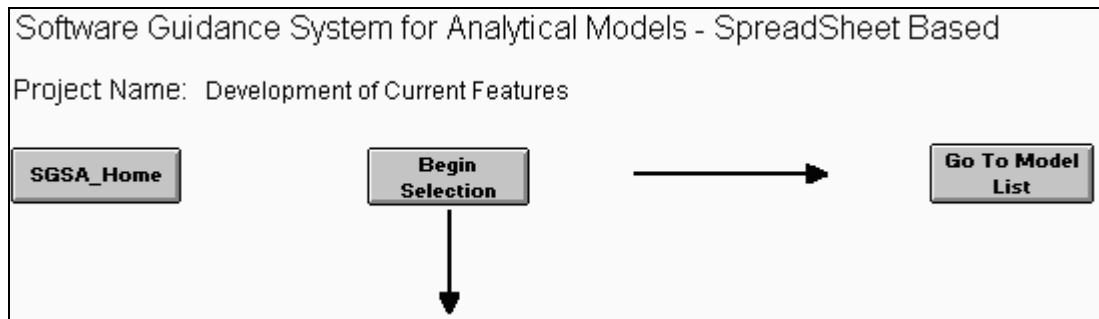
A demonstration of the prototype is shown in the following list:

1. Open the *MODELNDX.XLS* worksheet from Microsoft Excel for Windows (Version 4.0 or better). A window similar to Figure 4-2 should appear.
1. Choose the *SGSA\_Select* button to go to the model selection worksheet as shown in Figure 4-3.
1. Click the *Begin Selection* button to begin the selection as shown in Figure 4-3.
1. Choose a source sharp as shown in Figure 4-4.
1. Choose a transport dimension as shown in Figure 4-5.
1. Choose a source history as shown in Figure 4-6.

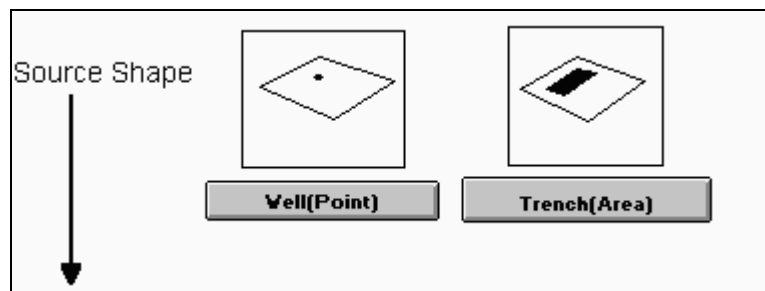
1. Choose a transport process as shown in Figure 4-7.
1. Choose an attenuation process as shown in Figure 4-8.
1. Click the *Go To Model List* button to go to the chosen model list as shown in Figure 4-9.
1. Click the *Run Selected Model* button to use the chosen model, as shown in Figure 4-10.
1. The result of the chosen model is shown in Figure 4-11.



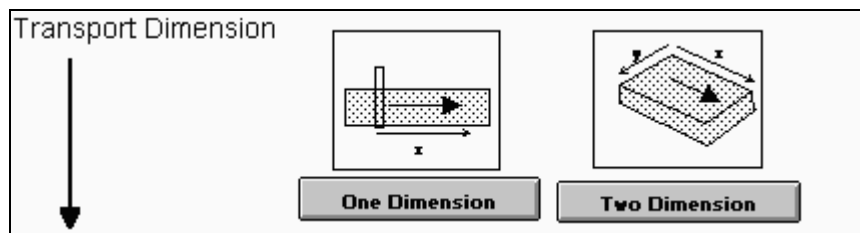
**Figure 4-2 The ExcelDSS main worksheet**



**Figure 4-3 The model selection worksheet**



**Figure 4-4 Choosing a source shape**



**Figure 4-5 Choosing a transport dimension**

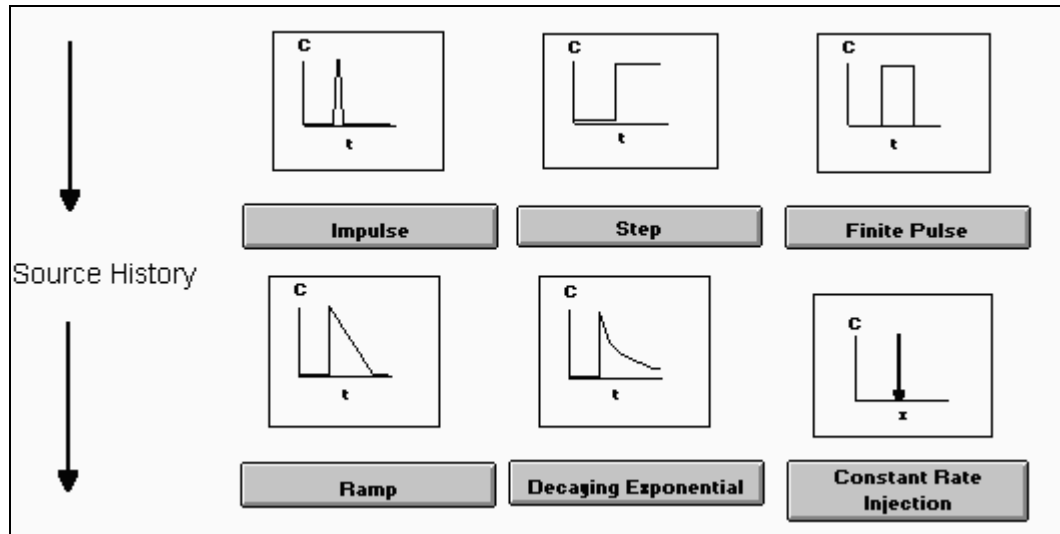


Figure 4-6 Choosing a source history

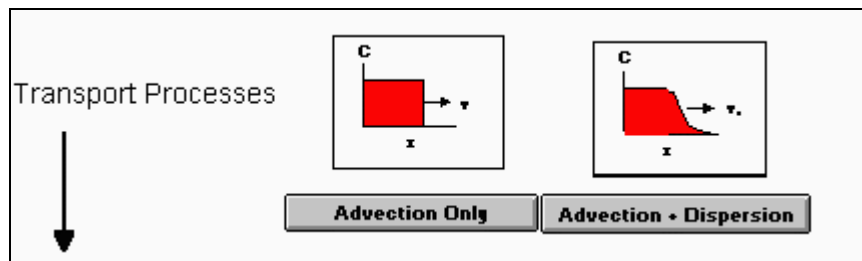


Figure 4-7 Choosing a transport processes

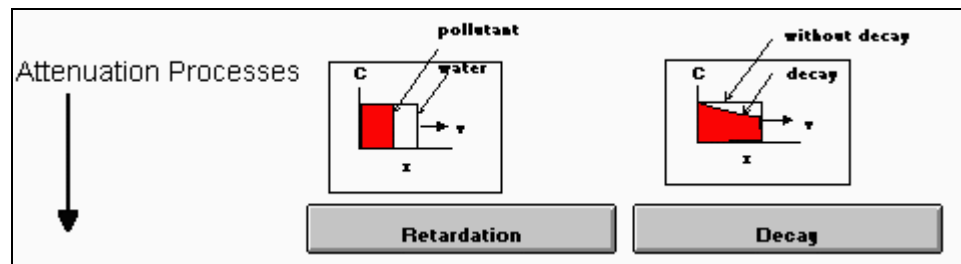


Figure 4-8 Choosing an attenuation processes

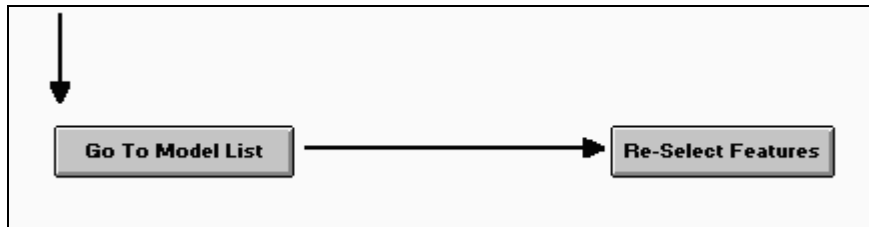


Figure 4-9 Getting to the chosen model

Analytical Model Database: EXCEL Models (all functions computed with MACROS or .DLL's)

**SGSA Contains an Appropriate Model : 1D,Step,Advection,Dispersion,Retardation**

Run Selected Model

Review Selected Model Documentation

Return to : SGSA\_Select

Return to : SGSA\_Home

Figure 4-10 Running the chosen model

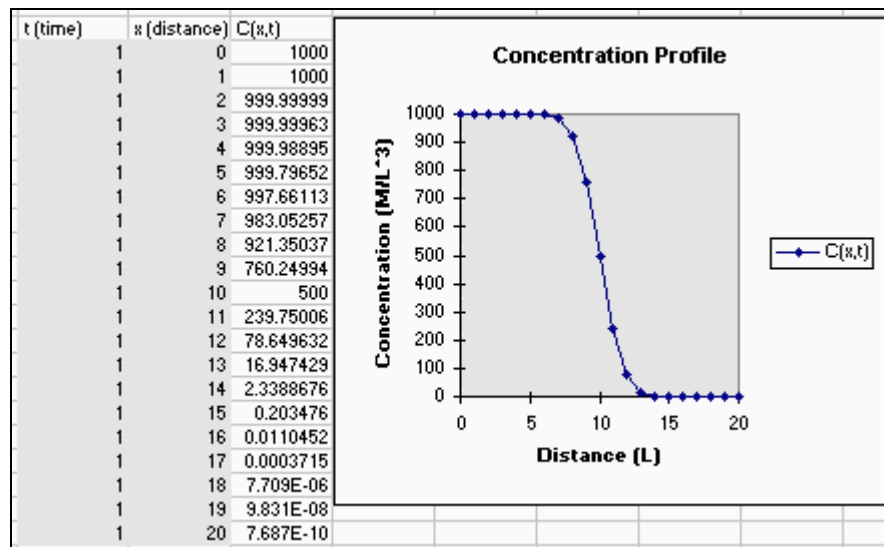


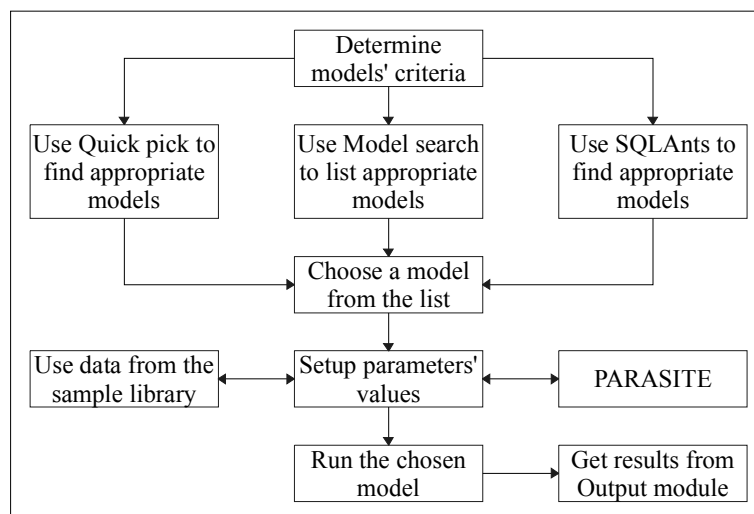
Figure 4-11 A model worksheet

## 4.4 Visual Basic Based Prototype - VBAnts

### 4.4.1 Introduction

The VBAnts prototype is a Microsoft Windows application. The VBAnts prototype consists of four components: a graphical user interface, a relational database, guidance engines, and a model library with more than 40 models. The graphical user interface and the guidance engines are the applications of Microsoft Visual Basic Version 3.0. The relational database is a database file of Microsoft Access. The contaminant transport models that were created by using Microsoft FORTRAN Version 5.1 are Microsoft Windows applications. The graphical user interface and the guidance engines are the components that most users can see and use. The relational database hides under the guidance engines' interfaces. Most end users only need to interact with the guidance engines. The experienced users will be able to access the relational database directly. This system is available for downloading in the ANTS web site.

Figure 4-12 shows the flowchart of the VBAnts prototype.



**Figure 4-12 The flowchart of the VBAnts prototype**

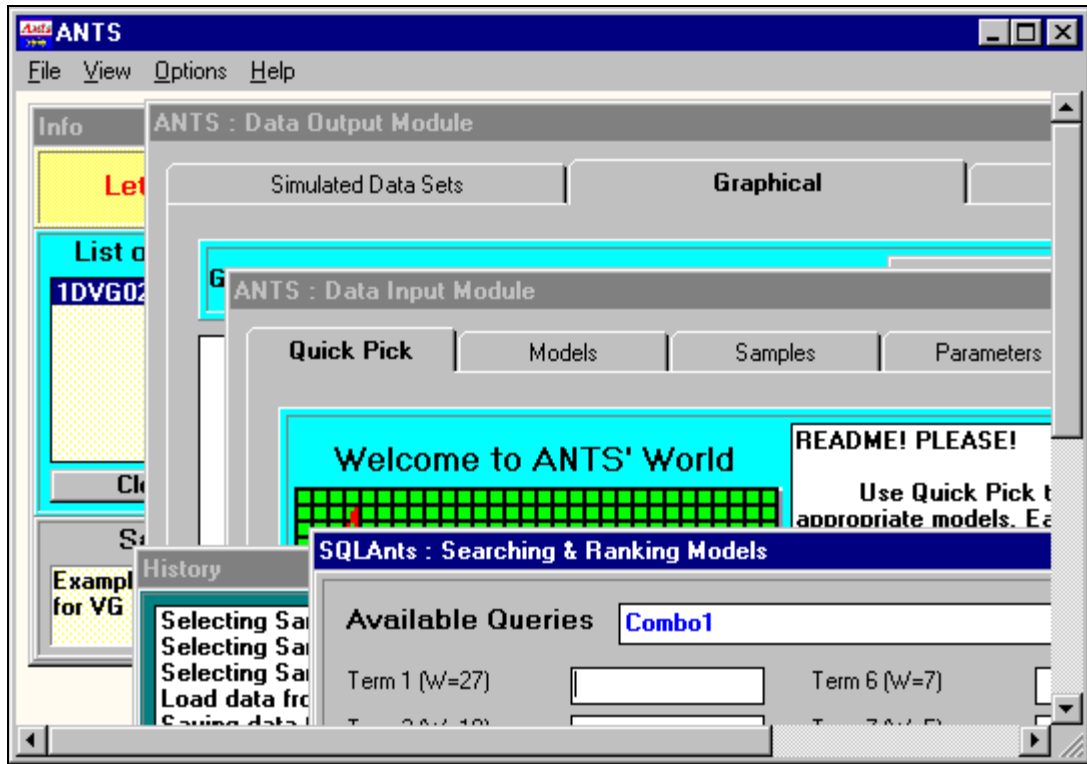
#### **4.4.2 Hardware and Software Requirements**

The hardware and software requirements to use the VBAnts prototype are as follows:

1. Intel 80486 CPU or better,
1. 8 MB RAM,
1. 15 MB hard disk storage space, and
1. Microsoft DOS 5.0 and Microsoft Windows 3.1 or better.

#### **4.4.3 VBAnts User Interface**

The main window of the VBAnts prototype is based on a multidocument interface (MDI) form. There are six subwindows inside the main window as follows: the about window, the info window, the history window, the data input module, the data output module, and the SQLANTS module. Figure 4-13 is a screen capture of the prototype.



**Figure 4-13 The VBANTS main window**

### Menu Bar

The menu bar at the top of the screen displays the menu topics. As the mouse is dragged across the menu bar (while holding down the left mouse button), each of these menus drops down a list of commands. Table 4-5 shows a summary of the menu commands, in the order in which they appear.

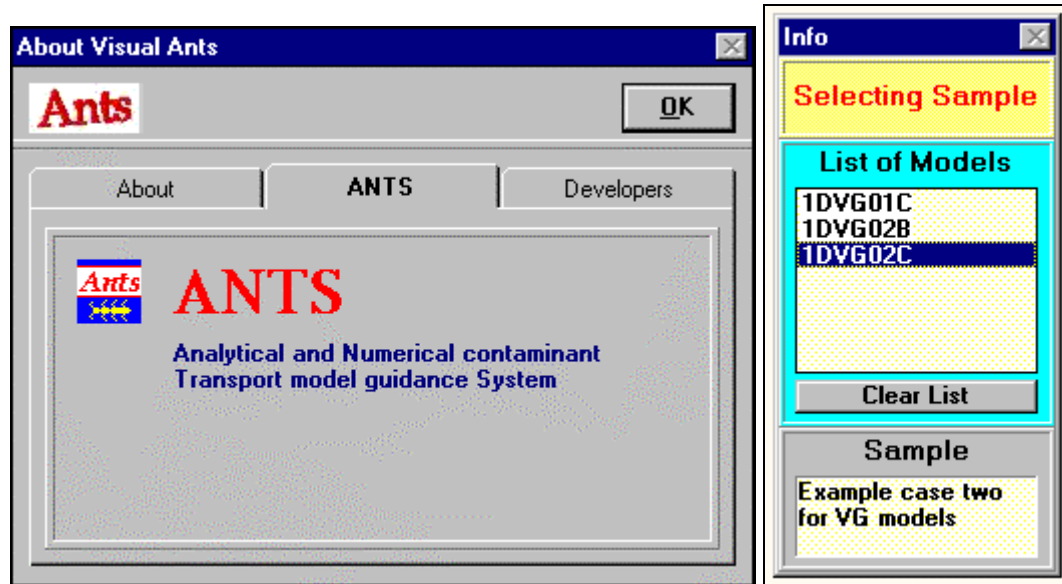
**Table 4-5 Summary of menu commands**

<b>Menu</b>	<b>Command Summary</b>
File	Perform basic file operations and program tasks.
View	Open a window or make it active, and arrange windows on the screen.
Option	Access the optional SQL Query window.
Help	Access the on-line help for VBANTS.



## The About Window

The about window, shown in Figure 4-14, contains information regarding to the purposes of the project.



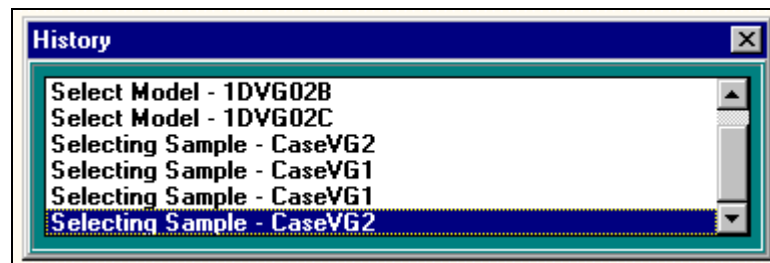
**Figure 4-14 A snapshot of the about and the info windows**

## The Info Window

The info window, also shown in Figure 4-14, contains vital information regarding to the status of the modeling process. It is organized to three panels. The top panel shows the current action of the user. The middle panel shows a list of the chosen models. The bottom panel shows that the name of the sample being chosen.

## The History Window

The history window, shown in Figure 4-15, contains a list of the user actions during the modeling process.

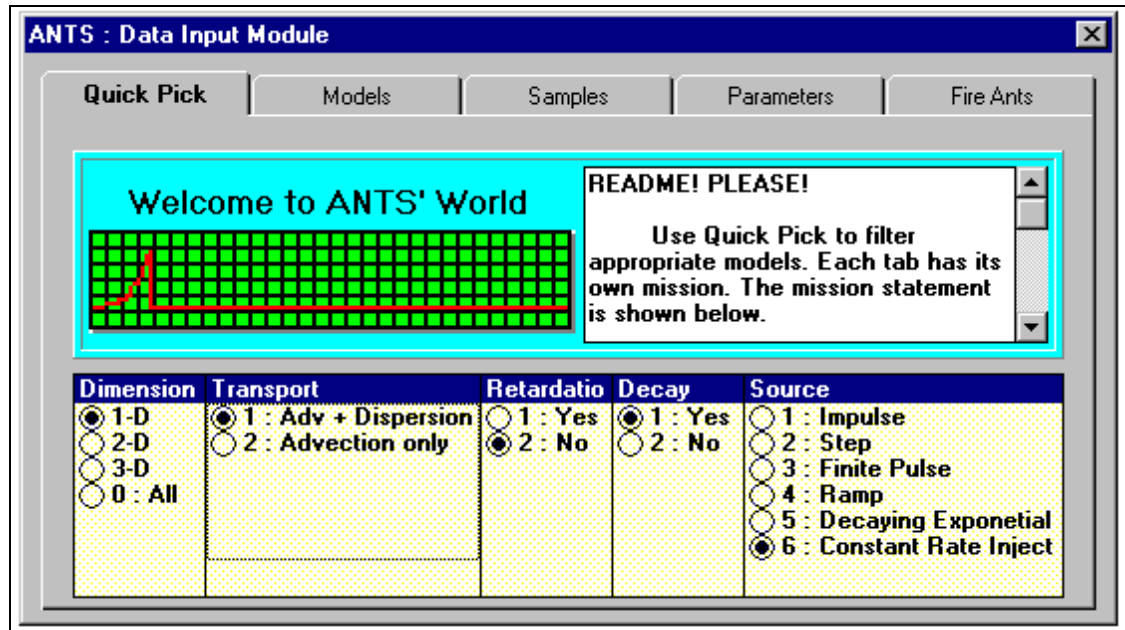


**Figure 4-15** A snapshot of the history window

## Data Input Module

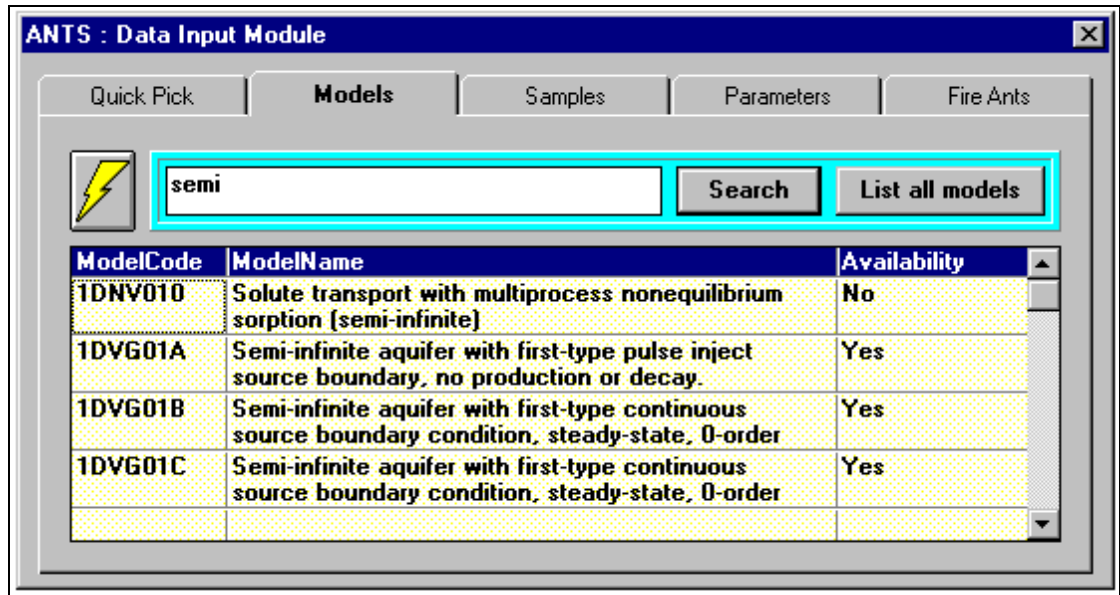
The most important component of the system is the data input module. The interface of the data input module is based on the tab concept as shown in Figure 4-16. Each tab has one purpose and one purpose only. A tab may consist of tables, text input boxes, buttons, or graphs. There are five tabs in the data input module. The functions of these tabs are described in the this section.

