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Compilation of Ground-Water Models

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COMPILATION OF GROUND-WATER MODELS

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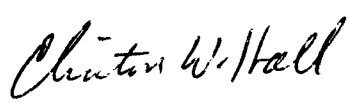
FOREWORD

EPA is charged by Congress to protect the Nation's land, air, and water systems. Under a mandate of national environmental laws focused on air and water quality, solid waste management and the control of toxic substances, pesticides, noise and radiation, the Agency strives to formulate and implement actions which lead to a compatible balance between human activities and the ability of natural systems to support and nurture life.

The Robert S. Kerr Environmental Research Laboratory is the Agency's center of expertise for investigation of the soil and subsurface environment. Personnel at the laboratory are responsible for management of research programs to: (a) determine the fate, transport and transformation rates of pollutants in the soil, unsaturated and the saturated zones of the subsurface environment; (b) define the processes to be used in characterizing the soil and subsurface environment as a receptor of pollutants; (c) develop techniques for predicting the effect of pollutants on ground water, soil and indigenous organisms; and (d) define and demonstrate the applicability and limitations of using natural processes, indigenous to the soil and subsurface environment, for the protection of this resource.

Ground-water modeling, as a computer-based methodology for mathematical analysis, is a tool for investigating and managing the mechanisms and controls of ground-water systems. These modeling codes are used for the evaluation of policies, actions, and designs that may affect such systems. Models are playing an important role in the determination of the physical and economical effects of proposed ground-water protection policy alternatives, and thus the protection of human and ecological health.

The model selection process for appropriate codes is a vital step to conducting these investigative and management alternatives for ground-water systems. This report presents the methodology used by the International Ground Water Modeling Center (IGWMC) to classify, evaluate and manage descriptive information regarding ground-water modeling codes for the purpose of model selection. Furthermore, the report provides an overview of available ground-water modeling codes and their major characteristics by presenting the classification approach taken by the IGWMC, and discusses different types of models and mathematical approaches invoked for developing the models. Separate sections discuss and review the different categories of ground-water models: flow models, transport models, chemical reaction models, stochastic models, models for fractured rock, and ground-water management models. The appendices include a listing and description from the IGWMC MARS database of selected models from each category.



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ABSTRACT

Ground-water modeling is a computer-based methodology for mathematical analysis of the mechanisms and controls of ground-water systems, and for the evaluation of policies, actions, and designs that may affect such systems. In addition to satisfying scientific interest in the workings of subsurface fluid flow and fluid-related mass-transfer and transformation processes, models assist in analyzing the responses of subsurface systems to variations in both existing and potential new stresses. Models play an increasingly dominant role in the determination of the physical and economical effects of proposed ground-water protection policy alternatives, and thus in the protection of human and ecological health. Furthermore, computer models are essential tools in the screening of alternative remediation technologies and strategies in cleaning up ground-water systems polluted in the (recent) past, in the sound design of ground-water resource development schemes for water supply, and for other land use modifications affecting ground-water systems.

To be able to select a computer code appropriate for the type of analysis to be performed, ground-water modelers need to have an overview of available computer codes and their characteristics. This report presents the methodology used by the International Ground Water Modeling Center to classify, evaluate and manage descriptive information regarding ground-water modeling codes for the purpose of model selection. Furthermore, the report provides an overview of available ground-water modeling codes and their major characteristics.

The report includes a section that defines ground-water modeling, presents the classification approach taken by the International Ground Water Modeling Center (IGWMC), and discusses different types of models and the mathematical approaches invoked for developing the models. Separate sections discuss and review the different categories of ground-water models: flow models, transport models, chemical reaction models, stochastic models, models for fractured rock, and ground-water management models. The appendices include a listing and description from the IGWMC MARS database of selected models from each category.

BACKGROUND AND REPORT ORGANIZATION

In the mid-1970's, by request of the Scientific Committee on Problems of the Environment (SCOPE), part of the International Council of Scientific Unions (ICSU), the Holcomb Research Institute (HRI) at Butler University, Indianapolis, Indiana, carried out a ground-water modeling assessment. This international study, funded in large part by the U.S. Environmental Protection Agency (EPA) through its R.S. Kerr Environmental Research Laboratory in Oklahoma, resulted in a report published by the American Geophysical Union (AGU) in its series, Water Resources Monographs. In 1985 a second edition of this monograph (AGU Monograph 5) was published, based on information collected at HRI through its International Ground Water Modeling Center (IGWMC) from its inception in 1978 until December 1983.

The Center was established at HRI as an international clearinghouse for ground-water models and a technology transfer center in ground-water modeling. Since 1983 the Center has been linked to the TNO Institute of Applied Geoscience, Delft, The Netherlands, which operates the European office of the IGWMC. Due to the closing of Holcomb Research institute by Butler University in the Summer of 1991, the IGWMC relocated its US office to the Colorado School of Mines (CSM), Golden, Colorado.

The Center operates a clearinghouse for ground-water modeling software, organizes and conducts short courses and seminars, and carries out a research program to advance the quality of modeling in ground-water management, in support of the Center's technology transfer functions. The Center's International Technical Advisory Committee provides guidance and active support to its program.

The present report contains the result of research and information processing activities performed by the IGWMC under a research and technology transfer cooperative agreement with the U.S. Environmental Protection Agency, initiated in 1988. Three other reports have been prepared under this cooperative agreement: " Modeling Multiphase Flow and Transport" by Aly I. El-Kadi, Osman A. Elnawawy, Pamela Kobe, and Paul K.M. van der Heijde, submitted to EPA in May 1991 (IGWMC Report Number GWMI 91-04), "Ground-Water Management Models", by Aly I. El-Kadi, Osman A. Elnawawy, and Paul K.M. van der Heijde, submitted to EPA in December 1991 (IGWMC Report Number GWMI 91-05), and "Quality Assurance and Quality Control in the Development and Application of Ground-Water Models" by Paul K.M. van der Heijde and Osman A. Elnawawy, submitted to EPA in September 1992 (IGWMC Report Number GWMI 92-03). The current report, together with the reports on management models and multiphase flow and transport, provides an overview of the status of major types of ground-water models. These reports present an update of Chapter 5 and the appendices of the report "Groundwater Modeling: An Overview and Status Report," prepared in 1988 under a previous cooperative agreement with the US EPA (Report EPA/600/2-89/028).

The review of models has been based on information gathered by the IGWMC through research and interviews on an on-going basis since 1978. To manage the rapidly growing amount of information, IGWMC

maintains a descriptive model information system, MARS (Model Annotation Search and Retrieval System). Currently, this database is installed on a microcomputer operating under MS-DOS. Detailed information on the reviewed models is presented in a series of tables, preceded by an introduction on model classification and principal characteristics of the described models.

The authors are grateful to Aly I. El-Kadi, Stan A. Williams, Milovan S. Beljin, and P. Srinivasan for their past contributions to the IGWMC model assessment studies; to Richard E. Rice for his contributions on geochemical equilibrium models; to Deborah L. Cave for her assistance in collecting model information and reviewing hydrogeochemical modeling literature; to Michael Stibitz for his assistance in processing model information; to David Dillon, Jeffrey Lewis and Manjit Trehan for database programming assistance; to Mary Willis, Amy Maxwell and Mary Pigman for word processing; to James N. Rogers for manuscript editing; and to Colleen Baker for graphics. Furthermore, authors wish to acknowledge the administrative and technical support provided by the Colorado School of Mines in completing this report.

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I. INTRODUCTION

Ground-water modeling is a computer-based methodology for mathematical analysis of the mechanisms and controls of ground-water systems, and for the evaluation of policies, actions, and designs that may affect such systems (van der Heijde *et al.* 1988). In addition to satisfying scientific interest in the workings of subsurface fluid flow and fluid-related mass-transfer and transformation processes, models assist in analyzing the responses of subsurface systems to variations in both existing and potential new stresses. Models play an increasingly dominant role in the determination of the physical and economical effects of proposed ground-water protection policy alternatives, and thus in the protection of human and ecological health. Furthermore, computer models are essential tools in the screening of alternative remediation technologies and strategies in cleaning up ground-water systems polluted in the (recent) past, in the sound design of ground-water resource development schemes for water supply, and for other land use modifications affecting ground-water systems.

Although a consensus may exist as to what ground-water modeling entails, the definition of a "model" *per se* is somewhat nebulous. In hydrogeology, the term "ground-water model" has become synonymous with conceptual ground-water models, mathematical ground-water models (including analytical and numerical models), computer models, and simulation models. Furthermore, the term "ground-water model" may apply to either a generic model or computer code (without site-specific data) or the representation of a site-specific system using such a generic code. The International Ground Water Modeling Center defines a model as a non-unique, simplified, mathematical description of an existing ground-water system, coded in a programming language, together with a quantification of the ground-water system the code simulates in the form of boundary conditions, system parameters, and system stresses. The generic computer code used in this problem-specific system simulation is sometimes referred to as a (ground-water) simulation code or a generic ground-water model. This use of the term "ground-water model" includes both the saturated and unsaturated zones.

Ground-water models are generally intended to perform as practical, descriptive, and predictive problem-solving tools. Most ground-water models are mathematical models in which the causal relationships among various components of the ground-water system and between the system and its environment are quantified and expressed in terms of mathematics and uncertainty of information. Mathematical models range from rather simple, empirical expressions to complex mechanistic, multi-equation formulations. As the problems encountered in protecting and remediating ground-water resources are highly complex in nature, their study requires cooperation between many disciplines. Routinely, simulations of the complex ground-water systems involved require characterization of hydrology, physical transport processes, geochemistry, contaminant chemistry and biochemistry in the near-surface and deep underground. Therefore, contemporary ground-water modeling is highly multidisciplinary in nature.

Models are useful tools for understanding the structure and dynamics of ground-water systems and the processes that influence their composition. Modeling serves as a means to ensure orderly interpretation

of the data describing a ground-water system, and to ensure that this interpretation is a consistent representation of the system. It can also provide a quantitative indicator for efficient resource utilization when additional field data collection is required and financial resources are limited. Finally, models can be used in what is often called the predictive mode by analyzing the response a system is expected to show when existing stresses vary and new ones are introduced, or by optimizing the response of the system by varying the stresses in a systematic way. Increasingly, the objectives behind the ground-water modeling efforts are protection and improvement of human health through providing good quality drinking water and reducing the risks resulting from exposure to contaminated ground water.

Where precise aquifer and contaminant characteristics have been reasonably well established, ground-water models may provide a viable, if not the only, method to predict contaminant transport and fate, locate areas of potential environmental risk, identify pollution sources, and assess possible remedial actions. Some examples in which mathematical models have assisted in the management of ground-water protection programs are (van der Heijde *et al.* 1988):

- Determining or evaluating the need for regulation of specific waste disposal, agricultural, and industrial practices

- Analyzing policy impacts, as in evaluating the consequences of setting regulatory standards and rules

- Assessing exposure, hazard, damage, and health risks

- Evaluating reliability, technical feasibility and effectiveness, cost, operation and maintenance, and other aspects of waste disposal facility designs and of alternative remedial actions

- Providing guidance in siting new facilities and in permit issuance and petitioning

- Developing aquifer or well head protection zones

- Assessing liabilities such as post-closure liability for waste disposal sites.

Computer-based ground-water modeling began in the mid 1960's and has gradually grown into a widely accepted and applied decision-support tool. In the last few years, modeling has been made easier, faster and "flashier" by rapidly evolving computer hardware and software technologies. The widespread availability of powerful desktop microcomputers and user-oriented software interfaces has made running ground-water computer codes a rather mundane task in hydrogeological assessments. The mechanics of entering data, running simulations, and creating high-quality graphics have become less time-consuming and less complex due to the availability of various, extensively supported window environments and expanded functionality, easy-to-debug, programming languages. These high-powered software development systems integrate

editing, compiling, and debugging functions with additional programming tools and libraries allowing efficient development of flexible, menu-driven software while facilitating achievement of high quality-assurance goals. Increased portability of the software due to the development of multi-platform operating systems such as UNIX, and standardization of high-level programming languages (e.g., FORTRAN 90) and the subsequent release of new compilers, makes it possible that software development groups are able to continue to improve the simulation components of the software. Furthermore, the use of object-oriented programming holds the promise of more flexibility regarding post-development expansion and maintenance, and in overall reliability and portability of the software (Gibson 1990, Mackie 1991).

Recently, geographical information systems (GIS) have become prominent tools in model preparation and evaluation of modeling results. Automatic allocation of model parameters is facilitated by overlaying the spatially organized geological and hydrological parameters with a model-defined computational mesh. The significance of the results of model simulations in the final decision-making process can be further enhanced by importing the raster- or vector-based simulation results back into a GIS and combining these with background maps of the area under study and other spatial information important for decision-making.

However, the reduction in time and effort in modeling due to new software developments does not mean that modeling has become a simple task; in fact, modeling is becoming more challenging as ground-water specialists are able to deal with increasingly complex mathematical descriptions of natural systems and resource management problems. In addition, these problems can be studied in much more detail by using high-order spatial and temporal resolution.

In-depth treatment of the theoretical basis of ground-water models can be found in NRC (1990), among others. Extensive discussion on modeling methodology is given in van der Heijde *et al.* (1988) and NRC (1990).

1.1 MODEL CLASSIFICATION

There are various kinds of ground-water models, designed to simulate different types of ground-water systems, and able to compute different variables. To identify the main attributes of a particular model, a classification system is needed. An early effort to classify ground-water models was published by Bachmat *et al.* (1978). This classification approach has been used, modified and expanded by various researchers (Mercer and Faust 1981, Simmons and Cole 1985, NRC 1990). The classification system presented here has been developed to enable the International Ground Water Modeling Center to systematically describe ground-water models in its computerized information system (see Table 1).

Ground-water models can be divided into various categories, depending on the purpose of the model, the nature of the ground-water system and the mathematical method(s) employed.

TABLE 1. GROUND-WATER MODEL CATEGORIES.

1. Objective-based model categories
   - applicability of the model to certain types of ground-water management problems
   - code development objective(s)
     - research
     - education/demonstration
     - general use
   - calculated variables
     - screening/ranking
     - prediction
     - backtracking
     - inverse or parameter estimation
     - optimization

2. Processed-based model categories
   - flow
     - saturated flow
     - unsaturated flow
     - vapor transport
     - multi-phase flow (water/air or vapor; water/NAPL; water/steam; salt water/fresh water
   - heat transport
   - hydrogeochemical speciation
   - solute transport and fate
     - conservative
     - nonconservative
     - coupled with hydrogeochemistry
   - matrix deformation due to fluid injection or withdrawal
   - coupling with external systems (e.g., surface water, plant uptake, atmosphere)

3. Physical-system-characteristics-based model categories
   - hydrogeological system
     - water-saturated vs. partially saturated
     - porous medium vs. fractured rock
     - single, simple system vs. multilayered system of aquifers and aquitards or soils
     - (leaky-) confined vs. phreatic aquifer conditions
     - heterogeneity, anisotropy
     - site, local, regional scale
   - flow conditions
     - laminar vs. turbulent
     - steady-state vs. time-varying conditions
   - fluid conditions
     - type of fluid (water, NAPL, vapor, steam)
     - varying vs. constant fluid viscosity
     - varying vs. constant fluid density
     - compressible vs. non-compressible fluid
   - boundary location and conditions
     - type of boundary condition (1st, 2nd, 3rd; flow, transport)
     - physical representation (recharge, stream, lake, seepage face, springs, point-,line-, or areal contaminant/heat source, diffuse source)

more.....

Table 1 - continued

4. Mathematics
   - general nature of equation
     - empirical vs. mechanistic
     - deterministic vs. stochastic
   - dimensionality of equations
   - solution method
     - analytical
       + single solution
       + superposition
       + semi-analytical solution
   - solution method - continued
     - numerical
       + spatial approximation (finite difference, finite element, boundary element, method of characteristics, random particle movement)
       + time-stepping scheme
       + matrix solution technique

1.1.1 Objective-Oriented Classification

The purpose of a model can be defined in terms of the applicability of the model to certain types of ground-water management problems, the code development objective(s), or in terms of the variables it calculates. Examples of modeling objectives from the perspective of ground-water management are:

- regional ground-water system characterization for resource development and protection planning
- optimal well-field design for water supply (effectiveness, impact)
- protection of well-fields against pollution from within aquifer or through confining layers
- construction site or mining site dewatering
- determination of contaminant movement from known source, such as a landfill, impoundment, or leaky underground storage tank
- design of waste storage facility
- exploring optimal design for hydraulic containment of a contaminant plume
- design of a pump and treat remediation action
- design of an in-situ biorestoration scheme
- design of a ground-water quality monitoring network
- risk assessment at a contaminated site
- feasibility study and design of an aquifer thermal storage system (ATES)
- assessment of impact of deep-well injection of waste
- screening or ranking of alternative policies, site-related risks, protection priority, engineering designs, etc.

A classification system based on management objectives should include such aspects as level of resolution required, accuracy acceptable, and other technical, scientific, social, and economic objectives. However, in general it is not practical to develop a classification system based on such management

objectives, as these are more easily taken into account in the code selection process than in model characterization.

Another objective-based approach is to analyze the development objectives for the model code. One can distinguish between three major development objectives: (1) to develop an educational tool (educational model), (2) to study quantitatively the fundamental nature of a ground-water system (research codes), and (3) to develop a code that can be applied routinely to various site-specific problems (general-use code).

Finally, an objective-based classification approach may be based on the variables which can be computed with the model. In this case, the major model types are (van der Heijde *et al.* 1985): (1) prediction models designed to predict the system responses, assuming the system parameters and system stresses are known; (2) backtracking models, determining system stresses when system parameters are known and the system responses are either known or bounded; and (3) inverse or parameter estimation models for the evaluation of system parameters when a history of stresses and responses are known. The most common variables computed by prediction models are hydraulic head, drawdown, pressure, velocity (vector), fluid flux (vector), stream- or pathlines, isochrones, contaminant fronts, contaminant concentration (in both liquid and solid phase), solute flux (vector), temperature, enthalpy, heat flux (vector), optimum location of sources and sinks, location of (saltwater/freshwater) interface, water balance, and chemical mass balance. Backtracking models are used specifically to determine system stresses and boundary conditions (e.g location and duration of contaminant source release, well-field pumping history, aquifer recharge rates). Inverse models are designed to determine the most likely distribution of system and process parameters (transmissivity, dispersivity, retardation coefficient).

1.1.2 Classification Based on the Nature of the Ground-Water System

The nature of the ground-water system is characterized by the system's hydrogeological characteristics (i.e. hydrogeologic schematization and geometry, parameter variability in space and time, boundary locations and conditions, and system stresses) and the physical, chemical, and biological processes that take place (type of processes, their spatial and temporal characteristics, and their relative importance). Accordingly, we distinguish between two classification types in describing the ability of models to represent the nature of the ground-water (or soil-water) system: (1) hydrogeology-based model types, and (2) process-based model types.

One way to distinguish between different types of ground-water models is based on the kind of hydrogeologic features they can simulate (see Table 1). Among others, distinction may be made between various kinds of hydrogeologic conceptualizations or zonings, e.g., saturated zone versus unsaturated zone, a single aquifer system versus a multilayered system of aquifers and aquitards (see Table 1). Another distinction is based on scale, e.g., site, local, or regional scale.

A classification based on processes distinguishes between flow, transport (solute and heat), fate of chemical compounds, phase transfers and other processes (Table 2 lists important processes encountered in ground-water systems. Flow models simulate the movement of one or more fluids in porous or fractured

rock. One such fluid is water; the others, if present, can be air, methane, or other vapors (in soil) or immiscible nonaqueous phase liquids (NAPLs) sometimes having a density distinct from water (LNAPLs, DNAPLs). A special case of multi-fluid flow occurs when layers of water of distinct density are separated by a relatively small transition zone, a situation often encountered when sea water intrusion occurs. Most flow models are based on a mathematical formulation which considers the hydraulic system parameters as independent field information and hydraulic head and flux as dependent variables. They are used to calculate steady-state distribution or changes in time in the distribution of hydraulic head or fluid pressure, drawdown, rate and direction of flow (e.g., determination of streamlines, particle pathways, velocities, and fluxes), travel times, and the position of interfaces between immiscible fluids (Mercer and Faust 1981, Wang and Anderson 1982, Kinzelbach 1986, Bear and Verruijt 1987). Inverse flow models simulate the flow field to calculate the spatial distribution of unknown system parameters using field information on the dependent variables such as hydraulic head and flux.

Two types of models can be used to evaluate the chemical quality of ground-water (e.g., Jennings *et al.* 1982, Rubin 1983, Konikow and Grove 1984, Kincaid *et al.* 1984): (1) pollutant transformation and degradation models, where the chemical and microbial processes are posed independent of the movement of the pollutants; and (2) solute transport models simulating displacement of the pollutants only (conservative transport), or including the effects of phase transfers, (bio-)chemical transformation and degradation processes (transport and fate; non-conservative transport). In fact, one may argue a third type exists, where a conservative solute transport model is coupled with a hydrogeochemical speciation model (Hostetler *et al.* 1988; Kinzelbach *et al.* 1989; Yeh and Tripathi 1989).

Hydrogeochemical speciation models represent the first type, as they consist solely of a mathematical description of equilibrium reactions or reaction kinetics (Jenne 1981, Rice 1986). These models, which are general in nature and are used for both ground water and surface water, simulate chemical processes in the liquid phase and sometimes between the liquid and solid phase (precipitation-dissolution; sorption) that regulate the concentration of dissolved constituents. They can be used to identify the effects of temperature, speciation, sorption, and solubility on the concentrations of dissolved constituents (Jenne 1981).

Solute transport models are used to predict movement and concentration of water-soluble constituents and radionuclides. A solute transport model requires velocities for the calculation of advective displacement and spreading by dispersion (Anderson 1984). If the velocity field is constant then it may be either calculated once using a program module or read into the program as data. If the velocity field is dependent on time or concentration, then calculation of velocities at each time step is required, either through an internal flow simulation module or an external, coupled flow module.

The nonconservative solute transport models include some type of solute transformation, primarily adsorption, radioactive decay, and simple (bio-)chemical transformations and decay (Cherry *et al.* 1984, Grove and Stollenwerk 1987).

The inclusion of geochemistry in solute transport models is often based on the assumption that the reaction proceeds instantaneously to equilibrium. Recently, various researchers have become interested in the kinetic approach that incorporates chemical reactions in transport model. This inclusion of

geochemistry has focused on single reaction such as ion-exchange or sorption for a small number of reacting solutes (Rubin and James 1973, Valocchi *et al.* 1981, Charbeneau 1981).

In some cases, comprehensive ground-water quality and risk assessment requires the simulation of temperature variations and their effects on ground-water flow and pollutant transport and fate. In the past, major heat transport model development focused on high-temperature geothermal systems. More recently, models have been developed to analyze aquifer thermal energy storage and shallow heat pump systems. A few highly specialized multipurpose prediction models can handle combinations of heat and solute transport, or heat transport and rock matrix displacement or solute transport and rock matrix displacement. Generally, these models solve the system of governing equations in a coupled fashion to provide for analysis of complex interactions among the various physical, chemical, and biological processes involved.

There are three major types of heat transport models in the subsurface: (1) transport through the fluid phase only, (2) transport through the solid phase only, and (3) transport through both the fluid and solid phase of the subsurface. Ground-water modeling deals primarily with model types 1 and 3. Within each of these two latter groups of models one may distinguish four more types of models: (1) low temperature, single phase heat transport without phase change (e.g., to evaluate heat-pump efficiencies), (2) low temperature, dual phase heat transport with two fluids (water and vapor, e.g., in soils), (3) low temperature, dual phase heat transport with phase change (freezing/thawing, e.g., for studying frost front propagation in soils), and (4) high-temperature, multi-phase (liquid/vapor) heat transport with phase change (steam/water; e.g., for evaluation of geothermal exploration potential). Typical processes incorporated include convection, dispersion, conduction, radiation, evaporation/condensation, and freezing/thawing.

Many models address the interaction between ground-water and the other components of the hydrologic cycle. These models describe only the inputs and outputs at interfaces with other components of the hydrologic cycle as dynamic stresses or boundary conditions. Increasingly, models are developed that simulate the processes in each subsystem in detail (e.g., Morel-Seytoux and Restrepo 1985; Prudic 1989). Two types of models fit this latter category: watershed models and stream-aquifer models (sometimes called conjunctive use models).

Watershed models customarily have been applied to surface water management of surface runoff, stream runoff, and reservoir storage. Traditionally, these models did not treat ground-water flow in much detail, in part because of the wide range of temporal scales involved. The subsurface components in these models were limited to infiltration and to a lumped, transfer function approach to ground-water (El-Kadi 1983, 1986).

With the growing interest during the 1970s in the conjunctive use and coordinated management of surface and subsurface water resources by responsible authorities, a new class of models was developed: the stream-aquifer models, where the flow in both the surface water network and the aquifers present could be studied in detail. Conjunctive use of water resources is aimed at reducing the effects of hydrologic uncertainty about the availability of water. For example, artificially recharged aquifers can provide adequate water supplies during sustained dry periods when surface water resources run out and nonrecharged aquifers do not provide enough storage.

TABLE 2. IMPORTANT PROCESSES IN GROUND-WATER MODELING

Flow:
- single fluid flow
- multifluid flow
  - multicomponent
  - multiphase
- laminar flow
  - linear/Darcian
  - nonlinear/non-Darcian
- turbulent flow

Transport:
- advection/convection
- conduction (heat)
- mechanical dispersion
- molecular diffusion
- radiation (heat)

Fate:
- hydrolysis/substitution
- dissolution/precipitation
- reduction/oxidation
- complexation
- radioactive decay
- microbial decay/biotransformation

Phase Transfers:
- solid⟷ gas: - (vapor) sorption
- solid⟷ liquid: - sorption
  - ion exchange
- liquid⟷ gas - volatilization
  - condensation
  - sublimation

Phase Changes:
- freezing/thawing
- vaporization (evaporation)/condensation

Conjunctive use models simulate more processes than those included in watershed models. Important processes include canal seepage, deep percolation from irrigated lands, aquifer withdrawal by pumping, ground-water inflow to or outflow from adjacent aquifers, evapotranspiration, artificial recharge, bank storage effects, and deep-well injection (El-Kadi 1986). The inclusion of detailed ground-water flow processes in watershed models increases significantly the complexity of model computations. Differences in temporal scale between surface and subsurface processes add to the complexities.

Recently, increased interest in such multi-system modeling has been motivated by the need to simulate the flow and chemical transport in systems with complex interaction between the surface water and subsurface water. This includes wetland systems, watersheds subject to nonpoint pollution from the use of agricultural chemicals, and regional systems where local soil and ground-water pollution contribute to the quality of surface water bodies. To model this type of problem, transport and fate processes are added to the multi-system flow models.

The flow and solute transport models may be embedded in a management model. The hydrologic system is described in terms of objective function(s) and constraints. For example in ground-water hydraulic management problems, the objective function is aimed at managing ground-water stresses such as pumping and recharge and the discretized ground-water flow equations are treated as part of the constraint set. The resulting equations are solved through an optimization technique such as linear and quadratic programming

(Gorelick 1983, Gorelick *et al.* 1983, Kaunas and Haimes 1985, Wagner and Gorelick 1987).

1.1.3. Classification Based on Mathematical Approaches

The classification scheme used by the IGWMC distinguishes three different classes in mathematical approaches: (1) the general nature of the governing equations; (2) the dimensionality in the space and time domain (for variables, parameters, and boundary conditions); and (3) the solution method employed.

In terms of spatial dimensionality, models may be capable of simulating systems in one, two, or three dimensions. In the time domain, they may handle either transient or steady-state simulations or both. Another distinction in the way models handle parameters spatially is whether the parameter distribution is lumped or distributed. Lumped parameter models assume that a system may be defined with a single value for the primary system variables, and the system's input-response function does not necessarily reflect known physical laws. In distributed-parameter models, the system variables often reflect detailed understanding of the physical relationships in the system and may be described with a spatial distribution. System responses may be determined at various locations.

Until recently, most ground-water modeling studies were conducted using deterministic models based on precise descriptions of cause-and-effect or input-response relationships. Increasingly, however, models used in ground-water protection programs reflect the probabilistic or stochastic nature of a ground-water system to allow for spatial and temporal variability of relevant geologic, hydrologic, and chemical characteristics (US EPA 1986a, El-Kadi 1987, Dagan 1989, NRC 1990).

Most mathematical models used in ground-water management are distributed-parameter models, either deterministic or stochastic. Their mathematical framework consists of one or more partial differential equations called field or governing equations, as well as initial and boundary conditions and solution procedures. Most models used in the field are based on a deterministic description of the processes governing flow and transport. Other models assume that the processes active in the system are stochastic in nature and hence the variables may be described by probability distributions. Consequently, system responses are characterized by statistical distributions estimated by solving the governing equation.

The governing equations for ground-water systems are usually solved either analytically or numerically. Analytical models contain a closed-form or analytical solution of the field equations subject to specified initial and boundary conditions. The analytical solution is continuous in space and time. Because of the complex nature of ground-water problems, the analytical solutions generally are available for problems that entail a simplifying nature of the ground-water system, its geometry, and external stresses (Walton 1984, van Genuchten and Alvas 1982).

In numerical models, a discrete solution is obtained in both the space and time domains by using numerical approximations of the governing partial differential equation. As a result of these approximations, the conservation of mass is not always assured (because of truncation and round off errors) and needs to be verified for each application. Spatial and temporal resolution in applying such models is a function of

study objectives and availability of data. If the governing equations are nonlinear, linearization often precedes the matrix solution (Remson *et al.* 1971, Huyakorn and Pinder 1983); sometimes solution is achieved using nonlinear matrix methods such as predictor-corrector or Gauss-Newton (Gorelick 1985).

Various numerical solution techniques are used in ground-water models. They include finite-difference methods (FD), integral finite-difference methods (IFDM), Galerkin and variational finite-element methods (FE), collocation methods, boundary (integral) element methods (BIEM or BEM), particle mass tracking methods (e.g., random walk method [RW]), and the method of characteristics (MOC) (Huyakorn and Pinder 1983, Kinzelbach 1986). Among the most used approaches are finite-difference and finite-element techniques. In the finite-difference approach a solution is obtained by approximating the derivatives of the PDE. In the finite-element approach an integral equation is formulated first, followed by the numerical evaluation of the integrals over the discretized flow or transport domain. The formulation of the solution in each approach results in a set of algebraic equations which are then solved using direct or iterative matrix methods.

In semi-analytical models, complex analytical solutions are approximated by numerical techniques, resulting in a discrete solution in either time or space. Models based on a closed-form solution for either the space or time domain, and which contain additional numerical approximations for the other domain, are also considered semi-analytical models. An example of the semi-analytic approach is in the use of numerical integration to solve analytical expressions for streamlines in either space or time (Javandel *et al.* 1984).

Recently, models have been developed for study of two- and three-dimensional regional ground-water flow under steady-state conditions in which an approximate analytic solution is derived by superposition of various exact or approximate analytic functions, each representing a particular feature of the aquifer (Haitjema 1985, Strack 1988, Rumbaugh 1991).

No universal model can solve all kinds of ground-water problems; different types of models are appropriate for solving different types of problems. It is important to realize that comprehensiveness and complexity in a simulation do not necessarily equate with accuracy.

1.2 MODEL INFORMATION SYSTEM

This section summarizes the development and operational design of the ground-water model referral database or computerized data directory MARS (Model Annotation Search and Retrieval System). Also discussed are the MARS database objectives, database design criteria, and database maintenance and updating procedures.

One of the IGWMC's primary objectives is assembling, organizing, analyzing, and disseminating information related to the development and use of computer-based simulation methodology (i.e., mathematical models) in response to changing water resources management demands and benefiting from computer technology development (van der Heijde 1987). Development of information sources, processing procedures and user feedback, together with an efficient computer-based system for information management and dissemination is crucial for such a facility to be successful.

In order to manage efficiently information concerning the rapidly increasing number of models, a standardized descriptive reporting system has been developed. Each model is described in an uniform way by a set of annotations describing its purpose, major hydrological, mathematical and operational characteristics, input requirements, simulative capabilities, level of documentation, availability, and applicability. A complete model annotation includes comments made by the model author and IGWMC staff concerning its development, testing, quality assurance and use, as well as names and addresses of users of the model, and model references.

1.2.1. Historic Development

In 1979, the Center established its first annotated database of information on ground-water models MARS (Version 1.0). The original descriptors resulted from the evaluation of a list of keywords used in a ground-water model review study conducted by the Holcomb Research Institute in 1975–1978 under auspices of SCOPE (Scientific Committee on Problems of the Environment [Bachmat *et al.* 1978]). The database was initially implemented on a UNIVAC 90/30 mainframe computer using software specially written for this purpose in the COBOL language. The information was stored in binary code [(0,1) = (no,yes) using a list of more than 200 descriptors, and as text fields (van der Heijde and Williams 1989). The data entered were based on an update of the results of a survey performed during the earlier study (Bachmat *et al.* 1978).

In 1982 this database was transferred to a DEC VAX 11/780 minicomputer and implemented with the VAX-based database management system DATATRIEVE-11. Although the data record structure was maintained, this conversion was used to add to and improve the list of model descriptors and to review the database contents resulting in MARS, Version 2.0. Since then, IGWMC staff has continually maintained, updated, and used the annotation system for storage of new information on ground-water models (covering all aspects of the aquatic subsurface including unsaturated and multiphase systems), and for retrieval of information for internal research and in response to external requests.

In the mid-1980s developments in modeling and computer technology led the IGWMC staff to review the annotation and software system then in use. The identified problem areas included:

- various types of models or model capabilities that were not adequately described;
- sluggish system behavior, especially when the database was searched;
- user interfaces were not intuitive and informative (not user-friendly);
- software was difficult to maintain, requiring expertise not always available at IGWMC or its host organizations;
- the system was only transferable to other DEC/VAX systems with DATATRIEVE resident under the DEC/VMS operating system;

- the software did not allow for decentralized updating of the database contents.

Rapid expansion of the kind of models the Center was asked to provide information on, and the increasing complexity of the models involved, required the descriptors to be expanded, regrouped, and hierarchically organized.

Modifications implemented included increasing the level of detail in the description of models for heat transport, transport of reactive solutes, transport in deformable and fractured rock and soils, biotransformation in subsurface transport, and optimal conjunctive use of ground-water and surface water. Categories to be added included hydrogeochemical models, ground-water parameter identification, and integral modeling of quantitative and qualitative aspects of ground-water and surface water systems.

The new system then would cover all subsurface flow and transport models including multiphase flow and vapor transport, and models simulating surface water/ground-water interaction and movement of water and dissolved chemicals between the subsurface and the atmosphere.

Furthermore, the Center needed a performance evaluation system to document usability and reliability of the models.

Because current users only indirectly access the Center's modeling information databases, the need to improve access has been recognized. One way to meet this need would be to make the database available in the microcomputer environment. However, the Center's experience has been that many current users of its model information service are primarily interested in selecting a model for a particular application. Often, these users are not familiar with the variety of available models or with the selection process, thus requiring IGWMC staff to provide additional assistance in analyzing the model requirements. In the design of the new version of the model information management system, procedures have been developed to facilitate such assistance, either provided directly by the Center's staff, or indirectly through implementation of new technologies, i.e. an experimental knowledge-based advisory system.

The new system has been implemented on a microcomputer operating under MS-DOS in the form of a relational database programmed in TurboPascal™ version 5.0 from Borland (van der Heijde and Williams 1989).

Based on the analysis of the needs for information on ground-water models, five types of potential model use have been identified:

- application to field problems in support of policy-making and resource management decisions;
- analyzing field and laboratory experiments as part of a research program;
- as basis for new model formulations and software development;
- in education regarding modeling principles and in training in the use of models;

- verification of and comparison with other models.

The content and structure of the database is thus a consequence of its primary objective: identification of models for any of the above uses. Furthermore, the following design criteria were formulated:

- assure completeness of data
- obtain a balance of information stored
- allow intuitive operation
- facilitate optimal user–computer interaction (e.g., effective screen layout, command structure, and command execution)
- permit efficient, useful, and "neat" reporting
- facilitate efficient searches
- facilitate efficient, multilocation updating of database content
- realize efficient internal data storage in terms of computer core memory use and mass storage
- facilitate fast operation (e.g., efficient CPU-mass storage device interaction)
- allow portability within the hardware–software environment in which the database is developed

The design criteria for the model referral database MARS are discussed in detail in van der Heijde and Williams (1989).

1.2.2 Database Management

Computer database management procedures emphasize data integrity and security, whether for referral information or actual data sets. This is accomplished by developing and enforcing strict data processing procedures that include authorization rules specifying that certain tasks be performed only by a specified group of users. External users, for example, are not allowed to write, modify, or delete data from the master database. Another important procedure requires routine data backup, thus allowing recovery of the database files in the event that their content is corrupted, destroyed, or lost.

At the IGWMC, the referral databases are backed up automatically when their contents are updated. In addition, the master database is backed up daily as part of institutional computer network backup

procedures. The daily backups are stored for at least one week, while once a week a backup is made to be stored for at least a month, etc.

To prevent program alteration, additional measures have been taken, including separation of program source codes from the user-accessible environment, using only executable images of the software. In addition, the operational software (both database management software and application programs) may be reloaded from backup in the event of data corruption.

As the MARS referral database might be distributed off-site, complete with search and report-generating software, procedures have been adopted to prevent data corruption off-site while maintaining the integrity of database content. To protect this content, only compiled versions of the search and report-generating software will be widely distributed, and database users will be provided periodically with updated data files and application programs to replace their previous versions.

1.2.3 Identification and Annotation of Models

The IGWMC staff continuously collects and analyzes information on models related to subsurface flow and transport phenomena. The initial information may come from open literature or from presentations and discussions at conferences, workshops, and other meetings, or may be obtained directly from researchers.

Once a model of interest is located, additional information is collected from the research team that developed the model, and from pertinent literature, to enable the Center's staff to include the model in the MARS database. In selecting a model for inclusion in the referral database, special attention is given to the importance of the model with respect to the kind of questions raised in model-based problem solving, and to the development status of the model (e.g., research instrument or deliverable versus generally applicable, well-tested and documented routine tool).

To assure consistency in the evaluation of the model information and in the data entered in the referral database, a standardized form, the MARS data entry form, has been designed (van der Heijde and Williams 1989). A complete data set annotation includes comments made by the original development team and the IGWMC staff, as well as bibliographic references regarding its development, theoretical foundation, updating, and use. After detailed evaluation of the model documentation by the Center's staff, the data is entered into MARS.

To ensure that the model description is correct and complete, a full report of the stored information is verified with the model author or custodian, if identified.

Once all the information describing a model is entered in the referral database, the information is checked for completeness and data entry errors.

Evaluation and verification of the information contained in the databases is a continuing process. In order to fulfill the growing and changing information needs of users, comprehensive and flexible procedures

for maintaining, updating, and expanding the databases have been adopted. Every few years the database structure (programs and record structure) and contents are reviewed and revised.

2. FLOW MODELS FOR POROUS MEDIA

Ground-water flow models simulate the movement of one or more fluids in porous or fractured rock systems. One fluid is always water and the other may be an immiscible liquid such as a nonaqueous phase liquid (NAPL). Most existing ground-water models consider only the flow of water in saturated or variably saturated porous systems. Increasingly, research is concerned with multiphase flow of immiscible liquids and water and with flow and transport in fractured media.

The mathematical model for ground-water flow is derived by applying principles of mass conservation (resulting in the continuity equation) and conservation of momentum (resulting in the equation of motion; Bear 1972, 1979). The equation of motion generally applicable in ground-water flow is Darcy's linear law for laminar flow, which originated in the mid-nineteenth century as an empirical relationship. Later, a mechanistic approach related this equation to the basic laws of fluid dynamics (Bear 1972). Some models use a nonlinear equation of motion to describe flow around well bores in large fissures and in very low permeable rocks (non-Darcian flow; Hannoura and Barends 1981, Huyakorn and Pinder 1983).

In order to solve the transient flow equation, both initial and boundary conditions are necessary (Franke *et al.* 1984). Initial conditions for saturated flow systems consist of given values for the piezometric head throughout the model domain. Initial conditions for variably saturated flow models are usually expressed in terms of pressure head. For most models, inclusion of initial conditions is only needed when transient simulations are performed. Boundary conditions for flow simulation may be any of three types: specified head (Dirichlet or first type), specified flux (Neumann type or second type), and head-dependent flux (Cauchy, mixed or third type) conditions. Boundary conditions are specified on the periphery of the modeled domain, either at the border of the modeled area or at locations within the system where system responses are fixed (e.g., connections with aquifer penetrating surface water bodies, or fluxes in/out of the system such as through wells).

Models exist for simulating flow under saturated or partially saturated (i.e., unsaturated) conditions. Models designed for saturated systems are not able to deal with unsaturated systems. Most of the models designed for partially saturated systems can handle variable saturation conditions, sometimes over a wide range from saturated or nearly-saturated to highly unsaturated conditions. The latter type of models use a single set of equations, generally based on the Richards equation or a variant of it (DeJong 1981, El-Kadi 1983). Models that have separate formulations for simulation of flow in the saturated zone and unsaturated zone are sometimes called coupled saturated-unsaturated zone models. Complex liquid wastes often consist of multiple miscible and immiscible chemical components of varying density and viscosity. Saltwater intrusion is another density-driven flow phenomenon that impairs parts of many coastal aquifers and, increasingly, deep continental freshwater aquifers. An evaluation of methods for analysis of saltwater intrusion is presented in Jousma *et al.* (1988). An overview of existing models for the latter type of use is given by van der Heijde and Beljin (1985).

IGWMC has compiled a comprehensive descriptive listing of models that address saturated, unsaturated, and multiphase flow. Appendix A of this report covers saturated flow models; Appendix B covers models for variably saturated flow; multiphase flow models are listed in Appendix I. The listings have

been compiled from the Center's MARS model referral database, and have been limited to those models that are documented and available for third-party use.

2.1. MATHEMATICAL FORMULATION FOR SATURATED FLOW

The flow of a fluid through a saturated porous medium can be derived by combining the mass conservation principle with Darcy's law resulting in (Bear 1979):

$$\nabla \cdot (K \nabla h) - W^* = S_s \frac{\partial h}{\partial t} \tag{1}$$

in which h is the hydraulic head, t is time, K is the hydraulic conductivity tensor, W^* is the source/sink term expressed as a volume flow rate per unit volume with positive sign for outflow and negative for inflow, and S_s is the specific storage that is defined as

$$S_s = \rho g(\alpha + n\beta) . \tag{2}$$

where ρ, α are the fluid density and compressibility, respectively, n, β are the aquifer porosity, and compressibility, respectively, and g is the gravitional acceleration.

Equation (1) can be written in a matrix form as

$$\frac{\partial}{\partial x_i}\left(K_{ij} \frac{\partial h}{\partial x_j}\right) - W^* = S_s \frac{\partial h}{\partial t} \tag{3}$$

where x_i are the spatial coordinates, t is time, $h=h(x_i, t)$ is the hydraulic head, K_{ij} is the hydraulic conductivity tensor. An overview of saturated flow models is presented in Appendix A.

2.2. MATHEMATICAL FORMULATION FOR UNSATURATED FLOW

Because air and water are immiscible fluids, when they coexist a discontinuity takes place between the two phases. The difference in pressure between the two fluids, called capillary pressure (P_c), is a measure of the tendency of the partially saturated medium to suck in water or to repel air. The negative value of the capillary pressure is called suction or tension. The capillary pressure head (ψ) is defined by (DeJong 1981):

$$\psi = \frac{P_c}{\rho g} \tag{4}$$

The hydraulic head is given by

$$h = z - \psi \tag{5}$$

in which z is elevation above an arbitrary datum.

The governing equation for unsaturated flow is derived by combining the mass balance principle with Darcy's law, ignoring compressibility of matrix, fluid, and air effects. The resulting equation, known as Richards' equation, is (DeJong 1981, El-Kadi 1983)

$$\nabla \cdot (K \nabla h) = F \frac{\partial h}{\partial t} \tag{6}$$

where $K = K(\theta)$ is the hydraulic conductivity, θ is volumetric water content, h is total head, t is time, and F is moisture capacity defined as

$$F = \frac{d\theta}{dh} = - \frac{d\theta}{d\psi} \tag{7}$$

The mathematical formulation and solution of the flow problem in the unsaturated zone require describing the hydraulic properties of soil, preferably in functional forms. The soil-water characteristic functions, $\psi(\theta)$ and $K(\theta)$, in which θ is the volumetric water content, is included in these properties. Hysteresis usually prevails in the relationship $\psi(\theta)$, i.e., a different wetting and drying curve. Soil air entrapment causes separation of the boundary drying and wetting curves at zero pressure. In fine-grained soils, subsidence or shrinking may cause the same effects. In general, simulation under hysteresis is difficult due to the existence of an infinite number of scanning, drying, and wetting curves, depending on the wetting-drying history of the soil. Examples of the generalized algebraic equations representing the moisture-characteristic curve with no hysteresis are given by Brooks and Corey (1964), Gardner (1958), Haverkamp *et al.* (1977), and van Genuchten (1978). An overview of variably saturated flow models is given in Appendix B.

2.3. MULTIPHASE FLOW

Fluids that migrate in the subsurface environment can be grouped with regard to their migration behavior as either miscible (mixes) with water or immiscible (does not mix) with water (Morel-Seytoux 1973, Parker *et al.* 1987). Miscible fluids form a single phase, while immiscible fluids form two or more fluid phases (a fluid is either a liquid or a gas). Such a grouping of fluids is essential for discussion purposes because the movement of two or more immiscible fluids is distinctly different from the simultaneous movement of miscible fluids. The flow of immiscible fluids gives rise to two-phase or multiphase flow and transport; miscible fluids give rise to single-phase flow and transport. The following discussion is based primarily on Kincaid and Mitchell (1986).

Migration patterns associated with immiscible fluids introduced at the soil surface (e.g., as a chemical spill) are schematically described by Schwille (1984). The extent and character of migration depends on the chemical characteristics, the source volume, the area covered by the source, the infiltration rate, and the retention capacity of the porous medium. Retention capacity is a measure of the volume of immiscible liquid or nonaqueous-phase liquid (NAPL) that can be held in the porous medium without appreciable movement. This volume is analogous to the volume of water prevented by the capillary force from draining because of the gravity force.

When the retention of the partially saturated soil column is not exceeded, the bulk of the liquid chemical contaminant will be retained in the soil column. Migration of the contaminant away from the spill site may occur as a result of its dissolution in water; it may also move in the gas phase. Contaminated soil water arriving at the water table will be carried down-gradient in the unconfined aquifer and in the capillary fringe. Figure 1 shows the ability of heterogeneous sediments within the partially saturated zone to laterally spread or broaden the contaminant plume with increasing depth. To estimate the retention capacity of the partially saturated soil column, the soil profile and moisture content must be known.

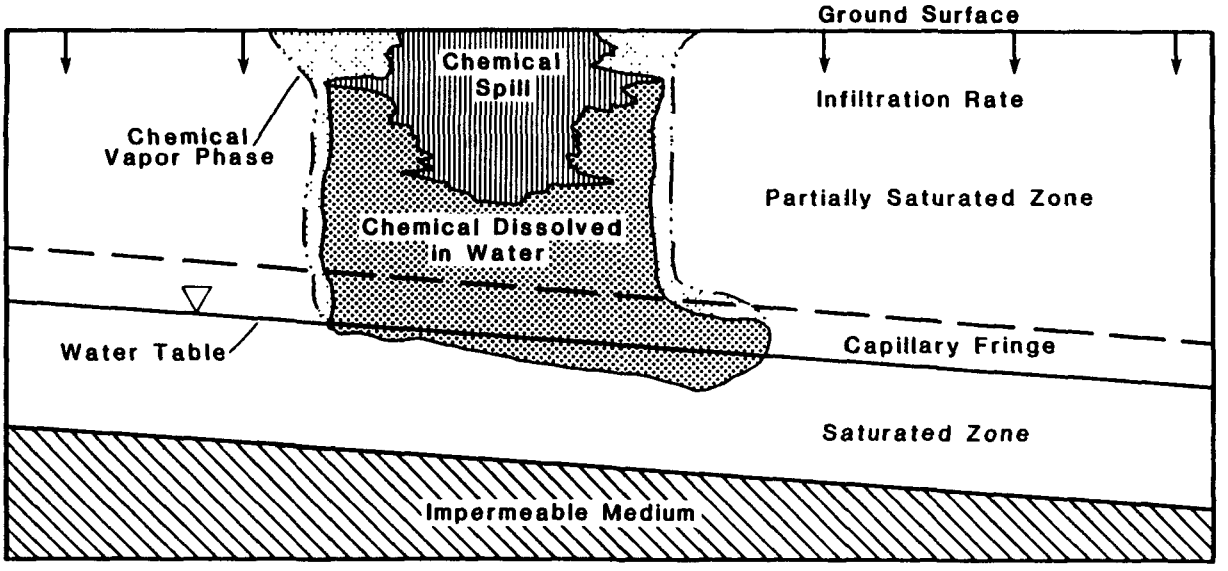

Figure 1. Schematic diagram of a chemical spill of a volume less than the retention capacity of the partially saturated soil profile (from Schwille 1984)

When the bulk volume of the chemical entering the soil exceeds the retention capacity of the partially saturated soil profile, the chemical will reach the water table in its liquid phase. Chemicals that are less dense than and immiscible in water (Light Nonaqueous Phase Liquids, LNAPLs) will remain in the capillary fringe of the partially saturated zone and near the water table in the saturated zone, as indicated in Figure 2. Examples of this type of pollutant are gasoline, jet fuel, and oil. Immediately beneath the spill, chemicals can be forced below the water table level and into the saturated zone by the pressure of the overlying liquid chemical mound (comparable to ground-water mounding in a phreatic aquifer resulting from recharge) replacing the water present. As the plume migrates down-gradient, the overlying pressure decreases and buoyant forces bring the lighter-than-water chemical up to the water table. The contamination will spread as a distinct liquid chemical phase at the water table, and if the chemical's solubility allows, partially as a dissolved constituent in the ground water. If the contaminant is volatile, it could also spread as chemical vapor phase. It should be noted that some fraction of the chemical will be held in the porous medium by

the retention capacity mechanism. Release of this fraction, as a dissolved constituent in soil water and ground water, will be a long-term process.

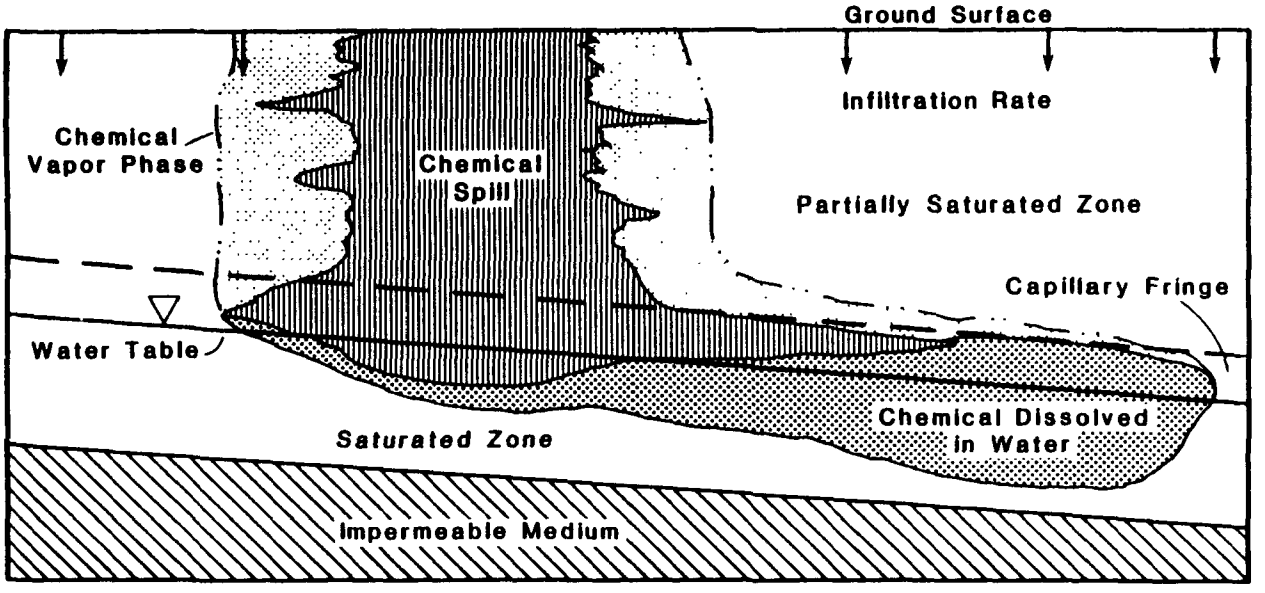

Figure 2. Schematic diagram of a lighter-than-water chemical spill of a volume greater than the retention capacity of the soil (from Schwille 1984)

As a substantial part of bulk volume of a heavier-than-water immiscible liquid (e.g., TCE) reaches the water table, the chemical will continue to move downward by displacing the ground water. These liquids are called Dense Nonaqueous phase Liquids (DNAPLs). Depending on the physical/chemical properties of the chemical with respect to the impermeable formation, the chemical may continue its downward migration or form a mound above the impermeable bottom of the aquifer. Chemicals lying on the aquifer bottom will migrate by following the relief of the bedrock or may enter the fractures in the bedrock. These various aspects of the migration of the heavier-than-water chemical are shown in Figure 3.

As occurred in the partially saturated zone, heterogeneity within the saturated zone will cause the contaminant to spread laterally as it migrates vertically. Note that the slope of the bottom topography (i.e., relief of the bedrock) may not coincide with the ground-water gradient; the chemical is driven by its own hydraulic gradient not the hydraulic gradient of the ground water, and, hence, the migration of the solvent phase may actually be in a direction opposite to ground-water flow.

The existence of distinct fluid phases competing for the same pore space is governed by mass and momentum balance equations and data that uniquely specify the balance between the fluids in the soil

environment. The wetting fluid is usually water; examples of a non-wetting fluid are mineral oil, chlorohydrocarbons, and soil air (Parker *et al.* 1987). Flow of each fluid is proportional to its potential gradient, the permeability of the medium, the fluid density and viscosity, and the portion of pore space (i.e., cross-sectional area) that the fluid occupies.

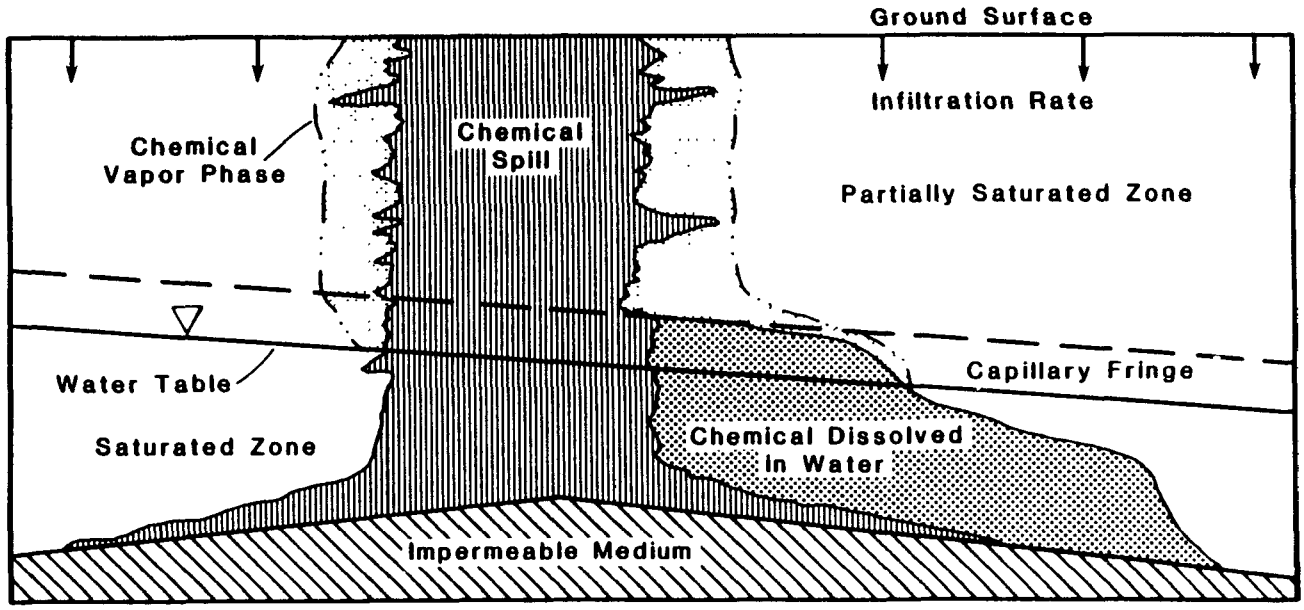

Figure 3. Schematic diagram of a heavier-than-water chemical spill of a volume greater than the retention capacity of the soil (from Schwille 1984)

A fluid mass balance and Darcy's equation can be written for each of the fluids (Bear and Bachmat 1990). When the detailed-flow phenomena in each fluid phase are of interest, as is the case with two liquids, the mass and momentum balance equations for each fluid should be solved. Consistent sets of saturation and potential for each fluid are obtained from such an analysis. However, when flow phenomena for only one of the two fluid phases are of interest, as is commonly the case with moisture movement in the partially saturated zone, the saturation and potential of the fluid of interest should be solved. The saturation of the second fluid can then be simply calculated given the porosity of the medium (i.e., given that it occupies the remaining pore space).

The relative permeability of the wetting and non-wetting fluids depends strongly on the degree of saturation (Dracos 1978, Parker *et al.* 1987). The curves describing the permeability of the fluids show the nonlinear behavior of fluids in a partially saturated environment. Unique curves exist for different fluids and media. In general, each fluid must reach a minimum saturation before it will flow. In the case of water and air, the minimum saturation for water is called the irreducible saturation. For moisture movement in the

vadose zone, soil physicists have found that irreducible saturation is actually a function of the suction pressure applied and the length of time one is willing to wait for the soil column to respond. Thus, irreducible saturation may not necessarily be single-valued. The wetting or non-wetting fluid must exceed its residual saturation before it will flow. Residual saturation is the measure of the ability of a soil to retain moisture and consequently the bulk of a chemical spill.

One of the more complex migration patterns that may occur involves three phases (Kuppussamy *et al.* 1987). Water and chemical would exist as liquid phases and soil air would exist as a gaseous phase. The flow process is more complicated than the two-phase situation, although the same principles of mass and momentum balance apply. The individual fluids are immobile over relatively large areas of the saturation triangle, as shown in Figure 4; a relatively small central region exists over which all three phases are simultaneously mobile.

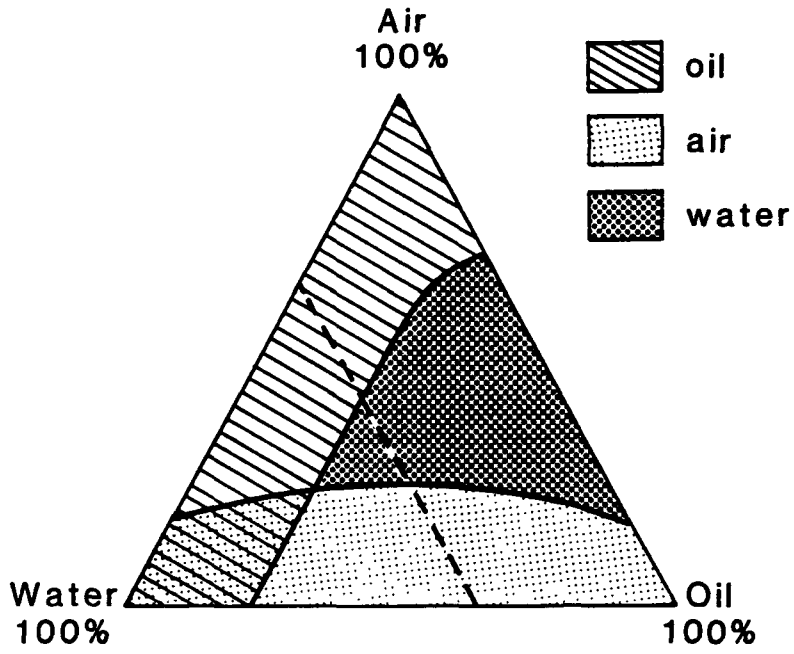

Figure 4. Funicular zones for three immiscible fluids

At low organic fluid saturations, a continuous organic phase may not exist and the organic fluid might be present as isolated globules surrounded by water. Such continuity is an essential assumption in virtually all existing models. In the current generation of models, discontinuity in a phase means that the relative permeability of the fluid goes to zero and that the model predicts no flow (Parker *et al.* 1987). In reality, however, migration of these isolated parcels of organic fluid can occur, resulting in a process termed "blob flow." This process is well known in tertiary oil recovery where the aim is to mobilize such "blobs," using injected surfactants and gases (e.g., Gardner and Ypma 1984). Existing mathematical models and codes cannot handle transport by way of globule migration.

2.3.1. Modeling Multiphase Flow

Models and codes for organic chemical migration are commonly categorized as (1) those for which fluid physics of immiscible organic liquids are emphasized, and (2) those for which organics appear as miscible constituents in which chemical/microbiological reactions for dilute levels of contamination are emphasized. Existing models and codes can be used to model selected phases to the extent that vapor phase exchange and transport, geochemical reactions, and microbiological degradation can be incorporated in existing codes (i.e., insofar as the mathematical equations are unchanged by the addition of these processes and reactions). These models are based on the assumption that for each phase continuous flow paths exist throughout the porous medium (Streile and Simmons 1986). A simplified version of such an approach is presented by Dracos (1978). The proposed model consists of vertical one-dimensional flow in the unsaturated zone through a column of radius R, under the source (Figure 5) and a two-dimensional horizontal model for the low density liquid atop the water table. For the miscible component in the plume a common two-dimensional solute transport model is used, taking the source term from the one-dimensional vertical column model. That it is not easy to make simplified modeling approaches work successfully for real-world phenomena is demonstrated by the Bartz and Käss experiment (Figure 6) in which the bulk oil continues to advance slowly after 120 days, but the outmost boundary of detectable solutes is retreating, resulting in a 120-day contour being located outside the 360-day contour (Dracos 1978).

Experimental models for more complex systems, documented recently, include finite-element formulations by Abriola and Pinder (1985a, 1985b) and Kuppusamy *et al.* (1987) and a finite-difference formulation by Faust (1985).

Models available for simulating NAPL contamination can be grouped into (1) sharp interface models, (2) capillarity models, and (3) interphase partitioning models. In the first category, it is assumed that sharp interfaces exist between various fluid phases. These models develop analytical and semi-analytical expressions for time versus infiltration and subsequent spreading of hydrocarbons. The second category of models solve numerically the partial differential equation describing the flow of the hydrocarbon coupled with functional relationships describing saturation and permeability. The third category includes the interphase partitioning of organics between the nonaqueous and water or vapor phases.

NAPL transport has been studied experimentally and modeled by a number of researchers; recent reviews have been introduced by Mackay *et al.* (1985), Abriola (1988), Parker (1989), and Mercer and Cohen (1990). Relevant studies include the work by van Dam (1967), Schwille (1971a,b,c, 1981, 1988), and Albertsen *et al.* (1986). These publications dealt mainly with analyzing the processes involved in the infiltration and subsequent spreading of light or heavy hydrocarbons. Modeling efforts include the work by van Dam (1967), Mull (1969, 1971, 1978), Dracos (1978), and Schiegg (1977), all of whom assumed sharp interfaces between various fluid phases. The studies by Mull, Dracos, and Schiegg developed analytical and semi-analytical expressions for time versus both infiltration and subsequent spreading of light hydrocarbons. El-Kadi (1991) adopted some of these formulations and examined the accuracy of the infiltration phase by comparing the results to those obtained by the numerical model of Kaluarachchi and Parker (1989) which included capillarity effects. As expected, the model is most accurate for NAPL infiltration into soil with a deep water table where pressure changes in soil-water are minimum. Corapcioglu and Hossain (1986) also

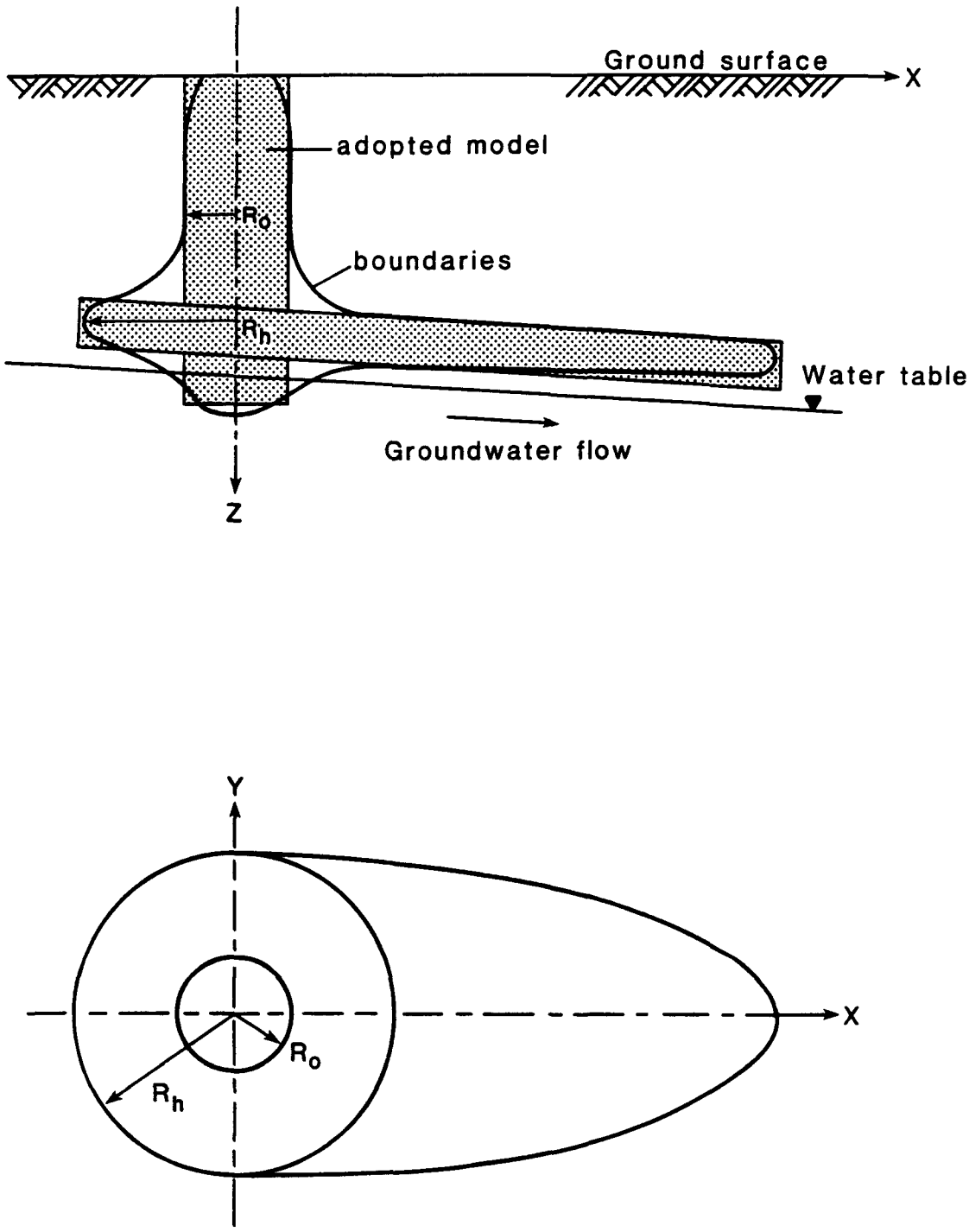

Figure 5. Schematized vertical infiltration and horizontal spreading of the bulk of a low density hydrocarbon atop the water table (after Dracos 1978).

adopted the sharp interface assumption to estimate infiltration of hydrocarbons and solved numerically a two-dimensional equation describing the dissolved phase.

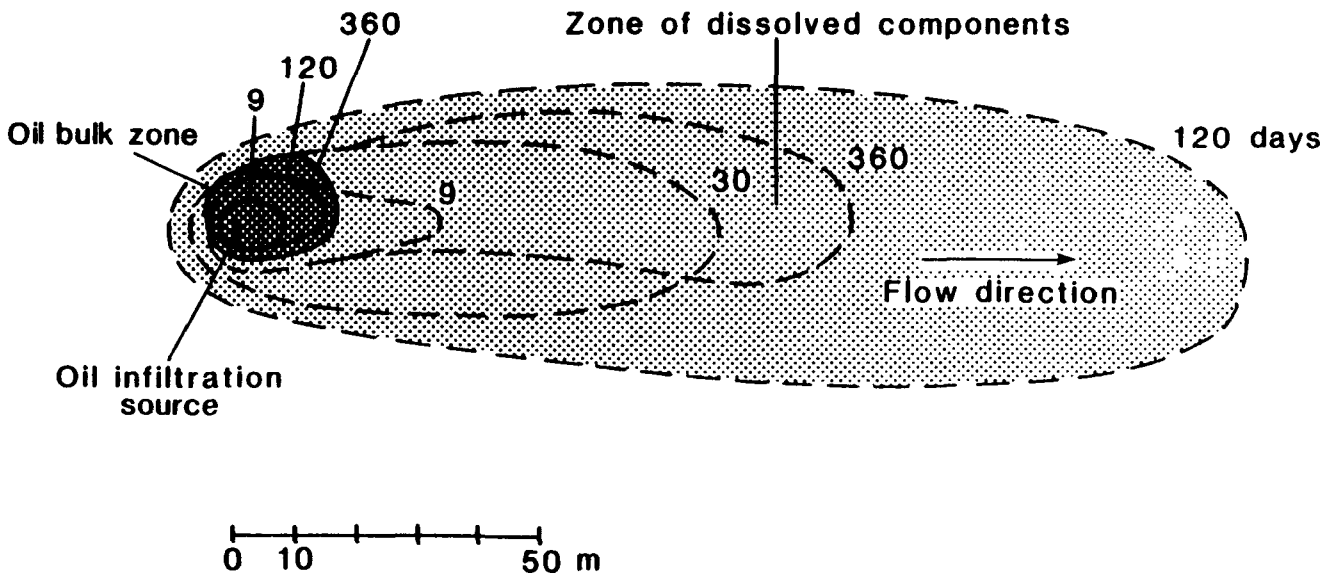

Figure 6. Oil bulk zone and spreading of dissolved components in ground water from a field experiment by Bartz and Käss (after Dracos 1978)

Models that include capillarity effects have been also introduced to reduce the limitations of the sharp interface approach. This category includes the work of Arthur D. Little (1983), Faust (1985), Osborne and Sykes (1986), Kuppusamy *et al.* (1987), and Kaluarachchi and Parker (1988). These models solve numerically a partial differential equation describing the flow of the hydrocarbon (i.e., mass balance combined with Darcy's law) coupled with functional relationships describing saturation and permeability.

A more refined category of NAPL models includes the interphase partitioning of organics between the nonaqueous and water or vapor phases (Corapcioglu and Baehr 1987, Baehr and Corapcioglu 1987, Baehr 1987, Allan 1986, and Abriola and Pinder 1985a,b,c). The formulations adopted usually result in a system of highly nonlinear partial differential equations that require an iterative numerical technique.

In the sharp interface approach, the migration process is divided into four phases: (1) infiltration, (2) intrusion and initial spreading, (3) final spreading, and (4) dissolved material migration (Figure 2). As Dracos (1978) indicated, such division is justified due to the difference in the time scale of each phase of the transport. The infiltration phase is fast and can be measured in hours. The early spreading, which depends

on pressure buildup, is one order of magnitude slower and thus can be measured in days. The last two phases are much slower and can be measured in months or even years. The sharp interface approach develops a time-distance profile for various stages from Darcy's law. The following assumptions are included in the formulation:

1. The NAPL gas phase is assumed to be at constant pressure, so only the liquid phase is modeled. Such an assumption is not generally valid due to the volatile nature of NAPL. However, ignoring the gas movement is likely to produce a more conservative estimate to travel times.

2. A sharp transition between NAPL-saturated and dry conditions is assumed; hence, the saturation-capillary relation is idealized as a rectangle, indicating that the pore system is either dry or saturated with the fluid. This assumption is generally acceptable for coarser material.

3. Only air is displaced by the infiltrating NAPL in the unsaturated zone. Air is also assumed to move freely under constant pressure, and water to be immobile. These conditions are generally acceptable in soils near dry conditions.

4. The displacement of fluids is assumed as piston flow; one fluid replaces the other, and hence only one mobile fluid exists in a given location. This type of flow is expected to be most accurate for coarse-textured soils or in situations where gravity or pressure predominates over capillarity.

5. Lateral spreading is ignored, i.e., the flow is assumed to be strictly vertical. Such an assumption is acceptable if the spill area is relatively large.

6. The water table is assumed to be too deep to have an influence on NAPL transport. This could be a serious limitation in some cases due to the large pressure gradient in water, which may affect NAPL movement.

7. Compressibility effects of matrix and fluids are ignored, which is a common assumption in the general treatment of transport in the unsaturated zone.

Interphase flow and transport models include the interphase partitioning of organics between the nonaqueous and water or vapor phases. The equations are derived from mass conservation principles by the application of volume-averaging techniques and the incorporation of various constitutive relations and approximations (Abriola and Pinder 1985a). Effects of matrix and fluid compressibilities, gravity, phase composition, interphase mass exchange, capillarity, diffusion, and dispersion are considered. The assumption of equilibrium leads to some simplification in the system of governing equations. Although this approach is more realistic in representing the physical phenomena of flow and transport in NAPL-air-water systems, its application is hindered by difficulties in solutions and by the data requirement. The governing equations are not given here because the system of governing equations is very involved.

A more detailed discussion of the mathematical formulations encountered in multiphase flow modeling is given in an earlier report by El-Kadi *et al.* (1991). Appendix I provides an overview of multiphase models.

3. TRANSPORT MODELS FOR POROUS MEDIA

3.1. SOLUTE TRANSPORT

The ground-water transport of dissolved chemicals and biota (e.g., bacteria and viruses) is directly related to the flow of water in the subsurface. Many of the constituents occurring in ground-water can interact physically and chemically with the solid phase (soil particles), and with various dissolved chemicals. As a consequence, their displacement is both a function of mechanical transport processes such as advection and dispersion, and of physicochemical interactions such as adsorption/desorption, ion-exchange, dissolution/precipitation, reduction/oxidation, complexation, and radioactive decay (Luckner and Schestakow 1991). Biotransformations taking place during transport can alter the composition of the ground-water significantly (Ward *et al.* 1985).

In modeling the transport of dissolved chemicals, the principle of mass conservation is applied to each of the chemical constituents of interest. The resulting equations include physical and chemical interactions, as between the dissolved constituents and the solid subsurface matrix, and among the various solutes themselves (Konikow and Grove 1984, Reilly *et al.* 1987, Bear and Bachmat 1990, Luckner and Schestakow 1991). These equations might include the effects of biotic processes (Molz *et al.* 1986, Borden and Bedient 1986, Srinivasan and Mercer 1988). To complete the mathematical formulation of a solute transport problem, equations are added describing ground-water flow and chemical interactions, as between the dissolved constituents and the solid subsurface matrix, and among the various solutes themselves. In some cases equations of state are added to describe the influence of temperature variations and the changing concentrations on the fluid flow through the effect of these variations on density and viscosity.

Under certain conditions such as low concentrations of contaminants and negligible difference in specific weight between contaminant and the resident water, changes in concentrations do not affect the flow pattern (homogeneous fluid). In such cases a mass transport model can be considered as containing two submodels, a flow submodel and a quality submodel. The flow model computes the piezometric heads. The quality submodel then uses the head data to generate velocities for advective displacement of the contaminant and spreading through dispersion. Transformations by chemical and microbial reactions may also be included. The final results are computed concentrations and solute mass balances. In cases of high contaminant concentrations in waste water or saline water, changes in concentrations affect the flow patterns through changes in density and viscosity, which affect the movement and spreading of the contaminant. To solve such problems through modeling, simultaneous solution of flow and solute transport equations or iterative solution between the flow and quality submodels is required (Huyakorn and Pinder 1983, Voss 1984, Kipp 1987).

Mass transport models which handle both advective and dispersive transport processes are sometimes called miscible transport models. Models that only simulate advective and dispersive displacements are called conservative models. Nonconservative models simulate both displacements and transformations of contaminants. Nonconservative solute transport models are often based on the assumption that the reactions proceed instantaneously to equilibrium. In general, the reaction rates depend

on the residence time for the contaminant. Recently, various researchers have become interested in the kinetic approach that incorporates chemical reactions in transport models (e.g., Brusseau *et al.* 1989, Valocchi 1989, Sardin *et al.* 1991).

The inclusion of geochemistry in solute transport models has focused on single reaction such as ion-exchange or sorption for a small number of reacting solutes. Because multicomponent solutions are involved in most contamination cases, there is a need for models that incorporate the significant chemical interactions and processes that influence the transport and fate of the contaminating chemicals. There are two approaches for modeling multicomponent solutions. In the first approach, the interaction chemistry may be posed independently of the mass transport equations. The most widely used form of this approach is the coupling of the transport equation with an equilibrium or kinetic phase exchange reaction such as the Langmuir or Freundlich isotherm (Jennings *et al.* 1982). The second approach is to insert all of the interaction chemistry directly into the transport equations (Jennings 1987).

Several difficulties impair both the credibility and the efficient use of mass transport models. One such difficulty is "numerical dispersion" in which the actual physical dispersion mechanism of the contaminant transport cannot be distinguished from the front-smearing effects of the computational scheme (Huyakorn and Pinder 1983). Another numerical problem influencing the results of solute transport modeling takes the form of spatial oscillations (overshoot and undershoot) near a concentration front, especially for advection-dominated transport, sometimes resulting in negative concentrations. A problem inherent to all numerical techniques, although of a different order of magnitude, is numerical inaccuracy. Numerical problems can often be mitigated by grid refinement or, in some cases, selection of an alternative method (Huyakorn and Pinder 1983). For particle-in-a-cell methods (e.g., random walk method and method of characteristics), higher accuracies can be obtained by increasing the number of particles in the system (Uffink 1983, Kinzelbach 1986).

Another issue is model dimensionality. Although a pollution problem is typically three-dimensional, vertical averaging is frequently used, resulting in the utilization of a two-dimensional, horizontal mass transport model that is generally connected with a hydraulic flow model. Such models tend to underestimate peak values and thus may fail to predict dangerous concentration levels and critical arrival times of pollutants in wells that become polluted by surface or near-surface sources.

It should be noted that multi-phase petroleum reservoir models do not appear to be readily applicable to organic transport analyses. These codes address only fluid flow phenomena and neglect entirely transport and attenuation phenomena. Petroleum reservoir simulators are useful in regard to the theory and numerical methods embodied for simulating multiphase, immiscible-fluid flow.

Appendix C presents an overview of available solute transport models.

3.1.1. Advection-Dispersion Equation

Processes that control the migration of solute include advection, hydrodynamic dispersion, geochemical and biochemical reactions and radioactive decay.

In the case of a conservative solute, no reactions occur between the solute and the solid phase. The rate of transport is equal to the seepage velocity. If the transport of solute is due only to advection, a sharp interface will separate the flow domain that contains the solute and the native ground-water. However, this interface does not remain sharp because hydrodynamic dispersion causes the solute spreading over a greater volume of aquifer than would be predicted by advection alone. This means that the travel time from the source to the point of observation for part of a pollutant release will be less than derived from calculations focussed on the center of the plume or based on a sharp front approach.

Advection--

Advection is the solute movement with the bulk flow of the fluid (water). Estimation of advection is based on fluid flow characteristics, flow paths, and velocity. Numerical models are often used as a substitute for field measurements to identify the flow field.

Dispersion--

Dispersion is considered to be caused by both microscopic and macroscopic effects (Dagan 1986). However, most studies of flow through porous media are conducted on a macroscopic scale where Darcy's law is valid. Hydrodynamic dispersion refers to the spreading of a solute at the macroscopic (Darcy) level by the combined action of mechanical dispersion and molecular diffusion (Bear 1972, 1979; Bear and Bachmat 1990; Battacharya and Gupta 1990; Moltyaner 1990). Mechanical dispersion is caused by the changes in the magnitude and direction of velocity across any pore cross-section at the microscopic level. Pores differ in size and shape, also causing variation in the maximum velocity within individual pores, in addition to velocity fluctuations in space with respect to the mean direction of flow. This results in a complex spatial distribution of the flow velocity. Molecular diffusion results from variation of solute concentration within the liquid phase and causes the solute to move from regions of higher concentration to regions of lower concentration.

In general, flux, Q_c, due to mechanical dispersion is estimated by analogy to Fick's law, i.e., flux is proportional to concentration gradient (Bear 1979). Combining expressions of both the diffusion and mechanical dispersion result in the equation

$$Q_c = -D' \nabla C \tag{8}$$

in which D' is the coefficient of hydrodynamic dispersion. D' is estimated as the sum of the coefficients of mechanical dispersion, D, and molecular diffusion, D_m. D is a tensor usually having longitudinal and transverse components. D_m is expressed generally as a function of the molecular diffusion coefficient of a chemical species in pure water and a tortuosity factor accounting for the pore system and the degree of saturation (Bresler and Dagan 1981, Gupta and Battacharya 1986), namely,

$$D_m = \eta_1 (\theta) D_m' \tag{9}$$

in which η_1 is the tortuosity factor, θ is volumetric water content and D'_m is the diffusion coefficient in pure water. One model for η_1 is

$$\eta_1 = \frac{\theta^{10/3}}{n^2} \tag{10}$$

where n is porosity. Equation (10) is similar to that concerning air diffusion, as proposed by Millington and Quirk (1961). Written in tensor form, the coefficient of hydrodynamic dispersion can be expressed as

$$D'_{ij} = D_{ij} + D_m \delta_{ij} \tag{11}$$

where D_{ij} is the coefficient of mechanical dispersion, D_m is the coefficient of molecular diffusion, and δ_{ij} is the unit tensor.

The contribution of molecular diffusion to hydrodynamic dispersion is small when compared to mechanical dispersion and for any practical purpose may be neglected. However, its effects cannot be neglected for underground injection of hazardous wastes where the injection rates are in the order of centimeters per year for very fine soils (e.g., clays).

The coefficient of mechanical dispersion is usually expressed as a function of the velocity of groundwater and to the fourth order tensor, α_{ijkm}, called the dispersivity of the porous medium (Bear 1972, 1979):

$$D_{ij} = \alpha_T \bar{V} \delta_{ij} + (\alpha_L - \alpha_T) \frac{\bar{V}_i \bar{V}_j}{\bar{V}} \tag{12}$$

where α_L and α_T are the longitudinal and lateral dispersivity, δ_{ij} is the Kronecker delta, $\bar{V}_i$ and $\bar{V}_j$ are components of the flow velocity in the i and j direction respectively, and $\bar{V} = |\bar{v}|$, the magnitude of the flow velocity or in Cartesian coordinates. In two-dimensions, equation (12) takes the form:

$$D_{xx} = \alpha_T \bar{V} + (\alpha_L - \alpha_T) \frac{\bar{V}_x^2}{\bar{V}} \tag{13a}$$

$$D_{xy} = D_{yx} = (\alpha_L - \alpha_T) \frac{\bar{V}_x \bar{V}_y}{\bar{V}} \tag{13b}$$

$$D_{yy} = \alpha_T \bar{V} + (\alpha_L - \alpha_T) \frac{\bar{V}_y^2}{\bar{V}} \tag{13c}$$

If one of the axes coincides with the direction of the average uniform velocity $\bar{V}$, for example the x-axis, equations (13a-c) become

$$D_L = D_{xx} = \alpha_L \bar{V} \tag{14a}$$

$$D_T = D_{yy} = D_{zz} = \alpha_T \bar{V} \tag{14b}$$

where D_L and D_T are the coefficients of longitudinal and transverse dispersion, respectively.

Dispersivity is influenced by vertical and horizontal permeability, permeability variations, and degree of stratification (Güven *et al.* 1984, Black and Freyberg 1987; Moltyaner 1990; Molz *et al.* 1990). Because large solute plumes encounter more permeability variations than small plumes, dispersivity tends to increase and approach some maximum asymptotic value (Gelhar *et al.* 1979). The difference between dispersivity values measured in the laboratory and evaluated in the field may be attributed to the effects of heterogeneity and anisotropy (Pickens and Grisak 1981a,b, Neuman *et al.* 1987). The values obtained from tracer tests are equivalent dispersivities that represent dispersion between the measuring point and the injection point (Anderson 1984).

Because of the difficulties in measuring dispersivity, both longitudinal and lateral dispersivities are often determined during calibration of the model. The common assumption is that the medium is isotropic with respect to dispersivity, which implies isotropy with respect to hydraulic conductivity. In practice, this is acceptable because most models used for solving field problems are two-dimensional with vertically averaged hydraulic properties and because generally the horizontal hydraulic conductivity is much larger than the vertical hydraulic conductivity. It should be noted that increasingly stochastic formulations are used to describe the dispersion process (Gelhar 1986, Smith and Schwartz 1980, Uffink 1983, Dagan 1989, Neuman *et al.* 1990).

The partial differential equation for solute transport, including dispersion, convection, and a sink/source term may be expressed as (e.g., Anderson 1984)

$$\underbrace{\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right)}_{[dispersion]} - \underbrace{\frac{\partial}{\partial x_i}(C\bar{v}_i)}_{[convection]} - \underbrace{\frac{C'W^*}{n}}_{[sink/source]} = \frac{\partial C}{\partial t} \tag{15}$$

where C is concentration of solute, C' concentration of solute in the source or sink fluid, D_{ij} coefficient of dispersion, and $\bar{v}_i$ seepage or pore velocity. The seepage velocity is calculated as

$$\bar{v}_i = -\frac{K_{ij}}{n}\frac{\partial h}{\partial x_j} = -\frac{q}{n} \tag{16}$$

The hydraulic head, h, is obtained by solving equation (1) or (6).

Adsorption--

Chemicals may partition between volatilized, adsorbed, and dissolved phases. An adsorbed chemical will migrate away from the source of pollution at a different rate than a nonsorbed chemical.

If adsorption/desorption between solid and liquid phase is considered, equilibrium-controlled equation (15) may be expressed as (Konikow and Grove 1984):

$$\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(C\bar{v}_i) - \frac{C'W^*}{n} = \frac{\partial}{\partial t}\left(C + \frac{\rho_b}{n}S\right) \tag{17}$$

where ρ_b is the dry bulk density of the solid and S is the concentration of solute adsorbed on the solid surface.

The relationship between adsorbed concentration (S) and liquid concentration at equilibrium (C) is called the adsorption isotherm:

$$S = S(C) \tag{18}$$

This relationship is obtained in laboratory experiments where the temperature is kept constant and the reactions are allowed to reach equilibrium. Several types of models for adsorption or ion exchange isotherms exist. Most frequently used isotherms are

Linear $$S = K_1 C + K_2 \tag{19}$$

Langmuir $$S = \frac{K_1 C}{1 + K_2 C} \tag{20}$$

Freundlich $$S = K_1 C^{K_2} \tag{21}$$

where K_1 and K_2 are empirically derived constants. The simplest isotherm is given as

$$S = K_d C \tag{22}$$

where K_d is the distribution coefficient:

$$K_d = \frac{\text{mass of solute on the solid phase per unit of solid phase}}{\text{concentration of solute in solution}}$$

Distribution coefficients for reactive nonconservative solutes range from values near zero to 10^3 ml/g or greater (Mercer *et al.* 1982b). All adsorption models represent reversible adsorption reactions. Generally two or more transport equations have to be solved for multi-ion transport problems.

By incorporating equation (22) into equation (17), the advection-dispersion equation takes the form:

$$\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(C\bar{v}_i) - \frac{C'W^*}{n} = R\frac{\partial C}{\partial t} \tag{23}$$

where R, the retardation coefficient, is given by

$$R = 1 + \frac{\rho_b}{n} K_d \tag{24}$$

As a result of sorption, solute transport is retarded with respect to transport by advection and dispersion alone. Sorption reduces the apparent migration velocity of the center of a plume or a solute front ($\bar{v}_s$) relative to the average ground-water flow velocity ($\bar{v}_{gw}$), or

$$R = \frac{\bar{v}_{gw}}{\bar{v}_s} \geq 1 \tag{25}$$

For K_d values that are orders of magnitude larger than 1, the solute is essentially immobile. Sorption capacity of geologic deposits is generally given in this order: gravel < sands < silts < clays ≤ organic material (Mercer *et al.* 1982b). If no sorption occurs, the retardation factor is equal to 1.

Transformation/Degradation--

Transformation processes determine the fate and persistence of chemicals in the environment. The key processes include biotransformation, hydrolysis, and oxidation/reduction. The transformation processes

are generally lumped as a reaction term in the solute transport equation. Reactions are usually represented by an effective rate coefficient which depends on a number of variables such as organic matter content, water content, and temperature. For simplification purposes, however, a first-order constant rate is usually employed in the analysis. For decay it is written as (Konikow and Grove 1984)

$$\frac{\partial C}{\partial t} = - \mu C \tag{26}$$

in which μ is the rate constant.

The solute (tracer) may undergo radioactive or biological decay

$$\frac{\partial C}{\partial t} = - \lambda C \tag{27}$$

where λ is the decay constant and can be calculated if the half-life of the tracer ($t_{1/2}$) is known:

$$\lambda = \frac{\ell n 2}{t_{1/2}} \cdot \tag{28}$$

Including decay and retardation and assuming decay rates are the same for sorbed and mobile species, equation (23) becomes

$$\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(c\bar{v}_i) - \frac{C'W^*}{n} - \lambda RC = R\frac{\partial C}{\partial t} \tag{29}$$

Biodegradation--

Biodegradation in ground-water refers to chemical changes in solute or substrate due to microbial activity. Reactions can occur in the presence of oxygen (aerobic) or in its absence (anaerobic). Research related to biodegradation include the work of Troutman *et al.* (1984), Borden *et al.* (1984, 1986), Borden and Bedient (1987), and Barker and Patrick (1985). Modeling efforts include the work of Sykes *et al.* (1982), Borden *et al.* (1984), Borden and Bedient (1986), Bouwer and McCarty (1984), Molz *et al.* (1986), and Srinivasan and Mercer (1988).