The *Quick Pick* tab contains three panels. The top panel includes a simple introduction of this module. The middle panel that is the *Quick Pick* panel that has a simple query interface with limited query choices. By clicking the *Option* buttons inside the *Quick Pick* panel, a user can filter for an appropriate model based on the dispersion type, the transport characteristic, and the source type of the model. The bottom panel contains several graphical icons that represent the characteristics of the model.



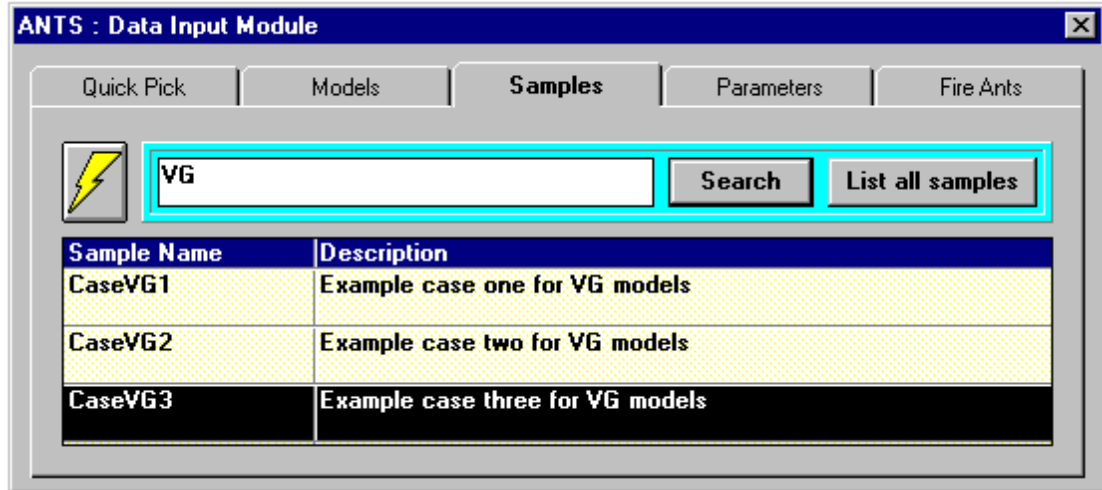
**Figure 4-16** A snapshot of the data input module window - Quick Pick

Figure 4-17 displays the *Models* tab. The tab contains three objects. The top-left object is the *Hint* button. Click the button to bring up a hint window. The top-right panel is a one-keyword search engine. Type in a keyword and click the *Search* button, the search engine will list all models related to the keyword. Click the *List all models* button to get a list of all models in the model library. The bottom portion is a table. This table shows some information related to the chosen models. To pick a model, move the mouse into the leftmost margin of the grid until a small checkmark appears. At that point, click the mouse button to select the model.



**Figure 4-17 A snapshot of the data input module - Models**

The *Samples* tab also contains three objects as shown in Figure 4-18. The top-left object is a hint button. Click the button to bring up a hint window. The top-right panel is a one-keyword search engine. Type in a keyword and click the *Search* button, the search engine will list all samples related to the keyword. Click the *List all samples* button to get a list of all samples. The bottom portion is a table. This table shows some information related to the chosen samples. To pick a sample, move the mouse into anywhere inside the row of the sample. At that point, click the mouse button to select the sample. The name of the selected sample will be listed on the info window. You can only choose one sample for each simulation.



**Figure 4-18 A snapshot of data input module window - Samples**

Figure 4-19 shows the *Parameters* tab. The top-left object is a *Hint* button. The top-right panel has three command buttons. The *Load Data* button loads the parameter values from the chosen sample. The *Update Change* button saves the current parameter values to a file. The *Load Parameter Guide* button opens the PARASITE parameter value assistant database. The purpose of the PARASITE database is to help users choose appropriate parameter values. The bottom portion is a table. This table shows necessary parameters used in a certain model.

The *Fire Ants* tab contains the *Fire Ants* button. Click the button run a simulation.

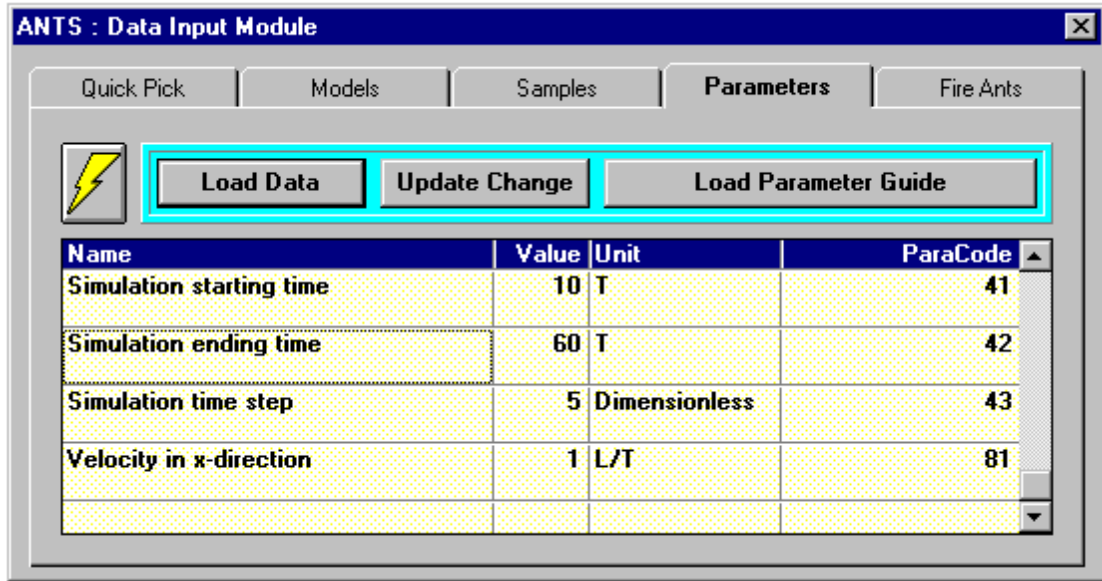
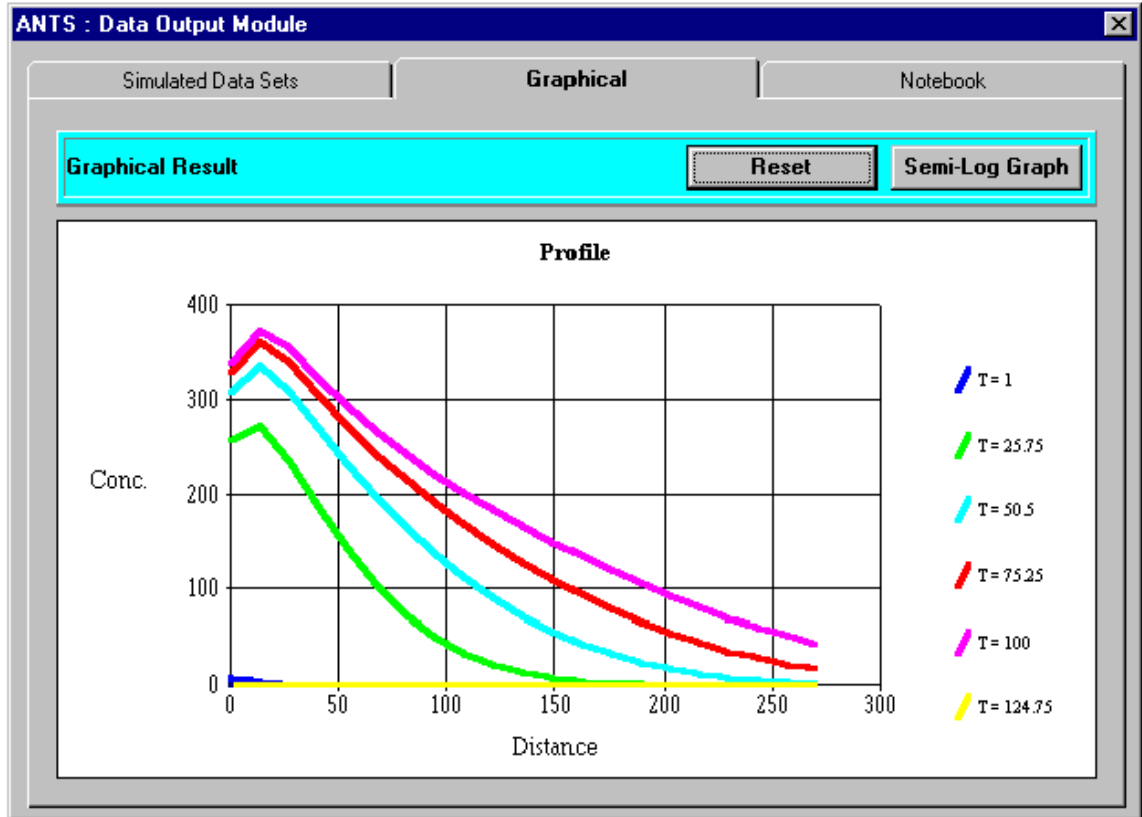


Figure 4-19 A snapshot of the data input module window - Parameters

## Data Output Module

Figure 4-20 shows the data output module. There are three tabs in the data output module. The *Simulated Data Sets* tab contains the output data. The *Graphical* tab shows the graphical output of the result from a simulation. The *Notebook* tab allows users to copy, paste, and store data.



**Figure 4-20 A snapshot of the data output module - Graphical**

#### **4.4.4 VBAnts Search Modules**

The VBAnts prototype uses the Microsoft JET engine to exchange information between its interface and its relational database. There are three guidance interfaces in the VBAnts prototype:

1. Quick Pick: As shown in Figure 4-16, this interface allows a user to find a model quickly. Its limitations are as follows: The user can only use its build-in options to find models. It is very difficult for a user to modify the interface.
1. One-keyword Search: As shown in Figure 4-17, this interface allows a user to select a model based on a keyword.

1. SQLAnts: As shown in Figure 4-21, a user can use the SQLAnts module to rank all models based on the user's requirements.

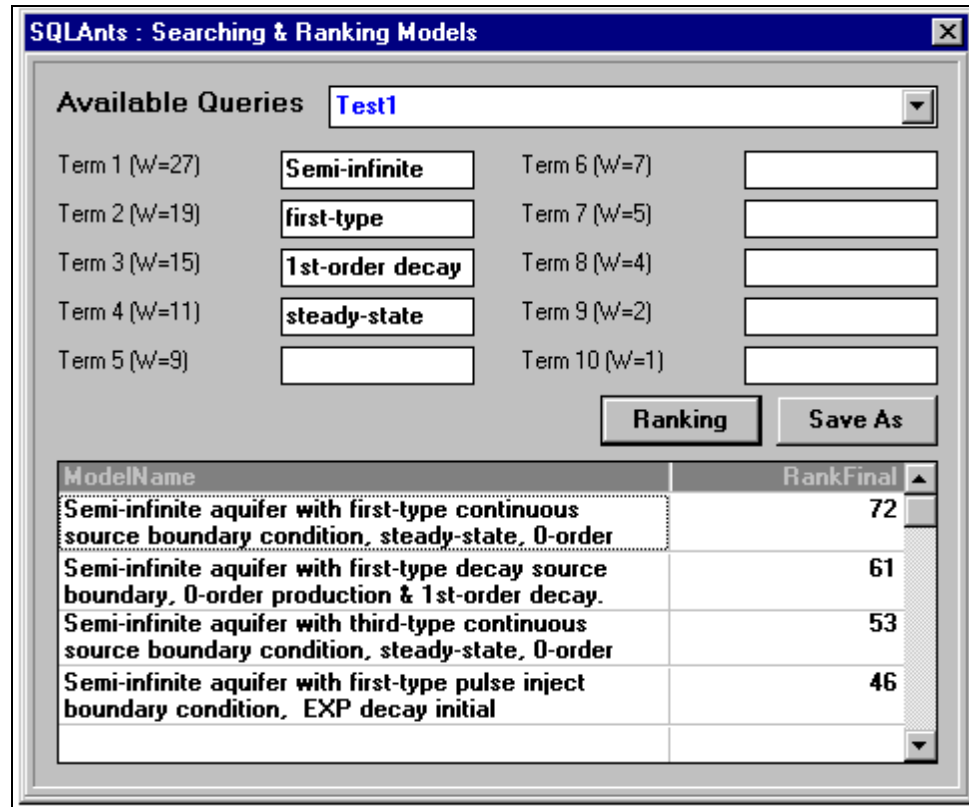


Figure 4-21 A snapshot of the SQLAnts

## 4.5 Summary

### 4.5.1 Objective Achievements of Two Prototypes

During the development of the prototypes, the following objectives were achieved:



1. The ExcelDSS and VBAnts prototypes have an analytical solution model library. A user can choose an appropriate analytical contaminant transport model from the model library. Currently there is no other program that serves this purpose.
1. The ExcelDSS and VBAnts prototypes are the Microsoft Windows and Microsoft Excel applications, respectively. Both systems are easier to use than the non-Windows FORTRAN-based programs that are available. Most potential users should feel comfortable to use the prototypes.
1. A large collection of analytical contaminant transport models was collected in the VBAnts prototype. The model library contains more than 40 analytical models.
1. Because the ExcelDSS and VBAnts prototypes were designed as highly modularized systems, many of their components such as the FORTRAN models, the model database, the SQL programs, and the Excel model worksheets can be used as standalone applications.

#### **4.5.2 Drawbacks and Problems Encountered**

The drawbacks of the ExcelDSS and VBAnts prototypes are as follows:

1. Both the ExcelDSS and VBAnts prototypes can not be accessed via the Internet.
1. The VBAnts prototype is a Microsoft Windows 3.1 / Windows 95 application. It may not be compatible with Microsoft Windows NT 4.0 or Microsoft Windows 98.
1. Most models in both systems are single chemical constituent models. The model library does not have heterogeneous media models, multiphase models, multiregion models, unsaturated zone models, or other models.
1. Planning for reversible user actions ensures that the system deals with the unintended error or action on the part of the user. In the ExcelDSS and VBAnts

prototypes, when mistakes are made during a model selection process, a user can not go back to the previous step. The user has to go back to the beginning of the selection process.

1. Nothing makes a user feel out of control more than a "fatal" error - by the system, or unintended by the user. The VBAnts prototype could crash by an unintended error or action on the part of the user.

These drawbacks were considered and addressed in the development of the Internet-based system.

# CHAPTER 5 SYSTEM DEVELOPMENT

## 5.1 Overview

The development of the Internet-based system is described in this chapter. The basic design requirements are described in the second section of this chapter. The hardware, and software selections of the system are defined in the third section of this chapter. Components of the system are described in the fourth section. The guidance modules are presented in the fifth section along with some screenshots. The concept of model visualization is presented in the sixth section. A demonstration session is shown in the last section to illustrate how one works with the system from a user's perspective.

## 5.2 Basic Design Requirements

The ANTS system must contain the following features in order to be fully functional:

1. guidance modules to help a user in selecting a most appropriate analytical contaminant transport model from a model library to predict the outcome of a contaminant transport problem,
1. a model library that contains a large collection of analytical solutions of contaminant transport models, and
1. ability to be used with or without much domain and computer knowledge.

### 5.3 Hardware and Software Selections

The Internet-based system has two parties involved: a web server and a web client. Figure 5-1 shows the architecture of the ANTS system. The web server has been provided in HTML, CGI, and Java. The web client can be any web browser. The model database was created by using Microsoft Access.

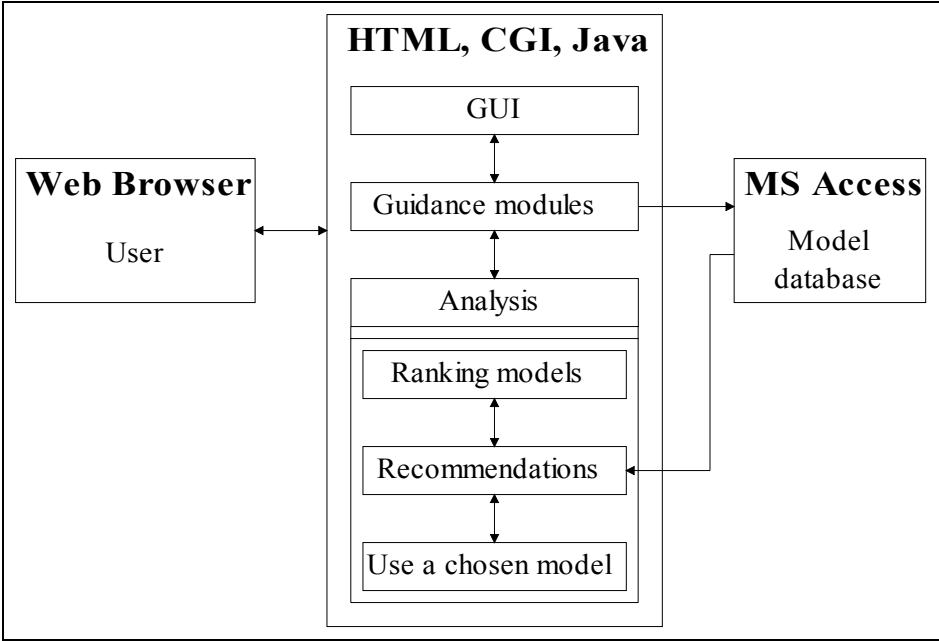


Figure 5-1 The ANTS architecture

#### 5.3.1 Web Server

A web server is a program that monitors for connections from a web browser, gets the information about the calling machine, searches the server configuration files to see if it has any instructions about accepting or denying requests from the machine that

is calling, and acts accordingly. The hardware and software selections for a web server machine are the following:

1. Pentium class CPU,
1. 32 MB RAM (minimum),
1. 100 MB hard disk storage space,
1. fast Internet connection (such as LAN),
1. Microsoft Windows NT 4.0 (or a higher version),
1. Microsoft Internet Information Server (or Netscape FastTrack Server),
1. CGI component (such as Perl or Microsoft FrontPage server extensions), and
1. Open Database Connectivity (ODBC).

### **5.3.2 Client**

Any online computer equips with a Java-enabled web browser should be able to use the Internet-based modeling guidance system. The two preferred web browsers for which the system is tested are Netscape Navigator for Windows Version 3.0 (or higher) and Microsoft Internet Explorer for Windows Version 3.0 (or higher).

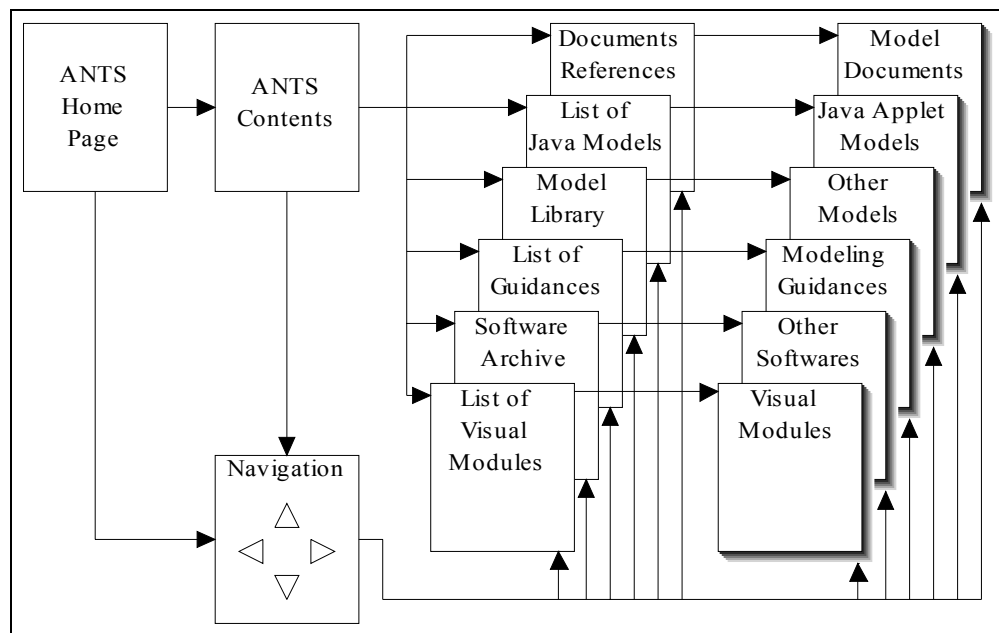
## **5.4 Components of the System**

The Internet-based system has four major components: a web-based graphical user interface, databases, a model library, guidance modules, and visualization modules.

### **5.4.1 Graphical User Interface Component**

In order to effectively use the Internet-based system to achieve a goal, a user must interact with the system via the graphical user interface component. Designing a

user-friendly graphical user interface is an important task in building the system. The graphical user interface in the system is a combination of many HTML web pages. This design allows the Internet-based system to have a universal appearance under different platforms. The web pages are classified into eight groups. The organization of the web pages is shown in Figure 5-2.



**Figure 5-2 The structure of the web pages in the system**

1. The index web pages include the home page, introduction pages, content pages, and list pages.
1. The documentation pages include model documents, model references, and tutorial pages. The tutorial pages contain information regarding basic concepts of contaminant transport modeling.

1. The Java model pages allow users to use online Java analytical solution models for solving contaminant transport problems.
1. The non-Java model pages allow users to download non-Java analytical models (such as the Microsoft Excel worksheets or the FORTRAN programs).
1. The modeling guidance pages are interactive guidance pages to help the user choose a model.
1. The model visualization pages display visual scenes of model characteristics.
1. The software archive pages allow users to download software available in the ANTS web site.
1. The navigation bar allows users to link to any web page in the system.