Studies indicate that the number of electrons must be conserved in all biochemical reactions (Srinivasan and Mercer 1988). In such reactions, a reduced product (called electron acceptor) exists whenever a product has carbon atoms in a higher oxidized state due to the loss of electrons. For example, in aerobic reactions oxygen is the electron acceptor and is reduced to water. In anaerobic systems NO_3^- is the electron acceptor and is reduced to NO_2^-, NO_2, or N_2.

Modeling approaches can be divided roughly into: (1) an approach that uses the biofilm concept to simulate the removal of organics by attached organisms (Molz *et al.* 1986), and (2) an approach that assumes that microbial population and growth kinetics have little effect on the contaminant distribution (Borden *et al.* 1984, Srinivasan and Mercer 1988). Both approaches apply Monod kinetics or a modified form of them, to reduce the required number of equations.

Application of the first approach results in a set of five coupled nonlinear equations that need to be solved simultaneously to calculate (Molz *et al.* 1986): (1) concentration of substrate; (2) concentration of oxygen; (3) substrate concentration within the colony; (4) oxygen concentration within the colony; and (5) number of organism colonies per unit volume of aquifer. Three of the five equations are partial differential equations and two are algebraic equations. Micro-colony kinetic parameters are needed for the analysis. The authors applied their approach to a one-dimensional problem for illustration purposes and performed a sensitivity analysis.

Application of the second approach by Borden and Bedient (1984) and Borden *et al.* (1986) has resulted in a two-dimensional model based on three partial differential equations describing contaminant concentration, oxygen concentration, and concentration of microbes in the solution.

Volatilization--

Volatilization is defined as the loss of a chemical in vapor from soil, water and plant surfaces. This process is controlled by the availability of vapor at the soil surface and the rate at which this vapor is carried to the atmosphere. In addition to the saturated vapor pressure of the chemical under consideration, a number of factors affect the actual volatilization rate from the soil surface, including soil and atmosphere characteristics, and management practices. Interaction among these components is also an important factor.

Generally, chemicals can partition into adsorbed, dissolved, and vapor phases. Under equilibrium conditions, the vapor pressure of a solute above its aqueous solution, C_G, is related linearly to the concentration in solution, C, by Henry's law (Fetter 1993)

$$C_G = K_H C \tag{30}$$

where K_H is Henry's constant. A similar relationship was described earlier regarding partitioning into adsorbed and dissolved chemicals.

Vapor movement from the soil to the atmosphere is usually modeled by applying Fick's Law of diffusion (Hern *et al.* 1986). Chemical movement in gaseous form through soil is described by an extension of the same law. The vapor flux is related to concentration gradient by

$$q_v = - \eta_2(a) D_G \nabla C_G \tag{31}$$

in which η_2 is a tortuosity factor and D_G is the dispersion coefficient in air. Millington and Quirk (1961) defined η_2 empirically, by

$$\eta_2 = \frac{a^{10/3}}{n^2} \tag{32}$$

in which a is air content and n is soil porosity. Equation (31) can be added to the general solute transport equation as a sink term.

Plant Processes--

Vegetation is an integral part of the terrestrial ecosystem. Chemicals applied to land surfaces may be intercepted by plant leaves where volatilization, photolysis, or biodegradation occur in addition to absorption by the plant. At a later time, chemicals initially intercepted may be washed off by rain or irrigation water and contribute to solute transport in the soil. Plant roots also affect the transport phenomena by uptaking the chemicals into the plant where they can accumulate in different parts of the plant. Chemicals may move to the leaves where they are subject to transformation and degradation processes. The remaining chemicals may return to the soil following plant death or leaf fall.

Additional modeling difficulties result from the dynamic nature of plants, caused by changes in their condition from the time of planting until harvesting. Also, stem and root penetration can influence the transport phenomena by changing the hydraulic properties of soil.

Plant models have been introduced by plant and soil scientists (see Thornley 1976, Tillotson *et al.* 1980, Campbell 1985). Molz (1981) compiled a list of extraction functions used by various researchers to represent water uptake by plant roots. An exponential depth function adequately describes the extraction patterns for a number of crops under relatively stable conditions, such as a fully developed crop under high frequency irrigation (Feddes *et al.* 1974). Models including relationships for plant uptake of dissolved chemicals are often based on the rates established for water uptake.

3.2. HEAT TRANSPORT

Analysis of heat transport in soils and ground-water aquifers is an important area of research and has many practical applications. Heat transport affects other transport processes directly and indirectly, e.g., contaminant transport. Conversely, heat transport might be affected significantly by other physical and chemical processes. Overlooking such interactive effects may lead to unacceptable errors. Direct effects on pollutant transport are attributed to, for example, changes in the soil/ground-water flow field due to freezing/thawing on the chemical transformation rates due to temperature changes. The indirect effects are due to the fact that some parameters are to a certain extent heat dependent (e.g., hydraulic conductivity).

Major research activities of heat transport processes took place in the 1970's and early 1980's, stimulated by the public interest in high temperature geothermal systems for energy production. Accordingly, attention has been paid to models for simulation of complex systems such as water-steam-rock (Grant *et al.* 1982). Further applications of research relevant to heat transport in the subsurface include aquifer thermal energy storage (Mercer *et al.* 1982a). There, warm waste water from cooling systems is injected into a confined aquifer during the warm season. During the cold season, warm water is recovered and utilized for heating purposes. The resulting cold water is reinjected far enough from the recovery well to prevent accelerating the cooling process of the warm water. An efficiency of heat recovery of up to 60% has been reported in the literature (Molz *et al.* 1978).

Another area of growing interest related to heat transport concerns modeling flow and solute transport under freezing/thawing soil conditions. Difficulties in mathematical formulation, in solution approaches, and

in parameter estimation are currently major hurdles toward the development of practical solutions to this complex problem.

Mathematical formulation of the general heat transport problem in the subsurface involves a coupled system of equations describing the flow of water and heat. The governing partial differential equations are nonlinear, because some parameters are a function of at least one dependent variable (temperature) interrelated by equation of state. In such a case, only numerical techniques might provide a solution. To solve the general equations analytically, a simplified subset of the general equations is required, resulting in separate, non-coupled solutions for flow and heat transport (Mercer *et al.* 1982a). The analytical solutions for flow assume isothermal conditions. The analytical solutions for heat transport assume a very simple and known flow field.

Numerical methods used in heat transport models were reviewed by Pinder (1979), Lunardini (1981), Mercer *et al.* (1982a), and Huyakorn and Pinder (1983); in more general terms, heat transport models were described in Bachmat *et al.* (1978), van der Heijde *et al.* (1985), and El-Kadi *et al.* (1988).

This section reviews briefly the theory of flow of water and solute in the subsurface under nonisothermal conditions. Details of the formulations may be found elsewhere (e.g., Lunardini 1981 and Farouki 1986). A list of available models is provided in Appendix D.

3.2.1. Heat Transport Equation

Ground-water may appear as ice, liquid, or steam, interacting with an aquifer. The heat transport equation is derived by applying the energy balance principles concerning the transport, storage, and external sources/sinks of heat. Dependent variables in this equation may be temperature or enthalpy. In general, a state of thermodynamic equilibrium is assumed, i.e., the temperature in different constituents (solids and fluids) is equal within the representative elementary volume for which the equations are derived. The processes that contribute to heat transport include conduction, convection, dispersion, radiation, evaporation/condensation, and freezing/thawing. Heat conduction occurs in all soil constituents, i.e., solids, water in different phases, and air. In air and vapor, heat conduction is caused by collision between molecules that increases their mean kinetic energy as heat moves from warmer to cooler regions. In liquid water, the same process occurs in addition to energy transfer by breaking and forming of hydrogen bonds. In crystalline solids, e.g., quartz, increased atomic vibration at one end will cause the neighboring atoms in the lattice to follow suit. Heat flux due to conduction is given by

$$Q_{cd} = \lambda_o \nabla T \tag{33}$$

in which T is temperature and λ_o is the thermal conductivity of the porous medium (water plus solid), defined as the rate which heat energy flows across a unit area of the soil due to a unit heat gradient in a porous matrix (Bird 1960).

Free or forced heat convection contributes to heat transfer. Free convection develops due to the existence of a temperature gradient resulting in density changes. On the other hand, forced convection is

due to currents of fluids that move through pores of soils as a result of head gradients. For a fluid with velocity v_w the convective flux is given by

$$Q_{cn} = v_w \rho_w C_w T \tag{34}$$

in which ρ_w and C_w are density and specific heat of the fluid, respectively.

Dispersion, sometimes referred to as lateral mixing or turbulent diffusion, is caused by mixing in the pore system. Dispersive heat flux is given by

$$Q_D = \rho_w C_w \delta \nabla T \tag{35}$$

in which δ is the heat dispersion coefficient

$$\delta = \beta |V_w| \tag{36}$$

where β is heat dispersivity analogous to solute dispersivity, field observations indicate in the same aquifer that their magnitudes may differ (de Marsily 1986).

Radiation, usually an unimportant process in heat transport in soils, is the emission of heat from bodies that have temperatures above absolute zero. Heat energy is emitted in the form of electromagnetic waves and travels across a vacuum as well as gases, liquids, or solids. The flow of heat depends mainly on the temperature of the radiating body, namely,

$$Q_R = \sigma \epsilon A (T - T_o)^4 \tag{37}$$

which is known as the Stefan-Boltzmann law. In equation (37), A is the surface area, σ is a constant, and ϵ the emissivity of the surface $(0 < \epsilon < 1)$.

Heat transport caused by evaporation/condensation is the result of the high latent heat (586 cal/g at 20°C). Local vapor pressure increases, causing water vapor to diffuse through interconnected pores to regions of lower pressure, where vapor may condense, releasing its latent heat. Heat flux due to evaporation/condensation is given by

$$Q_s = K_1 \cdot k_v \frac{x_w^s - x_w}{x_w^s} \delta' \tag{38}$$

in which K_1 is the heat flux needed for evaporation/condensation, k_v is a velocity coefficient, δ' is a control parameter that depends on the soil temperature, x_w is the value of the existing mole fraction of water in the soil-air, and x_w^s is the same value for air that is in equilibrium with the liquid water in the soil.

Phase change, in the form of freezing and thawing, is accompanied also by gain or loss of latent heat. Latent heat loss is necessary during ice formation. The apparent specific heat of freezing soil is given by

$$\bar{C} = C_s + C_w \theta_w + C_I(\theta_t - \theta_u) + L \frac{\partial \theta_u}{\partial T} \tag{39}$$

where C_s, C_w, and C_i are specific heat of solids, water, and ice, respectively, θ_t is the total moisture content, θ_u is the unfrozen moisture content, and L is the latent heat of freezing water. The expression in equation (39) is based on the assumption that the specific heat of unfrozen water is the same as that for water under standard conditions (20°C, 0,1 MPa).

Ignoring air movement, the general heat transport equation can thus be derived by applying the mass balance principal to yield

$$\nabla \cdot \{Q_{cd} + Q_D + Q_{cn}\} = \frac{\partial}{\partial t} \{ \sum [\theta_j \rho C_j T \} + S_h \qquad (40a)$$

or

$$\nabla \cdot \left\{ [\lambda_o + \rho_w C_w \delta] \nabla T + V_w \rho C_w T \right\} = \frac{\partial}{\partial t} \{ \sum [\theta_j \rho C_j T \} + S_h \qquad (40b)$$

in which S_h is a source/sink term that includes radiation, evaporation/condensation, or freezing/thawing effects. The subscript j in equation (40) refers to unfrozen water and ice (i.e., $j=w$ for water and $j=i$ for ice). Simplified versions of equation (40b) have been utilized in the analysis, especially in the absence of phase change processes. For example, for a fully saturated aquifer, if heat conduction and density changes are neglected, and if heat capacity was taken as constant, the equation becomes

$$C_w \left[\nabla \cdot (\delta \nabla T + V_w T) \right] = \alpha_h \frac{\partial T}{\partial t} + S_h \qquad (41)$$

in which α_h is the heat capacity of the aquifer.

3.3. VAPOR TRANSPORT

Soil Vacuum Extraction (SVE), or soil venting technology has recently received increasing attention as a relatively inexpensive method for cleaning up hazardous waste sites contaminated with volatile organic compounds (VOCs). This new technology is based on inducing an air flow through the soil, using a vacuum pump or blower, hence stripping and volatilizing the volatile organics from the soil matrix into the air stream (HMCRI 1991, Crow *et al.* 1985, NWWA 1991).

In addition to remediating soils via volatilization, soil vacuum extraction has the potential for enhancing abiotic or biotic degradation of contaminants because it can circulate air or other gases such as ozone at different depths.

In order to evaluate, utilize, and enhance the performance of soil vacuum extraction technology, it is important to understand the physical, chemical, and biological processes that control the transport and fate of volatile contaminants in the subsurface. These processes include multiphase flow (i.e., flow of air, water, and organic compounds), diffusion, dissolution, volatilization, etc. Because of the complex nature of the interactions among these processes, a need exists for laboratory and field studies in addition to mathematical model studies.

3.3.1. Physicochemical and Biological Processes

A number of studies have been documented as attempts to improve the understanding of the complex physicochemical and biological processes involved in soil venting. The processes involved in gas migration through the unsaturated zone are similar to those involved in contaminant transport in the subsurface. Gases are transported in soil by convection due to a pressure gradient, by diffusion due to a concentration gradient, and by compressibility and temperature effects. The governing equations describing contaminant transport in ground-water are adapted for describing gas movement in soil; however, they are usually formulated in terms of molar averaged quantities rather than mass averaged quantities (Mohsen *et al.* 1980, Metcalfe and Farquhar 1987). Metcalfe (1982) provided additional terms to account for the dissolution of the contaminant gas in the soil moisture and the movement of the dissolved phase of the gas due to downward-percolating rainwater, but these terms have not been validated with field data.

Soil characteristics influence the sorption behavior of organic vapors and thus affect the efficiency of vacuum extraction processes. As a result of using dry air for vacuum extraction, a dehydrated soil becomes a powerful adsorbent for organic vapors and hence reduces the efficiency of vacuum extraction processes. On the other hand, when water exists, it displaces the organic compound from the mineral surface and decreases the soil air conductivity. Therefore, humidified air can be used in a way to optimize the SVE processes and keep the soil permeability at a certain level (see Chiou and Shoup 1985).

3.3.2. Laboratory and Field Studies

Laboratory studies can provide quantitative information on individual processes (e.g., diffusion). However, the movement of the immiscible phase of an organic compound (e.g., gasoline) in the subsurface, and the effectiveness with which pools of the compound can be removed by venting, cannot be evaluated on a laboratory scale. Large physical models coupled with numerical modeling can be useful in examining the product movement, dissolution, volatilization, and weathering.

An example of laboratory studies was that performed by Houston *et al.* (1989). They developed a batch-type testing method for determining the adsorptive characteristics and equilibrium adsorption coefficients for gaseous chemical species on partially saturated soils. The effects of both water content and surface area on the adsorptive capacity of partially saturated soils for a gaseous component were investigated; equilibrium was reached in all tests. Houston *et al.* (1989) found that for a given soil, due to the decrease in the surface area of soil, the sorbed mass decreased with increasing water content, provided the solubility of the gas in water was low. They reported that other factors, such as the initial and final concentration of the gaseous pollutant, soil mineralogy, organic content, and degree of monolayer versus multi-layer adsorption, may be overshadowed by the available surface area for gas adsorption. Volatilization is shown to be a significant long-term transport mechanism, and biodegradation results in the escape of appreciable contamination to the atmosphere. Ostendorf and Kampbell (1989) have derived and field-calibrated a model of coupled hydrocarbon and oxygen transport in a microbiologically active vadose zone with a shallow water table.

Soil venting may be used to increase biodegradation (Hinchee 1989); based upon preliminary field work it appears that utilizing soil venting to deliver oxygen to contaminated vadose zone soils is feasible and the system becomes less oxygen-limited. Further work has been initiated by Hinchee (1991) to maximize biodegradation rates and minimize volatilization rates, with the objective of minimizing volatile hydrocarbon emissions.

3.3.3. Numerical Model Studies

Mathematical models can provide valuable assistance in assessing the migration of hazardous vapors in soil from spills of volatile chemicals, just as they have been helpful in solving the analogous problem of contaminant transport in ground-water. Mohsen *et al.* (1980) and Metcalfe and Farquhar (1987) developed mathematical models for simulating gas transport in porous media based on the continuum approach presented by Bear (1972) for contaminant transport in ground-water. The problem is formulated, however, in terms of molar averaged quantities rather than mass averaged quantities. Mohsen's model was applied to select an appropriate landfill size in a given plot of land; the results indicated that the depth of the landfill may serve as a first estimate of the trench depth. Metcalfe and Farquhar (1987) demonstrated that the reduction of the model from three to two dimensions, assuming uniformity along the landfill boundary, is applicable because the length of the waste disposal site boundary often exceeds gas excursion distances by an order of magnitude.

Sleep and Sykes (1989) have developed a model that simulates water phase flow and transport, and density-dependent gas flow and transport. The model incorporated rate expressions for dissolution, volatilization, and gas-liquid partitioning. The authors investigated the importance of including volatilization, gas-liquid partitioning, and advection in the gas phase for accurate determination of the fate of volatile organic compounds in variably saturated media. They reported that volatilization and gas-liquid partitioning, in combination with diffusion of organic vapors from the soil gas to the atmosphere, may be more important than dissolution in dissipating residual amounts of volatile organics immobilized in the unsaturated zone. They recommended laboratory and field studies on various fate processes for better understanding and for model verification and validation.

Johnson *et al.* (1990) developed a mathematical model that can be used as a screening tool to help determine if *in situ* soil venting will be a viable remediation option at any hazardous waste site. Three factors have been shown to have significant effect on the efficiency of any soil venting operation: vapor flow-rate, contaminant composition, and vapor flow-path relative to the contaminant location. The study presented equations that can be used as predictive tools to estimate the behavior of various aspects of the venting operation, such as vapor flow-rates as a function of well vacuum, or the change in residual composition with time. Examples of model predictions are presented, and the advantages and limitations of this remediation tool are illustrated. Thorstenson and Pollock (1989) noted the importance of including the Knudsen (1909) diffusion, the molecular and nonequimolar components of diffusive flux, and viscous flux in studying the multicomponent gas transport in unsaturated zones. They also discuss the adequacy of applying Fick's law to estimate the total fluxes of stagnant gas (e.g., nitrogen) versus non-stagnant gas. They demonstrated

that the error associated with estimating the total fluxes of nonstagnant relative to stagnant gases can vary from a few percent to orders of magnitude.

Other recently developed models include those by Lin and Kinzelbach (1990), Cho (1991), and Sabadell *et al.* (1991). The aforementioned studies and others demonstrate the mobility of volatile organic constituents in the unsaturated zone, a characteristic that can be exploited by the soil venting technology. The International Ground Water Modeling Center has compiled information regarding models that simulate the gaseous transport of volatile compounds in the unsaturated zone (Appendix E). These models can be invoked to assess the use of the venting technology in soil remediation.

4. HYDROGEOCHEMICAL MODELS

Hydrogeochemical models are used to analyze chemistry of subsurface aquatic systems independent of physical mass transport processes. The models can simulate chemical processes that regulate dissolved species concentrations, including mixing, adsorption, ion-exchange, oxidation-reduction reactions, complexation, and dissolution/precipitation reactions.

Hydrogeochemical codes may be used to determine what elements are expected to be mobile under given conditions of pH, oxidizing or reducing environment, and in the presence of mineral formations (Kincaid *et al.* 1984). When coupled with a transport code, they facilitate the simulation of the movement of metals from the surface (e.g. solid and liquid waste disposal facilities) through soil formations into or toward the ground water below. Their input requirements include one or more of the following information: initial concentration in the aqueous (dissolved) and solid (soil-matrix) phases, temperature, thermodynamics data base, and kinetic data base (Kincaid *et al.* 1984).

Coupling hydrogeochemistry and transport processes can be realized through the source/sink term in the transport equation for the chemical species under study. There are two processes that affect the sink/source term directly (Kincaid *et al.* 1984): adsorption/desorption and precipitation/dissolution. Other chemical processes may indirectly modify the source/sink term by affecting the processes mentioned above, (e.g., aqueous speciation, reduction/oxidation, hydration and ion interaction, kinetics, generation of gases, and isomorphic substitution).

The focus of this section is on thermodynamic models for systems at chemical equilibrium (though EQ3NR/6 and PROTOCOL [listed in Appendix G] contain submodels that do not require equilibrium assumptions). Equilibrium is rigorously defined for closed systems, (i.e., systems that cannot exchange matter with their surroundings). Since all natural ground-water systems are open systems, the time-invariant condition describing the chemical state of the ground-water system is steady-state, not equilibrium (Rice 1986). Therefore, application of thermodynamic equilibrium models to ground-water systems must be done with care. Although chemical equilibrium in some ground-water environments may be assumed for time scales of tens of hundreds of years (Morgan 1967), certain processes may not approach equilibrium for much longer periods of time; additionally, some reactions may be near equilibrium, while others in the same system are not.

Although a system may not be at equilibrium, the thermodynamic models may be used to indicate how close or far a reaction is from equilibrium. Although equilibrium models do not indicate the rate at which a reaction occurs, they do yield a description of the final state toward which the system is tending (Rice 1986).

Equilibrium models can be valuable tools in predicting the behavior of complex hydrogeochemical systems. They do have limitations, however, and only by understanding the conceptual as well as the computational model can they be properly applied and interpreted. To predict reliable results they need a complete complement of important aqueous complexes, accurate thermodynamic data bases and algorithms

for predicting adsorption/desorption of specific aqueous species and the transfer of elements into immobile mineral phases (Kincaid *et al.* 1984). The following discussion, based primarily on van der Heijde *et al.* (1988), deals with the basis for the theoretical derivation of the thermodynamic equilibrium models and limitations of those models. Nordstrom *et al.* (1979), Jenne (1981), Kincaid *et al.* (1984), and Nordstrom and Ball (1984) review the actual models and computer codes. An overview of currently available computer codes is included as Appendix G.

4.1. GIBBS FREE ENERGY AND EQUILIBRIUM CONSTANTS

In any system, a process is determined to be at equilibrium when the energy function is at a minimum. For a closed system at constant temperature T and pressure P, the energy associated with a hydrogeochemical process is described by the Gibbs free energy function (Denbigh 1971, Lewis and Randall 1961, Moore 1972), which is defined as the total Gibbs free energy of the products (final state) minus that of the reactants (initial state)

$$\Delta G = cG_C + dG_D - aG_A - bG_B \tag{42}$$

for the general chemical reaction

$$aA + bB \longleftrightarrow cC + dD \tag{43}$$

where upper case letters represent the species, and lower case letters the appropriate stoichiometric coefficients.

The Gibbs molar free energy for any individual species is related to the activity a_i of the species by the expression

$$G_i = G_i^o + RT \ln a_i \tag{44}$$

where G_i^o represents the free energy of the species in a standard state condition, and R is the gas constant.

The expression for ΔG in equation (42) can be rewritten in terms of equation (44) as

$$\Delta G = \Delta G^o + RT \ln \frac{a_C^c \, a_D^d}{a_A^a \, a_B^b} \tag{45}$$

At equilibrium, the ratio of activities raised to the power of the respective stoichiometric coefficients is equal to the equilibrium constant, K (law of mass action), and the change in total free energy, ΔG, is zero; therefore

$$\Delta G_r^\circ = -RT \ln K \tag{46}$$

4.2. ELECTROLYTES AND ACTIVITY COEFFICIENTS

Because equilibrium constants are defined in terms of activities, or effective solute concentrations, it is necessary to relate these quantities to experimentally measurable concentrations. The relationship (Moore 1972)

$$a_i = \gamma_i m_i \tag{47}$$

where γ_i is the activity coefficient and m_i the concentration of a component i considered to be the solute, is based on a standard state that obeys Henry's Law. The solution becomes ideal $(\gamma_i = 1)$ at low solute concentrations:

$$\lim_{m_i \to 0} \frac{a_i}{m_i} = 1 \tag{48}$$

If there are more than one solute in solution, all solutes must simultaneously conform to the limit in equation (48).

If the expression for activity in equation (47) is substituted into equation (44), the result may be written

$$G_i = G_i^\circ + RT \ln m_i + RT \ln \gamma_i \tag{49}$$

where the terms $G_i^\circ + RT \ln m_i$ represent the free energy of component i in an ideal solution, i.e., one that follows Henry's Law over the entire range of concentrations. Thus the term involving the activity coefficient is a measure of the real solution's deviation from ideality.

It is possible to calculate single-ion activity coefficients from only electrostatic considerations. This was first done successfully with the Debye-Hückel theory, which manages to provide surprisingly good results despite several contradictory and physically incorrect assumptions (Bockris and Reddy 1970). Essentially, the Debye-Hückel theory ignores short-range interactions between ions of the same charge, and thus predictions become less accurate with increasing solution concentrations. In such concentrated solutions ions with the same charge increasingly affect each other, and those with opposite charge form ion pairs through electrostatic attraction (Robinson and Stokes 1959).

Virtually all current computer models are based on the idea of ion pairing (Bjerrum 1926, Fuoss and Kraus 1933, Fuoss 1958). With the inclusion of these short-range ionic interactions, the modified Debye-Hückel equation for species *i* is

$$\log \gamma_i = - \frac{A_\gamma z_i^2 I^{1/2}}{1 + B_\gamma a_i I^{1/2}} \tag{50}$$

in which A_γ and B_γ are the Debye-Hückel constants that depend on dielectric constant and temperature and to a lesser extent pressure. z_i is the ionic charge, a_i an ion size parameter, and I the solution's ionic strength, defined by the expression

$$I = 1/2 \sum_i m_i z_i^2 \tag{51}$$

In equation (50) the numerator accounts for long-range coulombic interactions, the denominator for short-range interactions that arise from treating the ions as hard, finite-sized spheres. As a correction for short-range ion-solvent interactions as well as short-range ion-ion interactions that are not accounted for by the hard-sphere model, a linear term is often added empirically to equation (50). The extended Debye-Hückel equation which incorporates the linear term, is given by

$$\log \gamma_i = \frac{A_\gamma z_i^2 I^{1/2}}{1 + I^{1/2}} + b_i I \tag{52}$$

where b_i is an ion-dependent empirical constant. The Davies equation (Davies 1967), a modified form of the extended Debye-Hückel equation, given by

$$\log \gamma_i = - \frac{A_\gamma z_i^2 I^{1/2}}{1 + I^{1/2}} - 0.2I \tag{53}$$

is frequently used to determine γ_i, since it is supposedly applicable to solutions of ionic strength up to 0.5M (Stumm and Morgan 1981). The Debye-Hückel equation is valid only up to about 0.1M. Thus computer models that calculate activity coefficients by either (or both) of these equations are restricted to fairly dilute ground water.

4.3. OXIDATION-REDUCTION REACTIONS

Of all the reactions included in any computer model, only a small fraction consists of oxidation-reduction reactions (redox reactions). The model REDEQL-UMD (Harriss *et al.* 1984), for example lists only twenty-two redox couples, and the authors caution that the kinetics of many oxidation-reduction reactions may be slow.

The *emf* or Nernst potential *E* for any reaction involving electron transfer can be determined from the expression (Moore 1972)

$$E = E^{\circ} + \frac{RT}{nF} \ln \frac{a_C^c \, a_D^d}{a_A^a \, a_B^b} \qquad (54)$$

where n is the number of electrons transferred, F is the faraday, and the chemical notation refers to the general reaction in equation (43). The term E° is the standard emf of the redox reaction and can be calculated from the standard electrode potentials of the half reactions that sum to the overall reaction (Latimer 1952).

Because oxidation-reduction reactions can be characterized electrochemically in this manner, a ground-water system's "redox state" can be described in terms of a single parameter, either an overall Nernst potential, usually designated ***Eh*** (Freeze and Cherry 1979), or the negative logarithm of the electron activity designated ***pe*** (Truesdell 1968) in analogy with ***Ph***. The representation of the entire system by a single parameter like *pe* or ***Eh*** is based on the assumption that all the oxidation-reduction reactions occurring in the system are at equilibrium. Although this is not true (Morris and Stumm 1967, Jenne 1981, Wolery 1983), a particular redox couple may be used as an overall indicator of the redox state of the system (Liss *et al.* 1973, Cherry *et al.* 1979).

Lindberg and Runnells (1984) have quantitatively demonstrated the inaccuracy inherent in characterizing an entire ground-water system by a single redox parameter. The field-measured Eh value for each of approximately 600 water analyses was compared with the Nernst potential calculated from the data on ten different redox couples by means of the computer model WATEQFC (Runnels and Lindberg 1981). As these same authors (Lindberg and Runnels 1984) state: "The profound lack of agreement between the data points and the dashed line [which represents equilibrium points] shows that internal equilibrium is not achieved. Further, the computed Nernstian Eh values do not agree with each other. . . . If any measured Eh is used as input for equilibrium calculations, the burden rests with the investigator to demonstrate the reversibility of the system."

Because many of the important oxidation-reduction reactions are very slow and some are even irreversible, it is virtually impossible that any natural-water system can reach equilibrium with respect to all of its redox couples. Improvements in this area of computer modeling will require the inclusion of experimental data for each of the major redox couples in the water system under study.

4.4. LIMITATIONS OF HYDROGEOCHEMICAL MODELS

Each reaction in the set listed for a particular model must be characterized by an equilibrium constant. In any geological environment there is an extremely large number of possible reactions, and this is reflected by the databases of many of the models, some of which consist of several hundred reactions. These include not only reactions occurring solely in the aqueous phase, but also heterogeneous reactions between dissolved species and solid phases, such as precipitation/dissolution and ion exchange, as well as oxidation/reduction and degradation reactions that may be catalyzed by microorganisms in the soil.

At least three fundamental problems are associated with such tabulations of thermodynamic data. A particular species may simply be omitted from the database, so even though it is present in the physical system being modeled, it will obviously not appear in the final speciation results nor will its effect on the speciation of other elements. The program WATEQ3 (Ball *et al.* 1981), for example, is an extension of WATEQ2 (Ball *et al.* 1979) through the addition of several uranium species, but the expanded database does not include vanadium, which frequently occurs naturally with uranium. Thus the influence of minerals containing both elements cannot be taken into account.

Even when the database does contain particular minerals, thermochemical data for them may not be known with very great accuracy. This problem is frequently compounded by other uncertainties, i.e., non-stoichiometry, solution-dependent composition with respect to replaceable cations, meta-stable forms, and variation in free energy and solubility with the degree of crystallinity (Stumm and Morgan 1981).

Only a few models include thermodynamic data which have been checked for internal consistency. Because the data for a particular reaction may come from more than one source, there is no guarantee that all calculations were made with consistent values of the necessary auxiliary quantities or that the data satisfies the appropriate thermodynamic relationships. In a study done by Kerrisk (1981), experimental solubilities of $CaCO_3$, $CaSO_4$, and $BaSO_4$ in 0-4M NaCl solutions were compared to those calculated using four different computer models: WATEQF (Plummer *et al.* 1976), REDEQL.EPA (Ingle *et al.* 1978), GEOCHEM (Sposito and Mattigod 1980), and SENECA2, a modification of the earlier SENECA (Ma and Shipman 1972). Although the ionic strengths exceeded the limitations of the modified Debye-Hückel and Davies equations, the study indicated that results for the four models frequently differed even at low ionic concentrations. Calculations on $CaCO_3$ by GEOCHEM differed markedly from experimental observations even below 0.5M; one possible explanation for this is the inclusion of an equilibrium constant of about 4 for the formation of the ion pair $CaCl^+$. This particular ion pair is omitted from the other three computer models, and Garrels and Christ (1965) note that at ordinary temperatures chloride forms no significant ion pairs with any major cation of natural waters. This clearly points to some of the dangers inherent in the ion-air method employed in equilibrium models, and indicates another potential problem associated with the thermodynamic databases selected for the different hydrogeochemical models.

4.5. MODELING NON-DILUTE SOLUTIONS

A different approach to the problem of ionic interactions in solution is the specific-interaction model (Pitzer 1973), which has been applied to seawater (Whitefield 1975, Eugster *et al.* 1980) and hydrothermal brines (Weare 1981, Barta and Bradley 1985). It has been long assumed that results from the Debye-Hückel theory could be extended by the addition of power-series corrections (Weare *et al.* 1982):

$$\log \gamma_i = \log \gamma_i^{DH} + \sum_j B_{ij}(I) m_j + \sum_j \sum_k C_{ijk} m_j m_k \qquad (55)$$

where γ_i^{DH} is the Debye-Hückel activity coefficient and $B_{ij}(I)$ and C_{ijk} are the second and third virial coefficients respectively (Lewis and Randall 1961), the latter of which is required only for solutions of ionic strength greater than 3M. Pitzer (1973) has succeeded in modeling the second virial coefficient B_{ij} as a function of ionic strength and has also developed a Debye-Hückel term of the form

$$\log \gamma_i^{DH} = - \frac{A_\gamma Z_i^2 I^{1/2}}{1 + bI^{1/2}} + \frac{2}{b} \ln (1 + bI^{1/2}) \qquad (56)$$

which fits experimental data better than the extended Debye-Hückel term given by equation (52).

Although the specific-interaction model is more complex mathematically, it has the distinct advantage of not explicitly including ion pairs for ions that are only weakly associated, such as Ca^{2+} and Cl^-. Instead, the second virial coefficient accounts for these weak associations through dependence on the ionic strength (Weare *et al.* 1982). Weare and his coworkers (Harvie and Weare 1980, Eugster *et al.* 1980, Harvie *et al.* 1982, Harvie *et al.* 1984) have begun applying this model to simple electrolyte systems. The most complicated thus far is one containing only 11 different ionic species, but the preliminary results appear to be a significant improvement over calculations based on ion pairing. There is still considerable work to be done before the specific-interaction model can be applied to ground water in general, but it clearly has the advantage of being able to treat more concentrated solutions than ion-pair theory. Pitzer's equations have already been or are currently being incorporated into at least three hydrogeochemical models: EQ3NR (Wolery 1983), SOLMNEQ (Kharaka and Barnes 1973), and PHREEQE (Parkhurst *et al.* 1980).

4.6. NUMERICAL SOLUTION METHODS

Most of the existing hydrogeochemical speciation codes are based on a highly non-linear system of equations which do not include spatial or temporal dependence (Kincaid *et al.* 1984). Solving these sets of equations generally require two steps: reduction of the number of unknowns and solving the resulting set of simultaneous equations. The techniques for solving the systems of equations can be grouped into four categories: (1) iteration by simple back substitution; (2) predictive back-substitution; (3) mathematical minimalization techniques; and (4) integration of ordinary differential equations. A more detailed discussion of applicable solution methods can be found in Kincaid *et al.* (1984, Volume 1).

5. STOCHASTIC MODELS

Uncertainty due to the lack of information about the system or to the variable nature in space and time of certain properties or processes is increasingly incorporated in the analysis of ground-water systems. Incorporating information uncertainty in stochastic analysis can produce a best estimate of output (the mean) and a measure of the uncertainty of the estimate (the variance). On the other hand, if intrinsic uncertainty is included, the model results can describe head (for example) as a stochastic process resulting from an input (e.g., hydraulic conductivity) represented by a stochastic process. In other words, head is represented, as is the case with hydraulic conductivity, as a mean trend with superimposed fluctuations described by the covariance structure. Rather than a single answer that results from a deterministic model, the stochastic model provides a range of answers that can be expressed through a probability distribution function (PDF) or a number of the distribution moments. In addition, questions regarding spatial structure, statistical homogeneity, and ergodicity of the system (see, e.g., Bakr *et al.* 1978) need to be addressed if intrinsic uncertainty is incorporated.

Review of the stochastic approach to analyze uncertainty due to intrinsic heterogeneity have been presented by Neuman (1982), El-Kadi (1984), and Freeze *et al.* (1989), among others. Deterministic models fail because correct parameter values needed for models are not known at all locations other than those few available measurements. Research in stochastic analysis can be divided into (1) a geostatistical approach to estimate uncertainty in input parameters (e.g., Hoeksema and Kitanidis 1985), and (2) a simulation approach to assess the impact of uncertainty of these parameters on model results (e.g., Bakr *et al.* 1978). In addition, the stochastic analysis has been used to study the physics of flow and transport in fractured and porous media. For example, it can be used to illustrate how heterogeneities affect flow patterns (Smith *et al.* 1989), to analyze the impact of spatial variability on macroscopic dispersion (e.g., Gelhar and Axness 1983, Smith and Schwartz 1984), and to estimate effective parameters that allow the representation of the true heterogeneous media by an equivalent homogeneous one (e.g., El-Kadi and Brutsaert 1985).

Two issues stand central in the stochastic approach. The first issue is describing the spatial variability in probabilistic terms. In general, statistical distributions of model parameters can be estimated through the use of the geostatistical approach to analyze available data (e.g., Hoeksema and Kitanidis 1985). Given a set of data points located at random in space, the geostatistical approach (also known as kriging) offers a best linear unbiased estimation of a regionalized variable (e.g., hydraulic conductivity) at various locations. A spatial structure is used in the analysis, through the variogram which indicates the degree of correlation between values of the variable as a function of distance. In general, an assumed distribution of the variable (e.g., normal or log-normal) is employed and the first few moments of that distribution are used as input to the stochastic simulation model. These moments include the expected value, the variance, and covariance of the variable.

The second issue involves mathematical techniques to solve the stochastic equation. The available approaches can be divided into analytical, quasi-analytical, and numerical. The analytical techniques include derived distributions that provide an explicit expression of the PDF of the output variable (e.g., hydraulic head) as a function of the PDF for the input variable (e.g., hydraulic conductivity). This approach also

includes the spectral analysis technique (Bakr *et al.* 1978, Gelhar and Axness 1983) that estimates the expected value and covariance of output parameters.

The quasi-analytical techniques include finite-order (first- or second-order) or perturbation analyses (Sagar 1978, Dettinger and Wilson 1981). They also provide expressions for the first few moments within a finite-element or a finite-difference framework.

The numerical approach employs the Monte-Carlo technique, i.e., the repetitive solution of the deterministic problem for a large number of realizations, each with a set of parameters that is an equally probable representation of the actual set of parameters. The final product is a set of answers that can be analyzed to estimate the PDF or the first few moments of the distribution of the output variable. Example applications of the technique are presented by Smith and Freeze (1979) and El-Kadi and Brutsaert (1985).

A decision-theory framework based on the probabilistic structure of the measured variables can be used to assess the worth of data (Massman and Freeze 1987). An objective function that includes benefits, costs, and risks is optimized, allowing for assessment of the economic consequences of either planning alternative measurement strategies for a new site, or adding new measurements to an existing data collection strategy. When additional costs are no longer balanced by the risk reduction, additional measurements are not justified. This probabilistic modeling framework can also be used to make decisions regarding alternative actions, such as selecting between alternative sites for waste disposal or between alternative engineering designs for a specific site.

6. MODELS FOR FRACTURED ROCK

Fractured rocks can be classified according to the fracture system. Metamorphic and igneous rock are characterized by very low matrix porosities and permeability. Sedimentary rocks are characterized by a low- to high-porosity matrix with low or high permeability, depending on rock type. Understanding mechanisms of flow and mass transport in fractured rocks is critical, especially to the evaluation of the suitability of waste disposal sites in geologic media.

Flow in the fractured rocks is often characterized in a complex manner by the presence of discontinuities in the rock. These discontinuities can consist of cracks, fissures, fractures, joints, and shear zones occurring usually in sets with similar geometries (Witherspoon *et al.* 1987). Flow in such systems may take place through a channel network of interconnected fractures (Streile and Simmons 1986). Flow may also occur simultaneously through the porous component of the media, if present. In the latter case, the flow system is often referred to as a dual porosity system with matrix porosity as primary porosity and fracture porosity as secondary porosity.

In porous media, the size, shape, and degree of interconnection of the pores regulate the flow rate. The scale of these pores is small and for most purposes the medium may be treated as a continuum in which macroscopic flow properties are considered without regard to the actual flow paths of the individual fluid particles. In fractured rock, however, the scale of the pores (e.g., fracture space) can be large enough that the continuum approach is not always appropriate. In such cases, the network of individual fractures must be analyzed to understand macroscopic flow and transport properties (Endo and Witherspoon 1985).

Depending on the nature of the fracture system and the scale of analysis, Bear and Berkowitz (1987) distinguish four different conceptual models for flow (and transport) in fractured media:

Zone 1, the very near field, where flow can be assumed to occur in a single fracture with possible storage in the porous rock matrix block, if present;

Zone 2, the near field, where flow is assumed to occur in a well-defined set of fractures, with possible storage in the porous block, if present;

Zone 3, the far field, where flow (and storage) in two overlapping continua are considered: a network of fractures and porous blocks with exchange between them; and

Zone 4, the very far field, where the domain can be considered as a single continuum representing the properties of both the fractures and porous blocks.

Considering this classification, Zones 1 and 2 can be represented mathematically by a discrete fracture network model, Zone 3 by a double porosity (or *dual-porosity*) continuum model, and Zone 4 by a single porosity continuum model (*i.e.*, equivalent porous medium approach).

The major issues in analyzing fluid flow through a network of fractures, where the rock matrix is essentially impermeable, are determining the permeability of the fracture system and establishing whether or not such networks behave more or less as a porous medium. It is often observed in the field that rock masses contain sets of discontinuous fractures of finite size within a single plane. As a result, the degree of interconnection between the assemblage of discontinuous fracture planes has a major influence on the hydraulic conductivity of the total system (Witherspoon *et al.* 1987). The density, or number of fractures per unit volume of rock, is another important feature. Finally, the orientation will determine those directions along which the fluids may flow within the rock mass.

Flow in relatively large fissures requires a discrete fracture conceptualization where the flow within individual fractures is modeled directly as flow in an interconnected network of channels. The lack of precise information on the line configuration of fractures often leads to the need for stochastic representation of fracture geometry and distribution (Streile and Simmons 1986).

Contaminant and heat transport in fractured rock formations is governed by the same processes as in granular media: advection, mechanical dispersion, molecular diffusion, and chemical and biochemical reactions and in the case of heat transport, conduction. However, there are some differences in the effects that fractured media can have on these processes due to the need for a detailed description of the fluid velocities, the sparseness of the flow channels, their unequal distribution through the rock media, and in fractured porous rock the interaction between the fluid in the fractures and in the rock matrix. These effects are especially noticeable in observing dispersion and diffusion processes (Schwartz *et al.* 1983, Sudicky *et al.* 1985).

Although for the study of head distribution in a fractured system the calculation of fluxes is sufficient, for the simulation of solute and heat transport the velocity distribution needs to be known in detail. The velocities are determined by the active porosity (that part of the pore space in which the fluid movement takes place), which is often much smaller than the total porosity.

Mechanical dispersion in a single fracture consists of longitudinal dispersion only. Fracture width is generally too small to show any significant variation in the distribution of mass across the fracture. A major contributor to macroscopic dispersion in fractured media is the geometry of the network of interconnected fractures of limited extent (Smith and Schwartz 1984). The geometry directly determines the variability of the fluid velocity and the average path length through the interconnecting fractures. In general, the velocities in fractured rock are not normally distributed, precluding the use of a Gaussian dispersion model. Macroscopic dispersion is further complicated by local mixing at the connection between fractures.

Recent advances in laboratory and field studies along with simulation models of fluid flow and solute transport in fractured rocks have been documented in the literature. For example, Cacas *et al.* (1990) carried a large-scale experiment to investigate the flow and transport in fractured rocks. Haldeman *et al.* (1991) conducted a laboratory experiment to determine the flow and transport properties of a fractured porous tuff block. Rasmussen (1991) presented a laboratory flow experiment to demonstrate the interface

concept in unsaturated fractures. Cvetkovic (1991) studied the transport of reactive solute in individual fractures.

Mathematical models of flow in fracture systems have been based on the concept of a dual porosity medium (Grisak and Pickens 1981, Huyakorn *et al.* 1987). A few mathematical models exist for modeling flow and transport in saturated fractured and dual porosity media. Various analytical solutions for solute transport in simple fractured systems are brought together in the CRACK package (Sudicky 1986). These solutions include transport in a single fracture with matrix diffusion (but without dispersion along fracture axis), transport in a system of parallel fractures including matrix diffusion, and transport in a single fracture with matrix diffusion and radial diverging flow. A typical numerical model for flow and transport of heat and nonconservative solutes in fractured rock is the TRAFRAP-WT code developed for the International Ground Water Modeling Center (Huyakorn *et al.* 1987) This code is a two-dimensional finite-element code capable of treating both confined and water table aquifers. Fractured rock can be modeled as a system of discrete fractures or as a double porosity system by overlaying the two-dimensional element grid for the porous medium with one-dimensional line elements representing discrete fractures. This approach requires that the geometry of the fracture system be defined on an appropriate scale.