#### **5.4.2 Database Component**

The model database stores information regarding the properties of all models. The database was created by using Microsoft Access.

#### **5.4.3 Model Library Component**

The model library has a large collection of analytical solution models in three different formats:

1. The spreadsheet models: Twenty-two models are available as Microsoft Excel worksheets. These model worksheets can be downloaded from the ANTS web site.
1. The FORTRAN models: More than 60 models are available either as standalone Microsoft Windows applications or FORTRAN source codes. These models can be downloaded from the ANTS web site.

1. The Java applet models: More than 100 models are compiled as Java applets to be used via the Internet.

Most spreadsheet models are available as the FORTRAN models as well as the Java applet models. Most FORTRAN models are available as the Java applet models.

The model library not only consists of one-dimensional single chemical constituent models that are most commonly used in classrooms, laboratory, or fields, it also includes some multidimensional, multisite, multiregion, or heterogeneous media models that have these distinguishing characteristics and can be applied on specific problems. The current list of all models is attached in Appendix C.

#### **5.4.4 Guidance Module Component**

The guidance module component functions as a guide that can point users to an appropriate model. There are several guidance modules available in the system. As mentioned in Chapter 3, each guidance module has its own match strategy for finding an appropriate model. The guidance modules were created by HTML, CGI, and Java. The details of the guidance modules are described in the next section.

#### **5.4.5 Visualization Module Component**

The model visualization component was designed to help users understand the basic concepts of a particular model or a particular condition. The details of the model visualization component are described in the latter section.



## 5.5 Designs and Structures of Guidance Modules

### 5.5.1 Hierarchy Guidance Module

The hierarchy guidance module that is based on the hierarchy scheme described in Chapter 3 has a ten-layer model hierarchical tree. Ten properties were used to classify analytical solution models. The properties are as follows: *Models*, *Zone*, *Flow*, *Dispersion*, *Media*, *Component*, *Initial Conditions*, *Inflow Boundary Conditions*, *Outflow Boundary Conditions*, and *Source Type*.

Figure 5-3 shows three screenshots of the hierarchy guidance module. More than 80 analytical solutions of contaminant transport models were classified into the hierarchical model tree. Because the whole model tree is too large to fit in a single page (or a computer screen), the tree was divided into 16 subtrees. A synchronized hierarchical tree that contains 16 subtrees is shown in Figure 5-3(a). A screenshot of a subtree (Subtree 1-1) is shown in Figure 5-3(b).

To use the module, a user just follows the hierarchical tree with particular model properties in his (her) mind to advance to the next layer. The user should find a model in the end point of the tree. There is a help menu bar in every subtree as shown in Figure 5-3(c). The user can click a menu bar item to receive help information.

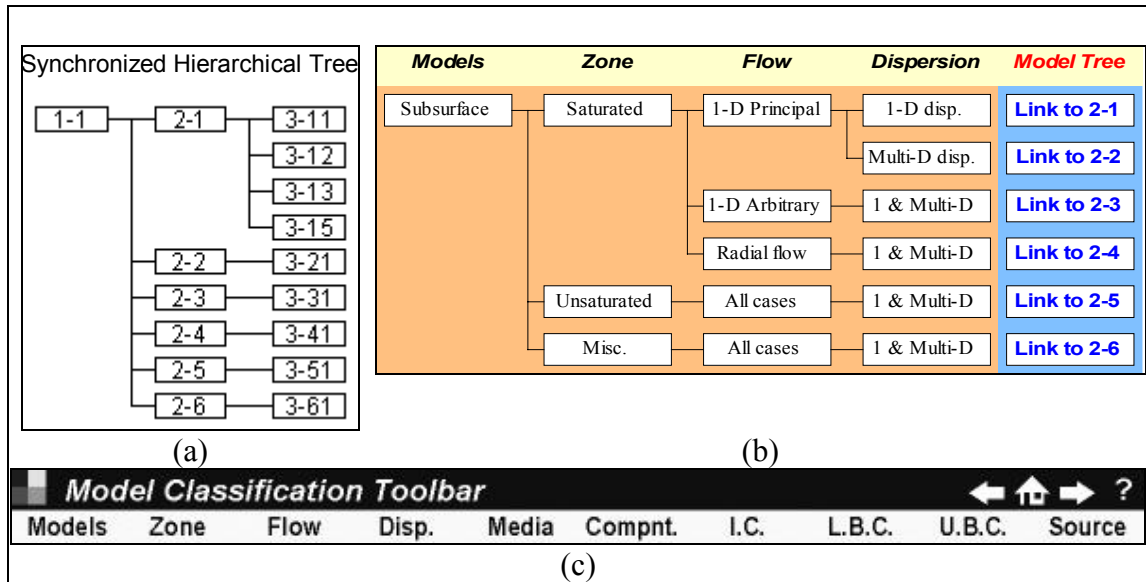
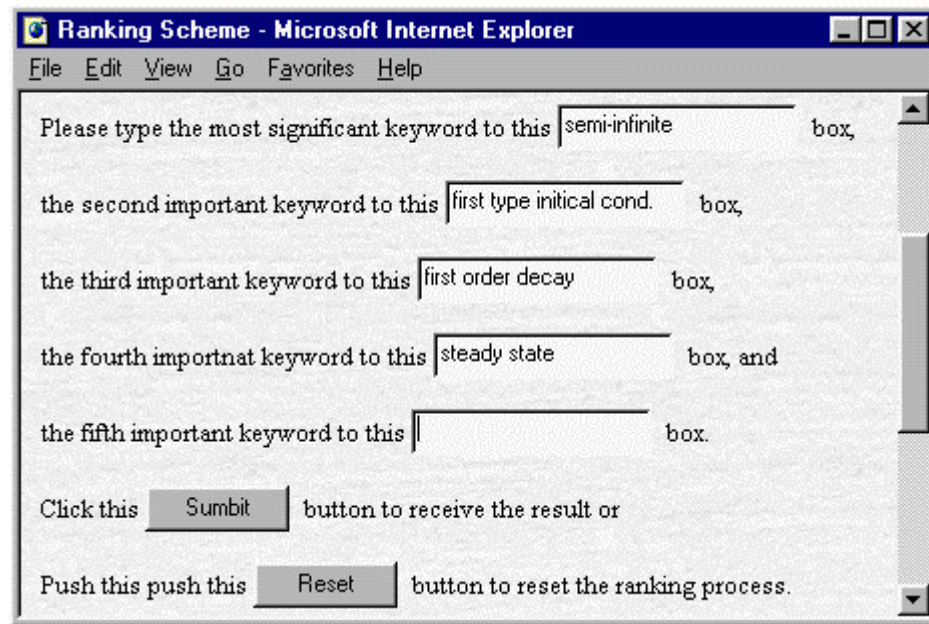


Figure 5-3 Structure of a hierarchical tree and a subtree (subtree 1-1)

### 5.5.2 Database Schemes

#### Ranking Module

A screenshot of the ranking module is shown in Figure 5-4. The ranking module has a five-keyword search engine that has a built-in SQL program overlaid by the ranking module web page. To use the module, a user adds keywords into five text boxes. The user then submits the requests by clicking the *Submit* button. The module will rank all models based on the user's requests. A ranked list of all models will show on a table in a new web page.



**Figure 5-4 A screenshot of the ranking scheme module**

### Querying Module

In the querying module, a user writes an SQL program to retrieve information from the model database. An SQL program that produces the same results as the ranking module in Figure 5-4 is shown in Figure 5-5.

```

UPDATE ModelRanking SET ModelRanking.Score1 = 50
WHERE ModelRanking.Abstract LIKE '%%textbox1%%';
UPDATE ModelRanking SET ModelRanking.Score1 = 40
WHERE ModelRanking.Abstract LIKE '%%textbox2%%';
UPDATE ModelRanking SET ModelRanking.Score1 = 30
WHERE ModelRanking.Abstract LIKE '%%textbox3%%';
UPDATE ModelRanking SET ModelRanking.Score1 = 20
WHERE ModelRanking.Abstract LIKE '%%textbox4%%';
UPDATE ModelRanking SET ModelRanking.Score5 = 10
WHERE ModelRanking.Abstract LIKE '%%textbox5%%';
UPDATE ModelRanking SET ModelRanking.FinalScore =
ModelRanking.Score1 + ModelRanking.Score2 +
ModelRanking.Score3 + ModelRanking.Score4 + ModelRanking.Score5;

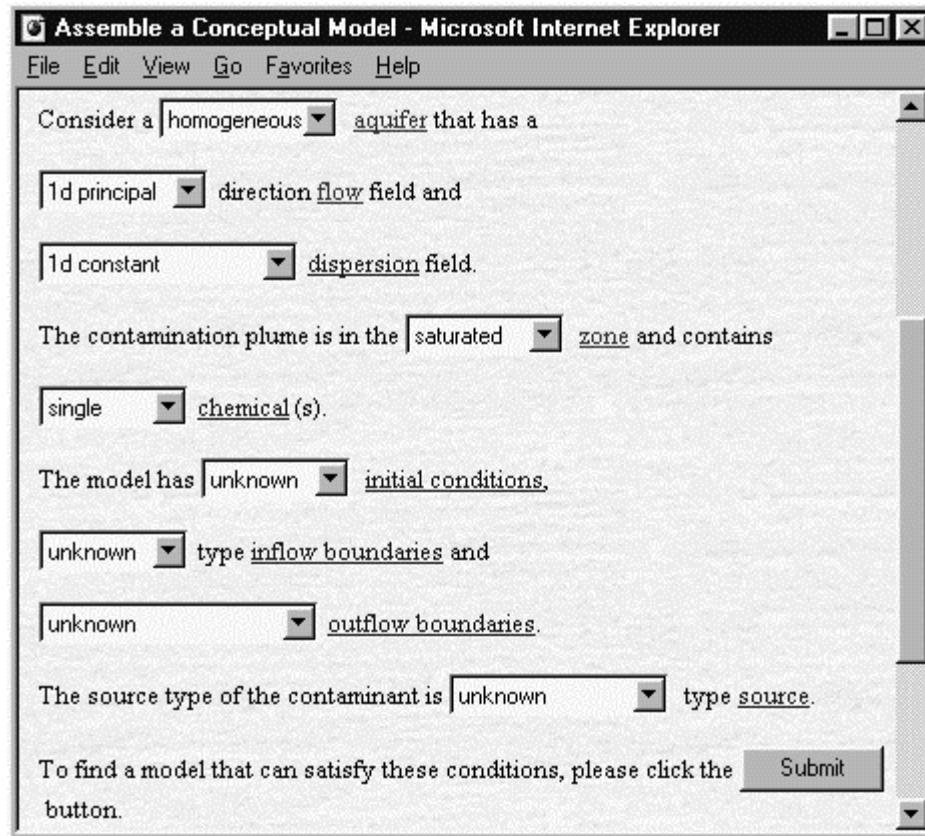
```

**Figure 5-5 An SQL program**

The SQL program is not as complicated as it seems. The user **UPDATES** six fields **WHERE** certain conditions must be met. The ranking module is more user-friendly than the querying module.

### **5.5.3 Scenario Module**

The scenario module is a form that is a collection of form fields on a page along with a form handler, a method of collecting information from the form. The form was created by using HTML and CGI. As shown in Figure 5-6, the module contains a series of form fields. Each form field has two parts: a label that contains a scenario question and a drop down menu that stores possible choices for the question. A user answers the questions by selecting options from the drop down menus to match a groundwater contaminant transport problem. The user then submits the form by clicking the “Submit” button. The system will return a list of appropriate models that can be used to simulate the user’s problem.



**Figure 5-6 A screenshot of the scenario scheme**

One problem in the scenario module is that not all scenario combinations match a model. There are ten scenario questions in the module as shown in Table 5-1. The number of the possible scenario combinations in this module is 23,040. There are only 120 models available in the model library. It is very likely that a user can not find a match model by choosing a particular scenario combination. To minimize this problem, the author suggests the following hints:

1. If a user is not sure about a particular question, choose the *unknown* option to bypass the question. A list of all available models in the database can be found by checking the *unknown* options to all questions.

1. The user should apply only one condition at the beginning of the search. Submit the request to see if any model will meet the scenario. Then add one condition at a time to narrow down the target.

**Table 5-1 A list of questions and choices in the scenario module**

<b>Scenario Questions</b>	<b>Choices</b>
What is the problem type?	<ul style="list-style-type: none"> <li>• Groundwater contaminant transport</li> </ul>
What kind of zone is the aquifer?	<ul style="list-style-type: none"> <li>• Saturated</li> <li>• Unsaturated</li> </ul>
What is the flow field type?	<ul style="list-style-type: none"> <li>• One-dimensional principal directional flow</li> <li>• One-dimensional arbitrary directional flow</li> <li>• Two-dimensional flow</li> <li>• Radial flow</li> </ul>
What is the dispersion type?	<ul style="list-style-type: none"> <li>• One-dimensional dispersion</li> <li>• Two-dimensional dispersion</li> <li>• Three-dimensional dispersion</li> </ul>
What kind of media does the aquifer have?	<ul style="list-style-type: none"> <li>• Homogeneous medium</li> <li>• Heterogeneous medium</li> <li>• Two-region medium</li> <li>• Layered soil medium</li> </ul>
How many chemicals are in the aquifer?	<ul style="list-style-type: none"> <li>• Single component</li> <li>• Multicomponent</li> </ul>
What are initial conditions?	<ul style="list-style-type: none"> <li>• Constant initial distribution</li> <li>• Decaying initial distribution</li> </ul>
What are inflow boundary conditions?	<ul style="list-style-type: none"> <li>• The first type</li> <li>• The third type</li> </ul>
What are outflow boundary conditions?	<ul style="list-style-type: none"> <li>• Semi-infinite</li> <li>• Finite domain</li> </ul>
What is the source type?	<ul style="list-style-type: none"> <li>• 15 different source types</li> </ul>

## 5.6 Model Visualization

The purpose of the model visualization is to help users understand the basic concepts of a particular model or a particular condition. The first part of the section describes the concepts of the model visualization. Two visualization modules, visual characteristics and visual model mosaic, are also described in this section.

### 5.6.1 Introduction

It is difficult to understand the meaning of a technical term or an equation without illustrations. Just as an example, what is the difference among the first type, the second type and the third type inflow boundary conditions? As the results from the user survey show in Chapter 3, very few respondents can answer this question. This section describes some model characteristics that may be difficult to understand without a graphical representation.

#### Inflow Boundary Conditions

The first type, the second type, and the third type inflow boundary conditions are described in this section. The first type inflow boundary condition, or the Dirichlet inflow boundary condition, prescribes the concentration along a portion of the boundary as

$$C = C_0(x, y, z), \quad (5-1)$$

where  $C_0$  is a given function of time and space for that particular portion of boundary.

The second type inflow boundary condition, or the Neumann inflow boundary conditions, prescribes the normal gradient of the concentration over a certain portion of the boundary. This boundary conditions can be given as

$$-D_x \frac{\partial C}{\partial x} = VC_0, \quad (5-2)$$

where  $C_0$  and  $D_x$  are the known measured concentration in the influent water and the dispersivity in the flow direction, respectively.

The third type inflow boundary condition, or the Cauchy inflow boundary conditions, prescribes the normal gradient of the concentration over a certain portion of the boundary. The flux of solute across the boundary is dependent upon the difference between a specified concentration value on one side of the boundary and the solute concentration on the opposite side of the boundary. This boundary conditions can be given as

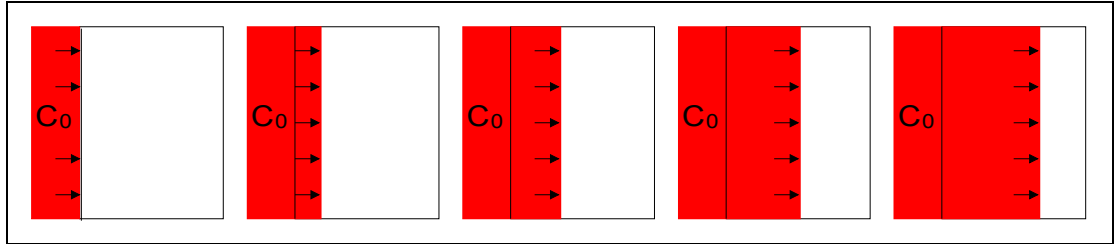
$$VC - D_x \frac{\partial C}{\partial x} = VC_0, \quad (5-3)$$

where  $C_0$  and  $D_x$  are the known measured concentration in the influent water and dispersivity in the flow direction, respectively.

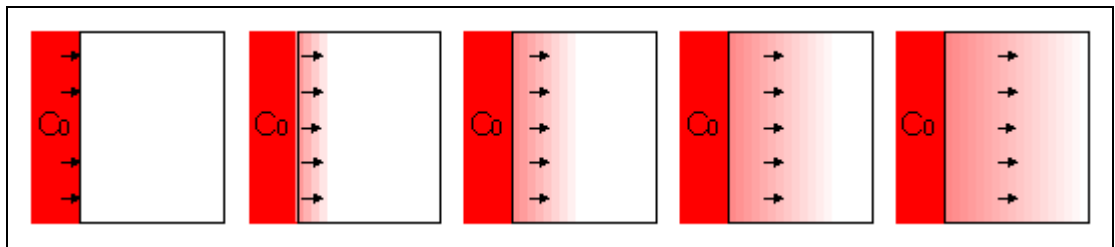
A domain novice is likely to have difficulty in understanding the differences among equations (5-1), (5-2), and (5-3). A conventional approach is to draw a graph to represent each condition. However, it is not easy to illustrate these three conditions in three graphs. A different approach was used in this research by creating a series of graphs to illustrate each condition. Figures 5-7, 5-8, and 5-9 show concentration advances of the first type, the second type, and the third type inflow boundary conditions, respectively. Figure 5-7 displays advection as the only mechanism in the concentration advance of the first type inflow boundary condition. Figure 5-8 displays diffusion as the only mechanism in the concentration advance of the second type inflow



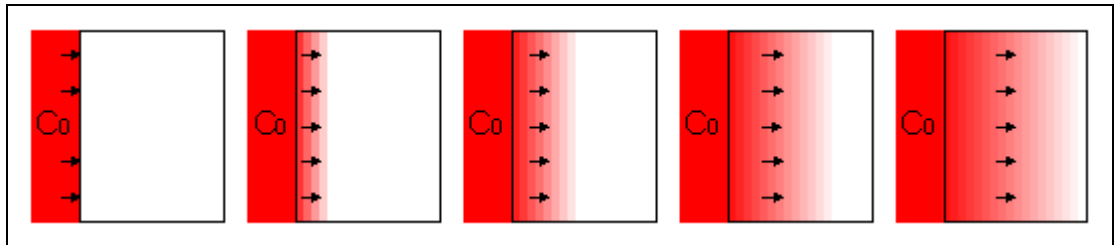
boundary condition. Figure 5-9 displays advection and diffusion as two mechanisms in the concentration advance of the third type inflow boundary condition.



**Figure 5-7 Concentration advance of the first type inflow boundary**



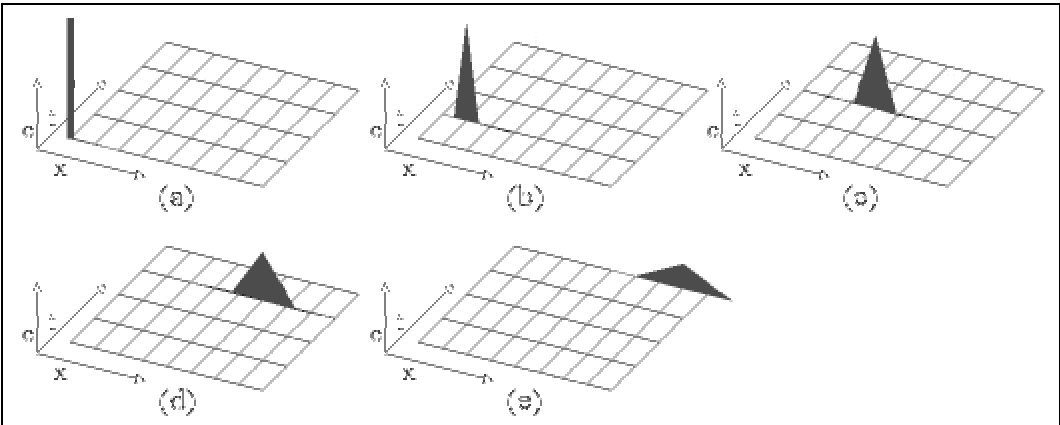
**Figure 5-8 Concentration advance of the second type inflow boundary**



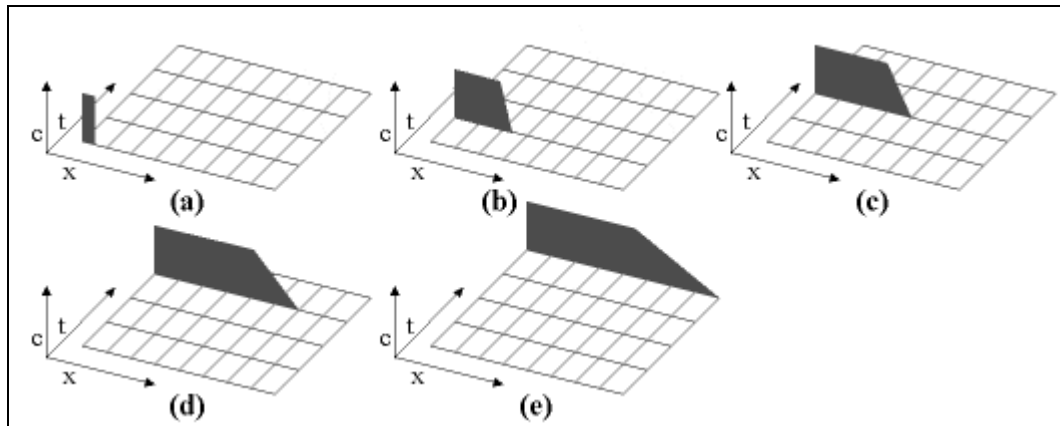
**Figure 5-9 Concentration advance of the third type inflow boundary**

### Contamination Source Types

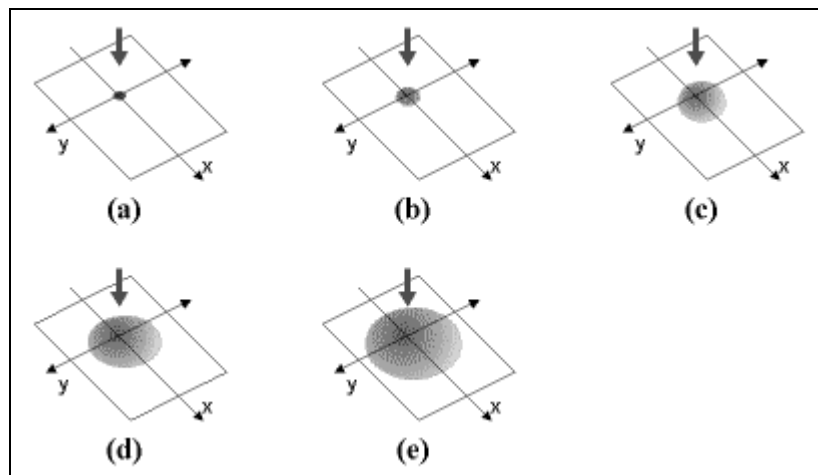
There are 15 contamination source types in the system. It may be difficult to understand a source type without a graphical representation. As an example, a user should be able to distinguish the differences among a one-dimensional instantaneous pulse injection, a one-dimensional continuous constant concentration injection, and a two-dimensional continuous point injection from Figures 5-10, 5-11, and 5-12. Figure 5-10 shows the advance of a one-dimensional instantaneous pulse injection source in a series of graphs. Each graph represents the advance of a pulse injection source in a particular time. Figure 5-11 shows the advance of a one-dimensional continuous constant concentration injection source in a series of graphs. Figure 5-12 shows the advance of a two-dimensional continuous point injection in a horizontal plane.