An example of a finite-difference model designed to handle solute and heat transport in fractured porous media is the FRASCL code (Fractured Media - Advanced Continuous Simulation Language) developed at the Idaho National Engineering Laboratory (Miller 1983, Clemo and Hull 1986). This code simulates the fractured system as discrete parallel-sided channels in the porous matrix. As with the TRAFRAP model this code allows for diffusion of chemical compounds from the liquid in the fractures into the matrix blocks. The porous aquifer is defined by a rectangular finite-difference grid of unit thickness. Fracture segments connect any two adjacent nodes (connectivity criterion), vertically, horizontally or diagonally, with a maximum of eight fracture segments converging at a single node. As in TRAFRAP, fractures can have any configuration of length, angle, and start and termination location, constrained only by the connectivity criterion. Aperture is constant in the individual fracture segments between two directly connected nodes, but may change in the fracture's continuation between the next set of nodes.

Recent review of approaches to modeling flow and transport in fractured rock is documented in van der Heijde *et al.* (1988). Additional information regarding the theory and mathematical formulations can be found in Bear and Berkowitz (1987), Chen (1989), Huyakorn and Pinder (1983), Evans and Nicholson (1987). The International Ground Water Modeling Center has compiled a descriptive listing of available models for flow and transport in fractured rocks (Appendix F).

7. GROUND-WATER MANAGEMENT

The management of ground-water resources is concerned with their efficient use in response to current and future demands, while protecting the integrity of the resources to sustain general environmental needs. Resource development may include determining the location, spacing, and sizing of wells, well fields, or other exploitation schemes, and time schedules for their operation. A successful well field project should consider, for example, excessive pumping that may reduce natural discharge of ground water to streams (baseflow) or capillary uptake in shallow aquifers, or that may cause land subsidence. Lowering the water table may increase the cost of pumping and reduce the economic benefit of a project. Quality-related issues may concern siting waste disposal facilities so that exposure, hazard, damage, and health risks are reduced while simultaneously minimizing costs. Another example involves the cleanup of hazardous chemicals in the subsurface within reasonable costs. In any of these examples, a decision made and implemented may have a profound and lasting effect both economically and environmentally. Various methods exist for evaluating alternative scenarios or designs which comprise solution strategies. Most commonly used are ranking and screening procedures based on absolute or relative criteria. Less common, at least in ground-water management, are optimization-based mathematical models. Among others, environmental objectives (e.g., those concerning water quantity and quality) and economic objectives (e.g., those concerning net benefits of a policy or engineering design) are expressed in mathematical terms, and the resulting mathematical models are used to make design or operational decisions.

Ground-water management problems can be formulated mathematically as one or more objective functions (e.g., environmental or economic objectives) that need to be optimized in order to estimate the values of decision variables (e.g., pumping rates, number and location of wells) subject to a set of constraints (e.g., maximum allowable pumping rates, minimum quality standards, limit on drawdown values, etc.). The resulting solution is optimal only with respect to the chosen mathematical models which represent an approximation of the real problem.

7.1. SOLUTION APPROACHES

Within the context of mathematical optimization the solution for an optimal strategy can be obtained by (1) a simulation approach which includes sampling and search procedures, or (2) a formal optimization approach which combines mathematical optimization with simulation.

In the simulation approach ground-water simulation models are used to evaluate alternative strategies through an iterative procedure. The values of decision variables are specified and the resulting objective functions are evaluated. The solution is repeated with all feasible values of decision variables. The main advantage of the simulation approach is the ability to handle highly nonlinear objective functions and constraints that might not be otherwise dealt with through the formal optimization approach. However, this approach may require a large number of model runs to account for all allowable values of the decision variables without the guarantee that an absolute optimal policy will be identified. The efficiency of the simulation approach may be enhanced through the use of a carefully designed computational scenario or through the solution of a simplified optimization problem in a preliminary screening phase.

An application of the simulation approach is the allocation problem as it pertains to ground-water (Loucks *et al.* 1983). It includes identifying a number of decision variables denoting pumping rates that should be assigned to water users, in order to maximize the net benefits. To eliminate the problem of overdrafting, the total drawdown at a specified time and location should not exceed a certain value.

For large-scale problems, systematic sampling and search procedures (Loucks *et al.* 1983) are used to identify an optimal solution by examining the system performance. Either a uniform grid or random sampling approach can be employed in evaluating the sensitivity surface. The uniform grid approach requires evaluating the objective function at uniformly spaced values of the decision variables (in the range of feasible values), a process that may require many simulations. On the other hand, the random approach consists of randomly choosing feasible values of the decision variables and requires sequential search procedures. Previous simulation results are utilized in the process to improve the performance as defined by the value of the objective function. The simplest approach is using trial-and-error; however, its success and efficiency depends on the modeler's understanding of the problem in adjusting the values of the decision variables in the right direction. A formal sequential search would include calculating the rate of increase of the objective function for a specified change in the value of the decision variables.

The mathematically formulated ground-water management problem, as an optimization problem, can be solved using a number of techniques including Lagrange multipliers, linear programming, mixed integer programming, dynamic programming, and quadratic programming. Details of these techniques may be found in Hillier and Lieberman (1980) and Loucks *et al.* (1983). An overview of these techniques is presented by El-Kadi *et al.* (1991). The Lagrange multipliers technique can be used directly in solving the optimization problem as formulated. Dynamic programming is suitable for allocation problems, capacity extension, and reservoir operation. Linear programming is an efficient technique that is suitable for solving optimization problems characterized by a linear objective function and linear constraints.

Other techniques used in ground-water applications include mixed integer programming and quadratic programming. Mixed integer programming deals with optimization problems which include decision variables that must assume integer values. For ground-water problems, such variables may include the number of wells needed to satisfy certain demands. Solution of the mixed integer problem is possible through a branch-and-bound algorithm (Dakin 1965, Hillier and Lieberman 1980). For a maximization problem, assuming that the lower bound on the optimal objective function is known, the technique involves trial and error that may be summarized as follows: (1) the set of all feasible solutions is partitioned into several subsets; (2) for each subset the upper bound on the objective function is obtained; (3) the subsets whose upper limit is smaller than the current lower bound on the objective function is excluded from further consideration; and (4) the process is repeated within each subset and for all remaining subsets until a feasible solution is obtained that identifies the overall optimal value of the objective function.

The quadratic programming term refers to the optimization of a quadratic objective function that is subjected to linear constraints. The quadratic programming problem can be solved by formulating the Kuhn-Tucker conditions (Kuhn and Tucker 1951). The problem reduces to finding a feasible solution to these conditions, provided that the objective function is concave. The problem reduces to a linear programming problem, which can be solved by using the modified simplex method (Bunday 1984, Kinzelbach 1986).

For a more in-depth discussion of solution techniques used in management models, see El-Kadi *et al.* (1991).

7.2. GROUND-WATER MANAGEMENT MODELS

As described by Gorelick (1983) and Datta and Orlob (1988), based on the purpose of the analysis, ground-water management models can be divided into water quantity or water quality models. Each group of models can deal with ground-water management only or with the integrated use of surface and ground-water resources. When the model aims at managing ground-water stresses, it is classified as a hydraulic management model. Ground-water policy evaluation and allocation models, on the other hand, include a significant economic component such as optimizing the net economic benefits, or optimizing the conjunctive use of surface and ground-water resources.

Based on the way hydrogeologic parameters (such as hydraulic head) are represented, ground-water management models can be classified into either lumped- or distributed-parameter models. In the lumped-parameter approach, the management problem is formulated by including explicit solutions of the ground-water problem (e.g., expressions relating head values to pumping rates) in the objective function or in the set of constraints. The distributed-parameter approach is based on the representation of the hydraulic processes through the use of the governing partial differential equations (PDEs). In general the planning formulation consists of a solution technique for the ground-water problem combined with an optimization scheme. A numerical solution technique is usually employed in the solution of the governing PDEs. Although their development and use may include certain difficulties due to complexity of the analysis, the distributed-parameter models have some advantages over lumped-parameter models insofar as they can handle realistic situations, as when parameter spatial variability exists.

Hydraulic models can be solved either by applying the embedding method or the response matrix method. In the first technique, numerical approximations of the governing PDEs are treated as constraints with decision variables, such as hydraulic head, and are estimated at nodes of the discretized flow domain. The optimization problem is generally formulated as a linear programming problem. The use of the embedding matrix technique usually defines the decision variables at all nodes; some of them may not be needed in the decision making. The technique is thus more suitable for relatively small aquifers where many nodes and wells are constrained.

In the response matrix approach, the simulation model is solved to estimate the unit response of the aquifer (e.g., for a unit pumping or recharge). Next, an assemblage of unit responses (called a response matrix) is formulated and incorporated in the management model. The problem can be formulated as linear, mixed integer, or quadratic programming. Constraint equations need to be formulated only for locations and times of interest; hence, the technique is superior to the embedding matrix approach in dealing with large-scale transient problems.

Policy evaluation and allocation models can be solved via a hydraulic-economic response approach, which is a direct extension of the response matrix approach. A second approach involves the use of linked

simulation-optimization, where the results of an external simulation model are used as an input to a series of subarea economic optimization models. The third method adopts a hierarchical approach that treats large systems as a series of independent systems with multiple objective functions.

Examples illustrating applications of the lumped- and distributed- parameter approaches to groundwater management problems are presented in El-Kadi *et al.*. An overview of available management models is presented in Appendix H.

8. CONCLUSION AND DISCUSSION

This report presents an overview of currently available computer-based simulation models for ground-water flow, solute and heat transport, and hydrogeochemistry in both porous media and fractured rock. Separate sections address multiphase flow and related chemical species transport, and ground-water management models. This report reflects the on-going ground-water modeling information collection and processing activities at the International Ground Water Modeling Center (IGWMC).

Systematically analyzing, evaluating and characterizing the capabilities and performance of mathematical models for studying such a complex system as encountered in managing and protecting ground-water resources is a highly challenging activity. In recent years the amount of information resulting from research in the many different disciplines involved has grown rapidly. Moreover, the character of the information available and searched for by the users of this information has changed and expanded. The IGWMC has responded to this challenge by focussing its research on code performance evaluation and the improvement of its information systems. Currently, a microcomputer-based database containing descriptions of more than 450 ground-water modeling codes is being tested. Plans are under development to bring this information system in a graphic microcomputer-based environment.

In the meantime, ground-water modeling continues to evolve. A wide range of flow characterizations are now possible. Many of the flow models include options for various types of time-varying boundary conditions, have the ability to handle a wide variety of hydrologic processes such as evapotranspiration, stream-aquifer exchanges, spatial and temporal variations in areal recharge and pumping or recharging wells. Some models have options to change the field parameters during the simulation runs, thus recognizing the potential influence of contaminants on the hydraulic parameters. Due to significant improvements in the mathematical formulation of the soil hydraulic characteristics, the treatment of boundary conditions and the numerical solution methods employed, models for simulating flow in the unsaturated zone have become more accurate, realistic and reliable.

However, it may be argued that the progress in understanding the transport and fate of contaminants has not yet resulted in a significant increase in the applicability of models to contamination problems. As the complexity of the physics and chemistry involved in the interaction between water, soil/rock matrix and the multi-component (sometimes immiscible) contaminant mixtures has not yet been resolved, models are lacking to adequately simulate many of the contaminant problems encountered in the field.

The same conclusion might be drawn for modeling flow and transport in fractured rock systems. Improved site characterization and stochastic analysis of fracture geometry, together with an improved capability to describe the interactions of chemicals between the active and passive fluid phases and the rock matrix, have facilitated increasingly realistic simulation of real-world fractured rock systems. However, lack of practical field characterization methods still impedes the routine use of such models in support of management's decision-making.

Finally, developments most promising for practical application may be found in the area of parameter estimation. Various geostatistic and stochastic approaches have become available together with new or

updated parameter estimation models and are increasingly used in the field, specifically in determining the distribution of hydraulic parameters.

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APPENDICES A through J

The following appendices contain descriptive listings of selected models from the IGWMC model information database. The models listed are considered by the authors to be relevant, available, and current. Additional information on the models is available from the IGWMC at the Colorado School of Mines, Golden, Colorado 80401. Model categories are: saturated ground-water flow (A), variable saturated flow (B), solute transport (C), heat transport (D), gas flow and vapor transport in the unsaturated zone (E), flow and transport in fractured rock (F), hydrogeochemical speciation (G), optimization for ground-water management (H), and multiphase flow of water and non-aqueous phase liquids (I). Some of the appendices are further divided based on dimensionality and mathematical method. Each appendix has two parts: a table with information for evaluating a model's usability and reliability and a summary of the model's characteristics and its contact address. Appendix J provides a cross-reference to all appendices.

The date listed for each model indicates the release date of the latest version of the code (either released by the original author or by a code custodian) for which information has been provided to IGWMC. Where possible the code custodian is listed as contact address; for some codes the distribution address is listed. Contact IGWMC for information on code distribution sources.

An important aspect of a model's use is its efficiency, which is determined by the human and computer resources required for its proper operation. A model's efficiency can be described by its usability, availability, modifiability, portability, and economy of computer use (van der Heijde et al. 1988). Another important issue is the model's reliability. In the appendices, usability and reliability are qualified by the following descriptors.

USABILITY

Pre- and Postprocessors

The presence of textual or graphic pre- and postprocessing software for the simulation code is rated as: not present [N], present [Y], or status unknown [U].

Documentation

As part of assessing the adequacy of the documentation, the presence of an adequate description of user's instructions and example datasets is indicated by yes [Y] or no [N]. Models having no published description of their theoretical basis are not listed in these appendices.

Support

Software support and maintenance is rated as: none [N], some available [Y], and unknown [U].

Hardware Dependency

In this report a modeling code's hardware and/or software dependency is indicated as present [Y] or not [N]. Hardware dependency may be due to the size of the source code, the way it has been designed and compiled, the use of specific peripherals, and graphics calls in the program. In addition, programs may be software-dependent, requiring specific program purchases to reside on the user's computer (e.g., graphics or mathematical routines).

RELIABILITY

Review

This report identifies peer-review of theory and coding. For each category the rating is: peer-reviewed [Y}, not peer-reviewed [N], and unknown [U]. A model is considered to be peer-reviewed if theory and code has been subject to a formal review process such as established by certain agencies (eg., U.S. EPA, U.S. Geological Survey). In addition, a model's theory is considered to be peer-reviewed if it has been published in a peer-reviewed publication.

Verification

A code's verification status is rated as: 1) code has been subject to extensive verification [E], e.g. tested for most of its functions and features, and verification results are available; 2) code has been subject to partial verification, e.g. tested for selected functions and features, or only selected verification tests are available [L -- limited]; 3) code verification results (if performed) are not available [N]; 4) IGWMC has no information regarding the code's verification [U]. It should be noted that most models have been verified only with respect to segments of their coding or for only a part of the tasks for which they were designed, and thus have been subject to only partial or limited verification.

Field Testing

In this report, model field testing, the application of codes to site-specific conditions for which extensive datasets are available, is rated as performed, either extensively or in a limited fashion [Y], not performed [N], or unknown [U].

Extent of Model Use

This report evaluates the extent of a model's use in four classes: many [M, >10], few [1-10], none [N], and unknown [U]. The evaluation is used on IGWMC's information regarding published reports, journal and proceedings papers, conference presentations, and non-published case history summaries provided by model authors and users.

AVAILABILITY

The programs listed are either general-use codes, or relatively easy-to-obtain research codes. Many of the codes are in the public domain, some are proprietary. In most case, the contact address listed is that of the code custodian or principal distributor.

For USGS software contact:

National Water Information System, Water Resources Division, U.S. Geological Survey, 437 National Center, 12201 Sunrise Valley Drive, Reston, VA 22092.

For EPA software contact:

Center for Subsurface Modeling Support (CSMoS), R.S. Kerr Environmental Research Lab., U.S. Environmental Protection Agency, P.O. Box 1198, Ada, OK 74820.

Center for Exposure Assessment Modeling (CEAM), Environmental Research Lab., U.S. Environmental Protection Agency, Athens, Georgia 30613-0801.

Many public domain and proprietary programs (including ready-to-run USGS and EPA software) are distributed by:

International Ground Water Modeling Center (IGWMC), Colorado School of Mines, Golden, Colorado 80401.

Another major source for groundwater software is:

Scientific Software Group, P.O. Box 23041, Washington, D.C. 20026-3041

IGWMC Key: 683 Model Name: IMAGEW-I Released: 1973
Author: White, W.A.

IMAGEW-I is an analytical well-field drawdown model for steady-state and time-varying pumping. The wells may be located in either a confined (Theis equation; no recharge) or an unconfined aquifer (Jacob's water-table correction for the non-steady-state Theis equation or Walton's modified steady-state solution for a water table aquifer with recharge). The model assumes that the aquifer is homogeneous and isotropic with respect to its parameters, and infinite in areal extent. Image well theory is used to simulate the effects of hydrogeologic boundaries.

Contact Address: Texas Dept. of Water Resources, P.O. Box 13087, Austin, TX 78758

IGWMC Key 1791 Model Name: SLAEM/SLW/SLWL/SYLENS Released: 1992
Author: Strack, O.D.L.

SLAEM and its predecessor SYLENS are models for analysis of two- and three-dimensional steady-state and transient groundwater flow in single or multi-layered aquifer systems based on the Analytical Element Method. SLAEM is an highly interactive graphic oriented program including many of the analytical elements available. The program includes transient wells, areal inhomogeneities, leaky or draining objects, variable infiltration (e.g. from rivers, lakes, and ponds). It allows analysis of flow in two aquifers separated by a thin confining layer. The model is especially suited to analyze flow in regional double aquifer systems with local interconnections. SLW and SLWL are scaled-down, educational versions of the SLAEM program.

Contact address: O.D.L. Strack, Univ. of Minnesota, Dept. of Civil Eng., Minneapolis, MN 55455

IGWMC Key: 1820 Model Name: FLOP/FLOP-LIESTE/FLOP-Z1/FLOP-ZN Released: 1820
Authors: Van den Akker, C., R. Lieste, and E.J.M. Veling.

The FLOP models are semi-analytical models for calculation of pathlines and residence times in groundwater systems. FLOP-LIESTE is designed for single (semi-) confined aquifers; FLOP-Z1 for a quasi three-dimensional semi-confined aquifer system; and FLOP-ZN for a multi-layered homogeneous aquifer system.

Contact Address: RIVM - National Institute for Health and Environment, P.O. Box 1, 3720 AB Bilthoven, The Netherlands

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IGWMC Key: 1822 Model Name: FRONT Released: 1981
Author: Van den Akker, C.

FRONT is a semi-analytical model for calculation of pathlines and residence times in a confined, isotropic, heterogeneous aquifer with steady-state or transient flow. The integration along the streamlines is performed with Runge-Kutta, restricting the maximum time step size with a user-provided error-criterion.

Contact Address: RIVM - Nat. Inst. for Health and Environment, P.O. Box 1, 3720 BA Bilthoven, The Netherlands

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IGWMC Key: 2120 Model Name: PATHS Released: 1980
Author: Nelson, R.W.

The PATHS program is an idealized hybrid analytical/numerical model for simulation of steady-state or transient, two-dimensional, saturated groundwater flow and single component transport. It includes an analytical solution of the flow equation and the Runge-Kutta solution for the pathline equations and the effects of equilibrium ion-exchange and linear adsorption. The model calculates pathlines, location/arrival time distribution, and location/outflow quantity distribution in a confined stratum of uniform vertical thickness. It assumes a uniform lateral flow gradient and superimposed leakage from a vertical, cylindrical fully penetrating pond or cavern and handles up to 35 fully penetrating wells or vertical line sources.

Contact address: Battelle Pacific NW Laboratories, P.O. Box 999, Richland, WA 99352

IGWMC Key: 2770 Model Name: CONFLOW Released: 1981
Author: Hertel Jr., E.S.

The computer code CONFLOW describes fluid flow between two wells in a confined homogeneous, isotropic region. The code uses superposition to solve Laplace's equation with impermeable boundaries and can assist in the design of flow experiments in geologic media. CONFLOW's output is a plot of the theoretical streamlines, the ratio between the time of first arrival for the confined region and the time of first arrival for unconfined two-well flow, and a value for the pressure drop function.

Contact address: E.S. Hertel Jr., Sandia National Laboratories, Albuquerque, NM 87185

IGWMC Key: 2791 Model Name: CRREL (Flow Lines Program) Released: 1984
Author: Daly, C.J.

CCREL is an analytical model to calculate and plot streamlines for flow in anisotropic, heterogeneous aquifers based on known head distribution.

Contact Address: R. Reynolds, U.S. Army Corps of Engineers, Cold Regions Research & Engineering Lab., Hanover, NH 03755

IGWMC Key: 3940 Model Name: RESSQ Released: 1985
Authors: Javandel, I., C. Doughty and C-F. Tsang

RESSQ is a semi-analytical model of 2-dimensional contaminant transport that calculates the streamline pattern in an aquifer, the location of contaminant fronts around sources at specified times, and concentration versus time at sinks. RESSQ assumes a homogeneous, isotropic confined aquifer of uniform thickness and a steady-state regional flow field. It can handle advection and linear equilibrium adsorption. Sources are represented by fully penetrating recharge wells and ponds, and sinks are represented by fully penetrating pumping wells.

Contact address: I. Javandel, Lawrence Berkeley Lab., Earth Sc. Div., Berkeley, CA 94720, or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 3943 Model Name: WHPA Released: 1992
Authors: Blandford T.N., and P.S. Huyakorn

WHPA is an integrated program of analytical and semi-analytical solutions for the groundwater flow equation coupled with pathline tracking. It is designed to assist technical staff with delineation of wellhead protection areas. Developed for the U.S. EPA's Office of Groundwater Protection, the package includes modules for capture zone delineation in a homogeneous aquifer with 2-dimensional steady-state flow with options for multiple pumping/injection wells and barrier or stream boundary conditions. Also included are modules for Monte Carlo analysis of uncertainty and a particle-tracking postprocessor for numerical flow models such as MODFLOW and PLASM, using a two-dimensional rectangular grid.

Contact address: P. Berger, U.S. Environmental Protection Agency, Office of Groundwater Protection, Washington, D.C., or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 4670 Model Name: DREAM Released: 1990
Authors: Bonn, B.A., and S.A. Rounds

DREAM is a menu-driven, user-interactive series of analytical programs for the calculation of drawdowns, water level elevations, steady-state velocities and streamlines in homogeneous and isotropic aquifers. The program uses a commercial contouring package for graphic display of results.

Contact address: Lewis Publishers, Inc. 2000 Corporate Blvd. N.W., Boca Raton, FL 33431

IGWMC Key: 4730 Model Name: GW-UN/DTCD Released: 1991
Authors: Karanjac, J. and D. Braticevic

The UN/DTCD Ground Water Software Series, currently, includes the following ten programs for general groundwater evaluation: 1) hydraulic conductivity calculations and conversions from grain size distributions, permeameters and pumping tests; 2) chemistry data base; 3) aquifer tests (Theis, Jacob, Hantush, recovery, Rushton's dug well test); 4) well construction and hydraulics (including well functions and step-drawdown test); 5) finite difference model for a confined aquifer; 6) a finite difference model for unconfined/confined aquifer; 7) water level data base and hydrograph presentation; 8) preprocessor for USGS 3D Flow Model for 2-layer system; 9) numerical model of a small island with salt-water/freshwater interface; and 10) lithology database and graphic display.

Contact address: Uri Golani, U.N., Dept. of Techn. Coop. for Developm., Water Resources Branch, United Nations Building DC-1, Room 745, New York, NY 10017

IGWMC Key: 5003 Model Name: MLU (Multi-Layer Unsteady-state model) Released: 1986
Author: Hemker, C.J.

MLU is a program for drawdown calculations and inverse modeling (aquifer tests) of transient flow in layered (up to 9 aquifers) and fissured (double porosity aquifer systems of (semi-)confined and unconfined conditions. The model is based on a series of analytical solutions.

Contact Address: Hemker, C.J., Elandsgracht 83, 1016 TR Amsterdam, The Netherlands

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IGWMC Key: 5004 Model Name: MFLOP (FLOw Pattern) Released: 1989
Author: Hemker, C.J.

MFLOP is a simple microcomputer program for the immediate generation of streamlines of well fields with superimposed uniform flow under confined conditions.

Contact address: C.J. Hemker, Elandsgracht 83, 1016 TR Amsterdam, The Netherlands.

IGWMC Key: 5100 Model Name: ANALYTICAL MODELS Released: --
Authors: --

The modular program ANALYTICAL MODELS can handle confined, unconfined, and leaky conditions. Module 1 creates time-drawdown data for observation wells. Aquifer parameters can be varied and graphed on the same chart. Module 2 graphs profiles along lines drawn on a map. Pumping wells and observation wells are shown. Module 3 creates contour and 3D maps of grids, up to 100x100, with 50 wells.

Contact address: Earthware of California, 30100 Town Center Drive, Laguna Niguel, CA 92677

IGWMC Key: 5130 Model Name: FINITE Released: --
Author: Koch, D.H.

FINITE is a program for simulation of the inflow to mines, dewatering schemes, the impact of excavations on groundwater levels, and any other hydrogeologic situation involving finite length lines of recharge or discharge. The program is based on the analytical solution by Muskat for steady-state flow to a finite length line sink in an infinite homogeneous confined or unconfined aquifer. The menu-driven program extends the Muskat algorithm to transient problems using the method of successive states, assuming that the potentiometric surface has a steady-state curvature at all points in time. Both constant head or constant flow sources or sinks may be simulated. This program handles up to 40 finite length line sources or.

Contact Address: Koch and Associates, 2921 Greenway Drive, Ellicot City, MD 21043

IGWMC Key: 5131 Model Name: LEAKY Released: --
Author: Koch, D.H.

LEAKY - Leaky Aquifer Analysis is a menu-driven, interactive program that uses the leaky well function developed by Hantush and Jacob to simulate the drawdowns from multiple wells in a leaky aquifer. Although this algorithm assumes infinite storage in the overlying bed, it is a useful approximation of the performance of an aquifer. By using the theory of superposition, one can simulate variable discharging wells, boundary conditions, and injection wells. The program permits the user to simulate up to 100 wells.

Contact Address: Koch and Associates, 2921 Greenway Drive, Ellicot City, MD 21403

IGWMC Key: 5140 Model Name: GLOVER Released: --
Author: Spinks, M.P.

GLOVER is an analytical model based on the Glover-Balmer equation for simulation of the depletion from or accretion to surface water due to pumping or recharging wells. The model is valid for a homogeneous, isotropic, twodimensional aquifer. Boundary conditions are either constant-head (e.g. fully penetrating rivers) or no-flux (e.g. impermeable boundary). The software provides various graphic input/output options.

Contact address: Microcode, Inc., 2473 Camino Capitan, Santa Fe, NM 87501

IGWMC Key: 5150 Model Name: HYDROPAL Released: --
Authors: --

HYDROPAL is an interactive, menu-driven set of analytical and numerical solutions of groundwater flow and contaminant transport problems. The numerical models are adaptations of the PLASM and RANDOM WALK models. The program creates ASCII output for postprocessing in a graphical package.

Contact address: Watershed Research Inc., 4779 126th St. N, White Bear Lake, MN 55110.

IGWMC Key: 5171 Model Name: THEIS Released: --
Author: Spinks, M.P.

THEIS is an analytical model for simulation of potentiometric surface drawdown or buildup effects due to pumping or injecting wells in a homogeneous, isotropic, twodimensional aquifer. Boundary conditions are either constant head or no-flux. User can specify grid for areal calculation of potentiometric surface changes.

Contact address: Microcode, Inc., 2473 Camino Capitan, Santa Fe, NM 87501

IGWMC Key: 5172 Model Name: THEIS2 Released: --
Authors: Koch, D.H.

THEIS2 is an aquifer analysis program which simulates up to 100 wells in a confined aquifer using the Theis equation. With a modification developed by Jacob, the equation can be used for unconfined aquifers. By using the theory of superposition, one can simulate variable discharging wells, boundary conditions, and injection wells. The program calculates drawdown at a particular time for an array of locations, or for a single location drawdown versus time.

Contact address: Koch and Associates, 2921 Greenway Drive, Ellicot City, MD 21043

IGWMC Key: 5176 Model Name: STREAMLINE Released: --
Authors: Koch, D.H.

This program computes and plots groundwater flow streamlines in a homogeneous, isotropic, and confined aquifer under influence of pumping wells and a uniform regional gradient. Travel times along a streamline or path line may also be computed.

Contact address: Koch and Associates, 2921 Greenway Drive, Ellicot City, MD 21043

IGWMC Key: 5300 Model Name: QUICKFLOW Released: 1991
Authors: --

QUICKFLOW is an interactive analytical model that simulates two-dimensional steady-state and transient ground-water flow. The steady-state module simulates flow in a horizontal plane using analytical functions developed by Strack (1989), including wells, uniform recharge, circular recharge/discharge areas, and line sources or sinks in confined and unconfined aquifers. The model generates streamlines, particle traces and head contours. The transient module calculates heads using equations developed by Theis (1935) and by Hantush and Jacob (1955) for confined and leaky confined aquifers, respectively, and includes a particle tracking option. Each module uses the principle of superposition to evaluate the effects of multiple wells in a uniform regional flow field.

Contact address: Geraghty & Miller, Inc., 10700 Park Ridge Blvd., Suite 600, Reston, VA 22091

IGWMC Key: 5391 Model Name: CSUPAW Released: 1985
Author: Sunada, S.K.

The interactive program CSUPAW (Colorado State University Pit And Well)allows the user to predict the response of a water-table to discharge from wells or artificial recharge of water from rectangular basins in a homogeneous aquifer of infinite areal extent, in a homogeneous stream-aquifer system, or in an aquifer having a vertical impermeable boundary. The model calculates discharge (recharge) to the stream in a stream-aquifer system at times specified by the user. Utilization of graphics allow visual evaluation of results. The program is based on Glover's (1960) analytical solution for recharge from a rectangular basin.

Contact Address: D.K. Sunada, Dept. of Civil Eng., Colorado State Univ., Fort Collins, CO 80523

IGWMC Key: 5570 Model Name: FLSTAT Released: 1988
Authors: Lieste, R., E.J.M. Veling, and C. van den Akker.

FLSTAT (FLow STATionary) is a program for forwards and backwards calculation of streamlines and residence times, given the two-dimensional areal distribution of hydraulic heads is known (from field measurements or flow model). It assumes a rectangular model domain with a grid of rectangular elements, which can be refined locally. The model requires as input the hydraulic conductivity in x- and y-direction and the porosity per element. The coupled differential equations are solved explicitly. The model includes an automatic time-step control routine. The streamlines are calculated from user-specified starting points. The program can provide plot output for hydraulic head contours, streamlines and isochrones.

Contact Address: R. Lieste, Nat. Inst. for Public Health and Environm. Protect., P.O. Box 1, 3720 BA Bilthoven, The Netherlands

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IGWMC Key: 5710 Model Name: AQMODEL Released: 1992
Author: O'Neill, G.T.

AQMODEL calculates drawdown, equipotentials (according to the Thiem formula) and stream functions (following McWhorter and Sunada) for a steady, uniform flow field, and drawdowns and equipotentials for unsteady flow fields with the Theis equation. The interactive program handles over 500 wells and can be used to determine capture zones and well head protection areas. The user can plot flow nets, contour maps of heads and other custom graphics using SURFER for IBM compatibles and or Spyglass Transform software for Macintosh.

Contact Address: WellWare, 3160 Woods Circle, Davis, CA 95616

IGWMC Key: 5790 Model Name: MAF (Multiple Aquifer Flow) Released: 1984
Authors: Roelse, A., and K. Maas.

The MAF program includes a number of analytical solutions for ground-water flow in systems comprising of multiple aquifers. The functions were derived through application of matrix functions in the superposition of linear closed-form solutions. Among others, the program includes generalized functions of De Glee, Mazure, Bosch, Theis, Hantush and Edelman for n-layer systems.

Contact Address: K. Maas, Provincial Dept. of Water Management Zeeland, P.O. Box 165, 4330 AD Middelburg, The Netherlands

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IGWMC Key: 5920 Model Name: TIM1/TIM2 Released: 1987
Authors: Jiin-Shuh, J., and D.I. Leap

TIM1 and TIM2 use the trajectory image method (TIM), a modeling technique based on image theory, to calculate heads, gradients, velocities, and flow directions. TIM is based on the concept that particles emitted by sources or absorbed by sinks may be reflected by impermeable boundaries, or they may be partially absorbed, reflected, and partially transmitted by boundaries of differing hydraulic conductivities. Particles move till their changes in head become negligible. The total head and gradients at each observation point are found by superposing heads and gradients of particle trajectories that pass through or close to the observation point. Combination of TIM with a boundary integral equation method (BIEM), resulting in TIMBIE, reduces computational requirements.

Contact Address: D.I. Leap, Dept. of Earth and Atmospheric Sciences, Purdue University, West Lafayette, IN 47907.

IGWMC Key: 6022 Model Name: THWELLS Released:1992
Author: van der Heijde, P.K.M.

THWELLS is an analytical model for transient groundwater flow in an isotropic homogeneous nonleaky confined aquifer with multiple pumping and injection wells using superposition of Theis solutions. Boundary effects can be included through use of image wells. The program includes a correction for a water table aquifer and superposition of local drawdown on a regional, sloping, stationary piezometric surface.

Contact address: Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401

IGWMC Key: 6023 Model Name: GWFLOW 1990
Author: van der Heijde, P.K.M.

GWFLOW is a menu-driven series of seven simple programs, each containing an analytical solution to a groundwater flow problem. The program contains solutions for transient drawdown in confined and semi-confined aquifers, including the effects of partially penetrating wells; circular recharge of a water table aquifer; and stream depletion resulting from pumping an aquifer.

Contact address: Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401

IGWMC Key: 6350 Model Name: WALTON35 Released: 1985
Author: Walton, W.C.

WALTON35 is a package containing a series of simple BASIC programs for simulating flow, solute transport, and heat transport in various types of aquifers. The programs are based on analytical and numerical solutions of the governing equations. Included are various analytical solutions for non-conservative solute transport in a homogeneous aquifer. The programs are interactive, simple to use, and easy to modify.

Contact address: Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401

IGWMC Key: 6351 Model Name: WELFUN/WELLFLO/CONMIG Released: 1989
Author: Walton, W.C.

The programs WELFUN, WELFLO and CONMIG calculate common well function values and simulate a wide range of ground-water flow and contaminant migration situations based on analytical solutions. The program options include: (1) drawdown or recovery due to multiple production and/or injection wells with variable discharge or recharge rates, drains, and mines; (2) confined, leaky confined, and water table conditions with barrier and/or recharge boundaries and discontinuities; and (3) development of localized contaminant plumes from slug or continuous source areas of various shape and sizes due to advection, dispersion, retardation caused by linear adsorption, and radioactive decay.

Contact address: Lewis Publ. Inc., 2000 Corporate Blvd., N.W. Boca Raton, FL 33431

IGWMC Key: 6352 Model Name: GWPT Released: 1987
Author: Walton, W.C.

GWPT is a series of analytical groundwater flow programs for use in aquifer test analysis. It includes models for pumping test design, semilog time-drawdown or distance-drawdown analysis, storativity analysis near a stream, stream depletion analysis and drawdown beneath a streambed. Furthermore, the package includes programs for calculation of the (confined aquifer) Well function, the partial penetration well function, the leaky aquifer well function, the well loss coefficient and other equations.

Contact address: Lewis Publishers, Inc., 2000 Corporate Blvd. N.W., Boca Raton, FL 33431

IGWMC Key: 6383 Model Name: HWELL Released: 1991
Author: Beljin, M.S.

HWELL is an interactive analytical model, developed to simulate steady-state or transient groundwater flow towards a horizontal well in a confined aquifer. The model can handle different vertical and horizontal hydraulic conductivities (anisotropy), and includes options for skinfactor and eccentricity of the well. The program also computes drawdown and specific capacity of a fully penetrating vertical well in the same aquifer. Performance of the two wells is compared by computing the specific capacity ratio as a function of screen length, hydraulic conductivity contrast, aquifer thickness, and other parameters. The program includes windows, mouse support and graphic output.

Contact address: M.S. Beljin, Univ. of Cincinnati, Dept. of Civil & Env. Eng., Cincinnati, OH 45221

IGWMC Key: 6570 Model Name: OPTP/PTEST Released: 1986
Authors: Paudyal, G.N., and A. Das Gupta

OPTP/PTEST is a fully interactive package consisting of two programs for determining optimal well discharge. PTEST computes the coefficients and exponent of the nonlinear drawdown equation using data from a step-drawdown test. OPTP computes the optimal discharge using a single-variable constrained nonlinear programming algorithm.

Contact address: A. Das Gupta, Asian Inst. of Technology, Div. of Water, P.O. Box 2754, Bangkok 10501, Thailand, or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 6590 Model Name: BEAVERSOFT Released: 1987
Authors: Bear, J. and A. Verruijt

BEAVERSOFT is a package of analytical and numerical solutions for groundwater flow and solute transport. It includes programs for steady and non-steady state two-dimensional flow in heterogeneous aquifers, for flow through dams, for transport of pollutants by advection and dispersion and for saltwater intrusion problems.

Contact address: Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401

IGWMC Key: 6604 Model Name: PAT Released: 1990
Authors: Kinzelbach, W. and R. Rausch

PAT is an analytical model for the computation and graphical representation of pathlines and travel times of groundwater in an infinite or semi-infinite, homogeneous and isotropic confined aquifer or in an infinite strip of such an aquifer. The computed steady-state flow field might include arbitrary pumping or injection wells superposed on a natural uniform regional flow. The model is screen-oriented and fully interactive.

Contact address: W. Kinzelbach, Geasamthochschule Kassel - Universitat, Moritzstrasze 21, D-3500, Kassel, Germany, or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 6681 Model Name: AQUIX Released: 1992
Authors: --

AQUIX is a series of programs for the interactive, forward and inverse modeling of pumping test data. It provides drawdowns in terms of aquifer storativity, transmissivity, leakage, anisotropy, and specific yield, depending on the model selected. A least squares, nonlinear curve fitting method is used to determine the best fit model parameters to the observed data. AQUIX include programs for partial penetrating wells, and for confined, leaky confined and unconfined aquifers. The models are based on Theis (1935), Hantush (1960, 1965), and Neuman (1975). The model comes with a sophisticated textual and graphic user-interface.

Contact address: R.S. Bell, Interpex Ltd., 715 14th Street, Golden, CO 80401

Appendix A.1: Saturated Flow; Analytical Models, Part 2: Usability and Reliability

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
683	IMAGEW-1	N	N	Y	Y	N	N	Y	N	Y	N	U
1791	SLAEM/SLW/ SLWL/SYLENS	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	M
1820	FLOP/ FLOP-LIESTE/ FLOP-Z1/ FLOP-ZN	Y	Y	Y	Y	Y	Y	Y	U	Y	Y	M
1822	FRONT	Y	Y	Y	Y	Y	Y	Y	U	Y	Y	M
2120	PATHS	Y	Y	Y	Y	Y	N	Y	Y	Y	Y	F
2770	CONFLOW	U	Y	Y	Y	Y	Y	Y	U	Y	U	U
2791	CRREL	U	Y	Y	Y	Y	U	Y	U	Y	U	U
3940	RESSQ	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	M
3943	WHPA	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	M
4670	DREAM	Y	Y	Y	Y	Y	Y	Y	N	Y	N	M
4730	GW-UN/DTCD	Y	Y	Y	Y	Y	Y	Y	N	Y	Y	M
5003	MLU	Y	Y	Y	Y	Y	Y	Y	U	Y	Y	U
5004	MFLOP	Y	Y	Y	Y	Y	Y	Y	U	Y	U	M
5100	ANALYTICAL MODELS	Y	Y	Y	Y	Y	Y	U	U	Y	U	M
5130	FINITE	Y	Y	Y	Y	Y	Y	U	U	Y	U	U
5131	LEAKY	Y	Y	Y	Y	Y	Y	U	U	U	U	U
5140	GLOVER	Y	Y	Y	Y	Y	Y	U	U	U	U	U
5150	HYDROPAL	Y	Y	Y	Y	Y	Y	U	U	Y	U	U
5171	THEIS	Y	Y	Y	Y	Y	U	U	U	U	U	U
5172	THEIS2	Y	Y	Y	Y	Y	Y	Y	U	U	U	U

KEY: Y = YES N = NO M = MANY F = FEW U = UNKNOWN

Appendix A.1, part 2 (continued)

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
5176	STREAMLINE	Y	Y	Y	Y	Y	Y	U	U	U	U	U
5300	QUICKFLOW	Y	Y	Y	Y	Y	Y	Y	U	Y	Y	M
5391	CSUPAW	Y	Y	Y	Y	Y	Y	Y	U	Y	Y	M
5570	FLSTAT	Y	Y	Y	Y	Y	Y	Y	U	U	U	U
5710	AQMODEL	Y	Y	Y	Y	Y	Y	Y	U	Y	U	U
5790	MAF	N	N	Y	Y	N	Y	Y	U	Y	U	U
5920	TIM1/TIM2	N	N	Y	Y	N	N	Y	N	Y	U	U
6022	THWELLS	Y	Y	Y	Y	Y	Y	Y	N	Y	N	M
6023	GWFLOW	Y	N	Y	Y	Y	Y	Y	N	Y	N	F
6350	WALTON35	Y	N	Y	Y	Y	N	Y	N	Y	N	F
6351	WELFUN/ WELLFLO/ CONMIG	Y	N	Y	Y	Y	Y	Y	N	Y	N	M
6352	GWPT	Y	Y	Y	Y	Y	Y	Y	N	Y	N	M
6383	HWELL	Y	N	Y	Y	Y	Y	Y	N	Y	U	U
6570	OPTP/PTEST	U	U	Y	Y	U	U	Y	U	U	U	F
6590	BEAVERSOFT	Y	N	Y	Y	Y	N	Y	Y	N	N	M
6604	PAT	Y	Y	Y	Y	Y	Y	Y	U	Y	U	F
6681	AQUIX	Y	Y	Y	Y	Y	Y	Y	U	Y	U	M

KEY: Y = YES N = NO M = MANY F = FEW U = UNKNOWN

Appendix A.2: Saturated Flow; Numerical Models For Two-Dimensional Flow in Horizontal or Vertical Plane, Part 1: Model Description

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IGWMC Key: 322 Model Name: PLASM Released: 1990
Authors: Prickett, T.A., and C.G. Lonnquist

PLASM (Prickett Lonnquist Aquifer Simulation Model) is a finite difference model for simulation of transient, two-dimensional or quasi-three-dimensional flow in a single or multi-layered, heterogeneous, anisotropic aquifer system. The original model of 1971 consisted of a series of separate programs for various combinations of simulation options. Later versions combined most of the options in a single code, including variable pumping rates, leaky confined aquifer conditions, induced infiltration from a shallow aquifer or a stream, storage coefficient conversion between confined and watertable conditions, and evapotranspiration as a function of depth to watertable. The model uses the iterative alternating implicit method (IADI) to solve the matrix equation.

Contact Address: T.A. Prickett and Assoc., Inc., 6 G.H. Baker Drive, Urbana, IL 61801, or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 514 Model Name: AQUIFEM Released: 1979
Authors: Pinder, G.F., and C.I. Voss

AQUIFEM is a two-dimensional finite element model for the simulation of transient, areal saturated groundwater flow in an isotropic, heterogeneous, confined, leaky-confined, or water table aquifer with areal recharge and distributed wells. It incorporates steady-state or transient leakage through confining layers. The model is based on ISOQUAD (1971); a water-balance calculation was added in 1974. This version, called AQUIFEM, includes groundwater velocity calculations and other modifications.

Contact Address: C.I. Voss, U.S. Geol. Survey, Water Resources Div., M.S. 431, Reston, VA 22092

IGWMC Key: 681 Model Name: GWSIM Released: 1974
Author: Knowles, T.R.

GWSIM (GroundWater SIMulation program) is a finite difference model for simulation of transient, two-dimensional, horizontal flow in a heterogeneous, anisotropic, single-layer aquifer. The program allows simulating flow in a confined, unconfined, or leaky confined aquifer. It uses an iterative alternating direction implicit procedure to solve the matrix equations.

Contact Address: Texas Dept. of Water Resources, P.O. Box 13087, Austin, TX 78758

IGWMC Key: 741 Model Name: USGS FRONT-TRACKING Released: 1983
Authors: Garabedian, S.P., and L.F. Konikow

USGS FRONT-TRACKING is a finite difference model for simulation of advective transport of a conservative tracer dissolved in groundwater under steady or transient flow conditions. The model calculates heads, velocities and tracer particle positions.

Contact Address: L.F. Konikow, U.S. Geological Survey, Water Resourc. Div., 431 National Center, Reston, VA 22092

IGWMC Key: 771 Model Name: USGS-2D-FLOW Released: 1976
Authors: Trescott, P.C., G.F. Pinder, and S.P. Larson.