**Figure 5-10 Advance of a one-dimensional instantaneous pulse injection**



**Figure 5-11 Advance of a one-dimensional continuous constant injection**

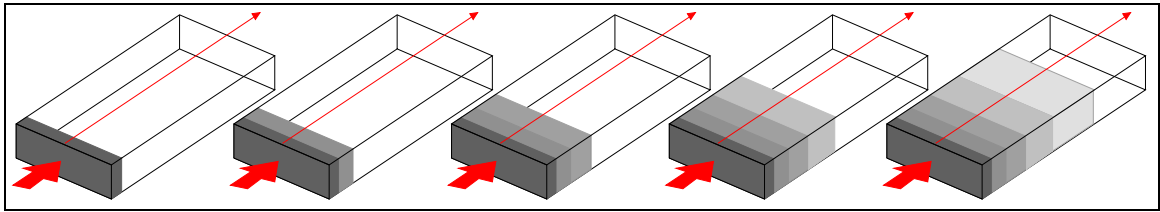


**Figure 5-12 Advance of a two-dimensional continuous point injection**

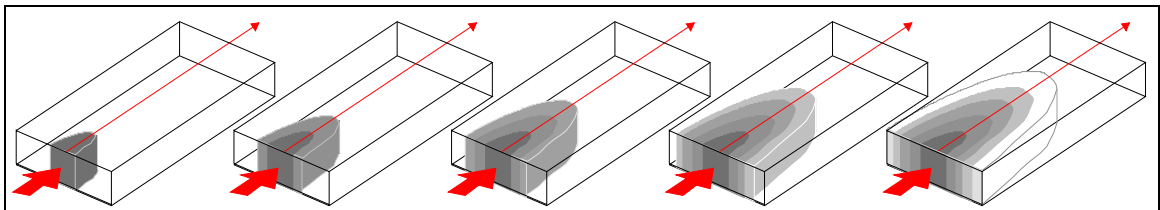
### Contamination Dispersion Type

There are three contamination dispersion types in the system. A user should be able to distinguish the differences among a one-dimensional dispersion, a two-dimensional dispersion, and a three-dimensional dispersion from Figures 5-13, 5-14, and 5-15. Figure 5-13 shows the advance of a one-dimensional dispersion in a series of

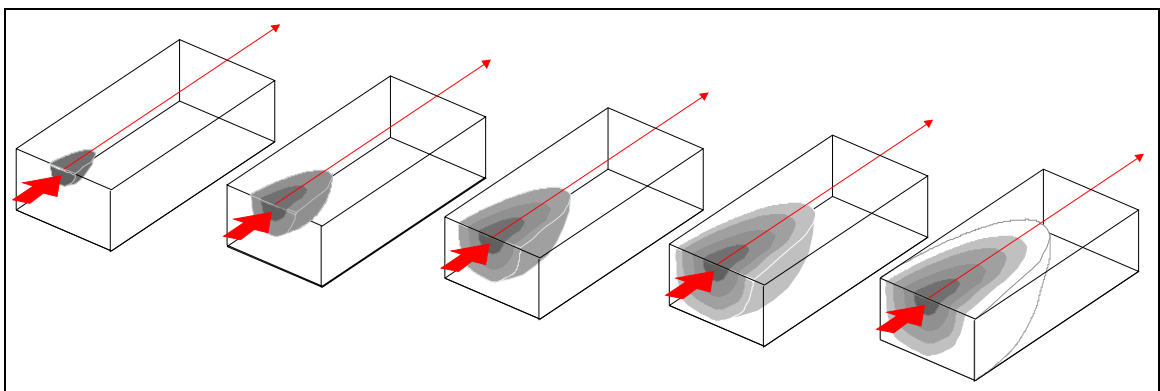
graphs. Figure 5-14 shows a two-dimensional dispersion in an aquifer. Figure 5-15 shows a three-dimensional dispersion in an aquifer.



**Figure 5-13 One-dimensional dispersion**



**Figure 5-14 Two-dimensional dispersion**



**Figure 5-15 Three-dimensional dispersion**

### **5.6.2 Visual Characteristics**

Most web browsers can display animated graphics interchange format (GIF) images. The GIF is a graphical file format commonly used to display indexed color images on the World Wide Web. The animated GIF is a file containing a series of GIF images that are displayed in rapid sequence by most web browsers, giving an animated effect. The visual characteristics take the advantage of the animated GIF image. In this approach, an animated GIF image was used to show a particular scenario such as the advance of a plume in a porous medium. Many animated GIF images were added into the system to help users understand the concept of groundwater contaminant transport. The author is unable to show animated effects of the visual model characteristics in the dissertation. The animated GIF images of the inflow boundary conditions can be found on the following web link:

[http://cleveland1.cive.uh.edu/ANTS/Guidances/mosaic/  
visual-boundarycondition.html](http://cleveland1.cive.uh.edu/ANTS/Guidances/mosaic/visual-boundarycondition.html).

The animated GIF images of the contamination source types can be found on the following web link:

[http://cleveland1.cive.uh.edu/ANTS/Guidances/mosaic/  
visual-sourceterm.html](http://cleveland1.cive.uh.edu/ANTS/Guidances/mosaic/visual-sourceterm.html).

The animated GIF images of the contamination dispersion types can be found on the following web link:

[http://cleveland1.cive.uh.edu/ANTS/Guidances/mosaic/  
visual-dispersion.html](http://cleveland1.cive.uh.edu/ANTS/Guidances/mosaic/visual-dispersion.html).

### **5.6.3 Visual Model Mosaic**

The visual model mosaic is used to help users understand the basic concepts of a model. A conventional approach is to draw a graph to represent a model. A different approach developed in this research is to use a visual model mosaic to represent a model. It is possible to represent a model by using the model mosaic that is a combination of visualized characteristics graphs. The major advantages of the mosaic approach are its reusable tiles and its dynamic results. A tile can be used in any model as long as the model has the characteristic. By using HTML and CGI, a model mosaic can be generated dynamically. In other words, a user can create a visual scene by picking parts.

A visual model mosaic is a conceptual graphical scene of a model. A visual model mosaic is a combination of 11 components that are GIFs. Each component represents a particular property of a model. A mosaic has three rows. The first row has three components: source term, initial condition, and model type. The second row has four components: inflow boundary condition, medium type, zone type, and outflow boundary condition. The last row also has four components: component type, dispersion type, flow type, and the legend of the mosaic. The geometric layout of a mosaic is shown in Figure 5-16.

source type		initial condition		model type
inflow boundary condition	medium type		zone	outflow boundary condition
component type	dispersion type	flow type		legend

**Figure 5-16 The layout of a visual model mosaic**

The combination of HTML and visual model mosaics provides a fast and easy way to generate a conceptual scene of a model. An example model mosaic of the J1DVG1014 model (van Genuchten and Alves, 1982) is shown in Figure 5-17.

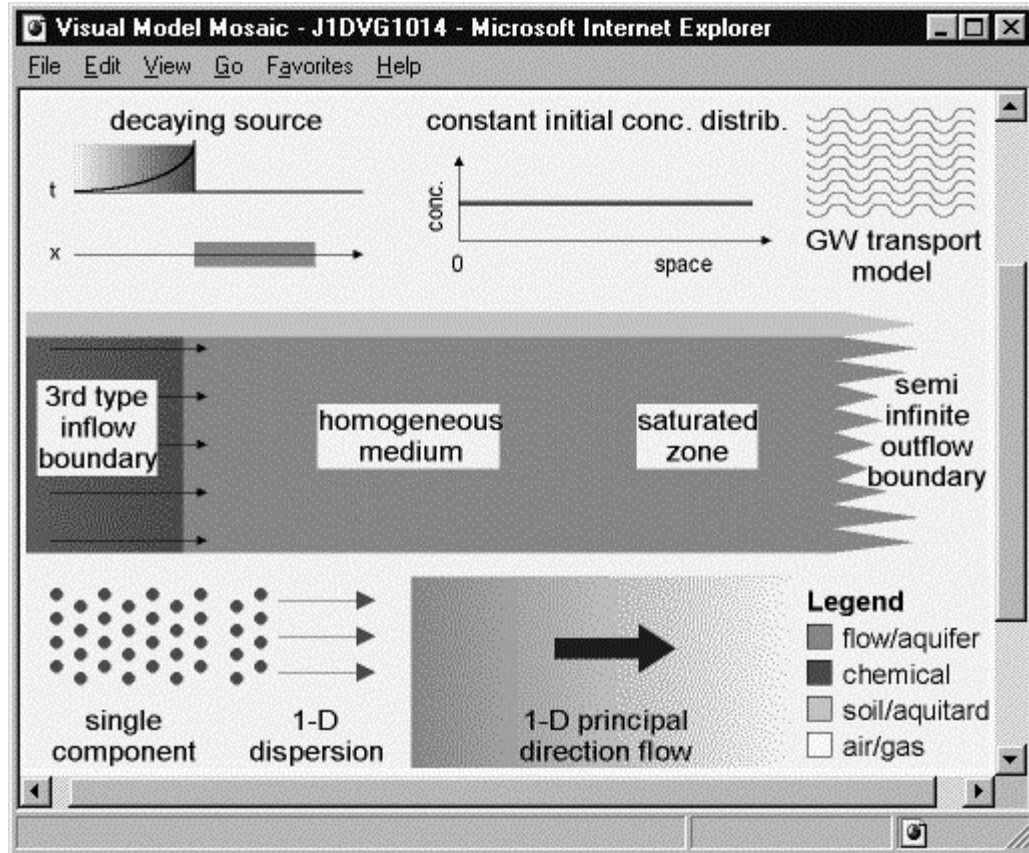


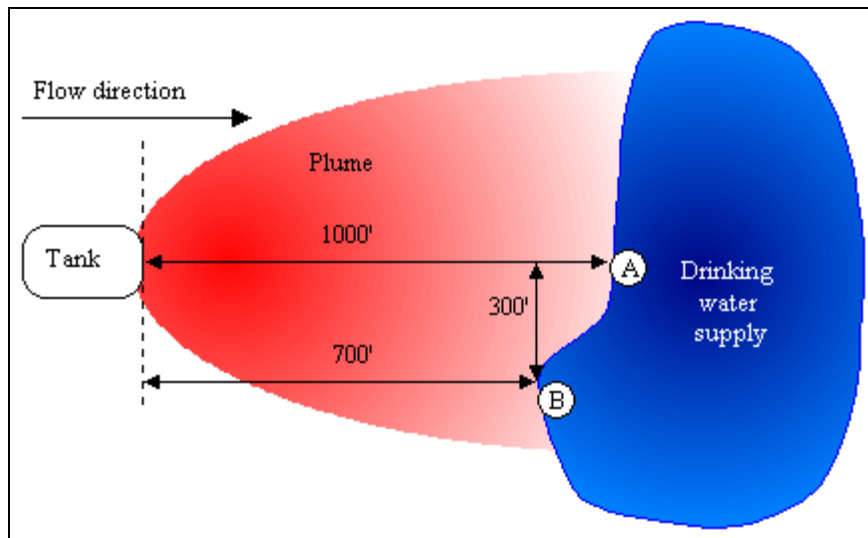
Figure 5-17 A screenshot of a visual model mosaic

## 5.7 Demonstration Session

A demonstration session is presented to illustrate the general features of the system. The hypothetical problem is a leak of gasoline from a storage tank for a period of 10 days, after which time it was halted and reported. A sand aquifer is assumed to underlie the site. The problem is to estimate the areal extent of dissolved benzene in the ground water at the time the leak was discovered. Figure 5-18 shows a leaking underground storage tank. The plume is moving toward a drinking water supply that is located in 1000 feet east of the underground tank. Local environmental agency needs to



find out how long will this plume reach the water supply. The maximum allowable dose is  $10 \text{ mg/m}^3$ .

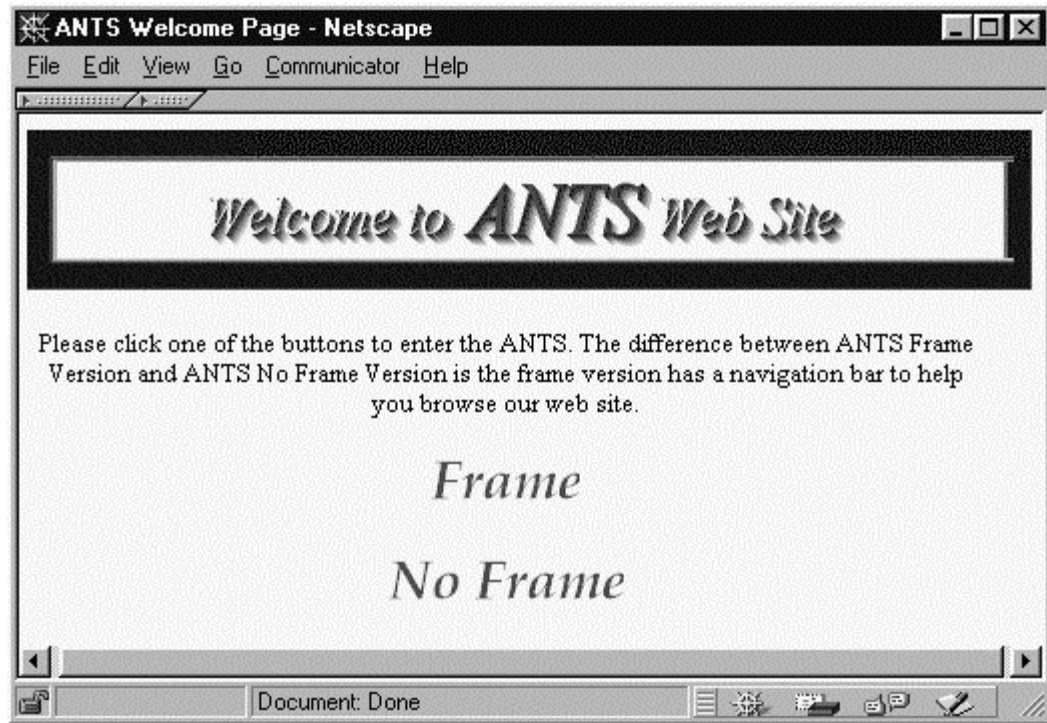


**Figure 5-18 A two-dimensional plane view of the problem**

To use the ANTS system, a user first connects the computer to the ANTS web site at

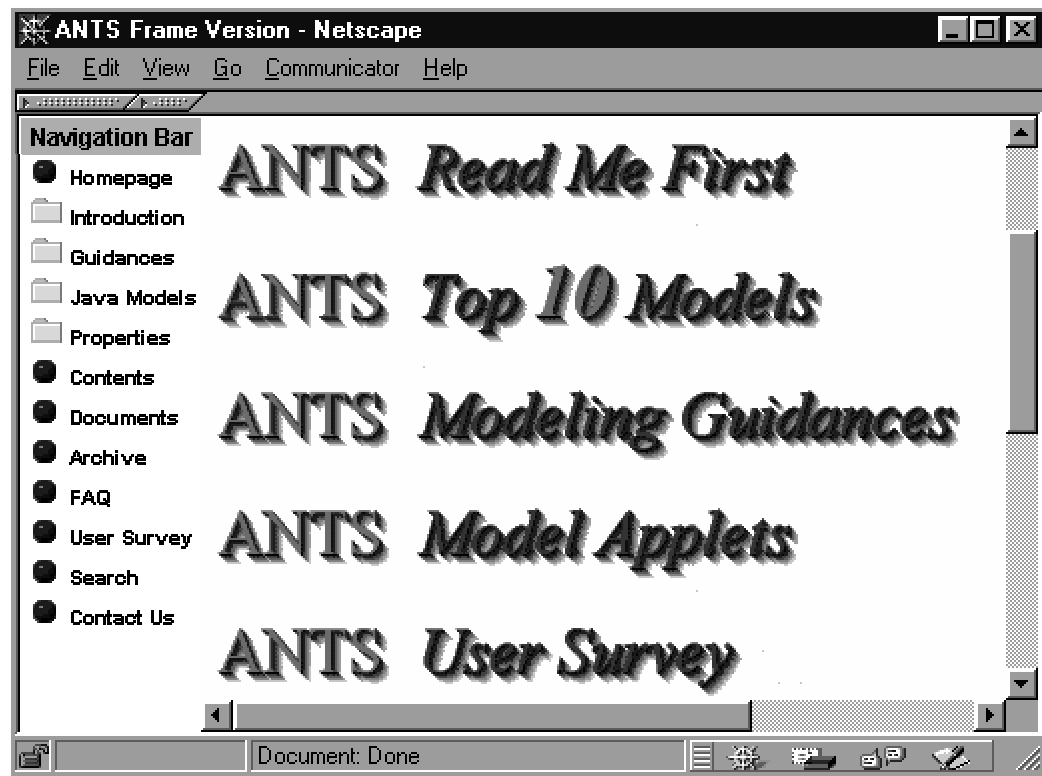
<http://cleveland1.cive.uh.edu/ANTS/ants-welcome.html>.

Figure 5-19 shows the ANTS welcome web page that should appear on the screen.



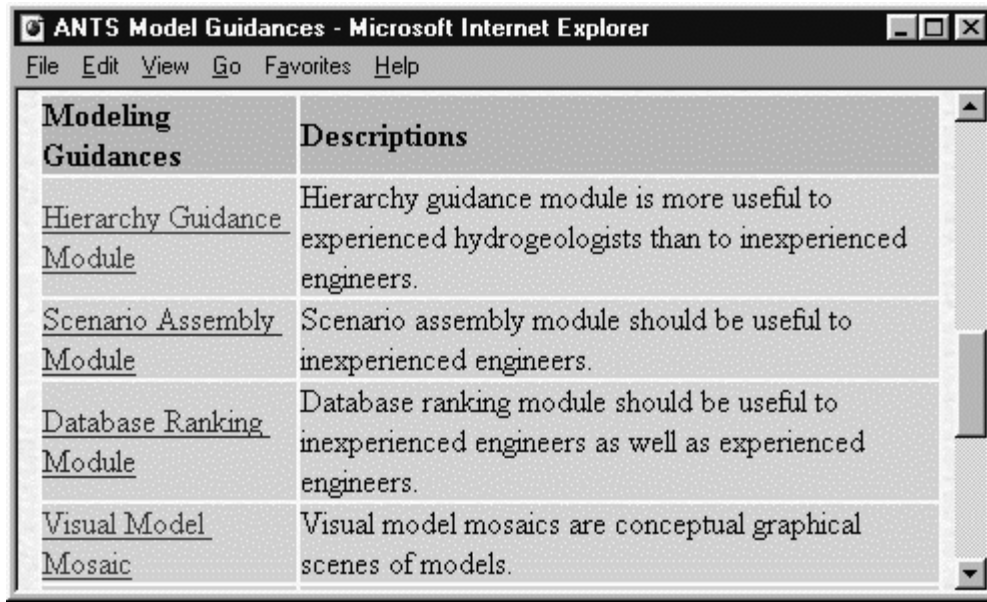
**Figure 5-19** A screenshot of the ANTS welcome web page

The user can choose to use the Frame version or the No Frame version of the ANTS system by clicking one of the buttons. The difference between the Frame version and No Frame version of the ANTS system is that the Frame version has a navigation bar to help a user browse the web site. If the user chooses the Frame version, the ANTS content window should appear as shown in Figure 5-20. The navigation bar is shown in the left side of the window. The user can use this navigation bar to browse the ANTS web site.



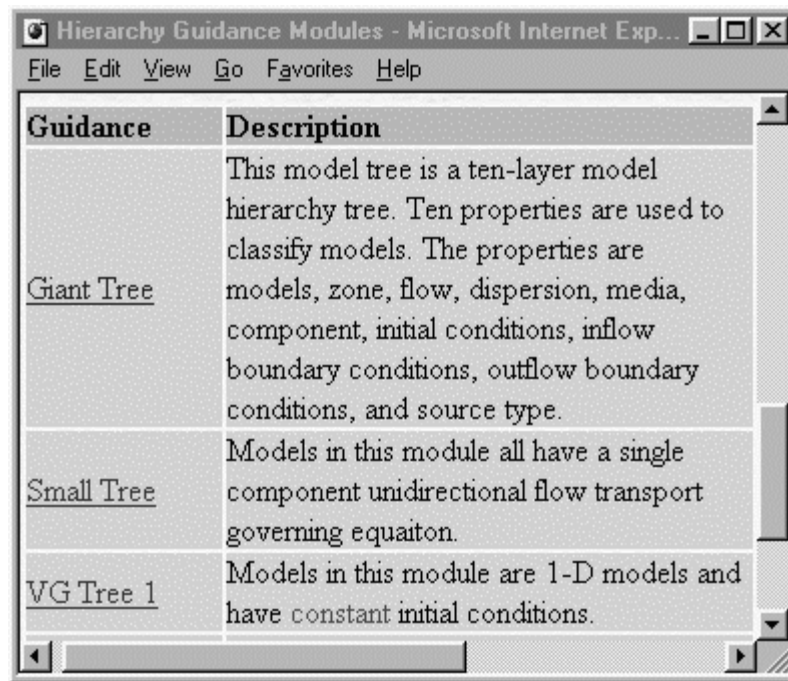
**Figure 5-20** A screenshot of the ANTS content web page

Next, The user clicks the ANTS *Modeling Guidances* item to choose a modeling guidance. The ANTS Model Guidances web page should appear as shown in Figure 5-21.