USGS-2D-FLOW is finite difference model to simulate transient, two-dimensional horizontal flow in an anisotropic and heterogeneous, confined, leaky-confined or water-table aquifer. It uses the iterative alternating-direction implicit approximation of the ground-water flow equation.

Contact Address: L.J. Torak, U.S. Geological Survey, Branch of Groundwater, M.S. 411 National Center, Reston, VA. 22092

IGWMC Key: 772 Model Name: SSIM3D Released: 1987
Authors: Trescott, P.C., S.P. Larson, and D.B. Sapik

SSIM3D is a modification of the USGS three-dimensional flow model developed by Trescott and Pinder (1975) to simulate steady flow of fresh water in a multiple aquifer system containing fresh water and static salt water. The two fluids are assumed immiscible, with constant densities and separated by a sharp interface. In addition to heads, boundary fluxes and global water balance, the finite difference model calculates the location of the interface.

Contact Address: District Chief, U.S. Geological Survey, 1201 Pacific Avenue - Suite 600, Tacoma, WA 98402

IGWMC Key: 1230 Model Name: AQU-1 Released: 1979
Authors: Rushton, K.R., and L.M. Tomlinson

AQU-1 is a simple finite difference model for simulation of transient, two-dimensional horizontal groundwater flow in a heterogeneous, anisotropic confined or leaky-confined aquifer.

Contact address: Rushton, K.R., University of Birmingham, Dept. of Civil Engineering, P.O. Box 363, Birmingham, Bl5 2TT, United Kingdom

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IGWMC Key: 1852 Model Name: SWIFT Released: 1982
Authors: Verruijt, A., and J.B.S. Gan.

SWIFT (Salt Water Interface by Finite element Technique) is a transient, cross-sectional finite element model to simulate flow of fresh and salt water in a confined, semi-confined or water-table aquifer of homogeneous permeability and porosity. The purpose of the model is the computation of the upconing of a sharp interface between the fresh and salt water.

Contact Address: Verruijt, A., Delft Technical University, Dept. Civil Engineering, Stevinweg 1, 2628 CN Delft, The Netherlands

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IGWMC Key: 2091 Model Name: VTTSS2 Released: 1979
Authors: Reisenauer, A.E., and C.R. Cole.

VTTSS2 is a finite difference model to predict steady-state hydraulic head in confined aquifer systems up to five layers. The solution is achieved by the Newton method for non-linear equations followed by direct Gaussian elimination. The model can handle cell-by-cell water budget computations and provides streamlines and traveltimes.

Contact Address: Cole, C.R., Battelle Pacific NW Laboratories, Water and Land Resources Division, P.O. Box 999, Richland, WA 99352

IGWMC Key: 2092 Model Name: VTT Released: 1979
Authors: Reisenauer, A.E., and C.R. Cole.

VTT (Variable Thickness Transient Groundwater Flow Model) is a finite difference model to calculate transient hydraulic head in confined or unconfined isotropic, heterogeneous, multi-layered aquifer systems. The model can calculate cell-by-cell water budgets and can generate stream-lines and travel times. Boundary conditions and aquifer stresses may be time-varying. The transient model is solved with the line successive over-relaxation method (LSOR).

Contact Address: Cole, C.R., Battelle Pacific NW Laboratories, Water and Land Resources Division, P.O. Box 999, Richland, WA 99352

IGWMC Key: 2140 Model Name: SWSOR Released: 1980
Authors: Mercer, J.W., and C.R. Faust

SWSOR is a finite difference model for simulation of two-dimensional areal, unsteady flow of saltwater and freshwater separated by a sharp interface in an anisotropic heterogeneous aquifer. There are two separate differential equations for flow of fresh water and of salt water. The model can handle water-table conditions or confined conditions with steady-state leakage of fresh water.

Contact Address: GeoTrans, Inc., 46050 Manekin Plaza, Suite 100, Sterling, VA 22170

IGWMC Key: 2510 Model Name: Quasi 3-D Multiaquifer Model Released: 1978
Author: Weeks, J.R.

This is an IADIP finite difference model to simulate transient or steady-state groundwater flow in isotropic, heterogeneous multi-aquifer systems using a quasi-three dimensional approach. Uniform recharge to each layer and distributed discharge can be simulated. Specified head boundaries can be simulated in the uppermost aquifer. Outflows to the specified head boundaries are computed for each time period and as cumulative volume of water.

Contact address: Weeks, J.R., U.S. Geological Survey, Box 25046, MS 412 Denver Federal Center, Lakewood, CO 80225

IGWMC Key: 2630 Model Name: AQUIFEM-1/AQUIFEM-N Released: 1989
Authors: Townley, L.R., J.L. Wilson, and A.S. Da Costa.

AQUIFEM-1/AQUIFEM-N is a finite-element model for transient, two-dimensional or quasi-three-dimensional groundwater flow in confined, leaky-confined, or unconfined single or multi-layered aquifers. Later versions allow for a wide variety of aquifer and boundary conditions and facilitate two-dimensional cross-sectional simulation, and simulation of groundwater discharge into streams, simulation of springs, partial penetrating wells and drains, and simulation of aquifer or aquitard pinch-outs. AQUIFEM-N is a multilayered version of AQUIFEM-1, developed by L. Townley at CSIRO, Australia. It includes grid generation and node renumbering programs, and allows plotting of grids, contours, flow lines, time series and cross-sections.

Contact Address: Ralph M. Parsons Lab. for Water Resources & Hydrodyn., Massachusetts Inst. of Technology, Cambridge, MA 02139 (single-layer version); CSIRO Division of Water Resources, Private Bag, PO Wembley, W.A. 6014, Australia (multi-layer version)

IGWMC Key: 2631 Model Name: SWIM Released: 1979
Authors: Sa da Costa, A.G., and J.L. Wilson

SWIM (Salt Water Intrusion Model) is a versatile finite element model for simulation of transient, horizontal flow of fresh and salt water separated by a sharp interface. The model can handle various aquifer conditions and boundary conditions.

Contact Address: Ralph M. Parsons Lab. for Water Resources and Hydrodynamics Dept. of Civil Engineering, Mass. Inst. of Technology, Cambridge, MA 02139

IGWMC Key: 2640 Model Name: TRIAG Released: 1979
Authors: Mallory, M.J., and T.J. Durbin

TRIAG is a Galerkin finite element model for simulation of steady and nonsteady-state ground-water flow in an isotropic, heterogeneous, two-aquifer system with leakage through the separating confining layer. The areal extent of the two aquifers do not have to coincide. Discharge and recharge can be varied spatially and with time. Evapotranspiration is treated as a linear function of depth to water. The model uses a backwards finite difference approximation for time.

Contact Address: Mallory, M.J., U.S. Geological Survey, Water Resources Division, 345 Middlefield Rd., Menlo Park, CA 94025

IGWMC Key: 2720 Model Name: INTERFACE Released: 1979
Author: Page, R.H.

INTERFACE is a finite element model to simulate transient flow of fresh and saline water as immiscible fluids separated by a sharp interface in an isotropic, heterogeneous, water table aquifer. The model can handle both confined and unconfined aquifers. The flow equations for the two fluids are coupled by assuming equality of pressures on either side of the interface.

Contact Address: Water Resources Program, Dept. of Civil Engineering, Princeton University, Princeton, NJ 08540

IGWMC Key: 2800 Model Name: SGMP Released: 1981
Authors: Boonstra, J., and N.A. De Ridder

SGMP is a polygon-based, integrated finite difference model for simulating steady-state or transient, two-dimensional, horizontal flow in a saturated, anisotropic and heterogeneous, confined, semi-confined or phreatic aquifer.

Contact Address: J. Boonstra, Internat. Inst. for Land Reclam. and Improvement, P.O. Box 45, Wageningen, The Netherlands

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IGWMC Key: 2870 Model Name: DISIFLAQ Released: 1980
Author: Berney, O.

DISIFLAQ (DIgital SImulation of FLow through a 2-layer AQuifer system) is a polygon-based finite difference model for steady-state or transient simulation of two-dimensional, horizontal groundwater flow in a one- or two-layer, isotropic, heterogeneous aquifer system. The model computes the position of the piezometric surface of the aquifer(s), the distribution of flux rates within the aquifers and across the leaky confining layer between or above the aquifers, the flux rates across the boundaries (springs, streams, etc.), and the distribution of storage changes in the aquifer(s). Also, the program computes the piezometric head variations in time for any point and aquifer.

Contact Address: Land and Water Developm. Div., U.N. F.A.O., Via Delle Terme Di Caracalla, 00100-Rome, Italy

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IGWMC Key: 3101 Model Name: GWFLOW/GWMESH/GWPLOT Released: 1991
Authors: Warner, J.W., and D.D. Walker

GWFLOW is a two-dimensional finite element flow model, based on a solution of the linearized Boussinesq equation using triangular elements and linear shape functions. The model has a choice of two solvers: a banded Gauss algorithm and a preconditioned conjugate gradient solver. A preprocessor, GWMESH, helps the user interactively design the mesh, organize the input data, interpolate non-uniform aquifer properties, and edit input for the GWFLOW model. The package also includes GWPLOT, a postprocessor and graphics program to view the mesh and provide for contouring of the simulation results.

Contact Address: J.W. Walker, Colorado State University, Ground Water Program, Engineering Research Center, Fort Collins, CO 80523

IGWMC Key: 3237 Model Name: PORSTAT/PORMC Released: 1983
Authors: Sagar, B., and P.M. Clifton

PORSTAT is a numerical model solving the two-dimensional stochastic groundwater flow equation, optionally coupled with the deterministic heat transfer and mass transfer equations using integrated finite differences coupled to a direct equation solver. The stochastic groundwater modeling is achieved by means of a second-order uncertainty analysis (using sensitivity coefficients), based on a Taylor series expansion of the state variables of interest (hydraulic heads and Darcian velocities) about the expected values of the model parameters. Uncertain variables which can be considered are hydraulic conductivities, specific storage,

(continued.....)

PORSTAT/PORMC -- continued

boundary conditions, and initial conditions. To assess the accuracy of PORSTAT, a Monte Carlo groundwater flow program (PORMC) was developed.

Contact Address: Rockwell Hanford Operations, Basalt Waste Isolation Project, P.O. Box 800, Richland, WA 99352

IGWMC Key: 3240 Model Name: GM5 (Groundwater Model 5) Released: 1982
Author: Liggett, J.A.

GM5 is a model using the boundary integral equation method (BIEM) for simulation of steady state or unsteady quasi-three-dimensional saturated groundwater flow in an anisotropic, heterogeneous, regional multi-aquifer system. The aquifers may be confined or unconfined. Boundary conditions include specified head and specified flux. The model has options for distributed recharge and point-specific pumping or injection wells.

Contact Address: Liggett, J.A., School of Civil and Environmental Engineering, Hollister Hall, Cornell University, Ithaca, NY 14853

IGWMC Key: 3241 Model Name: Seawater Intrusion with BIEM Released: 1983
Authors: Taigbenu, A.E., J.A. Liggett, and A.H-D. Cheng.

The purpose of this model is to simulate sea-water intrusion under transient confined and steady-state unconfined aquifer conditions using the Boundary Integral Equation Method.

Contact Address: Liggett, J.A., School of Civil and Environmental Engineering, Hollister Hall, Cornell University, Ithaca, NY 14853

IGWMC Key: 3350 Model Name: FEMSAT Released: 1978
Author: Van Bakel, P.J.T.

FEMSAT is a finite element model for simulation of transient two-dimensional horizontal flow in a saturated heterogeneous, anisotropic multi-layered aquifer system.

Contact Address: Van Bakel, P.J.T., Institute for Land and Water Management Research, P.O. Box 35, 6700 AA Wageningen, The Netherlands

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IGWMC Key: 3372 Model Name: AQUIFLOW Released: 1984
Authors: Yeh, G.T., and C.W. Francis

AQUIFLOW is a two-dimensional finite element model to simulate transient flow in horizontal, anisotropic, heterogeneous aquifers under confined, leaky or unconfined conditions.

Contact Address: Yeh, G.T., Penn State University, Dept. of Civil Eng., 225 Sackett Building, University Park, PA 16802

IGWMC Key: 3373 Model Name: FEWA Released: 1983
Authors: Yeh, G.T., and D.D. Huff

FEWA (Finite Element model of Water flow through Aquifers) is a two-dimensional finite element model to simulate transient vertically averaged flow in confined, leaky confined, or water table aquifers. The fluid flow is a function of pressure gradient and gravity. The model incorporates infiltration and evapotranspiration, leakage, and artificial injection and withdrawal. The aquifer may be partially confined and partially unconfined. The grid may include both quadrilateral and triangular elements. The resulting matrix equations are solved using a pointwise iteration solution strategy as optional alternatives to the direct solution method.

Contact Address: Yeh, G.T., Penn State University, Dept. of Civil Eng., 225 Sackett Building, University Park, PA 16802.

IGWMC Key: 3600 Model Name: SWIGS2D Released: 1982
Author: Contractor, D.N.

SWIGS2D is a two-dimensional finite element model to simulate transient, horizontal salt and fresh water flow separated by a sharp interface in an anisotropic, heterogeneous, confined, semi-confined or water table aquifer. The model solves the depth-averaged equations for continuity for fresh water and salt water simultaneously using linear, triangular elements. Boundary conditions of the Dirichlet and/or Neumann type can be applied. Pumping rates, recharge rates, and boundary conditions can be specified as function of time. The program can track the location of salt water toes and the fresh water toes (where the phreatic surface touches the impervious base). The program can provide the magnitude and direction of fresh and salt water velocities in each element.

Contact Address: Contractor, D.N., University of Arizona, Dept. of Civil Eng. & Mech. Eng., Tuscon, AZ 85721

IGWMC Key: 3640 Model Name: SEAWTR/SEACONF Released: 1980
Author: Allayla, R.I.

SEAWTR/SEACONF is a two-dimensional finite difference model for simulation of simultaneous horizontal flow of salt and fresh water separated by a sharp interface in a confined or water table aquifer with anisotropic and heterogeneous properties, including effects of capillary flow.

Contact Address: Colorado State University, Civil Engineering Department, Fort Collins, CO 80523

IGWMC Key: 3881 Model Name: 2-D Finite Element Galerkin Model Released: 1984
Author: Tracy, J.V.

This Galerkin finite element model simulates steady and transient two-dimensional ground-water flow in an irregularly shaped confined or unconfined aquifer. The aquifer's transmissive and storage properties may be heterogeneous. The model accounts for gains and losses from the river flow in each reach based on the incoming river and tributary flows and the gain/loss of the aquifer in each reach. With an estimate of river discharge, the river stage is computed for each reach using an input stage-discharge relationship.

(continued.....)

2D Finite Element Galerkin Model -- continued

The river-aquifer gains/losses are calculated as a function of streambed area, riverbed leakance values, and the head gradient between river and aquifer. Well discharge can vary and evapotranspiration is calculated monthly. BCs include specified flux and head.

Contact Address: U.S. Geol. Survey, WATSTORE Program Off., 437 Nat. Center, Reston, VA 22092

IGWMC Key: 4100 Model Name: MODFE Released: 1992
Authors: Torak, L.J., and R.L. Cooley

MODFE is a modular finite element model to solve two-dimensional steady-state or transient groundwater flow in (leaky) confined or unconfined, heterogeneous and anisotropic aquifers. The program uses triangular elements with linear basis functions and the extended Galerkin method of weighted residuals. Boundary conditions may be specified as a point, line, or areally distributed sources or sinks, depending on the nature of the field problem. Fluxes from these boundaries may be specified, or may be computed as a function of hydraulic head during the simulation (third type b.c.). Spatially distributed parameters may be specified for individual elements or for zones of elements. The discretized equations are solved using a modified incomplete-Cholesky, conjugate gradient method.

Contact Address: Torak, L.J., U.S. Geological Survey, Branch of Groundwater, M. S. 411 National Center, Reston, VA 22092, or WATSTORE Program Office, 437 National Center, Reston, VA 22092

IGWMC Key: 4160 Model Name: ST2D Released: 1985
Author: El-Kadi, A.I.

ST2D is a two-dimensional stochastic model to solve gravity drainage into adjoining streams using the Monte Carlo technique. The program consists of three sections: a generator for hydraulic conductivity realization, a deterministic finite element groundwater flow simulator, and a statistical analysis routine. The flow simulation is based on the two-dimensional Boussinesq equation with linearized hydraulic conductivity.

Contact Address: Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, CO 80401

IGWMC Key: 4530 Model Name: MAQWF Released: 1986
Authors: Contractor, D.N., S.M.A. El Didy, and A.S. Ansary.

MAQWF is a finite element model for simulation of transient two-dimensional horizontal flow in a multiple aquifer system with time-varying boundary conditions. The program handles both confined and unconfined aquifer conditions and allows local confined/unconfined conversion during the simulation. The model provides velocities to be used as input for a transport model.

Contact Address: Contractor, D.N., University of Arizona, Department of Civil Eng. and Mech. Eng., Tuscon, AZ 85721

IGWMC Key: 4640 Model Name: RAQSIM Released: 1985
Authors: Cady, R.E., and J.M. Peckenpaugh

RAQSIM (Regional AQuifer SIMulation) is a two-dimensional finite element model for transient regional aquifer simulation with support programs for evapotranspiration using the Jensen-Haise method, for infiltration, storage, and removal of water from the soil zone using climatic data, evapotranspiration data and soil characteristics, and for computing recharge and discharge from the groundwater system, including stream-aquifer flux.

Contact Address: District Chief, U.S. Geological Survey, 406 Federal Building, 100 Centennial Mall North, Lincoln, NE 68508

IGWMC Key: 4753 Model Name: AQ-FEM Released: 1989
Authors: Leijnse, A., and K. Kovar.

AQ-FEM is a finite element model for computation of the head distribution in a multi-layered, anisotropic heterogeneous aquifer-aquitard system. The model handles both steady-state and transient flow conditions. The program package consists of 3 modules: (1) AQ-EG is a finite element grid generator, (2) AQ-DD is used to allocate spatially variable data to the FEM grid, and (3) AQ-EP is the finite element simulator. The program is menu-driven and has extensive error checking, help features and graphic post-processing.

Contact Address: Nat. Inst. of Public Health and Environm. Protection, P.O. Box 1, 3720 Bilthoven, The Netherlands

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IGWMC Key: 4754 Model Name: AQ-EF Released: 1989
Authors: Leijnse, A., and K. Kovar

AQ-EF is a menu-driven, interactive computer program package for calculation of ground-water streamlines and isochrones in multi-layered, anisotropic heterogeneous aquifer-aquitard systems with steady-state or transient flow conditions. The program handles forward or backward particle tracking using the head distribution values computed by the program AQ-FEM. The package includes a module for plotting of the results.

Contact Address: Nat. Inst. of Public Health and Environm. Prot., P.O. Box 1, 3720 BA Bilthoven, The Netherlands

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IGWMC Key: 4900 Model Name: SLAM Released: 1990
Author: Aral, M.M.

SLAM (Steady Layered Aquifer Model) is a finite element groundwater model for simulation of steady-state flow in multilayered aquifers. The model can handle a system of up to five (leaky-)confined aquifers with the top aquifer either confined or unconfined.

Contact Address: Lewis Publishers, Inc. c/o CRC Publishers, Inc., 2000 Corporate Blvd., N.W., Boca Raton, FL 33431

IGWMC Key: 4901 Model Name: UNSTEADY FLOW Released: 1990
Author: Aral, M.M.

UNSTEADY FLOW is a finite element model for simulation of unsteady flow in multilayered aquifers. The model can handle up to 5 layers and allows for confined, semi-confined and water-table conditions.

Contact Address: Lewis Publishers, Inc. c/o CRC Publishers, Inc., 2000 Corporate Blvd., N.W., Boca Raton, FL 33431

IGWMC Key: 4920 Model Name: FLOWPATH Released: 1992
Authors: Franz, T., and N. Guiguer.

FLOWPATH is an easy-to-use program for the analysis of two-dimensional steady- state groundwater flow problems. The program calculates hydraulic head distributions, groundwater velocities, pathlines, travel times, capture zones, and wellhead protection areas in confined, leaky-confined or unconfined, anisotropic, heterogeneous aquifers. Pathlines are computed with a particle tracking method. The finite difference model can handle up to 10,000 nodes in an irregular grid, over 100 wells, and over 100 zones of different aquifer properties. The program has extensive and sophisticated post-processing capabilities.

Contact Address: Waterloo Hydrogeologic Software, 113-106 Seagram Drive, Waterloo, Ontario, Canada N2L 3B8

IGWMC Key: 5000 Model Name: MICROFEM Released: 1989
Authors: Hemker, C.J., and H. van Elburg

MICROFEM is a user-friendly series of programs to create and analyze a wide range of multi-layer steady-state groundwater flow problems using the finite element technique. The simulation technique is embedded in an elaborate, partially graphic, user-interface for data entry and editing; triangular element grid generation and optimization; and display of grid, contoured simulation results, flow-vectors, and flowlines. The model also calculates waterbalances and traveltimes. The program consists of three main programs and two optional utilities to plot graphics on a HP-plotter and to compile a new model data set by overlaying an existing model with a new network.

Contact Address: C.J. Hemker, Elandsgracht 83, 1016 TR Amsterdam, The Netherlands

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IGWMC Key: 5001 Model Name: FLOWNET Released: 1989
Authors: Van Elburg, H., C.J. Hemker, and G.B. Engelen

FLOWNET is used for interactive modeling of two-dimensional steady-state flow in an heterogeneous and anisotropic cross-section of the saturated zone. It generates a flownet, composed of flow lines and equipotential lines, obtained by a five-point finite difference approximation to calculate heads and linear interpolation to determine equipotential lines. The matrix equation is solved using the conjugate gradient method. The streamlines are determined from the flow function which in turn is determined using the adjoint function of the potential function. The model handles hydraulic head boundary conditions variable along the boundary. It has options for waterbalance calculations and HP-plotter output.

Contact Address: C.J. Hemker, Elandsgracht 83, 1016TR Amsterdam, The Netherlands

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IGWMC Key: 5030 Model Name: NUSEEP Released: 1990
Authors: --

NUSEEP is a collection of four IBM-PC compatible programs designed to allow for the rapid solution of steady-state groundwater flow problems in two dimensions using the boundary element method. The software computes piezometric head and boundary fluxes. The soil is presumed non-deformable, homogeneous and saturated. The solution of a groundwater flow problem begins with the construction of a boundary mesh and the specification of boundary conditions (boundary flux if heads are to be calculated, or heads if boundary flux is unknown). The software includes graphics post processing to create piezometric head contours and boundary configuration.

Contact Address: Northwestern Univ., Dept. of Civil Eng., 2145 Sheridan Road, Evanston, IL 60208

IGWMC Key: 5110 Model Name: AQUIFER Released: --
Authors: --

AQUIFER is a quasi three-dimensional finite difference groundwater flow model. It accepts real geologic columns in geologic terms at each node, using formation names for which the user defines the hydrogeologic parameters. Up to 12 pumping wells can be simulated with variable flow rates. The program handles rivers, lakes and other boundary conditions. The model switches automatically between confined and unconfined conditions at each node, dependent on the head and the geologic column.

Contact Address: J.C. Hall, Island Design, 518 Town Hill Road, New Hartford, CT 06057

IGWMC Key: 5160 Model Name: INTERSAT Released: --
Author: Voorhees, M.

INTERSAT is an interactive finite difference groundwater flow program for transient, quasi-three dimensional simulation of complex aquifers systems and boundary conditions. The program includes pre- and postprocessing as well as contour graphics. It has optional SIP and ADI solvers, calculates water budgets, and computes velocity distributions for use in a solute transport model.

Contact Address: ESE/Hydrosoft, 63 Sarasota Center Boulevard, #107, Sarasota, FL 34240

IGWMC Key: 5200 Model Name: FLOWNS Released: 1989
Authors: Bramlett, W., and R.C. Borden.

FLOWNS is a simple-to-use program for generating two dimensional flow nets for steady-state flow in any saturated rectangular domain with any combination of constant head or constant flux (including zero flux) boundary conditions. The domain might be either horizontally (areal) or vertically (cross-section) oriented. The program approximates with discrete values the continuous distributions of potential and stream function using finite difference approximations of the Laplace equation. The hydraulic conductivity distribution may be anisotropic and/or heterogeneous. A contouring program is required to generate the final stream and equipotential lines.

Contact Address: R.C. Borden, North Carolina State University, Civil Engineering Department, Box 7908, Rayleigh, NC 27695

IGWMC Key: 5230 Model Name: GEOFLOW Released: --
Authors: --

GEOFLOW is a computer program to solve two-dimensional, cross-sectional steady-state seepage problems. It can simulate confined and unconfined systems. The plotting option plots the finite element mesh, the top flow line, and specified equipotentials on the screen, printer and plotter. GEOFLOW is based on the finite element program FEDAR, originally developed at the University of California at Berkeley. Modifications provide solutions for flow, gradients, and heads. For unconfined flow the program modifies the position of the phreatic surface iteratively. The program includes an automatic mesh generator.

Contact Address: GEOCOMP Corporation, 66 Commonwealth Avenue, Concord, Mass. 01742

IGWMC Key: 5240 Model Name: CGAQUFEM Released: --
Authors: --

CGAQUFEM is a Galerkin finite element model for simulating 2-dimensional, transient groundwater flow in plan view. It computes the distribution of heads and groundwater velocities in a confined, unconfined or mixed aquifer. It can handle areal recharge when unconfined (or leakage through an aquitard from a water table aquifer if confined). Aquifer and aquitard thickness and hydraulic conductivity, initial head, recharge and pumping (injection) rates are node-wise variable. The matrix solution is provided by incomplete Cholesky decomposition and a conjugate gradient solver. The latter reduces core storage requirements significantly for large problems when compared to conventional solvers.

Contact Address: Waterloo Centre for Groundwater Research, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1

IGWMC Key: 5241 Model Name: FLONETS Released: --
Authors: --

FLONETS is 2-dimensional Galerkin finite element model for simulating steady-state groundwater flow in cross-section. It computes the distribution of heads, stream functions and groundwater velocities. It includes a mesh generation option for rectangular grids (it can seek the water table in this case). It can also read a manually generated grid. Vertical and horizontal hydraulic conductivity, porosity and principal direction angle are element-wise variable. Matrix solution is by the Cholesky decomposition method.

Contact Address: Waterloo Centre for Groundwater Research, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1

IGWMC Key: 5392 Model Name: CSUFDM Released: 1986
Authors: Close, B., J. Warner, G. Sunada, and D.K. Sunada

CSUFDM (Colorado State University Finite Difference Model) is a finite difference model for steady-state or transient two-dimensional areal flow in a single-layer heterogeneous, anisotropic confined, semi-confined, or unconfined aquifer. The model uses an implicit, central finite difference formulation for which is solved using Gauss elimination. The model employs a dynamic core allocation. The user can specify impermeable (no-flow), constant head, and underflow boundary conditions. The model calculates at any time interval

(continued.....)

CSUFDM -- continued

head distribution, discharge rates between grid cell, discharge to and from streams, mass balance, and difference in head between initial head and current head. The model has an interactive input and (graphic) output processor.

Contact Address: D.K. Sunada, Groundwater Program, Dept. of Civil Eng., Colorado State Univ., Fort Collins, CO 80523

IGWMC Key: 5540 Model Name: FRESAL Released: 1980
Author: Kovar, K.

FRESAL is a finite element model for calculation of the steady-state interface between salt and fresh water in the subsurface. The program can be used for problems dealing with a single aquifer, completely or partially overlain by a semi-permeable layer, or two aquifers separated by a semi-permeable layer. In the latter case, the saline-fresh water interface is situated in the lower aquifer, with only fresh water in the upper aquifer. The model assumes flow in the fresh water section to be horizontal and in the semi-permeable layer to be vertical. Saline groundwater flow is ignored. Density effects are introduced by using the saline groundwater potential.

Contact Address: National Inst. for Health and Environm. Prot., P.O. Box 1, 3720 BA Bilthoven, The Netherlands

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IGWMC Key: 5720 Model Name: JDB2D/3D Released: 1991
Author: Bredehoeft, J.D.

JDB2D/3D consists of two fairly simple, easy modifiable general-use computer programs for solving the 2D and quasi-3D formulation of the transient ground-water flow equation for (leaky-)confined aquifers. The governing equations are approximated using central finite differences for the spatial derivatives together with a block-centered formulation. Intercell transmissivities are taken as the harmonic mean of adjacent cell transmissivities. The FD equations are solved using the Strongly Implicit Procedure (SIP). The model requires a no-flow boundary around the area of computational interest, and assumes a leaky confining layer, an inactive source layer above the confining unit and pumping for every cell of interest. Source functions are used to approximate bc's other than no-flow.

Contact Address: J.D. Bredehoeft, U.S. Geol. Survey, Branch of Research, Menlo Park, CA 94025

IGWMC Key: 5730 Model Name: AQUAMOD Released: --
Authors: van Tonder, G., and H. van Rensburg.

AQUAMOD is a triangular 2-D finite element confined flow model. Abstraction rates may be changed at any time. Recharge is input by either supplying a constant value over the whole of the aquifer or a different recharge rate at each node. Dirichlet and Neumann boundary conditions can be handled. Output includes heads at each time step together with Darcian velocities. The program comes with a number of utilities: 1) GENDRIEH, which generates a simple triangular finite element mesh with rectangular sides; 2) TFEM, which generates a triangular finite element mesh from any given set of points using Delaney triangularization; KRIG,

(continued.....)

AQUAMOD -- continued

which uses ordinary or universal kriging to interpolate T and S values and water levels; and $) Bayes, for Bayes interpolation of water levels.

Contact Address: van Rensburg, H.J., Dept. of Water Affairs, Private Bag X313, Pretoria, South Africa

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IGWMC Key: 5750 Model Name: SHARP Released: --
Author: Essaid, H.I.

SHARP is a quasi-three-dimensional finite difference model for simulating freshwater and saltwater flow separated by a sharp interface in layered coastal aquifer systems. The interface tip and toe positions are tracked within each layer. The model accommodates multiple aquifers separated by confining layers, with spatially variable porous media properties. The uppermost aquifer can be confined, unconfined, or semi-confined with areally distributed recharge. Temporal variations in recharge and pumping are accounted for by multiple pumping periods. The boundary conditions which can be simulated include prescribed flux boundaries, constant freshwater head and/or constant saltwater head boundaries, and head-dependent flux boundaries in the upper-aquifer. Fresh water and salt water mass balances are calculated for each layer. The equations are solved using the strongly implicit procedure. The model is verified against experimental and analytical solutions.

Contact Address: H.I. Essaid, U.S. Geol. Surv., 345 Middlefield Road, MS 421, Menlo Park, CA 94025

IGWMC Key: 5810 Model Name: 2D Steady-State FE model Released: 1989
Author: Kuniansky, E.L.

This model program is a simple finite element model for simulation of two-dimensional steady-state ground-water flow in heterogeneous, anisotropic, confined aquifers. Constant head, constant flux, and head-dependent flux boundary conditions an be specified. The model uses triangular elements.

Contact Address: E.L. Kuniansky, Water Resources Div., U.S. Geological Survey, 8011 Cameron Road, Bldg. 1, Austin, TX 78753

IGWMC Key: 6030 Model Name: AQ/BASIC GWF Released: 1989
Author: Verruijt, A.

BASIC GWF is a simple finite element model for analysis of plane steady- or unsteady-state groundwater flow in an isotropic, heterogeneous, confined or unconfined aquifer. AQ is an updated version facilitating user-friendly interactive data entry and editing and graphic display of simulation results.

Contact Address: A. Verruijt, Technical University Delft, Dept. of Civil Eng., Stevinweg 1, 2628 CN Delft, The Netherlands

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IGWMC Key: 6353 Model Name: GWFL3D Released: 1989
Author: Walton, W.C.

GWFL3D is a finite difference model for simulation of transient groundwater flow in multilayered confined, leaky confined and water-table aquifer systems. The model allows for partially penetrating wells, well storage capacity, multi-aquifer production wells, flowing wells, mine excavations, induced infiltration from streams, subsurface drains, aquitard storativity and delayed gravity yield.

Contact Address: Lewis Publishers, Inc. c/o CRC Publishers, Inc., 2000 Corporate Blvd. N.W., Boca Raton, FL 33431

IGWMC Key: 6650 Model Name: GWPATH Released: 1990
Author: Shafer, J.M.

GWPATH is an interactive microcomputer-based software package for estimating horizontal or vertical fluid pathlines and traveltimes in fully saturated ground-water flow domains. The model is applicable to two-dimensional heterogeneous, anisotropic flow systems, and features forward and reverse pathline tracking, time-related capture zone analysis, and multiple pathline capture detection mechanisms. It requires as input a regular, cell-based distribution of observed or computed hydraulic heads.

Contact Address: J.M. Shafer, 1013 Devonshire Drive, Champaign, Illinois 61821

Note: See also Appendix C.2; many 2-D solute transport models include a flow simulation module.

Appendix A.2: Saturated Flow; Numerical Models For Two-Dimensional Flow in Horizontal or Vertical Plane, Part 2: Usability and Reliability

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
322	PLASM	Y	Y	Y	Y	N	Y	Y	U	E	Y	M
514	AQUIFEM	N	N	Y	Y	N	N	Y	U	E	U	F
681	GWSIM	N	N	Y	Y	N	N	Y	U	L	Y	F
741	USGS FRONT-TRACKING	N	N	Y	Y	N	Y	Y	U	L	U	F
771	USGS-2D-FLOW	Y	Y	Y	Y	Y	N	Y	Y	E	Y	M
772	SSIM3D	N	N	Y	Y	U	U	Y	U	L	U	U
1230	AQU-1	N	N	Y	Y	N	N	Y	U	L	U	M
1852	SWIFT	Y	Y	Y	Y	Y	Y	Y	U	L	U	U
2091	VTTSS2	U	U	Y	Y	U	N	Y	U	L	U	F
2092	VTT	Y	Y	Y	Y	U	N	Y	U	L	U	M
2140	SWSOR	N	N	Y	Y	N	N	Y	N	L	U	F
2510	Quasi-3-D Multiaquifer Model	N	N	Y	Y	N	N	Y	U	L	U	U
2630	AQUIFEM-1/ AQUIFEM-N	Y	Y	Y	Y	Y	Y	Y	U	E	U	M
2631	SWIM	N	N	Y	Y	N	N	Y	U	L	U	U
2640	TRIAG	N	N	Y	Y	N	N	Y	U	L	U	U
2720	INTERFACE	N	N	Y	Y	N	N	Y	U	L	U	U
2800	SGMP	N	N	Y	Y	Y	N	Y	U	L	U	M
2870	DISIFLAQ	N	N	Y	Y	Y	N	Y	U	L	U	M
3101	GWFLOW/ GWMESH/ GWPLOT	Y	Y	Y	Y	Y	U	Y	U	L	U	U

KEY: Y = YES N = NO L = LIMITED E = EXTENSIVE M = MANY F = FEW U = UNKNOWN

Appendix A.2, part 2 (continued)

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
3237	PORSTAT/ PORMC	N	N	Y	Y	Y	U	Y	U	L	U	U
3240	GM5	N	N	Y	Y	U	N	Y	U	L	U	U
3241	Seawater Intrusion with BIEM	N	N	Y	Y	U	N	Y	U	L	U	U
3350	FEMSAT	N	N	Y	Y	U	U	Y	U	L	U	U
3372	AQUIFLOW	N	N	Y	Y	Y	N	Y	U	L	U	F
3373	FEWA	N	N	Y	Y	Y	N	Y	U	L	U	F
3600	SWIGS2D	N	N	Y	Y	N	N	Y	U	L	U	F
3640	SEAWTR/ SEACONF	N	N	Y	Y	N	N	Y	N	L	U	U
3881	2-D Finite Element Galerkin Model	N	N	Y	Y	N	N	Y	U	L	U	F
4100	MODFE	Y	Y	Y	Y	Y	N	Y	U	E	U	M
4160	ST2D	N	N	Y	Y	N	N	Y	N	L	N	F
4530	MAQWF	N	N	Y	Y	N	N	Y	N	L	N	U
4640	RAQSIM	N	N	Y	Y	N	N	Y	N	L	N	F
4753	AQ-FEM	Y	Y	Y	Y	Y	Y	Y	U	L	U	M
4754	AQ-EF	Y	Y	Y	Y	Y	Y	Y	U	L	U	M
4900	SLAM	N	N	Y	Y	Y	Y	Y	U	L	U	M
4901	UNSTEADY FLOW	N	N	Y	Y	Y	Y	Y	U	L	U	M

KEY: Y = YES N = NO L = LIMITED E = EXTENSIVE M = MANY F = FEW U = UNKNOWN

Appendix A.2, part 2 (continued)

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
4920	FLOWPATH	Y	Y	Y	Y	Y	Y	Y	U	E	Y	M
5000	MICROFEM	Y	Y	Y	Y	Y	Y	Y	U	L	Y	M
5001	FLOWNET	Y	Y	Y	Y	Y	Y	Y	U	L	Y	M
5030	NUSEEP	Y	Y	Y	Y	Y	Y	Y	U	L	U	U
5110	AQUIFER	U	U	Y	Y	Y	Y	Y	U	L	U	U
5160	INTERSAT	Y	Y	Y	Y	Y	Y	Y	U	L	U	F
5200	FLOWNS	N	N	Y	Y	N	Y	Y	N	L	U	U
5230	GEOFLOW	Y	Y	Y	Y	Y	Y	Y	U	L	U	M
5240	CGAQUFEM	U	U	Y	Y	Y	U	Y	N	L	U	U
5241	FLONETS	U	U	Y	Y	Y	U	Y	N	L	U	U
5392	CSUFDM	Y	Y	Y	Y	Y	Y	Y	N	L	U	F
5540	FRESAL	N	N	Y	Y	Y	N	Y	N	L	N	F
5720	JDB2D/3D	N	N	Y	Y	Y	Y	Y	N	L	U	M
5730	AQUAMOD	Y	Y	Y	Y	Y	Y	Y	U	L	U	U
5750	SHARP	N	N	Y	Y	Y	N	Y	N	L	U	U
5810	2D Steady State FE Model	N	N	Y	Y	Y	N	Y	U	L	U	F
6030	AQ/BASIC GWF	Y	Y	Y	Y	Y	Y	Y	U	L	U	M
6353	GWFL3D	Y	Y	Y	Y	U	Y	Y	U	L	U	M
6650	GWPATH	N	N	Y	Y	Y	Y	Y	U	L	U	M

KEY: Y = YES N = NO L = LIMITED E = EXTENSIVE M = MANY F = FEW U = UNKNOWN

Appendix A.3: Saturated Flow; Numerical Models for Three-Dimensional Flow, Part 1: Model Description

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IGWMC Key: 510 Model Name: ISOQUOD Released: 1982
Authors: Pinder, G.F., and E.O. Frind

ISOQUOD is a finite element model to simulate transient three-dimensional groundwater flow in anisotropic and heterogeneous, confined or unconfined aquifers.

Contact Address: Water Resources Program, Department of Civil Engineering, Princeton University, Princeton, NJ 08540

IGWMC Key: 770 Model Name: USGS-3D-FLOW Released: 1982
Authors: Trescott, P.C., S.P. Larson, and L.J. Torak.

USGS-3D-FLOW is a widely used, general purpose finite difference model to simulate transient, three-dimensional and quasi-three-dimensional, saturated flow in anisotropic, heterogeneous (layered) groundwater systems. The flow system can be fully confined or the uppermost zone can be a water-table aquifer. The model simulates well discharge/recharge from any layer and recharge to the uppermost layer. The 1982 update extended the program to simulations involving leaky rivers, evapotranspiration as a linear function of depth to water, and discharge to drains and springs. (Replaced by MODFLOW).

Contact Address: L. Torak, U.S. Geological Survey, Branch of Groundwater, M.S. 411 National Center, Reston, VA 22092

IGWMC Key: 2072 Model Name: FE3DGW Released: 1985
Authors: Gupta, S.K., C.R. Cole, and F.W. Bond.

FE3DGW is a finite element model for transient or steady state, fully or quasi-three-dimensional simulation of flow in a large multi-layered groundwater basin. The code offers a wide choice of in specifying boundary conditions like prescribed heads, nodal injection or withdrawal, constant or spatially varying infiltration rates, and elemental sources or sinks. Support programs are included to plot the finite element grid, contour maps of input and output parameters, and vertical cross-sections. Also, there are support programs available for determining groundwater pathlines and travel times from a specified point. (Also distributed as part of CFEST).

Contact Address: Nat. Energy Software Ctr., Argonne Nat. Lab., 9700 S. Cass Ave, Argonne, IL 60439

IGWMC Key: 2090 Model Name: VTTSS3 Released: 1979
Authors: Reisenauer, A.E., C.R. Cole.

VTTSS3 (Variable Thickness Transient/Steady-State 3D model) is a finite difference model to predict steady-state hydraulic head in unconfined or (leaky-) confined, isotropic, heterogeneous, multi-layered aquifer systems. It can generate streamlines and traveltimes and has a separate module for cell-by-cell calculation of the water budget. Solving the steady-state equations is done with the Newton method and direct Gaussian elimination.

Contact Address: Cole, C.R., Battelle Pacific NW Laboratories, Water and Land Resources Div., P.O. Box 999, Richland, WA 99532

IGWMC Key: 2663 Model Name: Variable Density Model Released: 1984
Author: Kuiper, L.K.

Kuiper's model is an integrated finite difference model for the simulation of variable density, time dependant groundwater flow in three dimensions. The governing equation is the three-dimensional transient flow equation with fresh water head as dependent variable. The groundwater density, although variable in space, is approximately constant in time and known. The IFDM grid elements are rectangular when viewed from the vertical direction, but their top and bottom surfaces follow the curvature of the geologic strata. Solution methods employed are the line successive over-relaxation method, the strongly implicit procedure, and a conjugate gradient method.

Contact Address: Kuiper, L.K., U.S. Geological Survey, 211 East 7th Street, Austin, TX 78701

IGWMC Key: 2740 Model Name: NMFD-3D Released: 1980
Authors: Posson, D.R., G.A. Hearne, J.V. Tracy, and P.F. Frenzel

NMFD-3D (New Mexico Finite Difference 3-Dimensional Model) simulates non-steady state two-dimensional horizontal or fully-three-dimensional groundwater flow in multi-layered heterogeneous, anisotropic aquifer systems or three-dimensional saturated groundwater flow. The model includes an analytical-numerical approximation for transient leakage from confining beds and allows for both confined and water table conditions.

Contact Address: Posson, D.R., U.S. Geological Survey, P.O. Box 26659, Albuquerque, NM 87125

IGWMC Key: 2880 Model Name: GWHEAD Released: 1980
Authors: Beckmeyer, R.R., R.W. Root, and K.R. Routt

GWHEAD is a computer code for simulating transient three-dimensional groundwater flow in an anisotropic, spatially heterogeneous aquifer. The model solves the finite difference approximations using the strongly implicit solution procedure. The boundaries either may permit flow across them or may be impermeable. The top boundary represents the water table and its location is a function of the dependent head variable. Across this boundary the model allows vertical accretion (recharge). The code has been used to model leaky confined groundwater conditions and spherical flow to a continuous point sink, both of which have exact analytical solutions.

Contact Address: Code custodian, Waste Disposal Technology Division, E.I. du Pont de Nemours & Co., Savannah River Lab., Aiken, SC 29808

IGWMC Key: 3863 Model Name: SEEP(VM)-3D Released: 1983
Author: Desai, C.S.

SEEP(VM)-3D simulates three-dimensional confined, and steady and transient free surface seepage in porous bodies (dams, wells, slopes, drains, media with cracks) using a finite element technique with variable and moving mesh.

Contact Address: Desai, C.S., Univ. of Arizona, Dept. of Civil Eng. and Mech. Eng., Tuscon, AZ 85721

IGWMC Key: 3980 Model Name: MODFLOW Released: 1988

Authors: McDonald, M.G., and A.W. Harbaugh.

MODFLOW is a widely-used, modular, block-centered finite difference model for the simulation of two-dimensional and quasi- or fully-three-dimensional, transient groundwater flow in anisotropic, heterogeneous, layered aquifer systems. It calculates piezometric head distributions, flow rates and water balances. The model includes modules for flow towards wells, through riverbeds, and into drains. Other modules handle evapotranspiration and recharge. Various textual and graphic pre- and postprocessors are available. Additional simulation modules are made available by the authors and by third parties, including PATH3D, MODPATH, MT3D, STR1, Interbed Storage Packkage, and ZONEBUDGET.

Contact Address: A.W. Harbaugh, U.S. Geological Survey, Groundwater Branch, WRD WGS - Mail Stop 433, National Center, Reston, VA 22091

IGWMC Key: 3982 Model Name: PATH3D Released: 1990
Author: Zheng, C.

PATH3D is a general particle tracking program for calculating groundwater paths and travel times in transient three-dimensional flow fields. The program includes two major segments: 1) a velocity interpolator which converts hydraulic heads, as generated by the USGS three-dimensional modular flow model MODFLOW, into a velocity field, and 2) a fourth-order Runge Kutta numerical solver with automatic time steps size adjustment for tracking the movement of fluid particles.