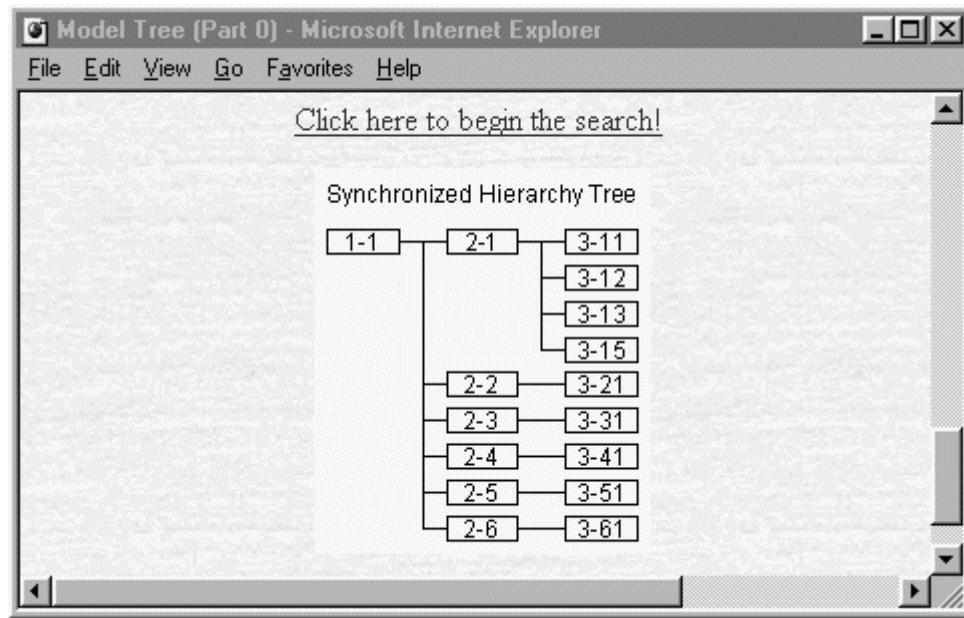
**Figure 5-21** A screenshot of the ANTS guidance web page

Next, the user chooses the [Hierarchy Guidance Module](#) Link. The Hierarchy Guidance Modules web page should appear as shown in Figure 5-22. First time users should read the page to understand the concept of the guidance modules.



**Figure 5-22** A screenshot of the hierarchy modules web page

Next, the user chooses the [Giant Tree](#) module to find an appropriate model. The following web page should appear. Read the page and click the [Click here to begin the search!](#) link to start a search.



**Figure 5-23** A screenshot of the synchronized hierarchical tree

To use the guidance, click the *1-1* button to advance to the next layer, as shown in Figure 5-24(a). By using the hierarchy modeling guidance, a possible model search path is shown in Table 5-2. The Java *J2DDR01P* model is chosen to solve the case. The subtrees involved in the search path is shown in Figure 5-24 series. A screen capture of the Java *J2DDR01P* model is shown in Figures 5-25 and 5-26.

**Table 5-2** A possible search path of the hierarchy modeling guidance

Steps	Actions	Reasons
Go to Subtree (1-1)	Choose Subtree (1-1)	The starting point
Choose Subtree (2-2)	Click <i>Link to 2-2</i> button to jump to Subtree (2-2)	A multidimensional dispersion model is needed.
Choose Subtree (3-21)	Click <i>Link to 3-21</i> button to jump to Subtree (3-21)	The aquifer is a homogeneous media.
Choose the Java <i>J2DDR01P</i> model	Click <i>J2DDR01P</i> button to activate the model applet	Contaminant source is a continuous source type.

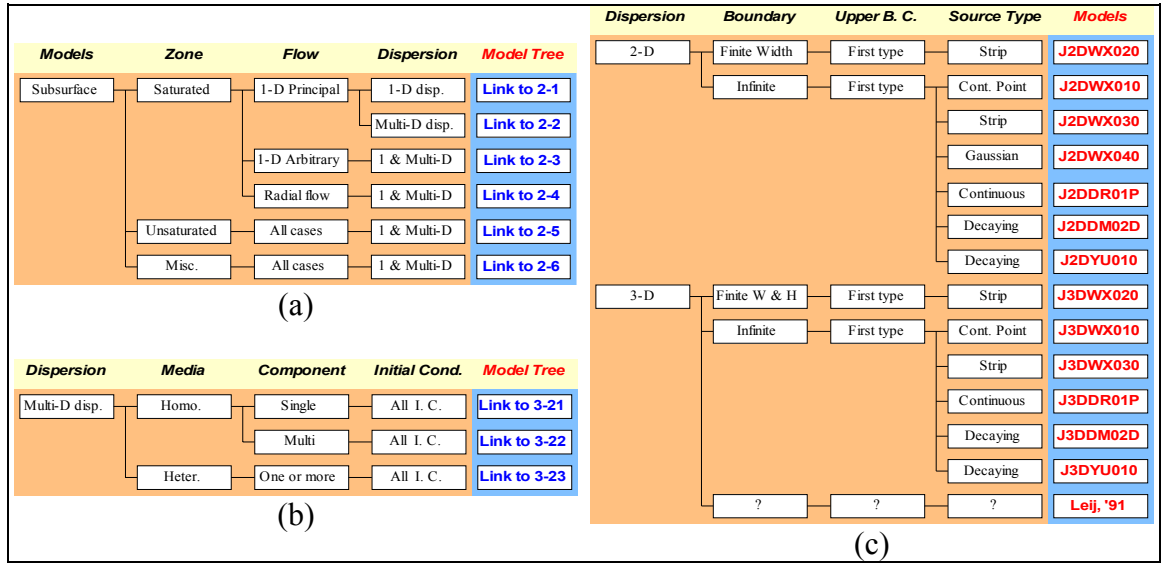
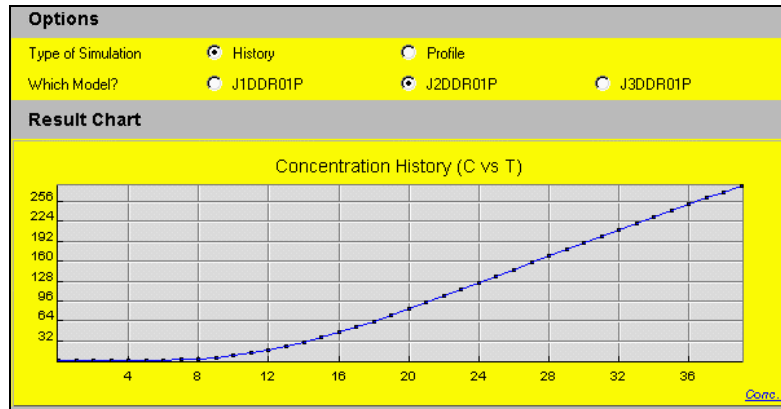


Figure 5-24 An example search path

ANTS Java Applet Model : JMDomenicoRobbins					
Parameters			Result		
Time Step	40	Dispersivity	60	10	7.86419
Starting Time	0	Dy	12	11	11.9545
Ending Time	40	Dz	0.1	12	16.9909
Obs. Point	100	Lambda	0.1	13	22.9257
	0			14	29.689
	0			15	37.1985
Y Location	0			16	45.3669
Z Location	0			17	54.1072
Aq. Width	80			18	63.3356
Aq. Thickness	60			19	72.9736
C0	1000			20	82.9489
Velocity	2			21	93.1959
				22	103.656
				23	114.275
				24	125.009
				25	135.814
				26	146.656
				27	157.504
				28	168.329

Run      Next      Reset

Figure 5-25 A snapshot of the Java J2DDR01P model



**Figure 5-26 A snapshot of the Java J2DDR01P model**

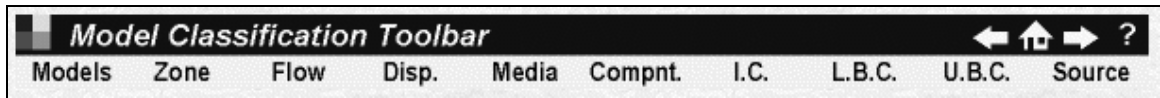
Table 5-3 contains the parameter values for two observation points. By using the *J2DDR01P* model, the times to reach 100 mg/m<sup>3</sup> in the observation points were computed. The results are 285 days and 290 days in the points A and B, respectively. The result data shown in the Figure 5-25 can be extracted to other programs (such as Microsoft Excel) for plotting.

**Table 5-3 Parameters and results of the example case**

Parameters	Point A	Point B
X Location	1000 ft	700 ft
Y Location	0 ft	300 ft
Aquifer Width	800 ft	800 ft
C0	1000 mg/m <sup>3</sup>	1000 mg/m <sup>3</sup>
Velocity	2 ft/day	2 ft/day
Dx	60 ft <sup>2</sup> /day	60 ft <sup>2</sup> /day
Dy	12 ft <sup>2</sup> /day	12 ft <sup>2</sup> /day
<b>Time to reach 10mg/m<sup>3</sup></b>	<b>285 days</b>	<b>290 days</b>

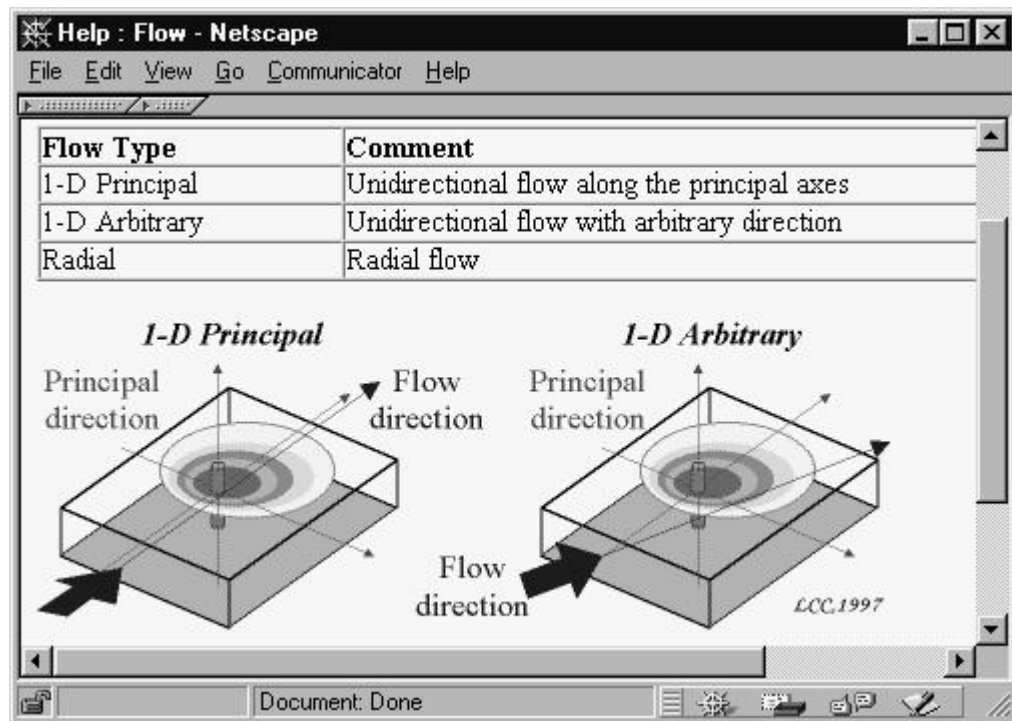
There is a help menu bar in every web page of the hierarchical tree, as shown in Figure 5-27.





**Figure 5-27** A screenshot of the help menu bar

The help web pages can be accessed by clicking items on the help menu bar. As an example, if the user clicks the flow button on the menu bar, the flow help web page should appear as shown in Figure 5-28.



**Figure 5-28** A snapshot of the flow help web page

# CHAPTER 6 CODE VALIDATION

## 6.1 Introduction

The computer code of an analytical solution of a groundwater contaminant transport model must be validated before being deployed. Without proper code validation, the analytical solution of the groundwater contaminant transport model could give erroneous and inconsistent results. Code validation is a procedure to determine whether or not the computer program (in these cases, Java applets) produces correct results when compared to accepted solutions. In developing the ANTS model library, a code validation was conducted to validate the analytical solution Java applet in the ANTS system.

The method used in the code validation is to compare the computed results from an ANTS model with the accepted results obtained for the same problem from other sources (such as the original reference journal for the particular model, numerical solutions, or other groundwater contaminant transport related literature).

## 6.2 Validation Process

Two sets of test cases were used to validate the ANTS models:

1. The basic cases are the example cases of from an ANTS model's reference. Every ANTS model has its own example cases. These cases are usually different from model to model.

1. The supplementary cases are a set of groundwater contaminant transport problems that were collected from groundwater contaminant transport related literatures. The problem set was used in the code validation process for some ANTS models.

The main goal of the code validation was to test that the ANTS models are correctly implemented in the system.

### 6.3 Reliability Index

The reliability of an analytical solution of an ANTS model is represented by a reliability index. The meanings of the reliability indexes are described in Table 6-1. The result of a test case is acceptable, if the following condition is met:

$$\left| \frac{R_t - R_o}{R_o} \right| \leq 0.05, \quad (6-1)$$

where  $R_t$  is the test result of the ANTS model and  $R_o$  is the accepted test result from the other source.

The possible reasons that a model has a low reliability index are as follows:

1. The incorrect implementation of the model is the main reason that the model has an undesirable reliability index. This type of error can be corrected over time as unreliable models are studied and corrected.
1. Undocumented limitations and constraints of the model are the other likely reason that the model created inconsistent results during the validation test.

**Table 6-1 The reliability index**

<b>Reliability index</b>	<b>Description</b>
AA	The model was tested by using the basic cases and the supplementary cases. The test results were acceptable. The model is very stable.
A0	The model was tested by using the basic cases. The test results were acceptable. The model is stable.
0A	The model was tested by using the supplementary cases. The test results were acceptable. The model is stable.
FA	The model was tested by using the basic cases and the supplementary cases. The results of the basic test cases were not acceptable. The results of the supplementary cases were acceptable. The model could produce inconsistent results under certain conditions. Use the model with caution.
AF	The model was tested by using the supplementary cases and the supplementary cases. The results of the basic test cases were acceptable. The results of the supplementary cases were not acceptable. The model could produce inconsistent results under certain conditions. Use the model with caution.
F0	The model was tested by using the basic cases. The results of some test cases were not acceptable. The model produces inconsistent results. Use the model with caution.
0F	The model was tested by using the supplementary cases. The results of some test cases were not acceptable. Use the model with caution.
FF	The model was tested by using the basic cases and the supplementary cases. The test results were not acceptable. Do not use this model.
00	The model has not yet been tested. Do not use this model.
NN	The model has not yet been implemented.

## **6.4 Model Reliability**

A model reliability matrix that describes the reliabilities of the ANTS models is shown in Table 6-2. This matrix identifies areas for future work: where the reliability of existing models can be improved and where new models can be added.

**Table 6-2 The model reliability matrix**

<b>Model name</b>	<b>Reliability index</b>	<b>Model name</b>	<b>Reliability index</b>
J1DBS03A	A0	J1DVG01B	AA
J1DBS03B	A0	J1DVG01C	AA
J1DBS04A	A0	J1DVG02B	AA
J1DBSO4B	A0	J1DVG02C	AA
J1DSR010	A0	J1DVG03B	AA
J1DSR020	A0	J1DVG03C	AA
J2DWX020	FA	J1DVG04B	AA
J2DWX010	FA	J1DVG04C	AA
J2DWX030	FA	J1DWX010	AA
J2DWX040	FA	J1DWX020	AA
J2DDRO1P	AA	J1DWX030	AA
J2DDM02D	AA	J1DWX040	AA
J2DYU010	AA	J1DDR01P	AA
J3DWX020	0A	J1DDM02D	AA
J3DYU010	AA	J2DCU010	AA
J3DEW020	0A	J2DCU020	AA
J1DVG01A	AA	J3DEW010	0A
J1DVG05B	AA	J3DEW030	0A
J1DVG05C	AA	J1DEL010	0A
J1DVG09A	AA	J1DEL020	0A
J1DVG07B	AA	J1DFR010	0A
J1DVG07C	AA	J1DFR020	0A
J1DVG14B	0A	J2DBR010	00
J1DVG14C	0A	J2DBR020	00
J1DVG03A	AA	J2DBR030	00
J1DVG11A	AA	J3DLE010	00
J1DVG15B	AA	J3DLE030	00
J1DVG13B	AA	J1DLP010	F0
J1DVG13C	AA	J1DLP020	F0
J1DVG02A	AA	J1DEL030	F0
J1DVG06B	AA	J1DZA010	F0
J1DVG06C	AA	J1DZA020	F0
J1DVG10A	AA	J2DZA010	F0
J1DVG04A	0A	J1DVGSP1	F0
J1DVG08B	0A	J1DVGSP2	F0
J1DVG08C	0A	J1DVGSP3	F0
J1DVG12A	0A	J1DVGSP4	F0

**Table 6-2 The model reliability matrix (continued)**

<b>Model name</b>	<b>Reliability index</b>	<b>Model name</b>	<b>Reliability index</b>
J1DVG15C	AA	Leij (1993)	NN
J1DVG16B	0A	Mironenko (1984)	NN
J1DVG16C	0A	Chen (1985)	NN
J1DVG05A	0A	Gureghian (1985)	NN
J1DVG06A	0A	Booker (1987)	NN
J1DVG07A	0A	Chen (1987)	NN
J1DVG08A	0A	Galya (1987)	NN
J1DVG09B	AA	Chen (1989)	NN
J1DVG09C	AA	Dillon (1989)	NN
J1DVG10B	AA	Brown (1990)	NN
J1DVG10C	AA	Yates (1990)	NN
J1DVG11B	AA	Bosma (1992)	NN
J1DVG11C	AA	Neville (1992)	NN
J1DVG12B	AA	Yates (1992)	NN
J1DVG12C	AA	Angelakis (1993)	NN
J1DBS01A	A0	Wallach (1993)	NN
J1DBS01B	A0	Illangasekare (1993)	NN
J1DBS02A	A0	Kool (1994)	NN
J1DBS02B	A0	Zaidel (1994)	NN
J3DWX010	0A	Domenico and Palciauskas (1982)	NN
J3DWX030	0A	Domenico and Palciauskas (1982)	NN
J3DDR01P	AA	Domenico and Palciauskas (1982)	NN
J3DDM02D	AA	Domenico and Palciauskas (1982)	NN
J3DEW040	0A	J1DHO010	NN

# CHAPTER 7 PRELIMINARY EVALUATION

## 7.1 Introduction

The purpose of this chapter is to provide a better sense of how and how well the system operates.

Decision-support systems must be verified and validated before being deployed. Without proper verification and validation, a decision-support system could give erroneous and inconsistent results. Verification is a procedure to check whether or not the system is functioning as intended. Validation is a procedure to determine whether or not the system performance meets application requirements in the real world. In developing the ANTS system, a preliminary evaluation was conducted to verify and validate the system.

There are several different methods to evaluate a decision-support system. One method is to compare results from the system with conclusive results obtained independently for the same problem from other systems. Another method is to set up a problem where a known correct answer is available in the form of a measurable, physical entity. The system was evaluated using the latter approach.

## 7.2 Evaluation Procedures

Test subjects were given the descriptions of seven contamination cases and were assigned the task of using the system to search appropriate models. A short survey with

16 questions was included in the evaluation. The short survey was used on verifying the results from the test cases.

The evaluation's main goals were to assess the present capabilities of the system and to identify those parts that required improvement. The evaluation also attempted to address the following issues:

1. Are the guidance modules in the system valid?
2. What is the most useful modeling guidance module?
3. Is the system sufficiently user-friendly so that it could be used without difficulty regardless of computer ability?
4. Which part of the system is most difficult?
5. What can be done to improve the system?
6. What are the effects of domain knowledge on the choices of the modeling guidance modules?

The testing procedure was neither rigorous nor comprehensive. This evaluation was a preliminary assessment of how the system could perform. The testers would only use the information that we provided. The test involved very small quantities of data.

### **7.3 Descriptions of Evaluation Cases**

The evaluation had two parts. The first part contains five cases. The testers had to find appropriate models for each case. The testers were required to answer two questions:

1. What model was chosen?
2. What modeling guidance module was used?



The descriptions of the cases are shown in Table 7-1. The main purpose of this part was to test the ability of the modeling guidance module to guide a user to an appropriate model.

**Table 7-1 Descriptions of the first five cases**

<b>Case</b>	<b>Description</b>
1	A fully penetrating well is injecting an instantaneous source into a confined aquifer. Assuming the aquifer is a homogeneous, isotropic aquifer with semi-infinite boundaries.
2	Same as Scenario 1. However, the simulation results of your chosen model does not match well with the result from field observation. One possible reason is that the dispersion of the aquifer may not be a constant value (i.e. a function of time or field distance.)
3	A fully penetrating well is injecting an exponential decaying discharge into a confined aquifer of uniform thickness that is a homogeneous, isotropic aquifer with infinite boundaries. Please choose a three-dimensional dispersion model to match the scenario.
4	A fully penetrating well is injecting a continuous constant discharge into a confined aquifer of uniform thickness that has a radial flow field.
5	A chemical is transported from a landfill to a homogeneous aquifer. The source injection can be thought as a constant plane (area) source injection.

The second part of the evaluation had two cases (Javandel et al. 1984). The descriptions of two cases are shown in Table 7-2. The main purpose of this part was to test the ability of the modeling guidance module in guiding a user to an appropriate model and to test the ability of testers to use the chosen model.