Contact Address: C. Zheng, S.S. Papadopulos & Assoc., Inc., 7944 Wisconsin Avenue, Bethesda, Maryland 20814

IGWMC Key: 4500 Model Name: FEM301 Released: 1985
Author: Kiraly, L.

FEM301 is a three-dimensional finite element model for simulation of steady state flow in an equivalent anisotropic porous medium intersected by linear or planar discontinuities. These discontinuities may be thin aquifers between aquitards or permeable shear zones. Such features are modeled with one- or two-dimensional elements embedded in the three-dimensional network. Post-processing routines include calculation and graphic display of pathlines and traveltimes within the three-dimensional network.

Contact Address: Hufschmied, P., Nat. Coop. for Storage of Radioactive Waste (NAGRA), Parkstrasse 23, CH-5401 Baden, Switzerland.

IGWMC Key: 4660 Model Name: FLOSA (FLOw Systems Analysis) Released: 1988
Authors: Zijl, W., and M. Nawalany

FLOSA is a series of finite element/finite difference models for simulation of two- and three-dimensional steady-state groundwater flow in anisotropic, heterogeneous porous media. The models are based on the use of flow velocity as dependent variable in the numerical solution. Separate programs exist for pathline generation and travel times calculation.

Contact Address: W. Zijl, TNO Inst. for Applied Geoscience, P.O. Box 6012, 2600 JA Delft, The Netherlands

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IGWMC Key: 4940 Model Name: DYNFLOW Released: 1992
Authors: Riordan, P.J., R.P. Schreiber, and B.M. Harley.

DYNFLOW (DYNamic groundwater FLOW simulation model) is a Galerkin finite element model for the simulation of transient and steady-state three-dimensional groundwater flow in multi-layered aquifer systems. The model handles 2D areal and cross-sectional and fully-3D situations, induced infiltration from streams, artificial and natural recharge or discharge, and heterogeneous, anisotropic aquifer hydraulic properties. It solves both linear (confined) and nonlinear (unconfined) aquifer flow equations, including the transition in time and/or space from confined to unconfined. The program has a "rising water" scheme to allow drainage to local streams if the piezometric head in a phreatic aquifer rises to the elevation of the stream bed. DYNFLOW has the following optional solvers: (1) gauss elimination, (2) successive overrelaxation with or without preconditioning, and (3) conjugate gradient with preconditioning.

DYNFLOW is part of DYN-SYSTEM, an integrated set of ground-water modeling programs used within the CDM company. Other components of the system are: DYNSWIM: 3-D sea water intrusion model; DYNAPL: 3-D two-phase (sharp interface) model; DYNPOTS: 3-D potential flow theory model; DYNCON: 3-D finite element mass transport model; DYN-EDM: environmental data manager. The DYN-SYSTEM includes various support programs and a model parameter optimization program.

Contact Address: B.M. Harley, Camp Dresser & McKee Inc., One Cambridge Center, Cambridge, MA 02142

IGWMC Key: 5560 Model Name: 3-D Free Surface FE Model Released: 1985
Authors: Durbin, T.J., and C. Berenbroeck.

This model utilizes the Galerkin finite element method for solving the equation of three-dimensional ground-water flow through a multi-aquifer system. The model handles deformation of the grid resulting caused by geometric changes of the ground-water system resulting from vertical movement of the water table during transient-state simulations. The three-dimensional grid is assembled from stacks of prismatic elements in each of which three tetrahedrons are fitted. This allows, among others, for layer pinch-outs. The model can handle a free-surface boundary at the top of the aquifer, prescribed hydraulic head and (zero) flux boundaries.

Contact Address: T.J. Durbin, U.S. Geological Survey, Federal Building, Room W-2234, 2800 Cottage Way, Sacramento, CA 95825

IGWMC Key: 5600 Model Name: STLINE Released: 1990
Authors: --

STLINE is a 3D particle tracking program using intercell flow rates computed by a finite difference model. The specific discharge vectors are converted to average linear flow velocities. Particle movements within the velocity field are computed by a linear interpolation scheme using a local coordinate system embedded in the global coordinate system of the numerical model. Intracell-particle translations and traveltimes are based on a linear variation in velocities in the cell. The trajectory of each particle is stored in memory as a series of particle translations each with a specific and accumulated travel time within the global coordinate system. Particle trajectories can be displayed in each of the three orthogonal planes of the Cartesian coordinate system.

Contact Address: D. Ward, GeoTrans, Inc., 46050 Manekin Plaza, Suite #100, Sterling, VA 22170

Note: See also Appendix C.3; some 3-D solute transport models include a sophisticated flow simulation module.

Appendix A.3: Saturated Flow; Numerical Models for Three-Dimensional Flow, Part 2: Usability and Reliability

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
510	ISOQUAD	N	N	Y	Y	N	N	Y	U	U	U	U
770	USGS-3D-FLOW	N	N	Y	Y	N	N	Y	Y	E	Y	M
2072	FE3DGW	Y	Y	Y	Y	Y	N	Y	Y	E	Y	M
2090	VTTSS3	N	N	Y	Y	N	N	Y	U	L	U	F
2663	Variable Density Model	N	N	Y	Y	N	N	Y	U	L	U	F
2740	NMFD-3D	N	N	Y	Y	N	N	Y	U	L	U	F
2880	GWHEAD	N	N	Y	Y	N	N	Y	U	L	U	F
3863	SEEP(VM)-3D	N	N	Y	Y	U	U	Y	U	L	U	F
3980	MODFLOW	Y	Y	Y	Y	Y	N	Y	Y	E	Y	M
3982	PATH3D	Y	Y	Y	Y	Y	Y	Y	U	L	Y	M
4500	FEM301	Y	Y	Y	Y	Y	N	Y	U	L	Y	F
4660	FLOSA	Y	Y	Y	Y	Y	Y	Y	U	L	U	F
4990	DYNFLOW	Y	Y	Y	Y	Y	Y	Y	Y	E	Y	M
5560	3-D Free Surface FE Model	N	N	Y	Y	N	N	Y	U	L	U	F
5600	STLINE	Y	Y	Y	Y	Y	Y	Y	U	L	U	F

KEY: Y = YES N = NO L = LIMITED E = EXTENSIVE M = MANY F = FEW U = UNKNOWN

Appendix A.4: Saturated Flow; Analytical Inverse Models (Aquifer Test Models), Part 1: Model Description

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IGWMC Key: 2801 Model Name: SATEM Released: 1989
Author: Boonstra, J.

SATEM (Selected Aquifer Test Evaluation Methods) is a set of four interactive microcomputer programs for analysis of aquifer tests in unconsolidated, confined, leaky confined or phreatic aquifers. These programs are: JACOB, HANTUSH, PARTIAL, and RECOVERY. For aquifers under fully confined or unconfined conditions SATEM allows for partial penetrating wells. The program has been designed to provide quick evaluation of the field data by using diagnostic plots, a method well-suited for sensitivity analysis. It can evaluate the drawdown data observed during pumping and residual drawdown data observed during recovery. The field data can be taken from observation and/or from the pumping well itself. SATEM includes a program for inputting field data and a program to set up hypothetical single well aquifer test data for instructional purposes.

Contact Address: J. Boonstra, Internat. Inst. for Land Reclamation and Improvement, P.O. Box 45, 6700 AA Wageningen, The Netherlands

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IGWMC Key: 3150 Model Name: HVRLV 1 Released: 1981
Authors: Weyer, K.U., and W.C. Horwood-Brown

HVRLV 1 is an interactive, user-oriented calculation of permeabilities from slug tests using Hvorslev's formulae for filters in uniform soil.

Contact Address: K.U. Weyer, Nat. Hydrology Research Inst., Ground Water Division, 101-4616 Valiant Drive N.W., Calgary, Alberta Canada, T3A OXG

IGWMC Key: 4751 Model Name: AQ-AT Released: 1989
Authors: Kovar, K., and A. Leijnse

AQ-AT is a computer program package for aquifer test analysis due to pumpage in a homogeneous infinite multi-layered aquifer-aquitard system. The menu-driven package includes modules for confined and leaky-confined systems and provides the best estimate for aquifer and aquitard parameters and corresponding uncertainty using least squares optimization. The program includes help screens and error checking. It has options for joint graphic display of observed drawdowns (input) and computed drawdowns using the estimated parameters.

Contact Address: K. Kovar, Inst. of Public Health and Environm. Protection, P.O. Box, 3720 BA Bilthoven, The Netherlands

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IGWMC Key: 5002 Model Name: MATE Released: 1985
Author: Hemker, C.J.

MATE (Microcomputer Aquifer Test Evaluation) is menu-driven, user-interactive program to evaluate aquifer parameters (transmissivity, storage coefficient, leakance) from pumping test data using the least-squares approach together with the Malquardt algorithm. The program can handle four types of aquifer parameter evaluations including: 1) steady-state flow in semi-confined aquifers (De Glee); 2) unsteady-state flow in (semi-)confined aquifers (Theis or Hantush well function); 3) recovery test in (semi-)confined aquifers (Theis or Hantush well function); and steady-state flow in multiple aquifer systems (Hemker).

Contact Address: C.J. Hemker, Elandsgracht 83, 1016 TR Amsterdam, The Netherlands

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IGWMC Key: 5003 Model Name: MLU (Multi-Layer Unsteady-state model) Released: 1986
Author: Hemker, C.J.

MLU is a program for drawdown calculations and inverse modeling (aquifer tests) of transient flow in layered (up to 9 aquifers) and fissured (double porosity aquifer systems) under (semi-)confined and unconfined conditions. The model is based on a series of analytical solutions.

Contact Address: C.J. Hemker, Elandsgracht 83, 1016 TR Amsterdam, The Netherlands

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IGWMC Key: 5040 Model Name: GWAP Released: 1989
Author: Dansby, D.A.

GWAP (Graphical Well Analysis Package) is a well test analysis package that provides a computer-based method of performing graphical curve matching. Data from the well test are plotted on the computer screen and then a type curve is selected, overlain, and matched to the data directly on the screen. GWAP supports confined-leaky aquifer (Hantush, 1956), unconfined aquifer (Neuman, 1975), large diameter well (Papadopulos and Cooper, 1967), and slug injection/withdrawal (Cooper et al., 1967) type curves.

Contact Address: Groundwater Graphics, 5209 Windmill Str., Oceanside, CA 92506

IGWMC Key: 5050 Model Name: HJ-MATCH Released: --
Author: Bump, A.C., and M.S. Ramesh

HJ-MATCH is an aquifer characterization program for fully penetrated, leaky, confined aquifers. HJ-MATCH computes the best values of aquifer transmissivity (permeability), storage coefficient (porosity-compressibility factor), aquitard hydraulic conductivity, and leakage factor in user-selected hydrology or petroleum terminology. The best values are determined automatically by matching pumping test data with families of type curves using non-linear relative least-squares matching. Completely automated, HJ-MATCH does not require initial estimates of hydrologic parameters. The program uses the Papadopulos method when drawdown data for at least three observation wells are available. The user-interactive program includes graphic output to screen, plotter, or printer.

Contact Address: In-Situ, Inc., P.O. Box 1, Laramie, Wyoming 82070

IGWMC Key: 5051 Model Name: PAPADOP Released: --
Authors: --

PAPADOP is an aquifer characterization program that calculates directional transmissivities (permeabilities) and frequency of direction of major transmissivity (permeability). The program uses multiwell test data to obtain directional transmissivity and storage coefficient in hydrologic units or directional permeability and porosity-compressibility factor in petroleum terminology. A method modified from the well-known Papadopulos method is used. The directional properties are computed for all three observation well combinations possible (up to 100 observation wells). The program can be used with almost any aquifer and well conditions (leaky or non-leaky, unconfined or confined, fractured, partially or fully penetrated).

Contact Address: In-Situ, Inc., P.O. Box 1, Laramie, Wyoming 82070

IGWMC Key: 5052 Model Name: STEP-MATCH Released: --
Authors: Bumb, A.C., and M.S. Ramesh

STEP-MATCH automates the processing and analysis of data from slug tests. The program plots field data in semilog form; calculates type curves representing various wellbore storage, skin and transmissivity values, and determines the "best" match using non-linear least squares and Taylor series approximation. The program includes a menu-driven, full screen editor environment and supports additional graphic programs available from the same vendor.

Contact Address: In-Situ, Inc., P.O. Box 1, Laramie, Wyoming 82070

IGWMC Key: 5054 Model Name: TS-MATCH Released: --
Authors: --

TS-MATCH is an aquifer characterization program for fully penetrated, non-leaky, confined aquifers. It computes the best values for transmissivity and storage coefficient or permeability and porosity-compressibility factor by matching the Theis exponential integral type curve with field pump test data. TS-MATCH uses full type-curve and non-linear relative least-squares matching. The program can compute directional transmissivities or permeabilities using the Papadopulos method when data from at least three observation wells are available.

Contact Address: In-Situ, Inc., P.O. Box 1, Laramie, Wyoming 82070

IGWMC Key: 5060 Model Name: PTDPS I Released: --
Author: Blair, A.W.

PTDPS I is a pumping test data plotting software for use with confined aquifers. It performs the following functions: (1) Cooper/Jacob confined aquifer trend, drawdown, and recovery graphs; (2) Thiem test-distance/drawdown analysis and trend and drawdown graphs; (3) Theis equation match point method trend and drawdown graphs; (4) step drawdown test trend and step drawdown graphs; (5) well and formation losses; (6) transmissivity and storage coefficient calculations; and (7) least squares or manual interactive graphic curve fitting.

Contact Address: A.W. Blair, IRRISCO, P.O. Box 5011, University Park, New Mexico 88003

IGWMC Key: 5061 Model Name: PTDPS II Released: --
Author: Blair, A.W.

PTDPS II is a pumping test data plotting software for use with unconfined/leaky aquifers with the following functions: (1) Cooper/Jacob unconfined aquifer trend, drawdown graphs; (2) Hvorslev slug (falling head) and bail (rising head) piezometer tests; (3) Hantush/Jacob leaky aquifer match point method trend and drawdown graphs; (4) transmissivity and storage coefficient calculated using least squares or manual interactive graphic curve fitting.

Contact Address: A.W. Blair, IRRISCO, P.O. Box 5011, University Park, New Mexico 88003

IGWMC Key: 5062 Model Name: PTDPS III Released: --
Author: Blair, A.W.

PTDPS III is a pumping test data plotting software for confined, leaky confined and unconfined aquifers. For confined aquifers the software performs the following functions: (1) Cooper/Jacob semilog method; (2) Theis well function match point method; and (3) Thiem distance/drawdown method. With unconfined aquifers the program handles the Cooper/Jacob semilog method. With leaky confined aquifers the program includes the Hantush/Jacob method. The program also performs: (1) step drawdown well/formation loss method; (2) Hvorslev's bail test method and slug test method; and (3) Bouwer and Rice piezometer functions.
Contact Address: A.W. Blair, IRRISCO, P.O. Box 5011, University Park, New Mexico 88003

IGWMC Key: 5070 Model Name: PUMPING TEST PROGRAM Released: --
Authors: --

This is a pumping test program package for analysis of drawdown and recovery tests. Hydrographs and site plans can be plotted and step tests analyzed. The programs will take the data from manual input or data loggers and will correct them for partial penetration or water table conditions. The aquifer coefficients can be calculated using straight line or least squares fit. It is possible to use only part of the graph for analysis.

Contact Address: Earthware of California, 30100 Town Center Drive, #196, Laguna Niguel, CA 92677

IGWMC Key: 5080 Model Name: PUMP Released: --
Author: Ulrick, J.

The Theis method pumping test analysis program PUMP matches a Theis curve to selected aquifer drawdown and recovery test data by Gauss-Newton non-linear regression. For a pumping well, corrections may be made for casing storage, water-table conditions, and well loss. The program is menu, driven and has full screen editing capabilities. Various options are available for graphic display and plotting of the results.

Contact Address: Ulrick & Associates, 1400 Grandview Drive, Berkeley, CA 94705

IGWMC Key: 5090 Model Name: WHIP Released: --
Authors: --

WHIP (Well Hydraulics Interpretation Program) is a menu driven interactive program which allows the user to design and interpret complex aquifer tests. The program handles simulation and analysis of aquifer tests with multiple pumping wells, time-varying pumping rates, and realistic pumped well conditions. WHIP uses numerical Laplace inversion techniques to solve the analytical equations of drawdown in homogeneous, vertically anisotropic, or double porosity aquifers.

Contact Address: G. Walter, Hydro Geo Chem Inc., 1430 N. 6th Avenue, Tuscon, AZ 85705

IGWMC Key: 5190 Model Name: PUMPING TEST PACKAGE Released: --
Authors: --

The PUMPING TEST PACKAGE calculates optimal values of aquifer parameters as transmissivity, storage coefficient, leakage coefficient, and hydraulic resistance from pumping test data as observed on one or more wells (up to 10 wells). The menu-driven program uses a non-linear regression technique and provides for error checking in input.

Contact Address: Rockware, Inc., 4251 Kipling Street, #595, Wheatridge, CO 80033

IGWMC Key: 5460 Model Name: Groundwater Discharge Tests Released: 1988
Author: Clarke, D.

This software is a menu-driven series of programs for designing and analyzing aquifer tests. It includes the following modules: (1) DTDHA - Discharge Test Data Handling and Analysis; this module uses the modified Sternberg and the Rorabaugh analysis for step-drawdown and recovery; (2) DRAWDOWN - drawdown in bounded or unbounded (leaky) confined aquifers using the Theis well function or the leaky confined aquifer well function; (3) NEUMAN - drawdown in an unconfined aquifer using Neuman's well function; (4) ANALYZE - determining transmissivity and storage coefficient for a (leaky) confined aquifer using least squares; and (5) various file manipulation and plotting utilities.

Contact Address: Clarke Computer Services, 20 Musgrave St., Crystal Brook, 5523, Australia

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IGWMC Key: 6025 Model Name: THCVFIT Released: 1992
Author: van der Heijde, P.K.M.

THCVFIT is an interactive program to determine transmissivity and storage coefficient from pump test data. This model replaces traditional curve-fitting by a graphics routine to match the Theis well function with field drawdown data. Match point and resulting parameters are listed.

Contact Address: Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401

IGWMC Key: 6080 Model Name: THEISFIT Released: 1991
Author: McElwee, C.D.

THEISFIT is a non-graphic, interactive program that calculates aquifer parameters by automatically fitting type curve and pump test data from pumping an isotropic heterogeneous nonleaky confined aquifer using a least squares method. The program has been designed to analyze data conforming to assumptions implicit in the Theis equation.

Contact Address: C.D. McElwee, Kansas Geological Survey, 1930 Avenue A, Campus West, University of Kansas, Lawrence, KS 66044, or Internat. Ground Water Modeling Ctr.

IGWMC Key: 6081 Model Name: TSSLEAK Released: 1992
Authors: Cobb, P.M., C.D. McElwee, and M.A. Butt

TSSLEAK is an interactive program for automated analysis of pumping-test data for a leaky-confined aquifer using a least-squares procedure for fitting the Hantush and Jacob equation to experimental time-drawdown data to obtain estimates for storage coefficient, transmissivity, leakage coefficient, and aquitard permeability. The program prompts for user-input and provides the results in ASCII text files.

Contact Address: C.D. McElwee, Kansas Geological Survey, 1930 Avenue A, Campus W, University of Kansas, Lawrence, KS 66044, or Internat. Ground Water Modeling Ctr.

IGWMC Key: 6082 Model Name: VARQ Released: 1987
Authors: Butt, M.A., and C.D. McElwee

VARQ is an interactive program to calculate aquifer parameters by automatically fitting pump test data with a Theis-type curve. It evaluates transmissivity and storage coefficient for a homogeneous, isotropic confined aquifer using a least-squares procedure. The program allows for variable discharge rates during the test. As a measure of error, the rms (root-mean-square) error in drawdown is calculated along with the correlation coefficient between pumping-test data and theoretically generated data, using the converged values of transmissivity and storage coefficient. Output is in tabular form.

Contact Address: C.D. McElwee, Kansas Geological Survey, 1930 Avenue A, Campus West, University of Kansas, Lawrence, KS 66044, or Internat. Ground Water Modeling Ctr.

IGWMC Key: 6382 Model Name: PUMPTEST Released: 1992
Author: Beljin, M.S.

PUMPTEST is an interactive program designed to determine aquifer parameters by analyzing aquifer test data using a least-squares fitting procedure. The package includes a program to evaluate transmissivity and storage coefficient based on Jacob's straight line method, a program to estimate transmissivity and storage coefficient from distance-drawdown data, and a program to estimate transmissivity from time-residual drawdown aquifer test data. Results are presented graphically and in ASCII format.

Contact Address: Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401

IGWMC Key: 6450 Model Name: TGUESS Released: 1985
Authors: Bradbury, K.R., and E.R. Rothchild

TGUESS is a simple interactive program for estimating transmissivity from specific capacity data. The program corrects for partial penetration and well loss. Output is in ASCII format.

Contact Address: K.R. Bradbury, Wisconsin Geological Survey, 1815 University Ave., Madison, WI 53705, or Internat. Ground Water Modeling Ctr.

IGWMC Key: 6580 Model Name: TIMELAG Released: 1987
Author: Thompson, D.B.

TIMELAG is an interactive program for evaluating permeability from single well tests based on the rate of water-level recovery after raising or lowering the water level in a well. Output is in ASCII format.

Contact Address: D. Thompson, SRW Associates, Inc., Robinson Plaza II, Suite 200, Pittsburgh, PA 15205, or Internat. Ground Water Modeling Ctr.

IGWMC Key: 6670 Model Name: AQTESOLV Released: 1992
Authors: --

AQTESOLV (AQuifer TEst SOLVer) is a user-friendly software package designed to assist in the analysis of pumping tests and slug tests. It computes and plots type curves for a number of different analytical solutions. The program allows the user to visually fit a type curve to time-drawdown data or provides least-squares based automatic estimation of aquifer properties. The options for constant-rate pumping tests include: (1) Theis, Cooper-Jacob and Theis recovery for confined aquifers; (2) Hantush for leaky aquifers; (3) Neuman, Theis and Cooper-Jacob for unconfined aquifers; and (4) Moench for fractured aquifers. For slug tests in confined aquifers the program provides the Cooper-Bredehoeft-Papadopulos method and for unconfined aquifers the Bouwer-Rice method.

Contact Address: Geraghty & Miller Modeling Group, 10700 Park Ridge Blvd, Suite 600, Reston, VA 22091

IGWMC Key: 6680 Model Name: SLUGIX/AQUIX-S Released: 1992
Authors: --

SLUGIX or AQUIX-S is an interactive, forward and inverse modeling program for analyzing slug test data. In the forward mode it provides the head response for a slug test for given aquifer storativity and transmissivity or hydraulic conductivity. The solution method of the inverse model is based on a non-linear least-squares fitting of the Cooper, Bredehoeft and Papadopulos model for a confined aquifer. The Bouwer and Rice model for an unconfined fully or partially penetrated aquifer and the Hvorslev models for a well point filter in uniform soil or at an impervious boundary use a real-time, interactive graphical curve fitting approach. The model comes with a sophisticated textual and graphic user-interface and report facilities.

Contact Address: T. Gilmer, EnviroTools Ltd, 27203 Armadillo Way, Evergreen, CO 80439

IGWMC Key: 6681 Model Name: AQUIX-T/AQUIX-4 Released: 1992
Authors: --

AQUIX-4 is a series of programs for the interactive, forward and inverse modeling of pumping test data with constant or variable flow rates and full recovery analysis. It provides drawdowns in terms of aquifer storativity, transmissivity, leakage, anisotropy, and specific yield, depending on the model selected. A least squares, nonlinear curve fitting method is used to determine the best fit model parameters to the observed data. AQUIX include programs for partial penetrating wells, and for confined, leaky confined and unconfined aquifers. The models are based on Theis (1935), Hantush (1960, 1965), and Neuman (1975). The model comes with a sophisticated textual and graphic user-interface and report facilities. AQUIX-T includes only the Theis varying rate recovery mode.

Contact Address: T. Gilmer, EnviroTools Ltd., 27203 Armadillo Way, Evergreen, CO 80439

IGWMC Key: 6730 Model Name: TENSOR2D Released: 1987
Authors: Maslia, M.L., and R.B. Randolph

TENSOR2D is a program for computing the components of the anisotropic transmissivity tensor of two-dimensional groundwater flow. To determine the tensor components using one pumping well and three observation wells, the type-curve and straight-line approximation methods are used. To determine the tensor components using more than three observation wells a weighted least-squares optimization method is used.

Contact Address: U.S. Geological Survey, Books and Open-File Reports Section, Federal Center, Box 25425, Denver, CO 80225

Appendix A.4: Saturated Flow; Analytical Inverse Models (Aquifer Test Models), Part 2: Usability and Reliability

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
2801	SATEM	Y	Y	Y	Y	Y	L	Y	N	Y	N	M
3150	HVRLV 1	N	N	Y	Y	Y	N	Y	N	Y	N	M
4751	AQ-AT	Y	Y	Y	Y	Y	Y	Y	U	Y	N	M
5002	MATE	Y	Y	Y	Y	Y	L	Y	U	Y	N	U
5003	MLU	Y	Y	Y	Y	Y	L	Y	U	Y	N	U
5040	GWAP	Y	Y	Y	Y	Y	Y	Y	U	Y	N	U
5050	HJ-MATCH	Y	Y	Y	Y	Y	Y	Y	U	Y	N	M
5051	PAPADOP	Y	Y	Y	Y	Y	Y	Y	U	Y	N	U
5052	STEP-MATCH	Y	Y	Y	Y	Y	Y	Y	U	Y	N	U
5054	TS-MATCH	Y	Y	Y	Y	Y	Y	Y	U	Y	N	M
5060	PTDPS I	Y	Y	Y	Y	Y	Y	Y	U	Y	N	U
5061	PTDPS II	Y	Y	Y	Y	Y	Y	Y	U	Y	N	U
5062	PTDPS III	Y	Y	Y	Y	Y	Y	Y	U	Y	N	U
5070	PUMPING TEST PROGRAM	Y	Y	Y	Y	Y	Y	Y	U	Y	N	M
5080	PUMP	Y	Y	Y	Y	Y	L	Y	U	Y	N	U
5090	WHIP	Y	Y	Y	Y	Y	Y	Y	U	Y	N	U
5190	PUMPING TEST PACKAGE	Y	Y	Y	Y	Y	Y	Y	U	Y	N	M
5460	GROUND WATER DISCHARGE TESTS	Y	Y	Y	Y	Y	L	Y	U	Y	N	U
6025	THCVFIT	Y	Y	Y	Y	Y	L	Y	N	Y	N	M
6080	THEISFIT	Y	N	Y	Y	Y	L	Y	N	Y	N	M

KEY: Y = YES N = NO L = LIMITED M = MANY F = FEW U = UNKNOWN

Appendix A.4, part 2 (continued)

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
6081	TSSLEAK	Y	N	Y	Y	Y	L	Y	N	Y	N	M
6082	VARQ	Y	N	Y	Y	Y	L	Y	N	Y	N	M
6382	PUMPTEST	Y	Y	Y	Y	Y	Y	Y	N	Y	N	M
6450	TGUESS	Y	N	Y	Y	Y	L	Y	N	Y	N	M
6580	TIMELAG	Y	N	Y	Y	Y	L	Y	N	Y	N	F
6670	AQTESOLV	Y	Y	Y	Y	Y	Y	Y	U	Y	N	M
6680	SLUGIX/AQUIX-S	Y	Y	Y	Y	Y	Y	Y	U	Y	N	M
6681	AQUIX-T/ AQUIX-4	Y	Y	Y	Y	Y	Y	Y	U	Y	N	M
6730	TENSOR2D	N	N	Y	Y	Y	N	Y	U	Y	N	U

KEY: Y = YES N = NO L = LIMITED M = MANY F = FEW U = UNKNOWN

Appendix A.5: Saturated Flow; Numerical Inverse Models, Part 1: Model Description

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IGWMC Key: 195 Model Name: NON-LINEAR FE/FD REGRESSION Released: 1985
Authors: Cooley, R.L., and R.L. Naff

An interactive, inverse groundwater flow model using non-linear regression and finite-element or (integrated) finite-difference simulation. It estimates areally distributed discharge and recharge, boundary fluxes and heads, vertical hydraulic conductance, and transmissivity distribution based on best fit hydraulic head distribution for steady state, horizontal groundwater flow in an anisotropic, heterogeneous aquifer. The regression is based on steady-state observed heads, prior estimates of the regression parameters and their reliability, and known fluxes into or out of the aquifer. Various statistics associated with the regression analysis are computed.

Contact Address: Cooley, R.L., U.S. Geol. Survey, m.s. 413, Federal Center, Denver, CO 80225

IGWMC Key: 3981 Model Name: MODINV Released: 1990
Authors: Doherty, J., R.E. Volker, and R.G. Pearson

MODINV (MODFLOW Parameter Optimization) is a parameter optimization program based on the USGS three-dimensional modular flow model MODFLOW. It accepts a wide variety of MODFLOW parameters for optimization, including recharge rates, hydraulic conductivity, transmissivity, EVT extinction depth, etc. The program requires preliminary parameters zoning and is based on the matching of calculated and observed heads according to a weighted least squares criterion. Optimization is achieved using the Gauss-Marquardt method. The program comes with a forward simulation version of MODFLOW and pre- and postprocessors including a mesh generation routine.

Contact Address: J. Doherty, Australian Centre for Tropical Freshwater Research, James Cook University, Townsville, Qld 4811, Australia

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IGWMC Key: 3987 Model Name: MODFLOWP Released: 1992
Author: Hill, M.C.

MODFLOWP is a new version of the USGS modular, 3-D finite difference flow model MODFLOW incorporating the new Parameter-Estimation Package. The model can be used to estimate various MODFLOW parameters by nonlinear regression. Parameters are estimated by minimizing a weighted least-squares objective function by the modified Gauss-Newton method or by a conjugate direction method. Any spatial variation in parameters can be defined by the user. Data used to estimate parameters can include existing independent estimates of parameter values, observed hydraulic heads or temporal changes in heads, and observed gains and losses along head-dependent boundaries. The performance of the code has been tested in models of both actual and hypothetical groundwater systems (see also remarks).

Contact Address: M.C. Hill, U.S. Geological Survey, Water Resources Division, Box 25046, M.S. 413, Denver Federal Center, Denver, CO 80225

Note: There are many more codes written for parameter estimation using numerical approximation of the governing equations and direct or indirect techniques to solve the inverse problem. Most of these codes are experimental and considered "research codes." In general they are not readily available.

Appendix A.5: Saturated Flow; Numerical Inverse Models, Part 2: Usability and Reliability

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
195	NON-LINEAR FE/FD REGRESSION	N	N	Y	Y	N	L	Y	U	Y	U	F
3981	MODINV	N	N	Y	Y	N	Y	Y	U	Y	U	F
3987	MODFLOWP	N	N	Y	Y	N	L	Y	U	Y	U	F

KEY: Y = YES N = NO L = LIMITED M = MANY F = FEW U = UNKNOWN

Appendix A.6: Saturated Flow; Pathline Models, Part 1: Model Description

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IGWMC Key: 741 Model Name: USGS FRONT-TRACKING Released: 1983
Authors: Garabedian, S.P., Konikow, L.F.

USGS FRONT-TRACKING is a finite difference model for simulation of advective transport of a conservative tracer dissolved in groundwater under steady or transient flow conditions. The model calculates heads, velocities and tracer particle positions.

Contact Address: L.F. Konikow, U.S. Geological Survey, Water Resourc. Div., 431 National Center, Reston, VA 22092

IGWMC Key: 1791 Model Name: SLAEM/SLW/SLWL/SYLENS Release: 1992
Author: Strack, O.D.L., et al.

SLAEM and its predecessor SYLENS are models for analysis of two- and three-dimensional steady-state and transient groundwater flow in single or multi-layered aquifer systems based on the Analytical Element Method. SLAEM is an highly interactive graphic oriented program including many of the analytical elements available. The program includes transient wells, areal inhomogeneities, leaky or draining objects, variable infiltration (e.g. from rivers, lakes, and ponds). It allows analysis of flow in two aquifers separated by a thin confining layer. The model is especially suited to analyze flow in regional double aquifer systems with local interconnections. SLW and SLWL are scaled-down, educational versions of the SLAEM program.

Contact Address: O.D.L. Strack, Univ. of Minnesota, Dept. of Civil Eng., 122 CME Building, Minneapolis, MN 55455

IGWMC Key: 1820 Model Name: FLOP/FLOP-LIESTE/FLOP-Z1/FLOP-ZN Released: 1988
Authors: Akker, C. Van Den, Lieste, R., Veling, E.J.M.

The FLOP models are semi-analytical models for calculation of pathlines and residence times in groundwater systems. FLOP-LIESTE is designed for single (semi-) confined aquifers; FLOP-Z1 for a quasi three-dimensional semi-confined aquifer system; and FLOP-ZN for a multi-layered homogeneous aquifer system.

Contact Address: RIVM - National Institute for Health and Environment, P.O. Box 1, 3720 AB Bilthoven, The Netherlands

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IGWMC Key: 1822 Model Name: FRONT Released: 1981
Author: Akker, C. Van Den

FRONT is a semi-analytical model for calculation of pathlines and residence times in a confined, isotropic, heterogeneous aquifer with steady-state or transient flow. The integration along the streamlines is performed with Runge-Kutta, restricting the maximum time step size with a user-provided error-criterion.

Contact Address: RIVM - Nat. Inst. for Health and Environment, P.O. Box 1, 3720 BA Bilthoven, The Netherlands

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IGWMC Key: 2072 Model Name: FE3DGW Released: 1983
Authors: Gupta, S.K., Cole, C.R., Bond, F.W.

FE3DGW is a finite element model for transient or steady state, fully or quasi-three-dimensional simulation of flow in a large multi-layered groundwater basin. The code offers a wide choice of in specifying boundary conditions like prescribed heads, nodal injection or withdrawal, constant or spatially varying infiltration rates, and elemental sources or sinks. Support programs are included to plot the finite element grid, contour maps of input and output parameters, and vertical cross-sections. Also, there are support programs available for determining groundwater pathlines and travel times from a specified point.

Contact Address: Nat. Energy Software Ctr./US DOE, Argonne Nat. Lab., 9700 S. Cass Ave, Argonne, IL 60439 (also included in CFEST code)

IGWMC Key: 2092 Model Name: VTT Released: 1979
Authors: Reisenauer, A.E., Cole, C.R.

VTT (Variable Thickness Transient Groundwater Flow Model) is a finite difference model to calculate transient hydraulic head in confined or unconfined isotropic, heterogeneous, multi-layered aquifer systems. The model can calculate cell-by-cell water budgets and can generate stream-lines and travel times. Boundary conditions and aquifer stresses may be time-varying. The transient model is solved with the line successive over-relaxation method (LSOR).

Contact Address: Cole, C.R., Battelle Pacific NW Lab., Water and Land Resources Division, P.O. Box 999, Richland, WA 99352

IGWMC Key: 2120 Model Name: PATHS Released: 1980
Authors: Nelson, R.W., Schur, J.A.

The PATHS program is an idealized hybrid analytical/numerical model for simulation of steady-state or transient, two-dimensional, saturated groundwater flow and transport processes of advection, sorption and ion exchange. It includes an analytical solution of the flow equation and the Runge-Kutta solution for the pathline equations and the effects of equilibrium ion-exchange and linear adsorption. The model calculates pathlines, location/arrival time distribution, and location/outflow quantity distribution in a confined stratum that is isotropic and homogeneous. It assumes a uniform lateral flow gradient and superimposed leakage from a vertical, cylindrical fully penetrating pond or cavern. The model can handle up to 35 fully penetrating wells or vertical line sources.

Contact Address: Battelle Pacific NW Laboratories, Land and Water Resources Div., P.O. Box 999, Richland, WA 99352

IGWMC Key: 2770 Model Name: CONFLOW Released: 1981
Author: Hertel, E.S., Jr.

CONFLOW describes fluid flow between two wells in a confined homogeneous, isotropic region. The code uses superposition to solve Laplace's equation with impermeable boundaries and can assist in the design of flow experiments in geologic media. CONFLOW's output is a plot of the theoretical streamlines, the ratio between the time of first arrival for the confined region and the time of first arrival for unconfined two-well flow, and a value for the pressure drop function.

Contact Address: Hertel, E.S., Jr., Sandia Nat. Lab., Albuquerque, NM 87185

IGWMC Key: 3940 Model Name: RESSQ Released: 1985
Authors: Javandel, I., Doughty, C., Tsang, C.F.

RESSQ is a semi-analytical model of 2-dimensional contaminant transport that calculates the streamline pattern in an aquifer, the location of contaminant fronts around sources at specified times, and concentration versus time at sinks. RESSQ assumes a homogeneous, isotropic confined aquifer of uniform thickness and a steady-state regional flow field. It can handle advection and linear equilibrium adsorption. Sources are represented by fully penetrating recharge wells and ponds, and sinks are represented by fully penetrating pumping wells.

Contact Address: Javandel, I., Lawrence Berkeley Lab., Earth Sciences Div., Univ. of California, Berkeley, CA 94720

IGWMC Key: 3943 Model Name: WHPA Released: 1992
Authors: Blandford, T.N., Huyakorn, P.S.

WHPA (Well Head Protection Area delineation model) is an integrated program of analytical and semi-analytical solutions for the groundwater flow equation coupled with pathline tracking. It is designed to assist technical staff with delineation of wellhead protection areas. Developed for the U.S. EPA's Office of Groundwater Protection, the package includes modules for capture zone delineation in a homogeneous aquifer with 2-dimensional steady-state flow with options for multiple pumping/injection wells and barrier or stream boundary conditions. Also included are modules for Monte Carlo analysis of uncertainty and a particle-tracking postprocessor for numerical flow models such as MODFLOW and PLASM, using a two-dimensional rectangular grid.

Contact Address: U.S. EPA, Off. of Groundwater Protection, Washington, D.C., or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 3982 Model Name: PATH3D Released: 1990
Author: Zheng, C.

PATH3D is a general particle tracking program for calculating groundwater paths and travel times in transient three-dimensional flow fields. The program includes two major segments: 1) a velocity interpolator which converts hydraulic heads, as generated by the USGS three-dimensional modular flow model MODFLOW, into a velocity field, and 2) a fourth-order Runge Kutta numerical solver with automatic time steps size adjustment for tracking the movement of fluid particles.

Contact Address: C. Zheng, S.S. Papadopulos & Assoc., Inc., 7944 Wisconsin Ave, Bethesda, MD 20814

IGWMC Key: 3984 Model Name: MODPATH Released: 1988
Author: Pollock, D.W.

MODPATH is a post-processing package to compute three-dimensional path lines based on the output from steady-state simulations obtained with the USGS MODFLOW groundwater flow model. The package consists of two FORTRAN 77 computer programs: 1) MODPATH, which calculates pathlines, and 2) MODPATH-PLOT, which presents results graphically. MODPATH uses a semi-analytical particle tracking scheme, based on the assumption that each directional velocity component varies linearly within a grid cell in its own coordinate direction. Data is input to MODPATH through a combination of files and interactive dialogue.

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MODPATH -- continued

The MODPATH-PLOT program comes in two versions, one for use with the DISSPLA graphics routines library, and one that uses the Graphical Kernel System (GKS).

Contact Address: U.S. Geological Survey, Water Resources Division, 411 National Center, Reston, VA 22092; Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401; or Scientific Software, Washington, D.C.

IGWMC Key: 4591 Model Name: MAGNUM-3D Released: 1985
Authors: Estey, S.A., Arnett, R.C., Aichele, D.R.

MAGNUM-3D is a three-dimensional finite element code for simulation of steady-state and transient groundwater flow. The model can handle complex anisotropic, heterogeneous hydrologic systems. Quadratic elements allow the user to model irregular boundaries and hydrogeologic structures in detail. Layer pinch-outs can be modeled using three-dimensional prism elements. Stress may be applied in the form of surface recharge due to precipitation or irrigation well discharge.

Contact Address: Sandra Estay or Deborah Aichele, BCS Richland, Inc., Richland, Washington 99352

IGWMC Key: 4660 Model Name: FLOSA Released: 1988
Authors: Zijl, W., Nawalany, M.

FLOSA (FLOw Systems Analysis) is a series of finite element/finite difference models for simulation of two- and three-dimensional steady-state groundwater flow in anisotropic, heterogeneous porous media. The models are based on the use of flow velocity as dependent variable in the numerical solution. Separate programs exist for pathline generation and travel times calculation.

Contact Address: W. Zijl, TNO Inst. for Applied Geoscience, P.O. Box 6012, 2600 JA Delft, The Netherlands

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IGWMC Key: 4752/54 Model Name: AQ-AS/AQ-EF Released: 1989
Authors: Kovar, K., Leijnse, A.

AQ-AS is a computer program package for calculation of ground-water streamlines and isochrones due to well pumpage and natural flow in homogeneous infinite multi-layered aquifer-aquitard systems. The program is based on superposition of analytical solutions and includes both forward and backward particle tracking using Runge-Kutta integration. The menu-driven interactive program computes and displays streamline geometry, traveltimes, and isochrones. It includes help screens and error checking.

AQ-EF is a menu-driven, interactive computer program package for calculation of ground-water streamlines and isochrones in multi-layered, anisotropic heterogeneous aquifer-aquitard systems with steady-state or transient flow conditions. The program handles forward or backward particle tracking using the head distribution values computed by the program AQ-FEM. The package includes a module for plotting of the results.

Contact Address: K. Kovar, RIVM -- Nat. Inst. of Public Health and Environm. Protection, P.O. Box 1, 3720 BA Bilthoven, The Netherlands

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IGWMC Key: 4920 Model Name: FLOWPATH Released: 1992
Authors: Franz, T., Guiguer, N.

FLOWPATH is an easy-to-use program for the analysis of two-dimensional steady- state groundwater flow problems. The program calculates hydraulic head distributions, groundwater velocities, pathlines, travel times, capture zones, and wellhead protection areas in confined, leaky-confined or unconfined, anisotropic, heterogeneous aquifers. Pathlines are computed with a particle tracking method. The finite difference model can handle up to 10,000 nodes in an irregular grid, over 100 wells, and over 100 zones of different aquifer properties. The program has extensive and sophisticated graphic pre- and post-processing capabilities.

Contact Address: Waterloo Hydrogeologic Software, 113-106 Seagram Drive, Waterloo, Ontario, Canada N2L 3B8

IGWMC Key: 4922 Model Name: FLONET Released: 1992
Authors: --

FLONET is a two-dimensional cross-sectional steady-state ground water flow model. It computes potentials, streamlines, and ground-water velocities in a vertical section through a confined or unconfined aquifer. The model is based on the dual formulation of potentials and stream functions using a finite element method. It can handle heterogeneous, anisotropic conditions. The principal direction of the hydraulic conductivity tensor can vary in space. The model can account for spatially variable leakage characteristics of under- and overlying aquitards. For unconfined aquifers, the model seeks the water-table iteratively. The model comes with a user-friendly interface and extensive graphics (contours, velocity plots, streamlines and flow nets.

Contact Address: Waterloo Hydrogeologic Software, 113-106 Seagram Drive, Waterloo, Ontario, Canada N2L 3B8

IGWMC Key: 5001 Model Name: FLOWNET Released: 1989
Authors: Van Elburg, H., Hemker, C.J., Engelen, G.B.

FLOWNET is used for interactive modeling of two-dimensional steady-state flow in an heterogeneous and anisotropic cross-section of the saturated zone. It generates a flownet, composed of flow lines and equipotential lines, obtained by a five-point finite difference approximation to calculate heads and linear interpolation to determine equipotential lines. The matrix equation is solved using the conjugate gradient method. The streamlines are determined from the flow function which in turn is determined using the adjoint function of the potential function. The model handles hydraulic head boundary conditions variable along the boundary. It has options for waterbalance calculations and HP-plotter output.

Contact Address: C.J. Hemker, Elandsgracht 83, 1016 TR Amsterdam, The Netherlands

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IGWMC Key: 5004 Model Name: MFLOP (FLOw Pattern) Released: 1989
Authors: Hemker, C.J.

MFLOP is a simple microcomputer program for the immediate generation of streamlines of well fields with superimposed uniform flow under confined conditions.

Contact Address: C.J. Hemker, Elandsgracht 83, 1016 TR Amsterdam, The Netherlands

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IGWMC Key: 5200 Model Name: FLOWNS Released: 1989
Authors: Bramlett, W., Borden, R.C.

FLOWNS is a simple-to-use program for generating two dimensional flow nets for steady-state flow in any saturated rectangular domain with any combination of constant head or constant flux (including zero flux) boundary conditions. The domain might be either horizontally (areal) or vertically (cross-section) oriented. The program approximates with discrete values the continuous distributions of potential and stream function using finite difference approximations of the Laplace equation. The hydraulic conductivity distribution may be anisotropic and/or heterogeneous. A contouring program is required to generate the final stream and equipotential lines.

Contact Address: R.C. Borden, North Carolina St. Univ., Civil Eng. Dept, Rayleigh, NC 27695

IGWMC Key: 5300 Model Name: QUICKFLOW Released: 1991
Authors: --

QUICKFLOW is an interactive analytical model that simulates two-dimensional steady-state and transient ground-water flow. The steady-state module simulates flow in a horizontal plane using analytical functions developed by Strack (1989), including wells, uniform recharge, circular recharge/discharge areas, and line sources or sinks in confined and unconfined aquifers. The model generates streamlines, particle traces and head contours. The transient module calculates heads using equations developed by Theis (1935) and by Hantush and Jacob (1955) for confined and leaky confined aquifers, respectively, and includes a particle tracking option. Each module uses the principle of superposition to evaluate the effects of multiple wells in a uniform regional flow field.

Contact Address: Geraghty & Miller, Inc., Modeling Group, 10700 Park Ridge Blvd., Suite 600, Reston, VA 22091

IGWMC Key: 5340 Model Name: CTRAN/W (Contaminant Transport) Released: 1992
Authors: --

CTRAN/W is a finite element model for simulation of steady-state and transient movement of contaminants through saturated/unsaturated soil. The model allows for advection, dispersion, adsorption and decay. It handles transient concentration and mass-flux boundary conditions. The program runs under Microsoft Windows 3.0. and uses a pull-down menu driven graphical interface with many graphical display and editing functions. It is integrated with SEEP/W, a two-dimensional finite element flow simulator. CTRAN can model contaminant movent by particle tracking from user-defined locations.

Contact Address: Geo-Slope International, #830, 633 - 6th Avenue S.W., Calgary, Alberta, Canada T2P 2Y5

IGWMC Key: 5501 Model Name: GEOTRACK Released: 1991
Author: Srinivasan, P.

GEOTRACK is a graphics software program used to display pathlines generated by the USGS particle tracking program , MODPATH, for ground-water flow simulations performed using the USGS three-dimensional finite difference flow model MODFLOW or the three-dimensional finite difference flow and transport model FTWORK. A simplified fence-diagram with hidden line removal can be constructed to be displayed together with the calculated pathlines. The program allows for importing a surface feature map showing buildings, trenches, roads, etc. The program allows the user to rotate the three-dimensional diagram in real time.

continued.....

GEOTRACK -- continued

Contact Address: GeoTrans, Inc., 46050 Manekin Plaza, Suite 100, Sterling, VA 22170

IGWMC Key: 5600 Model Name: STLINE Released: 1990
Authors: --

STLINE is a 3D particle tracking program using intercell flow rates computed by a finite difference model. The specific discharge vectors are converted to average linear flow velocities. Particle movements within the velocity field are computed by a linear interpolation scheme using a local coordinate system embedded in the global coordinate system of the numerical model. Intracell-particle translations and traveltimes are based on a linear variation in velocities in the cell. The trajectory of each particle is stored in memory as a series of particle translations each with a specific and accumulated travel time within the global coordinate system. Particle trajectories can be displayed in each of the three orthogonal planes of the Cartesian coordinate system.

Contact Address: GeoTrans, Inc., 46050 Manekin Plaza, Suite #100, Sterling, VA 22170

IGWMC Key: 5822 Model Name: SAFTAP Released: 1991
Authors: Huyakorn, P.S., Blandford, T.N.

SAFTAP (SAturated Flow and Transport And Particle tracking) simulates saturated groundwater flow and solute transport in 3D. It is composed of two separate modules: the flow and transport module FTM, and the particle tracking module PTM. FTM is a finite element code for multi-aquifer systems with a wide range of aquifer conditions (e.g., confined, unconfined or partially confined with storage conversion). It analyses 3D unconfined flow using a saturated-pseudo unsaturated modeling approach, allowing the prediction of the water table and flow rates without characterization of the unsaturated zone. Many types of steady-state or time-dependent boundary conditions can be used. Transport mechanisms considered include advection, dispersion, molecular diffusion, adsorption, and first-order degradation.

Contact Address: HydroGeologic, Inc., 1165 Herndon Parkway, Suite 900, Herndon, VA 22070

IGWMC Key: 6590 Model Name: BEAVERSOFT Released: 1992
Authors: Bear, J., Verruijt, A.

BEAVERSOFT is a package of analytical and numerical solutions for groundwater flow and solute transport. It includes programs for steady and non-steady state two-dimensional flow in heterogeneous aquifers, for flow through dams, for transport of pollutants by advection and dispersion and for saltwater intrusion problems.

Contact Address: Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401

IGWMC Key: 6603 Model Name: ASM Released: 1991
Authors: Kinzelbach, W., Rausch, R.

ASM (Aquifer Simulation Model) is a menu-driven numerical model for steady-state or transient groundwater flow and (uncoupled) solute transport. The two-dimensional block-centered finite difference equations for (leaky-)confined or unconfined flow are solved using either the IADI or PCG method. Pathlines and isochrones around pumping well are computed by point-tracking in the velocity filed using Euler integration.

continued.....

ASM -- continued

Solute transport is simulated by the random walk method based on the Ito-Fokker-Planck theory. The model can simulate variable well rates, constant flux and constant head boundaries, and constant or instantaneous contaminant sources. It includes various graphic display option to view the simulation results.

Contact Address: W. Kinzelbach, Gesamthochschule Kassel- Universitat, FB 14, Moritzstr. 21, D-3500 Kassel, Germany; or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 6604 Model Name: PAT Released: 1990
Authors: Kinzelbach, W., Rausch, R.

PAT is an analytical model for the computation and graphical representation of pathlines and travel times of groundwater in an infinite or semi-infinite, homogeneous and isotropic confined aquifer or in an infinite strip of such an aquifer. The computed steady-state flow field might include arbitrary pumping or injection wells superposed on a natural uniform regional flow. The model is screen-oriented and fully interactive.

Contact Address: W. Kinzelbach, Geasamthochschule Kassel - Universitat, Moritzstrasze 21, D-3500 Kassel, Germany; or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 6650 Model Name: GWPATH Released: 1990
Author: Shafer, J.M.

GWPATH is an interactive microcomputer-based software package for estimating horizontal or vertical fluid pathlines and traveltimes in fully saturated ground-water flow domains. The model is applicable to two-dimensional heterogeneous, anisotropic flow systems, and features forward and reverse pathline tracking, time-related capture zone analysis, and multiple pathline capture detection mechanisms. It requires as input a regular, cell-based distribution of observed or computed hydraulic heads.

Contact Address: J.M. Shafer, 1013 Devonshire Drive, Champaign, IL 61821

Appendix A.6: Saturated Flow; Pathline Models, Part 2: Usability and Reliability

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
741	USGS FRONT-TRACKING	N	N	Y	Y	N	L	Y	N	L	L	F
1791	SLAEM/SLW/ SLWL/SYLENS	Y	Y	Y	Y	Y	Y	Y	N	E	L	M
1820	FLOP series	Y	Y	Y	Y	Y	Y	Y	N	E	L	M
1822	FRONT	Y	Y	Y	Y	Y	N	Y	U	L	L	F
2072	FE3DGW	N	N	Y	Y	N	N	Y	U	E	L	M
2092	VTT	N	N	Y	Y	N	N	Y	U	L	U	F
2120	PATHS	U	U	Y	Y	U	U	Y	U	L	U	M
2770	CONFLOW	U	U	Y	U	U	U	Y	U	U	U	U
3940	RESSQ	Y	Y	Y	Y	Y	Y	Y	Y	E	L	M
3943	WHPA	Y	Y	Y	Y	Y	Y	Y	U	E	L	M
3982	PATH3D	Y	Y	Y	Y	Y	Y	Y	U	E	U	M
3984	MODPATH	Y	Y	Y	Y	Y	Y	Y	U	L	L	M
4591	MAGNUM-3D	U	U	Y	Y	U	U	Y	U	L	U	U
4660	FLOSA	Y	Y	Y	Y	Y	Y	Y	U	L	L	F
4752/54	AQ series	Y	Y	Y	Y	Y	Y	Y	U	L	U	U
4920	FLOWPATH	Y	Y	Y	Y	Y	Y	Y	U	L	L	M
4922	FLONET	Y	Y	Y	Y	Y	Y	Y	U	U	U	U
5001	FLOWNET	Y	Y	Y	Y	Y	L	Y	U	L	U	U
5004	MFLOP	U	U	Y	Y	Y	L	Y	U	U	U	U
5200	FLOWNS	U	U	Y	Y	U	U	Y	U	U	U	U

KEY: Y = YES N = NO L = LIMITED E = EXTENSIVE M = MANY F = FEW U = UNKNOWN

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
5300	QUICKFLOW	Y	Y	Y	Y	Y	L	Y	U	E	L	M
5340	CTRAN/W	Y	Y	Y	Y	Y	L	Y	U	U	U	U
5501	GEOTRACK	U	U	Y	Y	U	L	U	U	U	U	U
5600	STLINE	U	U	Y	Y	U	L	U	U	U	U	U
5822	SAFTAP	Y	Y	Y	Y	Y	L	Y	U	E	L	U
6590	BEAVERSOFT	Y	Y	Y	Y	Y	N	Y	Y	E	L	M
6603	ASM	Y	Y	Y	Y	Y	Y	Y	N	E	L	M
6604	PAT	Y	Y	Y	Y	Y	Y	Y	N	L	U	M
6650	GWPATH	Y	Y	Y	Y	Y	Y	Y	U	L	U	M

KEY: Y = YES N = NO L = LIMITED E = EXTENSIVE M = MANY F = FEW U = UNKNOWN

IGWMC Key: 21 Model Name: UNSAT2 Released: 1979
Authors: Neuman, S.P., R. A. Feddes, and E. Bresler.

UNSAT2 is a two-dimensional finite element model for horizontal, vertical, or axisymmetric simulation of transient flow in a variably saturated, nonuniform anisotropic porous medium. The governing equation is the Richard's equation expressed in terms of pressure head. Boundary conditions included are Dirichlet and Neumann, and seepage face. UNSAT2 is capable of simulating infiltration and evaporation as head-dependent conditions, determined after the fluid pressure is calculated. Evapotranspiration is simulated through user specified minimum allowed pressure head at the soil surface, maximum evaporation rate, and soil surface geometric data. User supplied input for simulation of evapotranspiration includes root zone geometric data, root effectiveness function, plant species wilting pressure, and maximum transpiration rate. The code can use both quadrilateral and triangular elements. Unsaturated hydraulic properties must be input in table form; internally, the code uses linear slopes between the data points for interpolation. UNSAT2 has a restart feature for simulating changing boundary conditions. The equation are solved with a band solver; nonlinearities are handled by a Picard iteration scheme.

Contact Address: S.P. Neuman, Dept. of Hydrology and Water Resources, University of Arizona, Tucson, AZ 85721

IGWMC Key: 120 Model Name: TRUST Released: 1984
Author: Narasimhan, T.N.

TRUST is an integrated finite difference simulator for computation of transient pressure head distributions in multidimensional, heterogeneous, variably saturated, deformable porous media with complex geometry. Deformation of the skeleton may be nonelastic. The polygon-based model considers pressure-dependent density variations. The code calculates internally hydraulic conductivity and fluid mass capacity from intrinsic permeability, fluid viscosity, fluid density, gravitational constants, void ratio, and compressibilities. The model allows for hysteresis. The governing equations are solved by an mixed explicit-implicit scheme, using a pointwise iterative solver. Optionally, a direct solver version is available form the author. This scheme recognized that regions with small time constants might be weakly coupled, resulting in a highly effective iterative solution algorithm. All boundaries of the flow domain are handled by a general head boundary algorithm. Thus, any boundary condition is developed by manipulating a conductance term that comprises the coefficient of the head differential between interior and exterior boundary node. In addition, TRUST can handle seepage faces. The recent versions of TRUST allow both harmonic and geometric means for the conductance term and includes an algorithm for automatically generating successive time step durations.

Modifications were made to the code to simulate flow in fractured unsaturated porous media. These modifications include additional characteristic curves and relative permeability curves, van Genuchten formulae for matrix blocks, gamma distribution formulae for discrete fracture grid blocks, hyperbolic characteristic curves of Pickens, and a new effective area factor. The new version of TRUST uses either the existing efficient iterative solver or a new direct solution.

Contact Address: Narasimhan, T.N., Dept. of Materials Sc. and Mineral Eng., University of California, Berkeley, CA 94720

IGWMC Key: 122 Model Name: FLUMP Released: 1981
Authors: Narasimhan, T.N., and S.P. Neuman

FLUMP is a finite element program for the computation of steady and nonsteady, two-dimensional areal or cross-sectional pressure-head distribution in heterogeneous, anisotropic, variably saturated porous media with complex geometry. FLUMP is especially suited for problems with moderate or high saturation. Some stability problems may be encountered while applying code to desiccated soils.

Contact Address: Narasimhan, T.N., Dept. of Materials Sc. and Mineral Eng., University of California, Berkeley, CA 94720

IGWMC Key: 1092 Model Name: FLO Released: 1985
Author: Vandenberg, A.

FLO simulates the elements of the hydrological cycle directly influenced by soil and surface drainage improvements. Total discharge from a drained plot includes surface runoff, and drain discharge is estimated. Detailed accounts of unsaturated flow is considered, including capillary forces and evapotranspiration.

Contact Address: Vandenberg, A., National Hydrology Research Institute, Inland Waters Directorate, Ottawa, K1A OE7 Ontario, Canada

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IGWMC Key: 1771 Model Name: MUST Released: --1985
Author: De Laat, P.J.M.

MUST (Model for Unsaturated flow above a Shallow water Table)is a finite difference model which simulates one-dimensional vertical, unsaturated groundwater flow, evapotranspiration, plant uptake, and interception of precipitation by plants.

Contact Address: De Laat, P.J.M, International Inst. for Hydraulic & Env. Eng., Oude Delft 95, Delft, The Netherlands

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IGWMC Key: 2071 Model Name: UNSAT1D Released: 1987
Authors: Gupta, S.K., C.S. Simmons, F.W. Bond, and C.R. Cole

UNSAT1D is a one-dimensional finite difference model for simulation of transient vertical unsaturated flow in a wide variety of geologic environments and boundary conditions. The program simulates infiltration, vertical seepage, and plant uptake by roots as function of the hydraulic properties of soil; soil layering; root growth characteristics; evapotranspiration rates; and frequency, rate, and amount of precipitation and/or irrigation.

Contact Address: Simmons, C.S., Battelle Pacific NW Laboratories, P.O. Box 999, Richland, WA 99352

IGWMC Key: 2062 Model Name: SOILMOP Released: 1982
Authors: Ross, D.L., and H.J. Morel-Seytoux

SOILMOP is an analytical model to predict ponding time, infiltration rate and amount, and water content profiles under variable rainfall conditions. The model solves a one-dimensional flow equation in a homogeneous soil. Air phase is also included.

Contact Address: Morel-Seytoux, H.J., Colorado St. Univ., Dept. of Civil Eng., Fort Collins, CO 80523

IGWMC Key: 2550 Model Name: SWACROP Released: 1983
Authors: Wesseling, J.G., P. Kabat, B.J. van den Broek, and R.A. Feddes

SWACROP (Soil WAter and CROP production model) is a transient one-dimensional finite difference model for simulation of the unsaturated zone, which incorporates water uptake by roots. The soil profile is divided into several layers (containing one or more compartments of variable thickness) having different physical properties. The partial differential equation for flow in the unsaturated system is solved using a implicit finite difference scheme. An explicit linearization of the hydraulic conductivity and soil water capacity is used. Knowing the initial conditions (i.e. water content or pressure head distribution profile) and top and bottom boundary conditions, the system of equations for all the compartments is solved for each (variable) timestep by applying the so-called Thomas tri-diagonal algorithm. The iteration procedure within each timestep allows calculation of all water balance terms for each time period selected.

For the top boundary condition data on rainfall, potential soil evaporation and potential transpiration are required. When the soil system remains unsaturated, one of three bottom boundary conditions can be used: pressure head, zero flux, or free drainage. When the lower part of the system remains saturated, one can either give the ground-water level or the flux through the bottom of the system as input. In the latter case the ground-water level is computed. The rate of vegetation growth, both potential and actual can be simulated in the crop growth submodel linked to the main water model in a complex dynamic way. However, both models can easily be run separately.

Contact Address: Winand Staring Centre, Dept. of Agrohydrology, Wageningen, The Netherlands

IGWMC Key: 2890 Model Name: SEEPV Released: 1980
Author: Davis, L.A.

SEEPV is a transient finite difference model to simulate vertical seepage from a tailings impoundment in variably saturated flow system; the program takes into consideration the interaction between an impoundment liner and the underlying aquifer.

Contact Address: Water, Waste and Land, Inc., 1311 S. College Ave., Fort Collins, CO 80524

IGWMC Key: 2983 Model Name: SOMOF Released: 1982
Author: Wesseling, J.W.

SOMOF is a finite difference model for the simulation of transient unsaturated soil moisture flow in a vertical profile. The model handles various processes, including infiltration from precipitation, capillary forces, evapotranspiration, gravity drainage, ponding, and plant uptake.

Contact Address: Wesseling, J.W., Delft Hydraulics Laboratory, P.O. Box 152, 8300 AD Emmeloord, The Netherlands

IGWMC Key: 3370 Model Name: FEMWATER/FECWATER Released: 1987
Authors: Yeh, G.T., and D.S. Ward

FEMWATER is a two-dimensional finite element model to simulate transient, cross-sectional flow in saturated-unsaturated anisotropic, heterogeneous porous media. The model is designed to treat both point sources/sinks and non-point sources/sinks, and to handle a wide variety of non-steady state boundary conditions, including a moving water-table and seepage faces. It allows three alternative approximations for the time derivative, has three options for estimating the non-linear matrix, and a direct and an iterative matrix solution option. Furthermore, the program includes automatic time-step adjustment and has an option to consider axisymmetric problems.

Contact Address: G.T. Yeh, Penn State University, Dept. of Civil Eng., 225 Sackett Bldg, University Park, PA 16802

IGWMC Key: 3377 Model Name: 3DFEMWATER Released: 1987
Author: Yeh, G.T.

3DFEMWATER is a three-dimensional finite element model for simulation of water steady state and transient flow through saturated-unsaturated media. The model is designed to handle anisotropic and heterogeneous geologic media, time-varying distributed and point sources and sinks, a wide variety of boundary conditions, including a moving water table and seepage faces. There are three options for estimating the nonlinear matrix, two options for solving the linearized matrix equation, and it includes automatic time step adjustment.

Contact Address G.T. Yeh, Penn State University, Dept. of Civil Eng., 225 Sackett Bldg, University Park, PA 16802

IGWMC Key: 3431 Model Name: UNSAT-1 Released: 1985
Author: Van Genuchten, M.Th.

UNSAT-1 is a Hermetian finite element solution to the Richards' equation for transient one-dimensional, variably saturated flow in layered soils. The model can handle both abrupt layering and smoothly changing profile properties.

Contact Address: Van Genuchten, M., USDA Salinity Laboratory, 4500 Glenwood Drive, Riverside, CA 92501, or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 3570 Model Name: INFIL Released: 1987
Author: Vauclin, M.

INFIL is a finite difference model which solves for ponded infiltration into a deep homogeneous soil. The model is based on the Philip series solution (1957) of a one-dimensional form of the Richards equation. Output includes water content profile and amount and rate of infiltration at different simulation times. The program, which requires the soil properties to be expressed in mathematical form, is designed to accommodate three different sets of these functions. They include the four parameter function of Vauclin (1979), the three parameter functions of Brutseart (1966 and 1967), and the two parameter function of Brooks and Corey (1964). A modified version by A.I. El-Kadi also includes a van Genuchten function (1978).

Contact address: M. Vauclin, Institute de Mecanique de Grenoble, BP 68, 38402 St. Martin D'Heres - Cedex France, or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 3660 Model Name: GRWATER Released: 1981
Authors: Kashkuli, H.A.

GRWATER is a finite difference model to predict the decline of ground water mounds developed under recharge in an isotropic, heterogeneous water table aquifer. The model has two modules, one for transient one-dimensional unsaturated flow above the water table which handles infiltration and evapotranspiration, and one for transient two-dimensional horizontal saturated flow in the aquifer.

Contact Address: D.K. Sunada, Dept. of Civil Eng., Colorado State University, Fort Collins, CO 80523

IGWMC Key: 4340 Model Name: UNSAT-H Released: 1985
Authors: Fayer, M.J., and G.W. Gee

UNSAT-H is a one-dimensional finite difference model for simulation of vertical unsaturated soil moisture flow. It simulates infiltration, drainage, redistribution, surface evaporation and plant water uptake from soil. The model's numerical technique is specially designed for arid zones characterized by very dry soils similar to the Hanford site (Washington).

Contact Address: Fayer, M.J., Battelle Pacific Northwest Lab., P.O. Box 999, Richland, WA 99352

IGWMC Key: 4380 Model Name: INFGR Released: 1985
Authors: Craig, P.M., and E.C. Davis

INFGR is one-dimensional model to estimate the infiltration rate using the Green and Ampt equation. The compression method is used to estimate infiltration during low rainfall periods. The model works well for determining infiltration but performs poorly in determining soil moisture content.

Contact Address: Davis, E.C., Oak Ridge National Lab., Environm. Sciences Div., Oak Ridge, Tennessee 37830

IGWMC Key: 4390 Model Name: FLOWVEC Released: 1983
Authors: Li, R-M., K.G. Eggert, and K.Zachmann

FLOWVEC utilizes a vector processor for solving three-dimensional, variably saturated flow problems. The model employs a finite difference technique in the formulation of the governing equations and a block implicit scheme in the solution.

Contact Address: R.-M. Li, Simons, Li and Associates, Inc., P.O. Box 1816, Fort Collins, CO 80522

IGWMC Key: 4400 Model Name: LANDFIL Released: 1984
Author: Korfiatis, G.P.

LANDFIL simulates the movement of moisture through the unsaturated zone using a finite difference solution for the one-dimensional flow equation. Conditions simulated are pertinent to landfills. Precipitation, evapotranspiration and redistribution are considered. Both lined and unlined landfills may be simulated.

Contact Address: G.P. Korfiatis, Stevens Inst. of Technology, Dept. of Civil Eng., Hoboken, NJ 07030

IGWMC Key: 4410 Model Name: HSSWDS Released: 1982
Authors: Perrier, E.R., and A.C. Gibson

HSSWDS is a one-dimensional, deterministic, water budget model to estimate the amount of moisture percolation through different types of landfill. The model was adopted from CREAMS, the U.S. Department of Agriculture hydrologic model. It includes recharge from precipitation including snowmelt, surface runoff and evapotranspiration.

Contact Address: Water Resources Eng. Group, Env. Lab., U.S. Army Engineer Waterways Experiment Station, Vicksburg, Mississippi 39185, or Municipal Env. Res. Lab., Solid and Hazardous Waste Res. Div., U.S. Env. Prot. Ag., Cincinnati, OH 45268

IGWMC Key: 4980 Model Name: PC-SEEP Released: 1992
Authors: Krahn, J., D.G. Fredlund, L. Lam, and S.L. Barbour

PC-SEEP is an interactive finite element program for simulating steady-state and transient groundwater flow in both the saturated and unsaturated zones. It can simulate surface infiltration and evapotranspiration and handle internal drains. PC-SEEP is designed to analyze seepage through earth dams, watertable location and fluctuations, and mounding of the watertable underneath a leaking waste pond. The model computes nodal pore-water pressures, hydraulic heads, velocities, flow directions and flow gradients. It includes postprocessors for finite element mesh plots, head contours and velocity vector plots. PC-SEEP provides options to use either an in-core or an out-of-core iterative solver for the nonlinear flow equations.

Contact Address: J. Krahn, Geo-Slope Programming Ltd., 7927 Silver Springs Road NW, Calgary, Alberta, Canada T3B 4K4

IGWMC Key: 5010 Model Name: SIMGRO Released: 1987
Author: Querner, E.P.

SIMGRO (SIMulation of GROundwater flow and surface water levels) simulates flow in the saturated zone, the unsaturated zone, and a surface water system. The saturated zone model consists of a quasi-threedimensional finite element model with an implicit calculation scheme. The unsaturated zone is modeled by means of two reservoirs, one for the root zone and one for the subsoil. The root zone is treated using a water balance model and includes storage and resulting change in phreatic level, capillary rise, percolation and evapotranspiration. The surface water system, representing a network of small channels, is considered as a single reservoir with criteria for water supply, discharge, water level control, and extraction for sprinkling.

Contact Address: E.P. Querner, Inst. for Land and Water Management Research (ICW), P.O. Box 35, 6700 AA Wageningen, The Netherlands

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IGWMC Key: 5057 Model Name: VADOSE Released: --
Authors: --

VADOSE is a 3-dimensional analytical model for flow into an unsaturated anisotropic or isotropic porous medium. It can predict the spread of a toxic solution seeping into the ground, or a lixiviant flowing in a heap leach. The saturation and/or the flow velocity can be calculated as a function of space and time for the leak configuration specified by the user. The leak configuration handled by the model can be a combination of point sources or rectangular sites (ponds, land treatment sites, sewage lagoons, or similar sites). The effect of each leak/flow is calculated and the final solution is obtained by superposition. Impermeable boundaries, vertical or horizontal, can be included. The model computes saturation, suction tension (capillary pressure), and velocities.

Contact Address: In Situ, Inc., P.O. Box 1, Laramie, WY 82070

IGWMC Key: 6400 Model Name: UNSAT Released: 1985
Authors: Khaleel, R., and T-C.J. Yeh

UNSAT is a Galerkin finite element model for solving the one-dimensional, transient flow equation in unsaturated porous media. It estimates the rate of infiltration into soil as well as the moisture distribution following infiltration. Both differential and cumulative mass balance errors are given to illustrate accuracy of the numerical scheme.

Contact Address: Khaleel, R., New Mexico Inst. of Mining and Technology, Dept. of Geoscience, Socorro, NM 87901

IGWMC Key: 6630 Model Name: WATERFLO Released: 1985
Author: Nofziger, D.L.

The WATERFLO model is based on a finite difference solution of the one-dimensional nonlinear Richards equation for simulation of water movement through homogeneous soils. The interactive microcomputer program can accommodate finite and semi-finite soil systems. It provides for the following boundary conditions at the soil surface: constant potential, constant flux density, rainfall or sprinkler infiltration rate, and mixed type (flux and potential boundary condition).

Contact Address: IFAS - Software Support, Univ. of Florida, Building 664, Room 203, Gainesville, FL 32611

Note: See also Appendix C.3; most solute transport models include a flow simulation module.

Appendix B.1: Variably Saturated Flow; Numerical Models, Part 2: Usability and Reliability

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
21	UNSAT2	N	N	Y	Y	N	L	Y	U	Y	Y	M
120	TRUST	Y	Y	Y	Y	N	L	Y	U	Y	Y	M
122	FLUMP	N	N	Y	Y	N	U	Y	U	Y	U	U
1092	FLO	N	N	Y	Y	N	U	Y	U	Y	U	U
1771	MUST	U	U	Y	Y	N	L	Y	U	Y	U	U
2071	UNSAT1D	Y	Y	Y	Y	Y	Y	Y	U	Y	U	M
2062	SOILMOP	N	N	Y	Y	N	N	Y	U	Y	N	U
2550	SWACROP	Y	Y	Y	Y	Y	Y	Y	U	Y	U	U
2890	SEEPV	U	U	Y	Y	U	U	Y	U	U	U	U
2983	SOMOF	U	U	Y	Y	U	U	U	U	U	U	U
3370	FEMWATER/ FECWATER	N	N	Y	Y	N	L	Y	U	Y	Y	M
3377	3DFEMWATER	N	N	Y	Y	N	L	Y	U	Y	U	U
3431	UNSAT-1	N	N	Y	Y	N	N	Y	U	Y	Y	M
3570	INFIL	Y	Y	Y	Y	Y	L	Y	U	Y	N	U
3660	GRWATER	N	N	Y	Y	U	U	Y	U	Y	U	U
4340	UNSAT-H	U	U	Y	Y	U	U	Y	U	Y	U	U
4380	INFGR	U	U	Y	Y	U	L	Y	U	Y	U	U
4390	FLOWVEC	U	U	Y	Y	U	U	Y	U	Y	U	U
4400	LANDFIL	U	U	Y	Y	U	U	Y	U	U	U	U
4410	HSSWDS	U	U	Y	Y	N	N	Y	U	U	U	U
4980	PC-SEEP	Y	Y	Y	Y	Y	Y	Y	U	U	U	U

KEY: Y = YES N = NO L = LIMITED M = MANY F = FEW U = UNKNOWN

Appendix B.1, part 2 (continued)

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
5010	SIMGRO	U	U	Y	Y	U	U	U	U	U	U	U
5057	VADOSE	U	U	Y	Y	U	U	U	U	U	U	U
6400	UNSAT	U	U	Y	Y	N	N	Y	U	Y	U	U
6630	WATERFLO	Y	Y	Y	Y	Y	L	Y	U	Y	Y	M

KEY: Y = YES N = NO L = LIMITED M = MANY F = FEW U = UNKNOWN

Appendix B.2: Variably Saturated Flow; Parameter Estimation Models, Part 1: Model Description

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IGWMC Key: 3433 Model Name: ONESTEP Released: 1985
Authors: Kool, J.B., J.C. Parker, and M.Th. Van Genuchten.

ONESTEP is a nonlinear parameter estimation model for evaluating soil hydraulic properties from one-step outflow experiments in the one-dimensional flow. The program estimates parameters in the van Genuchten soil hydraulic property model from measurements of cumulative outflow with time during one-step experiments. The program combines non-linear optimization with a Galerkin finite element model.

Contact Address: J.C. Parker, Virginia Polytechnical Inst., Dept. Soil & Environmental Science, Blacksburg, VA 24061, or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 5183 Model Name: SOILPROP Released: 1988
Authors: Mishra, S., J.C. Parker, and N. Singhal

SOILPROP is an interactive program to estimate soil hydraulic properties and their uncertainty from particle size distribution data. Properties estimated by the program are the saturated hydraulic conductivity and parameters in the van Genuchten and Brooks-Corey models which describe the relationship between soil water content, capillary pressure and relative permeability. SOILPROP is based on the premise that the soil-water retention function reflects a pore size distribution which in turn can be inferred from the grain size distribution. The Arya-Paris procedure is used to compute theoretical water content versus capillary pressure curve, which is then fitted to the two models. Covariances are estimated using a first-order error analysis procedure. The saturated hydraulic conductivity in SOILPROP is estimated from the user-specified porosity and grain-size distribution data using a Kozeny-Carmen type equation.

Contact Address: Environm. Systems & Technol., Inc., P.O. Box 10547, Blacksburg, VA 24062-0457

IGWMC Key: 5187 Model Name: FLOFIT Released: 1988
Authors: Kool, J.B., S. Mishra, and J.C. Parker

FLOFIT is a program to estimate unsaturated soil hydraulic properties and/or transport parameters from 1-dimensional vertical flow/transport experiments. Three modes of operation are possible: 1) flow properties may be estimated from transient flow data; 2) solute dispersion and linear adsorption parameters may be estimated from steady flow transport data; or 3) flow and transport parameters may be estimated simultaneously from transient unsaturated flow and tracer experiments. Hydraulic properties are described by a hysteric van Genuchten model and dispersion by a scale-dependent function. Hydraulic and/or transport parameters may differ between layers. Numerical inversion of governing equations is performed using an efficient Levensberg-Marquardt algorithm.

Contact Address: Environm. Systems & Technol., Inc., P.O. Box 10457, Blacksburg, VA 24062-0457

IGWMC Key: 6170 Model Name: FP Released: 1985
Authors: Su, C., and R.H. Brooks

FP is a program to determine the parameters of the retention function (the soil-water characteristic function) from experimental data. Based upon the Pearson Type VIII distribution function, a general retention function which relates the saturation to the capillary pressure in distributed soils has been formulated. This simple, yet complete function has been shown to describe the imbibition as well as the drainage branch of the retention curve. It is defined by four readily assessed parameters that either have physical significance themselves or may be used to determine some hydraulic properties of the soil. Please see "Remarks" for more information.

With the assumption that the Burdine integrals are adequate, a relative permeability function has been derived through the substitution of the retention function for the integrands in the Burdine Integrals. The permeability function is expressed in terms of the incomplete Beta function ration whose value may be conveniently found in some mathematical tables.

A general pore-sized distribution function of soils has been obtained from the retention function. The derivation of the pore-size distribution function enables more rigorous examination and further exploration of the theories concerning water movement in partially saturated soils. In this respect, an explanation of the phenomenon of air entrapment during imbibition has been offered through an energy concept based upon the pore-size distribution function along with the retention function. Two criteria of affinity have been established for porous media. Media are said to be affine if their corresponding pore-size distribution parameters are identical. The scaling factor for the external dimension of the model has been chosen to be the capillary pressure head at the inflection point of the retention curve, whose value is always finite. The analysis of the effect of the pore-size distribution parameters upon the retention, permeability, and diffusivity curves shows that the parameter governing the downward concavity of the retention curve is as important as that governing the upward concavity when it comes to computing the permeability values from the retention data.

Contact Address: Dept. of Agricultural Eng., Oregon State University, Corvallis, OR 97331, or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 6226 Model Name: SOHYP Released: 1986
Author: Van Genuchten, M. Th.

SOHYP is an analytical model for calculation of the unsaturated hydraulic conductivity function using soil moisture retention data. The basis of SOHYP is a relatively simple equation for soil moisture content-pressure head curve. The particular form of the equation enables one to derive closed-form analytical expressions for the relative hydraulic conductivity, when substituted in the predictive conductivity models of Burdine or Mualem. The resulting expressions for the hydraulic conductivity as function of the pressure head contain three independent parameters which may be obtained by fitting the described soil moisture retention model to experimental soil moisture retention data. The solution is based on automatic curve-fitting using a nonlinear least squares method.

Contact Address: USDA Salinity Laboratory, 4500 Glenwood Drive, Riverside, CA 92501, or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 6228 Model Name: RETC Released: 1991
Authors: Van Genuchten, M.Th., F.J. Leij, and S.R. Yates

RETC (Retention Curve Computer Code) uses theoretical methods to predict the soil water retention curve and the hydraulic conductivity curve from measured soil water retention data. It uses several analytical models to estimate water retention, unsaturated hydraulic conductivity or soil water diffusivity for a given soil. It includes the parametric equations of Brooks-Corey and van Genuchten, which are used in conjunction with the theoretical pore-size distribution models of Mualem and Burdine to predict unsaturated hydraulic conductivity from observed soil water retention data. RTC can be used in a forward mode and in a parameter fitting mode. In the forward mode it estimates the soil-water retention curve and hydraulic conductivity; in the parameter fitting mode it determines the analytical model parameters.

Contact Address: U.S. Dept. of Agriculture, U.S. Salinity Lab., Agric. Res. Service, 4500 Glenwood Drive, Riverside, Calif. 92501; Center for Subsurface Modeling Support (CSMOS), R.S. Kerr Environmental Research Laboratory, U.S. Environmental Protection Agency, P.O. Box 1198, Ada, OK 74820; or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 6330 Model Name: SOIL Released: 1987
Author: El-Kadi, A.I.

Using non-linear least-squares analysis, SOIL estimates soil-hydraulic properties. The code requires as input pairs of measured water content and suction. The model includes the methods of Brooks and Corey (1964) and Vauclin (1979) to estimate soil water characteristic function and the unsaturated hydraulic conductivity.

Contact Address: Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401

Appendix B.2: Variably Saturated Flow; Parameter Estimation Models, Part 2: Usability and Reliability

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
3433	ONESTEP	N	N	Y	Y	N	L	Y	U	Y	Y	U
5183	SOILPROP	Y	Y	Y	Y	Y	Y	Y	U	Y	Y	M
5187	FLOFIT	Y	Y	Y	Y	Y	Y	Y	U	Y	Y	M
6170	FP	N	N	Y	Y	N	U	Y	U	U	Y	U
6226	SOHYP	N	N	Y	Y	N	N	Y	U	Y	Y	F
6228	RETC	Y	Y	Y	Y	Y	L	Y	U	Y	Y	M
6330	SOIL	Y	Y	Y	Y	Y	L	Y	U	Y	Y	F

KEY: Y = YES N = NO L = LIMITED M = MANY F = FEW U = UNKNOWN

Appendix C.1: Solute Transport; Analytical Models For Saturated Zone, Part 1: Model Description

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IGWMC Key: 2037 Model Name: FRACSOL Released: 1981
Authors: G.E. Grisak and J.F. Pickens

FRACSOL is an analytical model for simulation of non-reactive advective-dispersive solute transport in planar fractures with diffusion into adjacent matrix blocks. The solution solves for the transient concentration distribution along the fracture as well as into the matrix.

Contact address: J.F. Pickens, Intera Technologies, Inc., 6850 Austin Center Blvd., #300, Austin, TX 78731

IGWMC Key: 2080 Model Name: GETOUT Released: 1983
Authors: H.C. Burkholder, M.O. Cloninger, W.V. Demier, G. Jansen

GETOUT is a one-dimensional analytical model of advective-dispersive radionuclide transport in ground-water subject to linear equilibrium sorption. The model handles radioactive decay for straight chains with a maximum of three nuclides in one chain.

Contact address: National Energy Software Center (NESC), Argonne National Laboratory, 9700 South Cass Avenue, Argonne, IL 60439

IGWMC Key: 2810 Model Name: WASTE Released: 1981
Authors: B. Ross and C.M. Koplik

WASTE is an analytical solution to compute one- or two-dimensional horizontal, or one-dimensional vertical, steady or unsteady transport of radionuclides in confined or semi-confined, anisotropic, heterogeneous, multi-aquifer systems. The model includes advection, dispersion, diffusion, linear adsorption, equilibrium ion exchange and first-order radioactive decay. It is part of the NUTRAN package for calculation of doses to humans from radionuclides carried out of deep geologic waste repositories by ground-water.

Contact address: Analytic Sciences Corporation, Energy & Environment Division, One Jacob Way, Reading, MA 01867

IGWMC Key: 3380 Model Name: GRDFLX Released: 1982
Authors: R.B. Codell, K.T. Key, and G. Whelan

The program GRDFLX consists of two analytical models: (1) GRND calculates the vertically averaged concentration at points in a uniform aquifer of finite thickness with constant physical transport properties; and (2) FLUX calculates the flux of radioactive liquid effluent passing a plane perpendicular to the ground-water flow direction. Both models assume a horizontal, limited area source. Radioactive decay is treated separately from the transport computations to facilitate analysis of releases of long decay chains. The models are based on Simpson's rule of integration. They include linear equilibrium adsorption (retardation) and three-dimensional dispersion.

Contact address: R.B. Codell, U.S. Nuclear Regulatory Commission, Div. of Eng., Off. of Nuclear Reactor Regulation, Washington, DC 20555.

IGWMC Key: 3432 Model Name: CXTFIT Released: 1984
Authors: J.C. Parker and M.Th. van Genuchten

The purpose of CXTFIT is to determine values for one-dimensional analytical solute transport parameters using a nonlinear least-squares inversion method. The analytical model includes advection, dispersion, diffusion, linear equilibrium sorption, first-order decay and zero-order production.

Contact address: J.C. Parker, Virginia Polytechn. Inst., Soil & Env. Sc. Dept., Blacksburg, VA 24061, or International Ground Water Modeling Center, Colorado School of Mines, Golden, CO 80401.

IGWMC Key: 4082 Model Name: LAYFLO Released: 1983
Authors: A.B. Gureghian and G. Jansen

LAYFLO is a one-dimensional, semi-analytical model for simulation of the migration of a three-member radionuclide decay chain in a multi-layered geologic porous medium. The advective-dispersive transport equation is solved using Laplace transformation. The model allows for two types of boundary conditions, i.e. a continuous source as well as a band release mode, respectively. The solution of the non-dispersive form of the mass transport equation can handle any number of layers, whereas for the general case the number of layers is restricted to six. A graphics program using the DISPLA package is provided with LAYFLO.

Contact address: Performance Assessment Dept., Off. of Nuclear Waste Isolation, Battelle Project Management Division, 505 King Avenue, Columbus, OH 43201

IGWMC Key: 4620 Model Name: MASCOT Released: 1986
Author: A.B. Gureghian

MASCOT is a program providing analytical solutions for multi-dimensional transport of a four-member radionuclide decay chain in an isotropic, homogeneous, confined ground-water system and includes linear equilibrium sorption. It computes the two- and three-dimensional space-time dependent convective-dispersive transport assuming steady-state, uniform ground-water flow. The model can handle a single or multiple finite line source or a Gaussian distributed source in the 2D case, and a single or multiple patch source or bivariate-normal distributed source in the 3D case.

Contact address: Battelle/OWTD, 7000 South Adams Str., Willowbrook, IL 60521

IGWMC Key: 4740 Model Name: SURMF Released: 1985
Authors: P.L. Chambre, T.H. Pigford, W.W-L. Lee, J. Ahn, et al.

SURMF is a series of analytical solutions for the dissolution and hydrogeologic near-field transport of radionuclides from geologic repositories of nuclear waste. The models calculate the total surface mass flux using the mass transfer theory from chemical engineering. The package includes models for advective-

(continued.....)

SURMF -- continued

dispersive radionuclide transport from various geometric waste forms through a backfill; transport through a backfill using a non-linear sorption isotherm; transport through a backfill, where the solubility, diffusivity and retardation coefficients are temperature dependent; a coupled near-field, far-field analysis where dissolution rates and migration are temperature dependent; 3D transport from a point source; and a general solution for the transport of radioactive chains.

Contact address: T.H. Pigford, Dept. of Nuclear Eng., Univ. of Calif., Berkeley, CA 94720

IGWMC Key: 4911 Model Name: OASIS Released: 1989
Authors: C.J. Newell, J.F. Haasbeek, L.P. Hopkins, S.E. Alder-Schaller, et al.

OASIS is a graphical decision support system for ground-water contamination modeling developed for the Macintosh II or SE personal computer using Hypercard software. OASIS is a collection of computer tools including extensive computerized documentation, two chemical databases, a hydrogeologic database derived from a survey of 400 sites across the US and DRASTIC aquifer vulnerability index system, a numerical 2-dimensional solute transport and biodegradation model --BIOPLUME II--, and an analytical solute transport model --ODAST. It includes extensive graphical pre- and postprocessing for BIOPLUME II. OASIS provides graphical and analytical support to decision makers and technical support personnel.

Contact address: P.B. Bedient, Rice Univ., Dept. of Env. Sc. and Eng., Houston, TX 77251

IGWMC Key: 5024 Model Name: PATHRAE Released: 1986
Authors: R.A. Fjeld, A.W. Elzerman, T.J. Overcamp, N. Giannopoulos et al.

PATHRAE is a computer code for assessing human health risk associated with low level radioactive waste disposal at municipal dumps and sanitary landfills. The code contains algorithms for analyzing ten different pathways including the subsurface transport of contaminants to a stream and migration to a well. The risk assessment procedure consists of: (1) specification of the source term, (2) analysis of environmental transport, and (3) estimation of the risk of health effects. Contaminant transport in the unsaturated zone is approximated by assuming plug flow resulting in a retarded contaminant entry in the saturated zone. Transport in the saturated zone is modeled as an analytical solution to the advective-dispersive transport equation including radioactive decay.

Contact address: R.Fjeld, Dept. of Env. Syst. Eng., Clemson Univ., Clemson, SC 29634-0919

IGWMC Key: 5055 Model Name: PLUME Released: --
Authors: --

PLUME is a two-dimensional analytical contaminant transport model. The dispersion of a contaminant in an aquifer is calculated as a function of time, distance, and direction of the contaminant source. Plumes from up to 50 rectangular sources can be modeled. Three types of contaminant sources can be considered: (1) an instantaneous source, (2) a source with a constant rate of contamination, and (3) a source with an exponentially declining rate of contamination. The concentration profile is given at a line of interest or at a fixed point as a function of time. The model includes the effects of regional ground-water flow, dispersion, linear adsorption, and radioactive decay, and conversion by first-order rate law. The output includes site layout and concentration contours.

Contact address: In Situ Inc., P.O. Box 1, Laramie, WY 82070

IGWMC Key: 5174 Model Name: FRACQUAL Released: --
Authors: --

FRACQUAL is a program that simulates the movement of a solute through a planar fracture in a fractured rock aquifer, including molecular diffusion into the non-fractured rock. In the program, the effects of advection, adsorption, decay, and diffusion into the rock matrix are simulated. The program uses the analytical equation of Tang, Frind, and Sudicky. Time-varying sources of contamination may be simulated using superposition.

Contact address: Koch and Assoc., 2921 Greenway Dr., Ellicot City, MD 21043

IGWMC Key: 5175 Model Name: POLLUT Released: --
Authors: --

POLLUT is an analytical model for two-dimensional simulation of a contaminant plume using the Wilson and Miller equation of 1978. The program computes the concentration at any point in space due to the continuous release of a solute at a point in an aquifer. The program includes the effects of advection (one dimension), dispersion (two dimensions), decay and linear adsorption. Up to 100 different continuous sources may be simulated using superposition for time-varying sources.