**Table 7-2 Descriptions of cases 6 and 7**

<b>Case</b>	<b>Description</b>
6	<p>Consider a shallow, homogeneous, isotropic aquifer with a thickness of 10 meters and a steady uniform average pore water velocity of 1 meter/day. A relatively long ditch cuts through this aquifer perpendicular to the direction of flow as shown in Figure 7-1(a). A nonreactive chemical waste is being continuously poured into the ditch. The rate of chemical waste inflow is about 0.1 m<sup>3</sup>/day per unit length of the ditch. The concentration of a certain nonreactive constituent in this waste is 10 kg/m<sup>3</sup>. A longitudinal dispersivity of 10 meters and porosity of 0.2 are assumed. Given these conditions, perform the following steps:</p> <ol style="list-style-type: none"> <li>1. find an appropriate analytical solution model to match this problem and</li> <li>2. determine how far downstream from the ditch a concentration of 0.1 ppm or more can be found after 1, 2, and 10 years.</li> </ol>
7	<p>Consider a relatively thin, shallow, homogeneous, isotropic aquifer having a steady, uniform seepage velocity of 0.1 meter/day. Liquid waste from a factory is being discharged into a surface impoundment 100 meters long and 5 meters wide as shown in Figures 7-1(b) and 7-1(c). The impoundment ditch is perpendicular to the direction of the groundwater flow. The waste liquid seeping from the bottom of this impoundment reaches the aquifer and creates a constant concentration of 1000 ppm of a certain solute species in the area beneath the ditch. The parameters are the same as the previous problem. The transverse dispersivity of the aquifer is about 1/10 the longitudinal value. Given these conditions, perform the following steps:</p> <ol style="list-style-type: none"> <li>1. find an appropriate analytical solution model to match this problem,</li> <li>2. estimating the variation of concentration downstream from the source 1 and 5 years after the contaminant reaches the aquifer, and</li> <li>3. given an allowable solute concentration for drinking water of 10 ppm, indicating the area of the aquifer downstream from the source where groundwater is considered to be contaminated 5 years after the solute reaches the aquifer.</li> </ol>

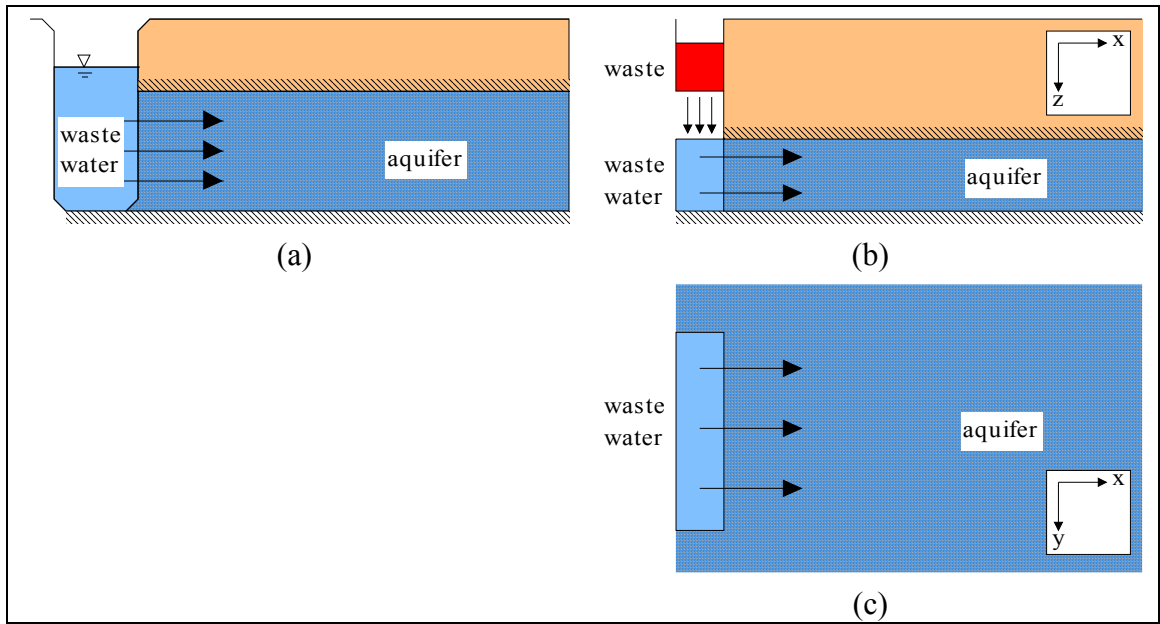


Figure 7-1 Layouts of cases 6 and 7

## 7.4 Test Subjects

The test subjects in the evaluation were classified into two areas, as shown in Tables 7-3 and 7-4. There were 13 test subjects in this evaluation. Nine subjects were graduate students. Most subjects obtained their knowledge from groundwater related classes.

Table 7-3 Background of test subjects

Background of the test subjects	Number
Academic Institute (school)	9
Government agency, petroleum company, consulting firm, others	4

**Table 7-4 Groundwater modeling knowledge source of test subjects**

<b>Groundwater modeling knowledge source of test subjects</b>	<b>Number</b>
School	9 (12 <sup>*</sup> )
Work experience	3
Short training class	1

\* Three test subjects marked two items.

Tables 7-5 and 7-6 show that nine test subjects had limited experience in groundwater contaminant transport modeling. These nine test subjects were classified as the novice test subjects (the novices). Four test subjects had more than three years experience in the domain field. These four test subjects were classified as the experienced test subjects (the experts).

**Table 7-5 Test subjects' experience in groundwater modeling**

<b>Experience in groundwater modeling</b>	<b>Number</b>
Less than 1 year	6
1 to 2 years	3
2 to 3 years	0
More than 3 years	4

**Table 7-6 Test subjects' domain knowledge**

<b>Domain knowledge</b>	<b>None</b>	<b>Novice</b>	<b>Average</b>	<b>Good</b>	<b>Expert</b>
Rate	0	3	6	3	1

Table 7-7 shows that all the test subjects had average or good computer skills. Ten out of 13 test subjects believed that they were capable in using spreadsheet programs. Nine out of 13 test subjects had average or good knowledge in using the

Internet. Only one test subject was a good programmer. The results show that a majority of the test subjects were casual computer users.

**Table 7-7 Test subjects' computer skills**

<b>Skills of</b>	<b>None</b>	<b>Novice</b>	<b>Average</b>	<b>Good</b>	<b>Expert</b>
Computer	0	0	7	6	0
Spreadsheet	0	3	3	7	0
Programming	0	7	5	1	0
Internet	0	4	5	4	0

The results in Tables 7-3, 7-4, 7-5, 7-6, and 7-7 suggest that a majority of the test subjects belonged to the NC user category that are novice engineers and casual computer users.

## **7.5 Evaluation Results**

### **7.5.1 Results of the Cases**

The results of the evaluation are shown in Tables 7-8, 7-9, and 7-10. Columns “Novice” and “Expert” in these tables contain the results of a particular module used or answered by the novice test subjects and the experienced test subjects, respectively.

Table 7-8 shows the results of the search modules used by the test subjects to find appropriate models. Sixty-five out of 98 models (66.3%) were chosen by the scenario module in the results of all the test subjects. Fifty-eight out of 70 models (82.9%) were chosen by the scenario module in the results of the novice test subjects. Nineteen out of 28 models (67.8%) were chosen by the hierarchy module in the results of the experienced test subjects.

**Table 7-8 Modules used by test subjects in finding appropriate models**

Case Domain	Hierarchy		Scenario		Ranking		Pick from list	
	Novice	Expert	Novice	Expert	Novice	Expert	Novice	Expert
1	3	2	7	2	0	0	0	0
2	2	3	8	1	1	0	0	0
3	1	3	9	1	0	0	0	0
4	0	4	11	0	0	0	0	0
5	1	2	9	1	0	0	0	1
6	1	2	8	1	0	0	0	1
7	2	3	6	1	0	0	1	0
<b>Subtotal</b>	<b>10</b>	<b>19</b>	<b>58</b>	<b>7</b>	<b>1</b>	<b>0</b>	<b>1</b>	<b>2</b>
<b>Total</b>	<b>29</b>		<b>65</b>		<b>1</b>		<b>3</b>	

Table 7-9 shows the results of the models chosen by the test subjects. Some test subjects used more than one module to find a model for each case. The results of all the test subjects show that 71 out of 95 (74.7%) chosen models were either the correct models or acceptable models. The results of the novice test subjects show that 47 out of 71 (66.2%) chosen models were either the correct models or acceptable models. The results of the experienced test subjects show that 22 out of 24 (91.7%) models were either the correct models or acceptable models.

**Table 7-9 Models chosen by test subjects**

Case	Correct model		Acceptable model		Wrong model		No match	
	Novice	Expert	Novice	Expert	Novice	Expert	Novice	Expert
1	5	3	3	1	2	0	0	0
2	4	4	0	0	4	0	2	0
3	6	4	0	0	2	0	2	0
4	7	4	0	0	3	0	0	0
5	5	4	0	0	3	0	1	0
6	8	3	0	1	1	0	0	0
7	5	4	0	0	2	0	2	0
<b>Subtotal</b>	<b>44</b>	<b>22</b>	<b>3</b>	<b>2</b>	<b>17</b>	<b>0</b>	<b>7</b>	<b>0</b>
<b>Total</b>	<b>66</b>		<b>5</b>		<b>17</b>		<b>7</b>	

Table 7-10 contains the results of the test subjects' answers of cases 6 and 7. The results of all the test subjects show 15 out of 26 (57.7%) answers were correct or reasonable. The results of the novice test subjects show 9 out of 18 (50%) answers were correct or reasonable. The results of the experienced test subjects show six out of eight (75%) were correct or reasonable.

**Table 7-10 Answers by test subjects**

Case	Correct answers		Reasonable answers		Incorrect answers		No answer	
	Novice	Expert	Novice	Expert	Novice	Expert	Novice	Expert
6	5	3	0	0	4	1	0	0
7	1	3	3	0	3	1	2	0
<b>Subtotal</b>	<b>6</b>	<b>6</b>	<b>3</b>	<b>0</b>	<b>7</b>	<b>2</b>	<b>2</b>	<b>0</b>
<b>Total</b>	<b>12</b>		<b>3</b>		<b>9</b>		<b>2</b>	

### **7.5.2 Result Analysis**

The results in Table 7-8 suggest that the scenario module was the most used guidance module among the novice test subjects. However, the hierarchy module was the most used module among the experienced test subjects. The different choices between the novice test subjects and the experienced test subjects may indicate that the hierarchy module is more suitable for the experienced domain users. These results also indicate that domain knowledge remains an important factor in selecting an appropriate guidance module.

The results in Table 7-9 suggest that the guidance modules were effective in choosing appropriate models for the novice test subjects and the experienced test subjects.

The results in Table 7-10 suggest that many test subjects did not have sufficient knowledge to find the correct solutions for two given cases, even though they were able to find the appropriate models. Most experienced test subjects were able to find the correct solutions for the given cases.

Although a majority of the test subjects had average computer skills as shown in Table 7-7, they were able to find the appropriate models for the test cases. These results indicate that computer skills were not an important factor in choosing an appropriate guidance module in this system.

### **7.5.3 Responses from Test Subjects**

The responses from the test subjects are shown in this section. Most test subjects thought the ANTS system was useful or very useful as shown in Table 7-11. Most test



subjects thought the design of the ANTS system was good or excellent as shown in Table 7-12.

**Table 7-11 Test subjects' opinions regarding usefulness of ANTS**

<b>Usefulness of ANTS</b>	<b>Don't know</b>	<b>Not useful</b>	<b>Sort of</b>	<b>Useful</b>	<b>Very useful</b>
ANTS	1	0	0	9	3

**Table 7-12 Test subjects' rates of ANTS**

<b>Rate of ANTS</b>	<b>Not very useful</b>	<b>Could be better</b>	<b>Average</b>	<b>Good</b>	<b>Excellent</b>
Interface	0	1	1	6	5
Guidance Modules	0	1	1	9	2
Java models	0	1	0	8	4
User friendliness	0	1	4	7	1
Model Library	0	1	3	7	2

The users' choices of the best features of the system are as follows:

1. The guidance modules were powerful and flexible. In most cases, the test subjects were able to find appropriate models by using one of the guidance modules.
2. The test subjects were very comfortable with the user interface of the system.
3. The test subjects found that the visual graphs and the animated graphs were very helpful in explaining model properties
4. The test subjects found that the system could be easily accessed via the Internet.

The test subjects suggested that there were some problems in the system. The problems and their solutions are as follows:

1. **Problem:** The scenario module seemed to be the best module for a user who is seeking an appropriate model. The problem was that the scenario module sometimes gave no results.

**Solution:** There was no appropriate model for some particular scenario combinations. The user could use the hierarchy module or the ranking module to find a model for the particular case.

2. **Problem:** The system needs to be more user-friendly by providing a step-by-step explanation on the importance and definition of model parameters.

**Solution:** The focus of the system is to choose an appropriate model. The system does not address the problem of setting up parameters. However, there are visual graphs and animated graphs available on the system. A step-by-step tutorial is also available on the system.

3. **Problem:** There was no output printing facility for Java applets.

**Solution:** Web browsers such as Netscape Navigator and Microsoft Internet Explorer can not yet print a Java applet. The solution of the problem is to use a third party screen capture program to capture and print the image. Numerical values in the Java applet can be cut-and-pasted into other programs.

4. **Problem:** Too many tools were provided to the users at the same time. The users may have difficulties to manage them.

**Solution:** This problem is sometimes called information overflow. The solution is to use the step-by-step tutorial that is available on the ANTS web site to understand the concept of the system.

5. **Problem:** There was no easy way to navigate though all web pages.

**Solution:** A navigation bar was added to the web site. The navigation bar gives the users an opportunity to navigate through the system from any page.

6. **Problem:** Most analytical solution models in the model library were over simplified for field cases.

**Solution:** Analytical solution models are simplified models of the field cases. The main reason to build the analytical solution library is to let the users have choices in matching a field problem to an appropriate model.

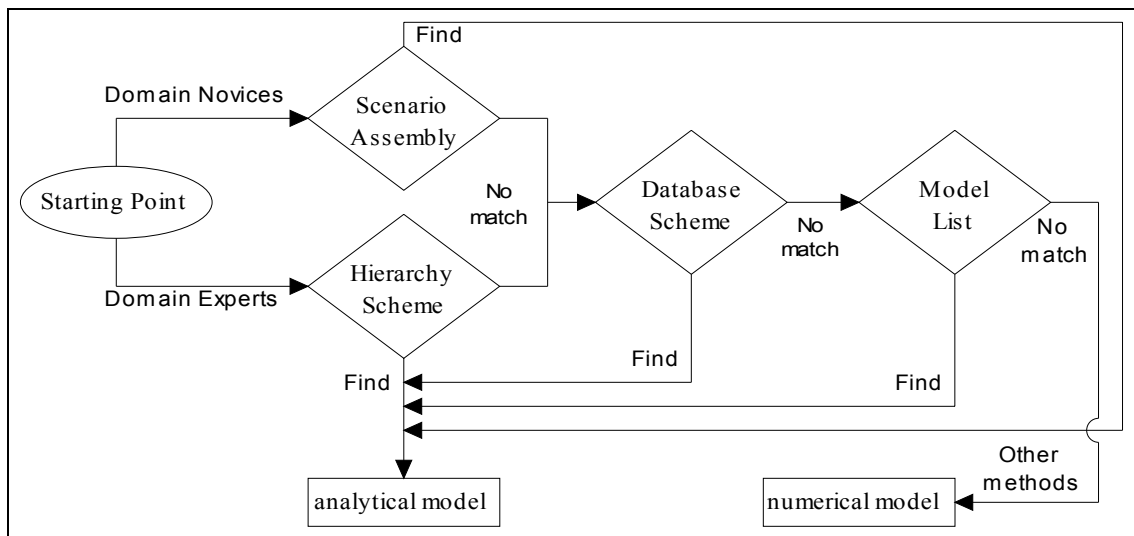
## 7.6 Target User Matrix

A target user matrix was created from the results of the evaluation as shown in Table 7-13. The target user matrix describes the degree of usefulness of the guidance modules to the four user groups. The number “1” means that the module is intended for the user group, so the module should be very useful for the group. The number “2” means that the module is not intended for the user group, but the module could be useful to the group. The number “3” means that the module is not intended for the user group. This matrix is used as a quick reference to choose a guidance module.

**Table 7-13 The target user matrix**

<b>User groups</b>	<b>EP</b>	<b>EC</b>	<b>NP</b>	<b>NC</b>
<b>Hierarchy module</b>	1	1	3	3
<b>Ranking module</b>	1	1	2	2
<b>Scenario module</b>	2	2	1	1
<b>Model visualization</b>	2	2	1	1

With several guidance modules available in the system, what guidance module should a user apply first? Figure 7-2 displays a flowchart of the recommended model search steps.



**Figure 7-2 The recommended model search steps**

The recommended search paths can be divided in two ways. For domain experts, the search steps are as follows:

1. A user first uses the hierarchy module to locate a model. If an appropriate model is found, the user can use the model to solve a groundwater contaminant transport problem. If not, go to the next step.
2. The user can use the ranking module to find a model. If an appropriate model is found, the user can use the model to solve the groundwater contaminant transport problem. If not, go to the next step.
3. The user looks at the list of the model library. If an appropriate model is found, the user can use the model to solve the groundwater contaminant transport problem. If

an appropriate model can not be found, the user should either simplify his problem or use a numerical model to solve the problem.

For domain novices, the recommend search steps are as follows:

1. A user first uses the scenario assembly module to assemble a scenario to find a model. If an appropriate model is found, the user can use the model to solve the groundwater contaminant transport problem. If not, go to the next step.
2. The user can use the ranking module to find a model. If an appropriate model is found, the user can use the model to solve the groundwater contaminant transport problem. If not, go to the next step.
3. The user looks at the list of the model library. If an appropriate model is found, the user can use the model to solve the groundwater contaminant transport problem. If an appropriate model can not be found, the user should either simplify his problem or use a numerical model to solve the problem

## **7.7 Summary**

A summary of the evaluation result analysis is as follows:

1. A majority of the test subjects belonged to the NC user category.
2. The guidance modules in the system were effective. In most cases, the test subjects were able to find an appropriate model. The results indicate that the system does match our expectation in finding appropriate models for the test cases.
3. The scenario module was the most used module in the system for the inexperienced domain users. The hierarchy module was more suitable for the experienced domain users. The results suggest that the degree of knowledgeableability of domain experience

can affect the system users' decisions in choosing a guidance module. The results also confirm the assumption made in Chapter 3 (Conceptual Framework) - an experienced user of the domain field approaches a contaminant transport problem different to a domain novice does.

4. The results of the evaluation indicate that computer skills were not an important factor in choosing an appropriate guidance module. The reason is that most users were familiar with the Internet. Since the ANTS system is an Internet-based system, they had no problem to use a web browser to explore the system.
5. The results suggest that the Internet-based system was well designed, so the system was used without difficulty regardless of computer ability and domain experiences. The system is sufficiently user-friendly.
6. The weak link of the system is how to setup a chosen model. As mentioned in the objectives and scope of the research, the system was not planned to address the problem in setting up model parameters. The results also suggest that the domain experts are more likely to setup a chosen model right.
7. Most test subjects agreed that the ANTS system could be a very useful tool in the field of groundwater contaminant transport modeling.

# CHAPTER 8 CONCLUSIONS

## 8.1 Objective Achievements

During the course of this research, the following objectives were achieved:

1. More than 100 analytical solutions of groundwater contaminant transport models were studied. The models were characterized into sets of property keywords. The results of the model characterization were stored in a model database. The model database is a very useful resource in the field of groundwater contaminant transport modeling.
2. A user survey was conducted to understand the needs of the potential users. The potential users were classified into a two-layer four-element user classification based on the results of the survey. Because the designs of the ANTS guidance modules was based on the needs of the four user groups in the user classification, the test subjects in the evaluation found that the ANTS guidance modules were very helpful in finding an appropriate model.
3. A modeling guidance system, ANalytical contaminant Transport modeling guidance System (or ANTS), for prediction of contaminant transport in groundwater was built. The ANTS system provides guidance modules for a user to select a most appropriate analytical contaminant transport model from a model library to predict the outcome of a groundwater contaminant transport problem. The system includes a model library that contains a large collection of analytical solutions of

contaminant transport models. Because the ANTS system was developed by using the Internet-based development toolkit, the system automatically inherits the advantages of Internet-based systems. The system is accessible by any user via the Internet. The system uses a web browser as its front end. The installation or maintenance of the system is performed on the server machine only. The system offers referable reusability. It means that any component of the system can become a link by the other web sites. Because the ANTS system has a hierarchical modular system structure, any modules of the ANTS system can be modified without changing the whole system.

4. A preliminary evaluation was conducted to validate the system. The results indicate that the system does match our expectation in finding an appropriate model for a groundwater contaminant transport case. A majority of the test subjects were able to find appropriate models for the test problems. The scenario module was the most used module in the system for the inexperienced domain users. The hierarchy module was more suitable for the experienced domain users. The results of the evaluation also indicate that computer skills were not an important factor in the system. The system is sufficiently user-friendly. The results of the evaluation suggest that the weak link of the system is how to setup a chosen model.

## **8.2 Innovations and Contributions**

ANTS is the first application to integrate groundwater contaminant transport modeling, decision-support systems, and Internet programming. There were many



innovations and contributions regarding the ANTS project to the field of groundwater contaminant transport modeling. The major ones are outlined below:

1. A new approach to model groundwater contaminant transport problems was introduced in this research. In the approach, a model is a result of a decision process. In the process, a user makes a series of decisions through a provided guidance module to find an appropriate model. Because groundwater contaminant transport models were divided to sets of model property keywords successfully, it is possible to identify a model by answering a series of questions. The approach worked very well for this research and may be applicable to other areas of natural resources modeling.
2. During the process of the model classification, several areas that have not yet had analytical solutions of groundwater contaminant transport models were identified. These areas can be used as research topics for other researchers.
3. A model classification scheme was introduced in the research. The scheme successfully classified groundwater contaminant transport models to sets of model property keywords. The scheme is applicable to other areas of natural resources modeling.
4. The ANTS system is the first Internet-based modeling guidance system. The ANTS system also has the first Internet-based groundwater contaminant transport model library. The significance of the system is not only that the ANTS system is the first Internet-based modeling system, but also one of the important web sites of sharing groundwater contaminant transport resources. The ANTS system marks the

beginning of modeling groundwater contaminant transport problems over the Internet. More than 600 users have accessed to the ANTS web site.

5. The evaluation suggested that the strategies of the guidance modules developed in the system were effective. These strategies are applicable to other areas of natural resources modeling.
6. The concept of the visual characteristics that show animated visual scenes is a significant contribution because of its potential usefulness in active-learning exercises and in distance instruction of groundwater contaminant transport modeling. Domain novices could learn the basic concepts of groundwater contaminant transport modeling by viewing these visual characteristics.

### **8.3 Problems Encountered**

It is obvious that the development of a decision-support system requires the devotion of great deal of time and effort. There were a lot of difficulties encountered during the research, and the major ones are listed below:

1. The research was conducted in a relatively new field. There was not much previous work in the Internet (or the World Wide Web), because the Internet-based development tools were not available until 1995. The rapid evolution of the Internet forced changes of the project directions during the course of the research. Three development toolkits were used to develop the system. The author had to adapt different concepts when different development toolkits were used. Some analytical solution models had been reprogrammed several times to be used in the current system.

2. The knowledge gathering process was the most difficult and time consuming part of the research. Only a limited number of previous studies tried to classify groundwater contaminant transport models. The limitations and constraints of many models were nowhere to be found. A few models did not have clear descriptions regarding the layouts of the models. Some analytical solution models could not be verified against their example cases, because there were insufficient parameters given in their literatures.
3. Finding potential test subjects was a difficult task. The author sent out 80 evaluation forms. There were only 17 users returned their evaluation forms. Only ten users completed all questions. Recruiting test subjects from the Internet was equally difficult. Although there were more than 600 hits on the ANTS web site, only three people completed all questions.
4. The ANTS system was developed by using the Internet-based development toolkit. A Java-enabled web browser is the only requirement to access the system. The system inherits advantages of an Internet-based system as well as limitations of an Internet-based system. A major limitation of the system is that most web browsers such as Netscape Navigator and Microsoft Internet Explorer can not yet print Java applets.

## **8.4 Future Extensions and Enhancements**

In the further development of the ANTS system, some suggestions are as follows:

1. The approach is potentially applicable to other areas of natural resources modeling. The potential advantages over other approaches to natural resources modeling are in: facilitating rapid model development and modification and providing a high degree of re-usability of models by sharing resources over the Internet.
2. This research did not answer a modeling problem: how to set up a model correctly? An Internet-based parameter assistant module is a logic choice to enhance the capability of the ANTS system.
3. Another interesting extension would be to combine the ANTS system with a specialized decision support system such as a GIS. The focus of GISs is on data selection, aggregation, parameter estimation, and output. A combination of GISs and the ANTS system could become capable of predicting groundwater contaminant transport for a region automatically.
4. No numerical groundwater contaminant transport model is available in the ANTS system. With a numerical model, ANTS could be used to solve complicated field problems.

## **8.5 Summary**

This chapter discussed objective achievements, innovations and contributions, problems encountered, and future extensions and enhancements for the ANTS system. Given the population of the Internet, the Internet-based ANTS system would be of tremendous use to environmental engineers, hydrogeologists, government regulation agencies, groundwater related professionals, and anybody interested in learning about groundwater contaminant transport modeling.

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## APPENDIX A GLOSSARY

### Computer Related

**ActiveX** Active X is based on OLE (Object Linking and Embedding), a technology developed by IBM and licensed by Microsoft. Microsoft has repackaged OLE in a new box called ActiveX. ActiveX is platform dependent. (Sun Microsystems, 1996)

**ARPANE** Advanced Research Projects Agency Network A pioneering long haul network funded by ARPA. It served as the basis for early networking research as well as a central backbone during the development of the Internet. The ARPANET consisted of individual packet switching computers interconnected by leased lines.

**Common Gateway Interface (CGI)** The Common Gateway Interface, or CGI, is a standard for external gateway programs to interface with information servers such as HTTP servers. A plain HTML document that the Web daemon retrieves is static, which means it exists in a constant state: a text file that doesn't change. A CGI program, on the other hand, is executed in real-time, so that it can output dynamic information. Basically any Webpage containing a form will require a CGI script or program to process the form inputs. (from the CGI reference <http://hoohoo.ncsa.uiuc.edu/cgi/overview.html>)

**CGI vs. Java** CGI and Java are fundamentally different, and for most applications are NOT interchangeable. Neither are the two isomorphic: you could in principle write a CGI program in Java, although it is hard to think of an instance where this would be the

best choice. CGI is a mechanism for running programs on a WWW server. Typical applications include accessing a database, submitting an order, or posting messages to a bulletin board. Java enables programs to run on the Client machine, and is suited to such tasks as detailed manipulation of an image. Alternatives to Java may include the X windows client/server protocol, use of browser plugins and helper applications, and other clientside languages such as SafeTCL and perl/penguin. In certain instances the two may be combined in a single application: for example a Java applet to define a region of interest from a geographical map, together with a CGI script to process a query for the area defined.

**Microsoft FrontPage Server Extensions** A set of programs and scripts that support FrontPage authoring and extend the functionality of a Web server.

**Geographic Information System (GIS)** A Geographic Information System, or GIS, is a computer system for managing spatial data. The word geographic implies that locations of the data items are known, or can be calculated, in terms of geographic coordinates (latitude, longitude). The word information implies that the data in a GIS are organized to yield useful knowledge, often as colored maps and images, but also as statistical graphics, tables, and various on-screen responses to interactive queries. The word system implies that a GIS is made up from several interrelated and linked components with different functions. Thus GIS have functional capabilities for data capture, input, manipulation, transformation, visualization, combination, query, analysis, modeling and output. A GIS consists of a package of computer programs with a user interface that provides access to particular functions. The purpose of GIS is to provide support for making decisions based on spatial data. (Bonham-Carter, 1994).

**Hypertext and Hypermedia** The operation of the Web relies on hypertext as its means of interacting with users. Hypertext is basically the same as regular text - it can be stored, read, searched, or edited - with an important exception: hypertext contains connections within the text to other documents. Hypermedia is hypertext with a difference - hypermedia documents contain links not only to other pieces of text, but also to other forms of media - sounds, images, and movies. Images themselves can be selected to link to sounds or documents.

**HyperText Markup Language (HTML)** HyperText Markup Language, or HTML, is a simple markup system used to create hypertext documents that are portable from one platform to another. HTML documents are SGML documents with generic semantics that are appropriate for representing information from a wide range of applications. HTML markup can represent hypertext news, mail, documentation, and hypermedia; menus of options; database query results; simple structured documents with in-lined graphics; and hypertext views of existing bodies of information. HTML has been in use by the World Wide Web (WWW) global information initiative since 1990.

**Java** Java is a language developed by Sun Microsystems which allows World Wide Web pages to contain code that is executed on the browser. It is a general-purpose concurrent class-based object-oriented programming language, specifically designed to have as few implementation dependencies as possible. Java allows application developers to write a program once and then be able to run it everywhere on the Internet.

**Java vs. ActiveX** ActiveX allows routines written in multiple languages (C, C++, Basic, and so on) to co-exist within a single application on a single platform (Microsoft

Windows). Java allows a single application to run on multiple platforms (Microsoft Windows, Macintosh, UNIX, Solaris, JavaOS, and so on). (Sun Microsystems, 1996)

**NSFNET** National Science Foundation Network The NSFNET is a highspeed "network of networks" which is hierarchical in nature. At the highest level is a network that spans the continental United States. Attached to that are mid-level networks and attached to the mid-levels are campus and local networks. NSFNET also has connections out of the U.S. to Canada, Mexico, Europe, and the Pacific Rim. The NSFNET is part of the Internet.

**Open Database Connectivity (ODBC)** A standard protocol for accessing information in SQL database servers, such as Microsoft SQL Server. You can install ODBC drivers that enable Microsoft Access to connect to these SQL database servers and access the data in the SQL databases.

**Structured Query Language (SQL)** The Structured Query Language, or SQL, that is marketed by IBM is derived from the SEQUEL language initially designed at IBM San Jose. A first version called SQUARE was designed as a research language to implement relational algebra with English sentences. A working group of ANSI standardized the SQL language for relational database manipulation. The SQL language may be considered as a particular syntax of relational algebra expressions, with complex conditions. Common SQL functions include select, insert, delete, and update.

**Virtual Reality Modeling Language (VRML)** VRML, the Virtual Reality Modeling Language, is an attempt to extend the web into the domain of three-dimensional graphics. VRML "worlds" can depict realistic or otherworldly places, which can contain objects that link to other documents or VRML worlds on the web. VRML is a file

format for describing 3D interactive worlds and objects. It may be used in conjunction with the World Wide Web. It may be used to create three-dimensional representations of complex scenes such as illustrations, product definition and virtual reality presentations. VRML is capable of representing static and animated objects and it can have hyperlinks to other media such as sound, movies, and image. Interpreters (browsers) for VRML are widely available for many different platforms as well as authoring tools for the creation VRML files.

**Visual Basic** Visual Basic (often abbreviated VB) is a programming language initially developed by Microsoft to provide programmers with a quick and easy method of developing Windows applications. VB provides the programmer with an integrated environment where one can use tools to create a point and shoot interface and use event driven programming techniques. A developer can quickly and easily create a user interface, then write the code to respond to specific events which occur as a result of user input. The integrated development environment (IDE) has sophisticated editing and debugging tools which allow you to attach code quickly to the interface created for each event which is applicable for any type of object on the interface.

**World Wide Web (Web or WWW)** The World Wide Web, Web or WWW, can be thought as the graphical Internet service that provides a network of interactive documents and the software to access them. It is based on documents called pages that combine text, pictures, forms, sound, animation, and hypertext links called hyperlinks. To navigate the Web, users surf from one page to another by pointing and clicking on hyperlinks in text or graphics. The Web has been used as a helpdesk, marketplace, art

gallery, library, community center, school, publishing house, and many other uses (Microsoft, 1997).

**Web Browser** A web browser is a program that navigates through the Web and displays pages. The web browser requests a page from a server based on its Internet address. It retrieves the document from the server and displays the contents.

**Web Server** A server on the Web stores pages and sends them to a browser when requested. Web servers are not simply file servers, however. They also run programs, called Common Gateway Interface (CGI) programs, based on requests from web browsers.

## **Groundwater Contaminant Transport**

**Volume-averaged vs. Flux-averaged concentrations (Dillon, 1989)** Volume-averaged concentration is the average concentration within a representative element (or unit) volume of porous medium. Flux-averaged concentration is the average concentration of water flowing through an element and reflects the range of velocities (hydrodynamic longitudinal dispersion) along flow paths between a source and an observation location. The difference between volume- and flux-averaged concentrations increases as the dispersion coefficient increases. The solute concentration of a sample from a bore or aquifer discharge point is most accurately described by a flux-averaged concentration.



# **APPENDIX B SURVEY RESULTS**

## **Introduction**

The purpose of this survey was to understand the computer skills and groundwater contaminant transport modeling knowledge of the potential users. A questionnaire was designed and intended for the general public and expert users who have been interacting with groundwater contaminant transport problems (industrial pollution cases, laboratory experiments, class work, etc.). The questionnaire was taken by a selected group of environmental engineering faculties and graduate students in the University of Houston. It was part of a research project on modeling contaminant transport problems on the Internet. The results of the survey that are presented in this section were analyzed and used to modify the potential user classification of the ANTS project.

One thing should be mentioned here is that several respondents picked more than one answer for some questions. It is possible that total percentages of answers are more than one hundred percents for some questions.

## **General Information**

A majority of the respondents were environmental engineering graduate students in the University of Houston. Most respondents obtained their knowledge of groundwater contaminant transport from classrooms rather than from their work

experience. All respondents had less than three years study or work experience in the domain field.

**Table B-1 The results of the survey - general information**

<b>Question</b>	<b>Number</b>	<b>Percentage (%)</b>
<b>What kind of company are you working for?</b>		
Academic research institute	11	64.71
Government agency	2	11.76
Petroleum company	0	0.00
Consulting firm	1	5.88
Self-employed	1	5.88
Other, Please specify:	2	11.76
<b>What is your job?</b>		
Professor / Researcher	2	11.76
Student	12	70.58
Civil engineer	1	5.88
Environmental engineer	2	11.76
Chemical engineer	0	0.00
Geologist	0	0.00
Water resource specialist	0	0.00
Other, Please specify:	0	0.00
<b>What is your major (if applicable)?</b>		
Civil Engineering	0	0.00
Environmental Engineering	16	94.12
Chemical Engineering	0	0.00
Geology Science	0	0.00
Chemistry	1	5.88
Other, Please specify:	0	0.00
<b>Where did you obtain your knowledge of groundwater contaminant transport?</b>		
Academic institute (class/classes)	15	88.24
Work experience	1	5.88
Short training class (less than 1 week)	0	0.00
Other, Please specify:	1	5.88
<b>How long have you been in the field of groundwater contamination?</b>		
< 1 year	6	35.29
1-2 year	3	17.65
2-3 year	3	17.65
> 3 year	2	11.76
Other, Please specify:	3	17.65

## **Computer Related**

The largest percentage (41.2%) of the respondents used the computer 10 to 20 hours per week with 29.4% using it more frequently and 29.4% less frequently. A majority of the respondents used PC and the Microsoft Windows/DOS operating system with some using Macintosh and Mac OS. Most users had ability to use Excel as a computation tool and had experience in writing computer programs. Most respondents always or frequently connected to the Internet. Netscape Navigator was the most used browser (76.5%) in this group with Microsoft Internet Explorer used by 17.6% of the respondents. Many (41.2%) users did not know if their browsers is Java-enabled or not. A majority (76.5%) of the respondents used the Internet search engines. Most respondents believed they were above average in using computers, Internet and spreadsheet programs. Most users were not comfortable about coding computer programs, using database, and writing SQL programs.

**Table B-2 The results of the survey - computer related**

<b>Question</b>	<b>Number</b>	<b>Percentage (%)</b>
<b>How much do you use a computer for work each week?</b>		
< 5 hour	0	0.00
5-10 hours	5	29.41
10-20 hours	7	41.18
> 20 hours	5	29.41
<b>What type of computer do you use?</b>		
PC	14	82.35
Macintosh	4	23.53
Unix Workstation	1	5.88
Other	0	0.00
<b>What type of operating system do you use?</b>		
MS Windows/DOS	13	76.47
Mac OS	3	17.65
Unix	2	11.76
Other	0	0.00
<b>Do you know how to write a Lotus 123 or Excel spreadsheet Macro program?</b>		
Yes	10	58.82
No	6	35.29
Not sure	0	0.00
Did not answer	1	5.88
<b>Have you coded a numerical integration computer program in any computer programming language?</b>		
Yes	9	52.94
No	6	35.29
Don't know	1	5.88
Did not answer	1	5.88
<b>How often do you use the Internet (World Wide Web)?</b>		
Always	3	17.65
Frequently	12	70.59
Occasionally	2	11.76
Never	0	0.00
<b>What browser do you normally use?</b>		
Netscape	13	76.47
Internet Explorer	3	17.65
Web Explorer	0	0.00
Other	1	5.88

**Table B-2 The results of the survey - computer related (continued)**

<b>Question</b>	<b>Number</b>	<b>Percentage (%)</b>
<b>Is your browser Java enabled?</b>		
Yes	10	58.82
No	0	0.00
Don't Know	7	41.18
<b>Do you know how to use Internet search engine?</b>		
Yes	13	76.47
No	2	11.76
Don't Know	2	11.76
<b>How would you rate your knowledge of computers?</b>		
None	0	0.00
Novice	0	0.00
Average	7	41.18
Good	8	47.06
Expert	2	11.76
<b>How would you rate your knowledge of spreadsheet programs?</b>		
None	1	5.88
Novice	2	11.76
Average	5	29.41
Good	6	35.29
Expert	3	17.65
<b>How would you rate your knowledge of Programming language?</b>		
None	3	17.65
Novice	4	23.53
Average	5	29.41
Good	5	29.41
Expert	0	0.00
<b>How would you rate your knowledge of the Internet?</b>		
None	0	0.00
Novice	2	11.76
Average	6	35.29
Good	7	41.18
Expert	1	5.88

**Table B-2 The results of the survey - computer related (continued)**

<b>Question</b>	<b>Number</b>	<b>Percentage (%)</b>
<b>How would you rate your knowledge of database programs?</b>		
None	4	23.53
Novice	3	17.65
Average	5	29.41
Good	4	23.53
Expert	1	5.88
<b>How would you rate your knowledge of Structured Query Language?</b>		
None	9	52.94
Novice	1	5.88
Average	4	23.53
Good	2	11.76
Expert	1	5.88

## **Contaminant Transport Modeling**

About one-half of (46.7%) the respondents believed that they had no problem to describe a model's governing equation, initial conditions, boundary conditions and source conditions. Most respondents had solved a groundwater contaminant transport problem by using an analytical solution or an approximate solution. About two-thirds of the respondents had not solved a groundwater contaminant transport problem by using a numerical solution (such as FDM/FEM). More than one-half of the respondents had solved a groundwater contaminant transport problem without knowing what method has been applied. Most respondents believed that they have no problem to identify a model's flow, dispersion, and source conditions. Only one person could identify the difference between a Dirichlet (the first type) inflow boundary condition and Cauchy (the third type) inflow boundary condition. Most respondents were not familiar with several popular groundwater and contaminant transport modeling programs. One-half of

the respondents might have difficulties to solve a two-dimensional dispersion, unidirectional flow groundwater contaminant transport model that has a decaying source. One-third of the respondents did not know if a contaminant transport model can produce a reasonable result or not. More than one-half of the respondents believed that their domain knowledge was above average.

**Table B-3 The results of the survey - modeling**

<b>Question</b>	<b>Number</b>	<b>Percentage (%)</b>
<b>Do you know the difference between a groundwater flow model and a groundwater contaminant transport model?</b>		
Yes	9	52.94
No	5	29.41
Did not answer	3	17.65
<b>By giving you a groundwater contaminant transport problem, can you describe what is its governing equation(s)?</b>		
Yes	7	41.18
Maybe	6	35.29
No way	2	11.76
Did not answer	2	11.76
<b>By giving you a groundwater contaminant transport problem, can you describe what is its initial condition(s)?</b>		
Yes	7	41.18
Maybe	7	41.18
No way	1	5.88
Did not answer	2	11.76
<b>By giving you a groundwater contaminant transport problem, can you describe what is its inflow boundary condition(s)?</b>		
Yes	7	41.18
Maybe	6	35.29
No way	2	11.76
Did not answer	2	11.76
<b>By giving you a groundwater contaminant transport problem, can you describe what is its outflow boundary conditions(s)?</b>		
Yes	7	41.18
Maybe	6	35.29
No way	2	11.76
Did not answer	2	11.76
<b>By giving you a groundwater contaminant transport problem, can you describe what is its source term(s)?</b>		
Yes	6	35.29
Maybe	7	41.18
No way	2	11.76
Did not answer	2	11.76



**Table B-3 The results of the survey - modeling (continued)**

<b>Question</b>	<b>Number</b>	<b>Percentage (%)</b>
<b>Have you solved a groundwater contaminant transport problem by using an analytical solution?</b>		
Yes	11	64.71
No	4	23.53
Did not answer	2	11.76
<b>Have you solved a groundwater contaminant transport problem by using an approximate solution?</b>		
Yes	8	47.06
No	7	41.18
Did not answer	2	11.76
<b>Have you solved a groundwater contaminant transport problem by using a numerical solution using finite different method?</b>		
Yes	6	35.29
No	9	52.94
Did not answer	2	11.76
<b>Have you solved a groundwater contaminant transport problem by using a numerical solution using finite element method?</b>		
Yes	3	17.65
No	12	70.59
Did not answer	2	11.76
<b>Have you solved a groundwater contaminant transport problem by using a computer program (but not sure what kind of solution)?</b>		
Yes	8	47.06
No	7	41.18
Did not answer	2	11.76
<b>Do you know the difference between an unidirectional and multidimensional flow?</b>		
Yes	15	88.24
No	1	5.88
Did not answer	1	5.88
<b>Do you know the difference between a one-dimensional and multidimensional dispersion?</b>		
Yes	14	82.35
No	2	11.76
Did not answer	1	5.88

**Table B-3 The results of the survey - modeling (continued)**

<b>Question</b>	<b>Number</b>	<b>Percentage (%)</b>
<b>Do you know the difference between a Dirichlet and Cauchy inflow boundary condition?</b>		
Yes	1	5.88
No	15	88.24
Did not answer	1	5.88
<b>Do you know the difference between the first and third type inflow boundary conditions?</b>		
Yes	1	5.88
No	15	88.24
Did not answer	1	5.88
<b>Do you know the difference between a pulse type and decaying type source injection?</b>		
Yes	11	64.71
No	5	29.41
Did not answer	1	5.88
<b>How would you rate your knowledge of the MODFLOW</b>		
None	9	52.94
Novice	4	23.53
Average	1	5.88
Good	2	11.76
Expert	0	0.00
Did not answer	1	5.88
<b>How would you rate your knowledge of the MOC</b>		
None	9	52.94
Novice	1	5.88
Average	4	23.53
Good	2	11.76
Expert	0	0.00
Did not answer	1	5.88
<b>How would you rate your knowledge of the Bioplume</b>		
None	14	82.35
Novice	1	5.88
Average	0	0.00
Good	1	5.88
Expert	0	0.00
Did not answer	1	5.88

**Table B-3 The results of the survey - modeling (continued)**

<b>Question</b>	<b>Number</b>	<b>Percentage (%)</b>
<b>How would you rate your knowledge of the MOFAT</b>		
None	15	88.24
Novice	1	5.88
Average	0	0.00
Good	0	0.00
Expert	0	0.00
Did not answer	1	5.88
<b>How would you rate your knowledge of the OASIS</b>		
None	15	88.24
Novice	1	5.88
Average	0	0.00
Good	0	0.00
Expert	0	0.00
Did not answer	1	5.88
<b>Assuming you do have all parameters' values, how long does it take for you to solve a two-dimensional dispersion, unidirectional flow, decaying source term groundwater contaminant transport model?</b>		
< 1 hour	0	0.00
1-4 hours	3	17.65
1 day	5	29.41
2 days	0	0.00
1 week	1	5.88
Infinity	0	0.00
Don't know	7	41.18
Did not answer	1	5.88
<b>Has the model that you manipulated done the job that it was supposed to (if applicable)?</b>		
Yes	5	29.41
Sort of	2	11.76
No	0	0.00
Don't know	5	29.41
Did not answer	5	29.41

**Table B-3 The results of the survey - modeling (continued)**

<b>Question</b>	<b>Number</b>	<b>Percentage (%)</b>
<b>How would you rate your knowledge of groundwater contaminant transport?</b>		
None	2	11.76
Novice	4	23.53
Average	6	35.29
Good	3	17.65
Expert	0	0.00
Did not answer	2	11.76

**ANTS Related**

**Table B-4 The results of the survey - ANTS**

<b>Question</b>	<b>Number</b>	<b>Percentage (%)</b>
<b>How would you rate the usefulness of having an Internet-based contaminant transport modeling system?</b>		
Very useful	2	11.76
Useful	7	41.18
Sort of	0	0.00
Not useful	0	0.00
Don't know	7	41.18
Did not answer	1	5.88

## Groundwater Contaminant Transport Modeling Questionnaire Version 1.01

This questionnaire is intended toward general public and expert users who have been interacting with groundwater contaminant transport problems (industrial pollution cases, laboratory experiments, class work, etc.). It is part of a research on modeling contaminant transport problems on the Internet. All answered questionnaires are confidential and will be used strictly as academic research material.

### General Information

What kind of company are you working for?

- Academic research institute*       *Government agency*       *Petroleum company*  
 *Consulting firm*       *Self-employed*       *Other, Please specify :*

What is your job?

- Professor / Researcher*       *Student*       *Civil engineer*  
 *Environmental engineer*       *Chemical engineer*       *Geologist*  
 *Water resource specialist*       *Government regulation agent*       *Other, Please specify :*

What is your major (if applicable)?

- Civil Engineering*       *Environmental Engineering*       *Chemical Engineering*  
 *Geology Science*       *Chemistry*       *Other, Please specify :*

Where did you obtain your knowledge of groundwater contaminant transport?

- Academic institute (class/classes)*       *Work experience*  
 *Short training class (less than 1 week)*       *Other, Please specify :*

How long have you been in the field of groundwater contamination?

- < 1 year*       *1-2 year*       *2-3 year*       *> 3 year*

### Computer Related

How much do you use a computer for work each week?

- < 5 hour*       *5-10 hours*       *10-20 hours*       *> 20 hours*

What type of computer do you use?

- PC*       *Macintosh*       *Unix Workstation*       *Other*

What type of operating system do you use?

- MS Windows/DOS*       *Mac OS*       *Unix*       *Other*

Do you know how to write a Lotus 123 or Excel spreadsheet Macro program?

- Yes*       *No*       *Not sure*

Have you coded a numerical integration computer program in any computer programming language?

- Yes*       *No*       *Don't know*

How often do you use the Internet (World Wide Web)?

- Always*       *Frequently*       *Occasionally*       *Never*

What browser do you normally use?

- Netscape*       *Internet Explorer*       *Web Explorer*       *Other*

Is your browser Java enabled?

- Yes*       *No*       *Don't Know*

Do you know how to use Internet search engine?

- Yes*       *No*       *Don't Know*

How would you rate your knowledge of :

- |   |                                      |  |   |                                      |  |
|---|--------------------------------------|--|---|--------------------------------------|--|
| 1. Computers?                               | <input type="checkbox"/> <i>None</i> | <input type="checkbox"/> <i>Novice</i> | <input type="checkbox"/> <i>Average</i> | <input type="checkbox"/> <i>Good</i> | <input type="checkbox"/> <i>Expert</i> |
| 2. Spreadsheet programs (Excel, Lotus 123)? | <input type="checkbox"/> <i>None</i> | <input type="checkbox"/> <i>Novice</i> | <input type="checkbox"/> <i>Average</i> | <input type="checkbox"/> <i>Good</i> | <input type="checkbox"/> <i>Expert</i> |
| 3. Programming language (Fortran, C, Java)? | <input type="checkbox"/> <i>None</i> | <input type="checkbox"/> <i>Novice</i> | <input type="checkbox"/> <i>Average</i> | <input type="checkbox"/> <i>Good</i> | <input type="checkbox"/> <i>Expert</i> |
| 4. Internet?                                | <input type="checkbox"/> <i>None</i> | <input type="checkbox"/> <i>Novice</i> | <input type="checkbox"/> <i>Average</i> | <input type="checkbox"/> <i>Good</i> | <input type="checkbox"/> <i>Expert</i> |
| 5. Database programs (Access, DBASE)?       | <input type="checkbox"/> <i>None</i> | <input type="checkbox"/> <i>Novice</i> | <input type="checkbox"/> <i>Average</i> | <input type="checkbox"/> <i>Good</i> | <input type="checkbox"/> <i>Expert</i> |
| 6. Structured Query Language (SQL)?         | <input type="checkbox"/> <i>None</i> | <input type="checkbox"/> <i>Novice</i> | <input type="checkbox"/> <i>Average</i> | <input type="checkbox"/> <i>Good</i> | <input type="checkbox"/> <i>Expert</i> |

**Contaminant Transport Modeling**

Do you know the difference between a groundwater flow model and a groundwater contaminant transport model?

- Yes  No

By giving you a groundwater contaminant transport problem, can you describe what is its : (assuming it is a unidirectional flow, single component problem)

- 1. governing equation(s)?  Yes  Maybe  No way
- 2. initial condition(s)?  Yes  Maybe  No way
- 3. inflow boundary condition(s)?  Yes  Maybe  No way
- 4. outflow boundary conditions(s)?  Yes  Maybe  No way
- 5. source term(s)?  Yes  Maybe  No way

Have you solved a groundwater contaminant transport problem by using a/an :

- 1. analytical solution?  Yes  No
- 2. approximate solution?  Yes  No
- 3. numerical solution using finite different method?  Yes  No
- 4. numerical solution using finite element method?  Yes  No
- 5. a computer program (but not sure what kind of solution)?  Yes  No

Do you know the difference between a :

- 1. unidirectional and multidimensional flow?  Yes  No
- 2. one-dimensional and multidimensional dispersion?  Yes  No
- 3. Dirichlet and Cauchy inflow boundary condition?  Yes  No
- 4. first and third type inflow boundary condition?  Yes  No
- 5. pulse type and decaying type source injection?  Yes  No

How would you rate your knowledge of the following groundwater related computer programs?

- 1. MODFLOW  None  Novice  Average  Good  Expert
- 2. MOC  None  Novice  Average  Good  Expert
- 3. Bioplume  None  Novice  Average  Good  Expert
- 4. MOFAT  None  Novice  Average  Good  Expert
- 5. OASIS  None  Novice  Average  Good  Expert

Assuming you do have all parameters' values, how long does it take for you to solve a two-dimensional dispersion, unidirectional flow, decaying source term groundwater contaminant transport model?

- < 1 hour  1-4 hours  1 day  2 days
- 1 week  Infinity  Don't know

Has the model that you manipulated done the job that it was supposed to (if applicable)?

- Yes  Sort of  No  Don't know

How would you rate your knowledge of groundwater contaminant transport?

- None  Novice  Average  Good  Expert

**ANTS Related**

How would you rate the usefulness of having a Internet-based contaminant transport modeling system?

- Very useful  Useful  Sort of  Not useful  Don't know

**Comment**

## APPENDIX C LIST OF MODELS

Table C-1 lists the contaminant transport models in the ANTS model library.

**Table C-1 List of the models in the model library**

<b>Name of the model</b>	<b>Authors of the model</b>	<b>Properties of the model</b>
J1DVG01A	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; radial flow in one-dimensional flow field; one-dimensional constant; homogeneous; single; constant; infinite; first; pulse; radial flow in one-dimensional flow field
J1DVG05B	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; radial; one-dimensional constant; homogeneous; single; constant; infinite; first; continuous; radial
J1DVG05C	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; radial; one-dimensional constant; homogeneous; single; constant; infinite; first; pulse; radial
J1DVG09A	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; homogeneous; single; mixing with continuous recharge; dilution process; average value approach
J1DVG13B	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; homogeneous; single; vertical and horizontal spreading; no longitudinal dispersion, only transverse dispersion
J1DVG13C	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; homogeneous; single; geometrical spreading; dilution process; average value approach
J1DVG02A	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; homogeneous; single; mixing with streams; dilution process; average value approach

**Table C-1 List of the models in the model library (continued)**

J1DVG06B	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; finite domain; third; decay; standard model set
J1DVG06C	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; finite domain; third; pulse; standard model set
J1DVG10A	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; finite domain; third; pulse; standard model set
J1DVG14B	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; finite domain; third; decay; standard model set
J1DVG14C	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; finite domain; third; decay; standard model set
J1DVG03A	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; decaying; semi-infinite; first; pulse; standard model set
J1DVG07B	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; decaying; semi-infinite; third; pulse; standard model set
J1DVG07C	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; finite domain; third; pulse; standard model set
J1DVG11A	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; decaying; finite domain; third; pulse; standard model set



**Table C-1 List of the models in the model library (continued)**

J1DVG15B	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; semi-infinite; third; decay; standard model set
J1DVG15C	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; steady state; semi-infinite; first; pulse; standard model set
J1DVG04A	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; steady state; semi-infinite; first; pulse; standard model set
J1DVG08B	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; steady state; semi-infinite; third; pulse; standard model set
J1DVG08C	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; steady state; semi-infinite; third; pulse; standard model set
J1DVG12A	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; steady state; finite domain; first; pulse; standard model set
J1DVG16B	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; decaying; finite domain; first; pulse; standard model set
J1DVG16C	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; semi-infinite; third; decay; standard model set
J1DVG05A	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; semi-infinite; first; pulse; standard model set

**Table C-1 List of the models in the model library (continued)**

J1DVG06A	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; semi-infinite; first; pulse; standard model set
J1DVG07A	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; semi-infinite; first; decay; standard model set
J1DVG08A	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; semi-infinite; first; decay; standard model set
J1DVG09B	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; semi-infinite; first; decay; standard model set
J1DVG09C	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; semi-infinite; third; pulse; standard model set
J1DVG10B	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; finite domain; first; pulse; standard model set
J1DVG10C	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; semi-infinite; third; pulse; standard model set
J1DVG11B	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; finite domain; first; decay; standard model set
J1DVG11C	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; steady state; semi-infinite; first; pulse; standard model set

**Table C-1 List of the models in the model library (continued)**

J1DVG12B	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; semi-infinite; third; decay; standard model set
J1DVG12C	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; steady state; finite domain; first; pulse; standard model set
J1DBS01A	Basha and El-Habel (1993)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; finite domain; first; pulse; standard model set
J1DBS01B	Basha and El-Habel (1993)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; finite domain; first; pulse; standard model set
J1DBS02A	Basha and El-Habel (1993)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; finite domain; first; decay; standard model set
J1DBS02B	Basha and El-Habel (1993)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; finite domain; first; decay; standard model set
J1DBS03A	Basha and El-Habel (1993)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; semi-infinite; third; pulse; standard model set
J1DBS03B	Basha and El-Habel (1993)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; steady state; semi-infinite; first; pulse; standard model set
J1DBS04A	Basha and El-Habel (1993)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; steady state; finite domain; third; pulse; standard model set

**Table C-1 List of the models in the model library (continued)**

J1DBSO4B	Basha and El-Habel (1993)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; steady state; finite domain; third; pulse; standard model set
J1DSR010	Serrano (1992)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; steady state; finite domain; third; pulse; standard model set
J1DSR020	Serrano (1992)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; steady state; finite domain; first; pulse; standard model set
J2DWX020	Wexler (1989)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; steady state; finite domain; first; pulse; standard model set
J2DWX010	Wexler (1989)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; steady state; finite domain; third; pulse; standard model set
J2DWX030	Wexler (1989)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; steady state; semi-infinite; third; pulse; standard model set
J2DWX040	Wexler (1989)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; semi-infinite; first; pulse; standard model set
J2DDRO1P	Domenico and Robbins (1985)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; steady state; semi-infinite; third; pulse; standard model set
J2DDM02D	Domenico and Robbins (1987)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; semi-infinite; both; pulse; two-region

**Table C-1 List of the models in the model library (continued)**

J2DYU010	Yuan (1995)	groundwater contaminant transport; saturated; radial; specified; homogeneous; single; constant; semi-infinite; specified; well injection; radial flow well injection; simultaneous diffusion
J3DWX020	Wexler (1989)	groundwater contaminant transport; saturated; one-dimensional principal; two-dimensional constant; homogeneous; single; constant; infinite; first; continuous; two-dimensional model
J3DWX010	Wexler (1989)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; semi-infinite; first; continuous; one-dimensional continuous source
J3DWX030	Wexler (1989)	groundwater contaminant transport; saturated; one-dimensional principal; three-dimensional constant; homogeneous; single; constant; infinite; first; continuous; three-dimensional model
J3DDR01P	Domenico and Robbins (1985)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; chain; constant; semi-infinite; both; pulse; sequential first-order decay chain reactions
J3DDM02D	Domenico and Robbins (1987)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; chain; constant; semi-infinite; both; pulse; sequential first-order decay chain reactions
J3DYU010	Yuan (1995)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; chain; constant; semi-infinite; both; pulse; sequential first-order decay chain reactions
J3DEW020	Ellsworth and Butters (1993)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; chain; constant; semi-infinite; both; pulse; sequential first-order decay chain reactions

**Table C-1 List of the models in the model library (continued)**

J3DEW040	Ellsworth and Butters (1993)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; chain; constant; semi-infinite; both; pulse; sequential decay chain reactions in multilayered medium
J3DEW010	Ellsworth and Butters (1993)	groundwater contaminant transport; saturated; vertical; one-dimensional constant; homogeneous; single; constant; semi-infinite; third; landfill; landfill
J3DEW030	Ellsworth and Butters (1993)	groundwater contaminant transport; saturated; radial; specified; homogeneous; single; constant; semi-infinite; third; continuous and pulse well injection; radial flow well injection
J1DEL010	Eldor and Dagan (1972)	groundwater contaminant transport; saturated; specified; three-dimensional constant; homogeneous; single; constant; semi-infinite; third; horizontal plane; horizontal plane source
J1DEL020	Eldor and Dagan (1972)	groundwater contaminant transport; saturated; radial; specified; homogeneous; single; constant; semi-infinite; specified; well injection; radial flow well injection
J1DLP010	Lerner and Papatolios (1993)	groundwater contaminant transport; saturated; two-dimensional flow; two-dimensional constant; homogeneous; single; constant; semi-infinite; first; horizontal strip; two-dimensional horizontal strip
J1DLP020	Lerner and Papatolios (1993)	groundwater contaminant transport; saturated; one-dimensional principal; three-dimensional constant; homogeneous; single; constant; finite width and height; first; area; area (plane) source in a finite width and height aquifer
J1DEL030	Eldor and Dagan (1972)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; finite domain; first; pulse; same as J1DVG07C
J1DZA010	Zaidel and Russo (1993)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; finite domain; third; pulse; same as J1DVG08C

**Table C-1 List of the models in the model library (continued)**

J1DZA020	Zaidel and Russo (1993)	groundwater contaminant transport; saturated; one-dimensional principal; three-dimensional constant; homogeneous; single; constant; infinite; first; area; area (plane) source in an infinite aquifer
J2DZA010	Zaidel and Russo (1993)	groundwater contaminant transport; saturated; one-dimensional principal; three-dimensional constant; homogeneous; single; constant; infinite; first; continuous point; continuous point source in a three-dimensional space
J2DBR010	Bear (1987)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; semi-infinite; first; pulse; same as J1DVG05C
J2DBR020	Bear (1987)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; semi-infinite; third; pulse; same as J1DVG06C
J2DBR030	Bear (1987)	groundwater contaminant transport; saturated; one-dimensional principal; two-dimensional constant; homogeneous; single; constant; infinite; first; gaussian; gaussian distribution concentration strip (line) source
J1DFR010	Fry and Istok (1993)	groundwater contaminant transport; saturated; one-dimensional principal; two-dimensional constant; homogeneous; single; constant; infinite; first; strip; strip (line) source in an infinite aquifer
J1DFR020	Fry and Istok (1993)	groundwater contaminant transport; saturated; one-dimensional principal; two-dimensional constant; homogeneous; single; constant; infinite; first; continuous point; continuous point source in a horizontal plane
J3DLE010	Leij (1991)	groundwater contaminant transport; saturated; one-dimensional principal; two-dimensional constant; homogeneous; single; constant; finite width; first; strip; strip (line) source in a finite width aquifer

**Table C-1 List of the models in the model library (continued)**

J3DLE030	Leij (1991)	groundwater contaminant transport; unsaturated; one-dimensional principal; one-dimensional constant; heterogeneous; multi; constant; semi-infinite; first; pulse; unsaturated zone volatile solvent
Leij1993	Leij, Toride, and van Genuchten (1993)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional distance-dependent; heterogeneous; single; constant; semi-infinite; both; specified; distance-dependent dispersion
J1DVGSP1	Van Genuchten (1985)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; heterogeneous; single; constant; semi-infinite; specified; specified; layered soils
J1DVGSP2	Van Genuchten (1985)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; multi; constant; semi-infinite; specified; specified; multichemicals
J1DVGSP3	Van Genuchten (1985)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional distance-dependent; heterogeneous; single; constant; semi-infinite; third; instantaneous; distance-dependent dispersion
J1DVGSP4	Van Genuchten (1985)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional distance-dependent; heterogeneous; single; constant; semi-infinite; first; continuous; distance-dependent dispersion
Mironenko1984	Mironenko and Pachevsky (1984)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional distance-dependent; heterogeneous; single; constant; semi-infinite; both; specified; distance-dependent exponential dispersion
Chen1985	Chen (1985)	groundwater contaminant transport; unsaturated; heterogeneous;



**Table C-1 List of the models in the model library (continued)**

Gureghian1985	Gureghian and Jansen (1985)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional time-dependent; heterogeneous; single; constant; semi-infinite; third; instantaneous; exponential time-dependent dispersion
Booker1987	Booker and Rowe (1987)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional time-dependent; heterogeneous; single; constant; semi-infinite; first; continuous; exponential time-dependent dispersion
Chen1987	Chen (1987)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional time-dependent; heterogeneous; single; constant; semi-infinite; first; continuous; asymptotic time-dependent dispersion
Galya1987	Galya (1987)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional time-dependent; heterogeneous; single; constant; semi-infinite; third; instantaneous; asymptotic time-dependent dispersion
Chen1989	Chen (1989)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional time-dependent; heterogeneous; single; constant; semi-infinite; first; continuous; linear time-dependent dispersion
Dillon1989	Dillon (1989)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional time-dependent; heterogeneous; single; constant; semi-infinite; third; instantaneous; linear time-dependent dispersion
Brown1990	Brown and McWhorter (1990)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; heterogeneous; single; constant; semi-infinite; third; instantaneous; constant time-dependent dispersion

**Table C-1 List of the models in the model library (continued)**

Yates1990	Yates (1990)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; heterogeneous; single; constant; semi-infinite; first; continuous; constant time-dependent dispersion
Bosma1992	Bosma and van der Zee (1992)	groundwater contaminant transport; saturated; one-dimensional arbitrary; three-dimensional constant; homogeneous; single; specified; infinite; third; pulse; three-dimensional model with arbitrary flow direction
Neville1992	Neville (1992)	groundwater contaminant transport; saturated; one-dimensional arbitrary; three-dimensional constant; homogeneous; single; constant; infinite; third; pulse; three-dimensional model with arbitrary flow direction
Yates1992	Yates (1992)	groundwater contaminant transport; saturated; one-dimensional principal; three-dimensional constant; homogeneous; single; specified; infinite; third; pulse; three-dimensional model
Angelakis1993	Angelakis, Kadir, and Rolston (1993)	groundwater contaminant transport; saturated; one-dimensional principal; three-dimensional constant; homogeneous; single; constant; infinite; third; pulse; three-dimensional model
Wallach1993	Wallach (1993)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; finite domain; third; specified; aqueous concentration rate limited desorption and decay
Illangasekare1993	Illangasekare, Brannon, and Amadei (1994)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; finite domain; third; specified; sorbed concentration rate limited desorption and decay
Kool1994	Kool et al. (1994)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; semi-infinite; third; specified; two region
Zaidel1994	Zaidel and Russo (1994)	groundwater contaminant transport; saturated; radial; one-dimensional constant; homogeneous; single; constant; area; first; pumping well; radial

**Table C-1 List of the models in the model library (continued)**

J1DVG01B	Van Genuchten and Alves (1982)	groundwater contaminant transport; saturated; radial; one-dimensional constant; homogeneous; single; constant; area; first; pumping well; radial
J1DVG01C	Van Genuchten and Alves (1982)	groundwater contaminant transport; specified; vertical; one-dimensional constant; specified; single; constant; semi-infinite; third; specified; chemical transfer from soil to runoff
J1DVG02B	Van Genuchten and Alves (1982)	groundwater contaminant transport; unsaturated; one-dimensional principal; one-dimensional steady state; heterogeneous; single; constant; finite domain; first; vertical extended; one-dimensional unsaturated zone
J1DVG02C	Van Genuchten and Alves (1982)	groundwater contaminant transport; unsaturated; one-dimensional principal; one-dimensional steady state; heterogeneous; single; constant; finite domain; first; plane source; one-dimensional unsaturated zone
J1DVG03B	Van Genuchten and Alves (1982)	groundwater contaminant transport; unsaturated; one-dimensional principal; two-dimensional steady state; heterogeneous; single; constant; finite depth; first; pulse; two-dimensional unsaturated zone
J1DVG03C	Van Genuchten and Alves (1982)	groundwater contaminant transport; specified; specified; specified; specified; single; constant; semi-infinite; specified; specified; numerical solution
J1DVG04B	Van Genuchten and Alves (1982)	groundwater contaminant transport; both; specified; specified; specified; single; constant; semi-infinite; both; horizontal plane; numerical solution
J1DVG04C	Van Genuchten and Alves (1982)	groundwater contaminant transport; unsaturated; one-dimensional principal; two-dimensional steady state; heterogeneous; single; constant; finite depth; first; pulse; two-dimensional unsaturated zone
J1DWX010	Wexler (1989)	groundwater contaminant transport; saturated; one-dimensional principal; three-dimensional constant; homogeneous; single; constant; infinite; first; decay; three-dimensional model with exponentially decaying source

**Table C-1 List of the models in the model library (continued)**

J1DWX020	Wexler (1989)	groundwater contaminant transport; saturated; one-dimensional principal; two-dimensional constant; homogeneous; single; constant; infinite; first; decay; two-dimensional model with exponentially decaying source
J1DWX030	Wexler (1989)	groundwater contaminant transport; saturated; one-dimensional principal; three-dimensional constant; homogeneous; single; constant; infinite; first; decay; three-dimensional model with exponentially decaying source
J1DWX040	Wexler (1989)	groundwater contaminant transport; saturated; one-dimensional principal; two-dimensional constant; homogeneous; single; constant; infinite; first; decay; two-dimensional model with exponentially decaying source
J1DDR01P	Domenico and Robbins (1985)	groundwater contaminant transport; saturated; one-dimensional principal; one-dimensional constant; homogeneous; single; constant; semi-infinite; first; decay; one-dimensional decaying source
J1DDM02D	Domenico and Robbins (1987)	groundwater contaminant transport;
Domenico and Palciauskas (1982)	Domenico and Palciauskas (1982)	groundwater contaminant transport;
Domenico and Palciauskas (1982)	Domenico and Palciauskas (1982)	groundwater contaminant transport;
Domenico and Palciauskas (1982)	Domenico and Palciauskas (1982)	groundwater contaminant transport; saturated; homogeneous; single; constant;
Domenico and Palciauskas (1982)	Domenico and Palciauskas (1982)	groundwater contaminant transport; saturated; homogeneous; single; constant;

**Table C-1 List of the models in the model library (continued)**

J2DCU010	Cleary and Unga (1978)	groundwater contaminant transport; saturated; one-dimensional principal; two-dimensional constant; homogeneous; single; constant; specified; specified; decay; two-dimensional model with exponentially decaying source
J2DCU020	Cleary and Unga (1978)	groundwater contaminant transport; saturated; one-dimensional arbitrary; two-dimensional constant; homogeneous; single; constant; specified; specified; decay; two-dimensional model with exponentially decaying source
J1DHO010	Hoopes and Harleman (1967)	groundwater contaminant transport; saturated; radial; one-dimensional constant; homogeneous; single; constant; infinite; specified; continuous; radial flow model