Contact address: Koch and Assoc., 2921 Greenway Dr., Ellicot City, MD 21043

IGWMC Key: 5210 Model Name: PULSE Released: --
Author: L.S. Slotta

PULSE is a one-dimensional analytical model for solute transport in confined or unconfined aquifers, calculating concentration distribution in space and time. It simulates the fate of a contaminant initially present as a distributed rectangular pulse. The model assumes no contaminant sources or sinks present. Longitudinal dispersion, adsorption and first-order loss (decay) is included. The model presents tabular output of contaminant concentration values at various distances from origin of pulse and for various times.

Contact address: Slotta Engineering Assoc., Inc., P.O. Box 1376, Corvallis, OR 97339

IGWMC Key: 5211 Model Name: CXPMPM Released: --
Author: L.S. Slotta

CXPMPM is an analytical model for simulation of solute transport in confined or unconfined homogeneous, isotropic aquifers. It calculates concentration distributions in space and time due to one-dimensional advection, longitudinal dispersion, linear adsorption, and first-order loss (decay) for up to 250 areal contaminant sources. The inlet boundary is a time-dependent concentration flux (constant, exponentially decreasing, skewed or bell shaped distributions). The model provides tabular and graphical output of results.

Contact address: Slotta Engineering Assoc., Inc., P.O. Box 1376, Corvallis, OR 97339

IGWMC Key: 5212 Model Name: TDPLUME/TWODPLME Released: --
Author: L.S. Slotta

TDPLUME/TWODPLME are two-dimensional analytical solute transport models for confined or unconfined aquifers, the contaminant being convected and dispersing in X (flow direction) and Y (orthogonal to the flow direction in a horizontal plane) directions. Two scenarios can be considered: initial distribution of contaminant as a number of up to 250 rectangles with specified concentration, or a number of constantly emitting chemical sources (line sources: TDPLUME, or large rectangular sources: TWODPLME). The models are based on one-dimensional stationary ground-water flow, and include lateral and transverse dispersion, linear adsorption, and first-order loss (decay). Calculation of concentration distribution in time and space.

Contact address: Slotta Engineering Assoc., Inc., P.O. Box 1376, Corvallis, OR 97339

IGWMC Key: 5242 Model Name: BLOB3D Released: --
Authors: --

BLOB3D is an analytical model simulating 3-dimensional transient solute transport from a parallelopiped source in a finite thickness medium. It assumes known constant, uniform ground-water velocity field. It computes the concentration of the solute at any point in time and for any distance from the source. It can handle source or solute decay and solute retardation.

Contact address: R.G. McLaren, Waterloo Centre for Groundwater Res., Univ. of Waterloo, Waterloo, Ontario, Canada N2L 3G1

IGWMC Key: 5243 Model Name: CRAFLUSH Released: --
Authors: --

CRAFLUSH is an analytical model for simulating 2-dimensional, transient solute transport in a series of parallel fractures. It can handle longitudinal dispersion and diffusion of solute into the rock matrix. It computes concentration of the solute at any time and distance from source.

Contact address: R.G. McLaren, Waterloo Centre for Groundwater Res., Univ. of Waterloo, Waterloo, Ontario, Canada N2L 3G1

IGWMC Key: 5245 Model Name: HPATCH3D Released: --
Authors: --

HPATCH3D is an analytical model for 3-dimensional, transient advective-dispersive solute transport from a horizontal patch source which can be located at any depth in an aquifer with finite thickness. The model assumes constant, uniform ground-water velocities. It computes the concentration of the solute at any time and distance from the source and handles both source and solute decay and solute retardation.

Contact address: R.G. McLaren, Waterloo Centre for Groundwater Res., Univ. of Waterloo, Waterloo, Ontario, Canada N2L 3G1

IGWMC Key: 5246 Model Name: LINE2D Released: --
Authors: --

LINE2D is an analytical model for simulating 2-dimensional, transient advective-dispersive solute transport with a vertical line source at x=0 in a finite thickness aquifer. The model assumes constant, uniform groundwater velocities. It computes the concentration of a solute at any time and distance from the source. It can handle both source and solute decay and solute retardation.

Contact address: R.G. McLaren, Waterloo Centre for Groundwater Res., Univ. of Waterloo, Waterloo, Ontario, Canada, N2L 3G1

IGWMC Key: 5247 Model Name: PATCH3D Released: --
Authors: --

PATCH3D is an analytical model for 3-dimensional, transient advective-dispersive solute transport from a vertical patch source at x=0 in a finite thickness aquifer. The model assumes constant, uniform groundwater velocities. It computes the concentration of the solute at any time and distance from the source. It can handle both source or solute decay and solute retardation.

Contact address: R.G. McLaren, Waterloo Centre for Groundwater Res., Univ. of Waterloo, Waterloo, Ontario, Canada N2L 3G1

IGWMC Key: 5248 Model Name: SUPER1D Released: --
Authors: --

SUPER1D is an analytical model for simulating one-dimensional, transient advective-dispersive solute transport based on the Ogata-Banks solution with superposition. It computes the concentration and flux of a solute at any time and distance from the source. The source strength may vary with time. The model can handle solute retardation.

Contact address: R.G. McLaren, Waterloo Centre for Groundwater Res., Univ. of Waterloo, Waterloo, Ontario, Canada N2L 3G1

IGWMC Key: 5310 Model Name: PRZMAL Released: --
Authors: J. Wagner and C. Ruiz-Calzada

PRZMAL is an aquifer linkage model for US EPA's Pesticide Root Zone Model (PRZM). It connects PRZM with the analytical three-dimensional advective-dispersive transport model PLUME 3D developed at Oklahoma State University. This linkage allows the user to predict non-conservative contaminant movement from the point of application, in a continuous manner, into and within the aquifer.

Contact address: J. Wagner, Oklahoma State Univ., School of Chem. Eng., Stillwater, OK 74074

IGWMC Key: 6011 Model Name: RWH Released: 1992
Author: P.K.M. van der Heijde

RWH simulates solute transport in homogeneous isotropic, confined aquifers. It accounts for regional groundwater flow and the superposed effects of production and injection wells. The effects of wells is based on the Theis equation. The transport equation is solved via the particle-in-a-cell technique for convection and the random walk technique for dispersion. Options for retardation and first-order decay are included. The program utilizes screen graphics as the primary output device. It can be used for both educational purposes and initial definition of more complex problems.

Contact address: Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401

IGWMC Key: 6020 Model Name: PLUME Released: 1991
Author: P.K.M. van der Heijde

PLUME is an analytical model to calculate two-dimensional vertically averaged or three-dimensional concentration distribution in a homogeneous aquifer with a continuous solute injection in a one-dimensional regional flow field. It includes the simulation of dispersion, retardation, and radioactive decay. The source is either a line source at a specified depth in the three-dimensional version or a vertically averaged area source of specified width in the two-dimensional version. The source strength may vary in time. The program uses Simpson's rule of integration and includes a subroutine to calculate concentration values on a user-defined grid base.

Contact address: Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401

IGWMC Key: 6024 Model Name: PLUME2D Released: 1986
Author: P.K.M. van der Heijde

PLUME2D provides an analytical solution to calculate concentration distribution in a homogeneous, nonleaky confined aquifer with uniform regional flow. The model uses the well-function for convection and dispersion of a solute in a system with continuous injecting, fully penetrating wells. The program based on the corrected Wilson and Miller solution (1978), has an option for retardation and first-order decay.

Contact address: Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401

IGWMC Key: 6100 Model Name: GROUND Released: 1982
Authors: R.B. Codell, K.T. Key and G. Whelan

GROUND is an analytical model for calculation of the flux into a river and the concentration at points downgradient of a source with a single radioactive contaminant released from a vertical plane. The model is developed for the limiting case of unidirectional advective transport with three-dimensional dispersion in an isotropic aquifer. Furthermore, the model includes first-order decay and linear equilibrium adsorption as represented by the retardation coefficient. The point concentration model uses Simpson's rule quadrature of an arbitrary pulse release into a confined aquifer.

Contact address: R.B. Codell, U.S. Nuclear Regulatory Commission, Div. of Eng., Off. of Nuclear Reactor Regulation, Washington, DC 20555.

IGWMC Key: 6120 Model Name: AT123D Released: 1987
Author: G.T. Yeh

AT123D is a generalized analytical transient, one- two-, and/or three-dimensional computer code developed for estimating the transport of chemicals in a homogeneous aquifer system with uniform flow. The model handles various source configurations and release characteristics. The transport mechanisms include advection, hydrodynamic dispersion, linear adsorption, first-order decay/degeneration, and chemical losses to the atmosphere.

Contact address: G.T. Yeh, Dept. Civil Eng., Penn. State Univ., University Park, PA 16802, or Internat. Ground Water Modeling Center, Colorado School of Mines, Golden, CO 80401.

IGWMC Key: 6220 Model Name: ONE-D Released: 1982
Authors: M.Th. van Genuchten and W.J. Alves

ONE-D is a package of five analytical solutions to the one-dimensional convective-dispersive solute transport equation with linear equilibrium adsorption, zero-order production, and first-order decay in a semi-infinite homogeneous aquifer with a uniform flow field. The five solutions are based on different governing equations and boundary conditions.

Contact address: M.Th. van Genuchten, U.S. Salinity Lab., U.S. Dept. of Agriculture, 4500 Glenwood Drive, Riverside, CA 92501, or International Ground Water Modeling Center, Colorado School of Mines, Golden, CO 80401.

IGWMC Key: 6227 Model Name: CFITIM Released: 1981
Author: M.Th. van Genuchten

CFITIM is a program for the estimation of the parameters for one-dimensional non-equilibrium convective-dispersive solute transport in saturated porous media from miscible displacement experiments using least squares analysis.

Contact address: M.Th. van Genuchten, U.S. Salinity Lab., U.S. Dept. of Agriculture, 4500 Glenwood Drive, Riverside, CA 92501, or International Ground Water Modeling Center, Colorado School of Mines, Golden, CO 80401.

IGWMC Key: 6250 Model Name: WELL Released: 1982
Author: L.W. Gelhar

WELL is a program to determine the tracer concentration evolving in a pumping-recharge well system when an instantaneous pulse of conservative tracer is introduced in the recharge well. The program is based on the numerical approximation of a closed-form solution of the governing convective-dispersive equation for transport in a homogeneous aquifer.

Contact address: L.W. Gelhar, Dept. of Civil Eng., Mass. Inst. of Techn., Cambridge, MA 012139, or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 6310 Model Name: LTIRD Released: 1985
Authors: I. Javandel, C. Doughty and C.F. Tsang

LTIRD simulates advective-dispersive transport in a radial flow field, calculating the dimensionless concentration of a particular solute, injected into an aquifer, as a function of dimensionless time for different values of dimensionless radius. It assumes a fully penetrating injection well with constant injection rate and concentration at source, a homogeneous and isotropic aquifer of uniform thickness, and zero background concentration. The evaluation of the analytical solution is based on numerical inversion of the Laplace transform.

Contact address: I. Javandel, Lawrence Berkeley Lab., Earth Sc. Div., Berkeley, CA 94720, or Internat. Ground Water Modeling Center, Colorado School of Mines, Golden, CO 80401.

IGWMC Key: 6311 Model Name: TDAST Released: 1985
Authors: I. Javandel, C. Doughty and C.F. Tsang.

TDAST evaluates an analytical solution to the two-dimensional convective-dispersive solute transport equation. The model includes decay (both at the source and in the aquifer), and linear equilibrium adsorption. It calculates C/CO at any point downstream from a finite strip source (orthogonal to direction of flow) at any specified time. It assumes a homogeneous, isotropic aquifer of uniform thickness, a uniform flow field, and zero background concentration.

Contact address: I. Javandel, Lawrence Berkeley Lab., Earth Sc. Div., Univ. of Calif., Berkeley, CA 94720, or International Ground Water Modeling Center, Colorado School of Mines, Golden, CO 80401.

IGWMC Key: 6312 Model Name: ODAST Released: 1985
Authors: I. Javandel, C. Doughty and C.F. Tsang.

ODAST is an analytical solution to the one-dimensional convective-dispersive transport of a nonconservative solute in a homogeneous, isotropic aquifer with a uniform flow field. The model includes decay at the solute source and in the aquifer, and linear equilibrium adsorption. It calculates C/CO at any point downstream from the contaminant source at any specified time and assumes zero background concentration.

Contact address: I. Javandel, Lawrence Berkeley Lab., Earth Sc. Div., Berkeley, CA 94720, or Intern. Ground Water Modeling Ctr., Col. Sch. of Mines, Golden, CO 80401.

IGWMC Key: 6350 Model Name: WALTON35 Released: 1985
Author: W.C. Walton

WALTON35 is a package containing a series of simple BASIC programs for simulating flow, solute transport, and heat transport in various types of aquifers. The programs are based on analytical and numerical solutions of the governing equations. Included are various analytical solutions for non-conservative solute transport in a homogeneous aquifer. The programs are interactive, simple to use, and easy to modify.

Contact address: Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401

IGWMC Key: 6351 Model Name: WELFUN/WELFLO/CONMIG Released: 1989
Author: W.C. Walton

The programs WELFUN, WELFLO and CONMIG calculate common well function values and simulate a wide range of ground-water flow and contaminant migration situations based on analytical solutions. The program options include: (1) drawdown or recovery due to multiple production and/or injection wells with variable discharge or recharge rates, drains, and mines; (2) confined, leaky confined, and water table conditions with barrier and/or recharge boundaries and discontinuities; and (3) development of localized contaminant plumes from slug or continuous source areas of various shape and sizes due to advection, dispersion, retardation caused by linear adsorption, and radioactive decay.

Contact address: Lewis Publ. Inc., 2000 Corporate Blvd., N.W. Boca Raton, FL 33431

IGWMC Key: 6380 Model Name: SOLUTE Released: 1991
Author: M.S. Beljin

SOLUTE is an interactive program of eight analytical solutions for conservative and non-conservative solute transport in saturated ground-water systems. The solutions vary according to dimensionality, type of source and initial and boundary conditions. The package includes screen graphics.

Contact address: Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401

IGWMC Key: 6590 Model Name: BEAVERSOFT Released: 1987
Authors: J. Bear and A. Verruijt

BEAVERSOFT is a package of analytical and numerical solutions for ground-water flow and solute transport. It includes programs for steady and non-steady state two-dimensional flow in heterogeneous aquifers, for flow through dams and for conservative and non-conservative advective-dispersive transport of pollutants.

Contact address: Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401

IGWMC Key: 6600 Model Name: CATTI Released: 1988
Authors: J.P. Sauty and W. Kinzelbach

CATTI (Computer Aided Tracer Test Interpretation) is a program for the interpretation of tracer test data based on an analytical solution of the nonconservative advective-dispersive solute transport equation. It computes breakthrough curves based on instantaneous or continuous injection of tracer into a homogeneous aquifer with either 1D-2D uniform flow or axisymmetric flow for 1 or 2 layers. CATTI allows interactive modification of transport parameters and immediate visualization of breakthrough curves. The program is also capable of automatic parameter identification by non-linear least-squares estimation methods.

Contact address: Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401

IGWMC Key: 6601 Model Name: EPA-VHS Released: 1989
Author: P.K.M. van der Heijde

EPA-VHS (Vertical-Horizontal Spread model) is an analytical solute transport model to predict maximum concentration of a pollutant at a prescribed distance downstream from a continuous source (compliance point). It is based on a solution for the transport of a conservative constituent in a homogeneous, isotropic aquifer with one-dimensional, horizontal steady-state flow and dispersion perpendicular to the flow path. The model assumes zero retardation, a continuous input at maximum extraction levels, and saturated soil conditions. This program contains two versions: (1) the original VHS model as published by Domenico and Palciauskas (1982), and (2) the modified EPA version as published in the Federal Register, Nov. 27, 1985.

Contact address: Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 6660 Model Name: CRACK Released: 1988
Author: E.A. Sudicky

The CRACK package contains 4 analytical models for mass transport in fractured porous media: (1) transport in a single fracture including matrix diffusion with and without dispersion along fracture axis (models CRACKD and CRACKD0, respectively); (2) transport in a system of parallel fractures including matrix diffusion with no dispersion along fracture axis (PCRACK0); (3) and transport in a single fracture with matrix diffusion and radial diverging flow (RCRACK). The package includes a plotting routine for concentration vs. time at different locations or concentration vs. position for different times (PLOTC).

Contact address: Waterloo Center for Groundwater Research, Univ. of Waterloo, Waterloo, Ontario, Canada N21 3G1

IGWMC Key: 6700 Model Name: MYGRT Released: 1989
Authors: K.V. Summers, S.A. Gherini, M.M. Lang, M.J. Ungs, et al.

MYGRT is an interactive, menu-driven microcomputer code to predict the migration of both inorganic and organic solutes through the saturated ground-water zone, downgradient of sources such as waste disposal sites or spills. The processes included are advection, dispersion, retardation and decay. The code is based on analytical solutions and can simulate problems in one or two dimensions using either horizontal or vertical views. The code includes various options for tabular and graphic display of the results.

Contact address: Electric Power Res. Inst., Software Center, 1930 Hi Line Drive, Dallas, TX 75207

Appendix C.1: Solute Transport; Analytical Models For Saturated Zone, Part 2: Usability and Reliability

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
2037	FRACSOL	U	U	U	U	U	L	Y	U	Y	U	U
2080	GETOUT	U	U	Y	Y	N	L	Y	Y	Y	L	M
2810	WASTE	U	U	Y	Y	N	L	Y	U	Y	L	U
3380	GRDFLX	N	N	Y	Y	N	N	Y	U	U	U	U
3432	CXTFIT	Y	Y	Y	Y	Y	Y	Y	U	Y	L	M
4082	LAYFLO	N	N	Y	Y	N	U	Y	U	Y	Y	U
4620	MASCOT	N	N	Y	Y	N	L	Y	Y	Y	N	F
4740	SURMF	N	N	U	Y	N	L	Y	U	U	U	U
4911	OASIS	Y	Y	Y	Y	Y	L	Y	U	Y	Y	F
5024	PATHRAE	N	N	Y	Y	N	U	Y	U	Y	U	U
5055	PLUME	Y	Y	Y	Y	Y	Y	U	U	U	U	F
5174	FRACQUAL	Y	Y	Y	Y	Y	Y	U	U	U	U	F
5175	POLLUT	Y	Y	Y	Y	Y	Y	U	U	U	U	F
5210	PULSE	Y	Y	Y	Y	Y	Y	U	U	U	U	F
5211	CXPMPM	Y	Y	Y	Y	Y	Y	U	U	U	U	F
5212	TDPLUME/ TWOPLME	Y	Y	Y	Y	Y	Y	U	U	U	U	F
5242	BLOB3D	U	U	Y	Y	U	L	Y	U	U	U	U
5243	CRAFLUSH	U	U	Y	Y	U	L	Y	U	U	U	U
5245	HPATCH3D	U	U	Y	Y	U	L	Y	U	U	U	U

KEY: Y = YES N = NO L = LIMITED M = MANY F = FEW U = UNKNOWN

Appendix C.1, part 2 (continued)

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
5246	LINE2D	U	U	Y	Y	U	L	Y	U	U	U	U
5247	PATCH3D	U	U	Y	Y	U	L	Y	U	U	U	U
5248	SUPER1D	U	U	Y	Y	U	L	Y	U	U	U	U
5310	PRZMAL	U	U	Y	U	Y	L	U	U	U	U	U
6011	RWH	Y	Y	Y	Y	Y	Y	Y	N	Y	N	M
6020	PLUME	Y	Y	Y	Y	Y	Y	Y	N	Y	L	M
6024	PLUME2D	Y	N	Y	Y	Y	Y	Y	N	Y	L	M
6100	GROUND	N	N	Y	Y	N	N	Y	U	Y	U	U
6120	AT123D	Y	Y	Y	Y	N	L	Y	Y	Y	L	M
6220	ONE-D	N	N	Y	Y	N	L	Y	N	Y	U	M
6227	CFITIM	N	N	Y	Y	N	L	Y	U	Y	L	M
6250	WELL	N	N	Y	Y	N	N	Y	Y	Y	L	F
6310	LTIRD	N	N	Y	Y	N	L	Y	Y	Y	L	M
6311	TDAST	N	N	Y	Y	N	L	Y	Y	Y	L	M
6312	ODAST	N	N	Y	Y	N	L	Y	Y	Y	L	M
6350	WALTON35	Y	N	Y	Y	Y	L	Y	N	Y	N	M
6351	WELFUN/ WELFLO/ CONMIG	Y	Y	Y	Y	Y	L	Y	Y	Y	N	M

KEY: Y = YES N = NO L = LIMITED M = MANY F = FEW U = UNKNOWN

Appendix C.1, part 2 (continued)

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
6380	SOLUTE	Y	Y	Y	Y	Y	Y	Y	N	Y	L	M
6590	BEAVERSOFT	Y	Y	Y	Y	Y	L	Y	Y	Y	L	M
6600	CATTI	Y	Y	Y	Y	Y	Y	Y	N	Y	L	M
6601	EPA-VHS	Y	N	Y	Y	Y	L	Y	N	Y	N	M
6660	CRACK	Y	Y	Y	Y	Y	L	Y	U	Y	L	M
6700	MYGRT	Y	Y	Y	Y	Y	Y	Y	Y	Y	L	M

KEY: Y = YES N = NO L = LIMITED M = MANY F = FEW U = UNKNOWN

Appendix C.2: Solute Transport; Two-Dimensional Numerical Models for Saturated Zone, Part 1: Model Description

Note: Some two-dimensional models may also be used for simulation of one-dimensional systems or for simulation of radial-symmetric problems; most models for dual porosity media may also be used for simulation of regular porous media systems (see Appendix F); some transport models can handle either solute transport or heat transport, or even both in a single simulation; there are some one- and two-dimensional variably saturated models which may also be used for simulation of systems under fully saturated conditions (see Appendix C.4).

IGWMC Key: 251 Model Name: WTQUAL1 Released: 1981
Authors: McWhorter, D.B., Sunada, D.K.

WTQUAL1 is a finite difference model for simulation of transient, two-dimensional horizontal flow and solute transport in confined, semi-confined or water-table aquifers with water quality problems caused by mining activities or natural contamination.

Contact Address: Sunada, D.K., Colorado State Univ., Dept. of Civil Eng., Fort Collins, CO 80523

IGWMC Key: 588 Model Name: SEFTRAN Released: 1986
Authors: Huyakorn, P.S., Ward, D.S., Rumbaugh, J.O., Broome, R.W.

SEFTRAN (Simple and Efficient Flow and TRANsport model) is a concise finite element model to simulate transient two-dimensional fluid flow and transport of non-conservative contaminants or heat in isotropic, heterogeneous aquifers. It can solve the flow and transport equations in an areal plane, a vertical cross-section, or an axisymmetric configuration. Line elements may be used to simulate discrete fractures or rivers.

Contact Address: D.S. Ward , GeoTrans, Inc., 46050 Manekin Plaza, Suite 100, Sterling, VA 22170

IGWMC Key: 680 Model Name: GWSIM-II Released: 1981
Author: Knowles, T.R.

GWSIM-II is a finite difference model for simulation of steady-state or transient, two-dimensional groundwater flow and conservative solute transport in an anisotropic, heterogeneous, (leaky) confined or unconfined aquifer. The model can handle a combination of confined and unconfined conditions. The uncoupled finite difference equations for flow and transport are solved using the iterative alternating direction implicit (IADI) method, together with Gauss elimination.

Contact Address: Texas Dept. of Water Resources, Texas Natural Resources Information System, P.O. Box 13087, Austin, TX 78711

IGWMC Key: 740 Model Name: USGS-2D-TRANSPORT/MOC/KONBRED Released: 1989
Authors: Konikow, L.F., Bredehoeft, J.D.

MOC is a two-dimensional model for the simulation of non-conservative solute transport in heterogeneous, anisotropic aquifers. It computes changes in time in the spatial concentration distribution caused by convective transport, hydrodynamic dispersion, mixing or dilution from recharge, and chemical reactions. The chemical reactions include first-order irreversible rate reaction (e.g. radioactive decay),

(continued.....)

USGS-2D-TRANSPORT -- continued

equilibrium-controlled sorption with linear, Freundlich or Langmuir isotherms, and monovalent and/or divalent ion-exchange reactions. MOC solves the finite difference approximation of the groundwater flow equation using iterative ADI and SIP. It uses the method of characteristics followed by an explicit procedure to solve the transport equation.

Contact Address: L.F. Konikow, U.S. Geological Survey, Groundwater Branch WRD, 431 National Center, Reston, VA 22092; or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 742 Model Name: MOCDENSE Released: 1992
Authors: Sanford, W.E., Konikow, L.F.

MOCDENSE is a numerical model to simulate conservative (non-reactive) convective-dispersive solute transport one or two constituents in groundwater where there is two-dimensional, cross-sectional, density-dependent flow. The model is a modified version of the USGS two-dimensional solute transport model MOC by Konikow and Bredehoeft, which uses a combination of the finite difference method and the method of characteristics to solve the flow and transport equations. It solves for fluid pressure and solute concentration. Density is a function of concentration of one of the constituents. The model is applicable to situations where in addition of the density controlling species movement and concentration of another dissolved species needs to be predicted.

Contact Address: L.F. Konikow, U.S. Geological Survey, National Center, Reston, Virginia; or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 1010 Model Name: GGWP Released: 1983
Authors: Miller, I., Marlon-Lambert, J.

GGCP (Golder Groundwater Computer Package) is an integrated suite of computer programs for steady-state or transient finite element simulation of two-dimensional, vertical or axisymmetric and quasi-three dimensional flow and transport of reactive solutes in anisotropic, heterogeneous, multi-layered aquifer systems. Auxiliary computer programs are included for semi-automatic mesh generation, input preparation, and presentation of model results (contour and vector plots). Confined, leaky-confined and unconfined flow problems are simulated with the programs AFPM (Aquifer Flow in Porous Media) and FPM (Flow in Porous Media). They can handle a moving phreatic surface, evaporation, and interaction with surface flows. The transport program (SOLTR) includes convection, dispersion, dilution, sorption and radioactive decay.

Contact Address: Golder Associates , Inc., 4104 148th Ave. NE, Redmond, WA 98052

IGWMC Key: 2120 Model Name: PATHS Released: 1980
Authors: Nelson, R.W., Schur, J.A.

The PATHS program is an idealized hybrid analytical/numerical model for simulation of steady-state or transient, two-dimensional, saturated groundwater flow and transport processes of advection, sorption and ion exchange. It includes an analytical solution of the flow equation and the Runge-Kutta solution for the pathline equations and the effects of equilibrium ion-exchange and linear adsorption. The model calculates pathlines, location/arrival time distribution, and location/outflow quantity distribution in a confined stratum

(continued.....)

PATHS -- continued

that is isotropic and homogeneous. It assumes a uniform lateral flow gradient and superimposed leakage from a vertical, cylindrical fully penetrating pond or cavern. The model can handle up to 35 fully penetrating wells or vertical line sources.

Contact Address: Water & Land Resources Div., Battelle Pacific NW Laboratories, P.O. Box 999, Richland, WA 99352

IGWMC Key: 2690 Model Name: RANDOM WALK/TRANS Released: 1981
Authors: Prickett, T.A., Naymik, T.G., Lonnquist, C.G.

RANDOM WALK/TRANS is a numerical model to simulate two-dimensional steady or transient flow and transport problems in heterogeneous anisotropic aquifers under water table and/or confined or leaky confined conditions. The model calculates heads, velocities and concentrations for transport processes of advection, dispersion, diffusion, sorption and decay. Flow is simulated using a finite difference approach and the resulting set of equations is solved with the iterative alternating direction implicit method. Advective transport is solved with a particle-in-a-cell method, while the dispersion is analyzed with the random walk method.

Contact Address: Illinois State Water Survey, P.O. Box 5050, Sta. A, Urbana, IL 61820; or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 3084 Model Name: CHNTRNS Released: 1987
Authors: Noorishad, J., Carnahan, C.L., Benson, L.V.

CHMTRNS is a temperature-dependent non-equilibrium reactive chemical transport code, based on the CHEMTRN code (Miller and Benson) developed in the early 1980's. Equations solved include mass balance, aqueous species transport, non-equilibrium reactions, transport of hydrogen and hydroxide ions, equilibrium complexation, dissolution and precipitation, ion exchange, redox reactions, and heat transport. The code is capable of simulating kinetic calcite and silicate dissolution, irreversible glass dissolution, oxidation and reduction, and stable carbon isotope fractionation during transport. The code can handle Neumann and Dirichlet boundary conditions and includes a mesh generation scheme. The 1-D transport equation is solved using a upstream weighted finite difference algorithm.

Contact Address: Noorishad, J., Lawrence Berkeley Laboratory, Earth Sciences Division, Univ. of Calif., Berkeley, CA 94720

IGWMC Key: 3220 Model Name: GEOFLOW Released: 1982
Authors: Haji-Djafari, S., Wells, T.C.

GEOFLOW is a Galerkin finite element model to simulate steady or non-steady, groundwater flow and solute mass transport in two-dimensional groundwater systems. The aquifer can be confined, semiconfined (leaky), or unconfined and its properties can be anisotropic and heterogeneous. Multiple wells with time-dependent flow rates can be specified. The model includes geochemical reactions such as adsorption, acid neutralization, and radioactive decay. The model comes with a graphical postprocessor to produce contours, velocity vectors, and isopachs.

Contact Address: D'Appolinia Waste Management Services, Inc., 10 Duff Road, Pittsburg, PA 15235

IGWMC Key: 3233 Model Name: PORFLOW - II (2D) Released: 1988
Author: Runchal, A.K.

PORFLOW II (2D) is an integrated finite difference model for analysis of coupled, steady-state or transient, 2-dimensional horizontal, vertical or radial, density dependent flow and heat and/or mass transport in anisotropic, heterogeneous, non-deformable saturated porous media with time dependent aquifer and fluid properties. User interface is based on the FREEFORM language with simple English commands.

Contact Address: Analytic & Computational Research, Inc., 1931 Stradella Road, Bel Air, CA 90077

IGWMC Key: 3376 Model Name: FEMA Released: 1985
Authors: Yeh, G.T., Huff, D.D.

FEMA (Finite Element model of Material transport through Aquifers) is a two-dimensional finite element model for simulation of solute transport in heterogeneous, anisotropic porous media. The advective-dispersive transport model includes radioactive decay, sorption and biological and chemical degradation, consolidation, and natural and artificial sources and/or sinks. The model grid may include both quadrilateral and triangular elements. FEMA solves the solute transport equation only, requiring the velocity field to be generated by the accompanying flow model FEWA.

Contact Address: Yeh, G.T. , Penn State University, Dept. of Civil Eng., 225 Sackett Building, University Park, PA 16802.

IGWMC Key: 3378 Model Name: AQUITRAN Released: 1989
Authors: Yeh, G.T., Francis, C.W.,

AQUITRAN is a two-dimensional, vertically averaged solute transport model based on an orthogonal-upstream weighing finite element scheme, which results in a matrix amenable to successive over-relaxation (SOR) solution strategies. The model considers advection, dispersion, sources/sinks, first-order decay, and linear equilibrium adsorption. The model needs a hydraulic head distribution as generated by the complementary model AQUIFLOW by Yeh (1984). The set of weighing functions are developed for line, quadrilateral and triangular elements. For large problems, when SOR iteration must be employed to solve the matrix equation, the orthogonal-upstream weighing scheme provides the only scheme resulting in convergent SOR computations for all Peclet numbers.

Contact Address: Oak Ridge National Laboratory, Environm. Sciences Div., Oak Ridge, TN 37831

IGWMC Key: 3610 Model Name: CHEMTRN/THCC Released: 1986
Authors: Miller, C.W., Benson, L.V., Carnahan, C.L.

CHEMTRN is a one-dimensional simulation of advective-diffusive-dispersive transport of a reactive chemical in a saturated porous medium by simultaneously solving the mass action, transport and site constraint equations. Sorption is modeled by ion exchange and surface complexation. The code allows precipitation and dissolution processes. The activity coefficient is computed by Davies equation. THCC is a modified version of CHEMTRN including redox reactions. THCC uses a one-step algorithm to incorporate chemical reactions directly into the chemical transport equations and solve then simultaneously.

Contact Address: Lawrence Berkeley Laboratory, Earth Sciences Division, Berkeley, CA 94720

IGWMC Key: 3790 Model Name: PORFLO Released: 1985
Authors: Runchal, A.K., Sagar, B., Baca, R.G., Kline, N.W.

PORFLO is an integrated finite difference model for transient two-dimensional or axisymmetric simulation of coupled buoyancy driven groundwater flow, heat transfer and radionuclide transport in layered geologic systems. Heat transfer processes include storage, advection, conduction, dispersion and heat generation. Fluid flow processes include storage, inflows and outflows, pore pressure buildup, buoyancy driving force and temperature dependent hydraulic conductivity. Density is a function of concentration. Mass transport processes can handle multi-phase conditions and include storage, advection, dispersion, diffusion, sorption, retardation, dissolution, decay, and mass release.

Contact Address: N.W. Kline, Boeing Computer Services Richland, P.O Box 300, Richland, WA 99352

IGWMC Key: 3831 Model Name: SATRA-CHEM Released: 1986
Authors: Lewis, F.M., Voss, C.I., Rubin, J.

SATRA-CHEM is a hybrid Galerkin finite-element and integrated finite difference model for simulation of horizontal or cross-sectional two-dimensional flow and multi-solute transport in fully saturated porous media. The constant-density model is a modification of the USGS' SATRA model, which in itself is a simplified version of SUTRA. SATRA-CHEM incorporates equilibrium controlled reactions: (1) linear sorption and up to two aqueous complexations, and (2) binary ion-exchange and a single complexation reaction involving one of the exchanging species. The time derivative is approximated using a backwards finite-difference scheme.

Contact Address: U.S. Geological Survey, WATSTORE Program Office, 437 National Center, Reston, VA 22092

IGWMC Key: 3868 Model Name: MAST-2D Released: --
Author: Desai, C.S.

MAST-2D is a finite element solution of the coupled two-dimensional transient seepage and convective-dispersive mass transport equations for a saturated porous media. The coupling occurs through changes in density of the liquid with time as a function of concentration. The model, applicable to two-dimensional cross-sectional problems, uses quadrilateral 4-node elements with bilinear variation of concentration, fluid pressure and two components of velocity. The assemblage equations are solved using a Crank-Nicolson scheme. The model has been designed for analysis of density-varying transport problems such as saltwater intrusion and pollutant transport.

Contact Address: Desai, C.S., University of Arizona, Department of Civil and Mechanical Engineering, Tuscon, AZ 85721

IGWMC Key: 3940 Model Name: RESSQ Released: 1985
Authors: Javandel, I., Doughty, C., Tsang, C.F.

RESSQ is a semi-analytical model of 2-dimensional contaminant transport that calculates the streamline pattern in an aquifer, the location of contaminant fronts around sources at specified times, and concentration versus time at sinks. RESSQ assumes a homogeneous, isotropic confined aquifer of uniform thickness and

(continued.....)

RESSQ -- continued

a steady-state regional flow field. It can handle advection and linear equilibrium adsorption. Sources are represented by fully penetrating recharge wells and ponds, and sinks are represented by fully penetrating pumping wells.

Contact Address: Javandel, I., Lawrence Berkeley Laboratory, Earth Sciences Division, University of California, Berkeley, CA 94720; or Internat. Ground Water ModelingCtr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 4320 Model Name: SOTRAN Released: 1983
Authors: Nwaogazie, I.L.

SOTRAN is a finite element solute transport model for two-dimensional unconfined aquifer systems using linear or quadratic isoparametric quadrilateral elements and including linear equilibrium adsorption, first-order biodegradation and radio-active decay.

Contact Address: Nwaogazie, I.L., University of Port Harcourt, Department of Civil Engineering, PMB 5323 Port Harcourt, Nigeria

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IGWMC Key: 4360 Model Name: IONMIG Released: 1984
Authors: Russo, A.J.

IONMIG is a finite difference model to calculate two-dimensional far-field convective-diffusive transport of decaying radionuclides through a saturated porous medium. Nuclide adsorption coefficient is a function of concentration and temperature. Planar or axisymmetric two-dimensional geometries can be treated with either explicit or implicit solvers. The model requires for input temperature and velocity distributions as generated by the related code MARIAH.

Contact Address: Russo, A.J., Sandia National Laboratories, Fluid Mechanics and Heat Transfer Div. 1512, Albuquerque, NM 87185

IGWMC Key: 4450 Model Name: TRANQL/MICROQL Released: 1985
Authors: Cederberg, G.A., Street, R.L., Leckie, J.O.

TRANQL is a finite element transport model for simulation of multi-component solute transport with equilibrium interaction chemistry coupled with one-dimensional advective-dispersive finite element transport. Significant equilibrium reaction such as complexation, ion exchange, competitive adsorption, and dissociation of water may be included. It includes to models for ion-exchange, the constant capacity model and the triple-layer model. The model has been applied to cadmium, chloride, and bromide transport in a one-dimensional column.

Contact Address: G.A. Cederberg, 2305 A 37th Street, Los Alamos, NM 87544

IGWMC Key: 4694 Model Name: SAFTMOD Released: 1988
Authors: Huyakorn, P.S., Buckley, J.E.

SAFTMOD is a finite element model for simulating flow and solute transport in the saturated zone of an unconfined groundwater system. It performs two-dimensional simulations in either the X-Y or X-Z plane of the porous medium. It also can perform axisymmetric simulations. Both single and leaky two-aquifer systems can be handled with recharge from infiltration or precipitation and well pumping or injection. Transport include hydrodynamic dispersion, advection, linear equilibrium sorption, and first-order decay. Parent/daughter transformations are also simulated. Boundary conditions include prescribed head, volumetric water flux, concentration, and solute mass flux.

Contact Address: HydroGeologic, Inc., 1165 Herndon Parkway, Suite #900, Herndon, VA 22070

IGWMC Key: 4910 Model Name: BIOPLUME II Released: 1987
Authors: Rifai, H.S., Bedient, P.B., Bordon, R.C., Haasbeek, J.F.

BIOPLUME II is a two-dimensional solute transport model to compute changes in concentration over time due to advection, dispersion, mixing, and retardation. The model simulates the transport of dissolved hydrocarbons under influence of oxygen-limited biodegradation. It also simulates reaeration and anaerobic biodegradation as a first order decay in hydrocarbon concentrations. BIOPLUME II is based on the USGS 2D solute transport model MOC (Konikow-Bredehoeft). It solves the transport equation twice: once for hydrocarbon and once for oxygen. The model assumes an instantaneous reaction between oxygen and hydrocarbon. It can simulate natural biodegradation processes, retarded plumes, and in-situ bioremediation schemes.

Contact Address: H.S. Rifai, Rice University, Dept. of Environm. Sciences and Eng., P.O. Box 1892, Houston, Texas 77251; EPA/CSMoS, or IGWMC.

IGWMC Key: 4911 Model Name: OASIS Released: 1989
Authors: Newell, C.J., Haasbeek, J.F., Hopkins, L.P., Alder-Schaller, S.E. et Al.

OASIS is a graphical decision support system for groundwater contamination modeling developed for the Macintosh II or SE personal computer using Hypercard software. OASIS is a collection of computer tools including extensive computerized documentation, two chemical databases, a hydrogeologic database derived from a survey of 400 sites across the US and DRASTIC aquifer vulnerability index system, a numerical 2-dimensional solute transport and biodegradation model --BIOPLUME II--, and an analytical solute transport model --ODAST. It includes extensive graphical pre- and postprocessing for BIOPLUME II. OASIS provides graphical and analytical support to decision makers and technical support personnel. See also remarks.

Contact Address: P.B. Bedient, Rice University, Dept. of Environm. Sciences and Eng., P.O. Box 1892, Houston, Texas 77251-1892

IGWMC Key: 4930 Model Name: TARGET-2DH Released: 1985
Authors: Moreno, J.L., Asgian, M.I., Lympany, S.D., Pralong, P-J. et al.

TARGET-2DH is one of five models of the TARGET series (Transient Analyzer of Reacting Groundwater and

(continued.....)

TARGET-2DH -- continued

Effluent Transport). It simulates two-dimensional, vertically averaged, confined and unconfined transient groundwater flow and solute transport in a single heterogeneous, anisotropic aquifer using a hybrid finite difference method. The transport is based on the solution of the advective-dispersive transport equation for a single non-conservative contaminant with linear equilibrium adsorption (retardation). The solution method used is based on an iterative alternating direction implicit method.

Contact Address: Dames & Moore, 1125 17th Str., #1200, Denver, CO 80202

IGWMC Key: 4932 Model Name: TARGET-2DM Released: 1985
Authors: Moreno, J.L., Asgian, M.I., Lympany, S.D., Pralong, P-J. et al.

TARGET-2DM is one of five models of the TARGET series (Transient Analyzer of Reacting Groundwater and Effluent Transport). It simulates quasi-three dimensional, confined and unconfined transient groundwater flow and solute transport in a multi-layered heterogeneous, anisotropic aquifer/aquitard system using a hybrid finite difference method. The transport is based on the solution of the advective-dispersive transport equation for a single non-conservative contaminant with linear equilibrium adsorption (retardation). The solution method used is based on an iterative alternating direction implicit method.

Contact Address: Dames & Moore, 1125 17th. Str., #1200, Denver, Colorado 80202

IGWMC Key: 5018 Model Name: AQUA Released: 1991
Authors: Kjaran, S.P., Egilson, D., Sigurdson, S.Th.

AQUA is a program package developed for solving steady-state and transient two-dimensional ground-water flow and transport problems using the finite element method. The model can be applied to either confined or unconfined aquifers allowing for heterogeneity and anisotropy of aquifer hydraulic parameters and time-varying infiltration and pumping. Processes included in the simulation of transport of heat and dissolved chemicals are convection, decay, adsorption and velocity dependent dispersion. For heat transport conduction is included. The AQUA package includes various graphic pre- and post processors facilitating interactive grid design and data entry for areal and cross-sectional problems.

Contact Address: Vatnaskil Consulting Engineers, Armuli 11, IS-108 Reykjavik, Iceland; or Scientific Software, Washington D.C.

IGWMC Key: 5120 Model Name: FEMSEEP Released: --
Author: Meiri, D.

FEMSEEP is a 2-D finite element flow and solute transport model, combined with particle tracking for solving steady state and transient planar and cross-sectional groundwater flow in heterogeneous, anisotropic aquifers. The aquifer can be under confined, unconfined or leaky confined conditions. The flow model can be solved in terms of hydraulic head, drawdown, or stream function. Flow b.c.'s may include prescribed head, prescribed flux, or mixed head-flux. The solute transport model accounts for advection, dispersion, and retardation. Transport b.c.'s may have prescribed concentrations or mass flux. FEMSEEP supports a movable grid for cross-sectional phreatic surface simulation and includes a preprocessor for grid design and data preparation and a graphic postprocessor.

Contact Address: D. Meiri, Ebasco Environmental, 111 N. Canal Street, Chicago, IL 60606, or Sceintific Software, Washington, D.C.

IGWMC Key: 5244 Model Name: CFEMTRAN Released: --
Authors: --

CFEMTRAN is a Galerkin finite element model for simulating 2-dimensional, transient solute transport in cross-section. It computes solute concentration distribution by solving the advection-dispersion equation. The program includes a mesh generation option for rectangular grids. It can also read manually generated grid data. The groundwater velocities are element-wise variable and can be read directly from a FLONETS output file. The model can handle solute decay and retardation. The matrix solution is by Cholesky decomposition.

Contact Address: Waterloo Centre for Groundwater Research, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1

IGWMC Key: 5270 Model Name: MADPD Released: 1988
Authors: Syriopoulou, D., Koussis, A.D.

MADPD (Matched Artificial Dispersivity - Principal Direction Method) is a two-dimensional finite difference model for solute transport in saturated, steady groundwater flow systems with a known pore velocity distribution. The model is tailored to advection-dominated conditions. The methodology combines the Principal Directions of transport formulation with a fractional time stepping algorithm that incorporates a highly efficient advection-dispersion step. The code can accommodate space-variable geohydrological parameters, sources of time-varying strength distributed on entry boundaries, and solute undergoing first-order decay and linear adsorption. The model can use one- or two-dimensional grids and cartesian or curvilinear coordinates.

Contact Address: Koussis, A.D., Vanderbilt University, Dept. of Civil and Environm. Eng., Nashville, TN 37235

IGWMC Key: 5330 Model Name: CANSAZ (EPACMS) Released: 1989
Authors: --

EPA's CANSAZ (Combined Analytical-Numerical Saturated Zone model) was developed to simulate the migration of contaminants beneath surface impoundments where hydraulic mounding occurs. The model combines an analytical solution for two-dimensional steady-state ground-water flow, coupled with both an analytical and a numerical three-dimensional contaminant transport model. It includes the monte carlo technique to account for uncertainty in parameter distribution. It was meant for use in the development of national regulation under RCRA. It should not be used for site-specific application.

Contact Address: Z. Saleem, U.S. Environmental Protection Agency, Office of Solid Waste (OS-331), 401 M Str. S.W., Washington, D.C. 20460

IGWMC Key: 5530 Model Name: SANDWICH Released: 1985
Authors: P.S. Huyakorn et al.

SANDWICH is a 3D finite-element model for analyzing groundwater flow and contaminant transport in

(continued.....)

SANDWICH -- continued

multi-layered confined/unconfined aquifer systems. The model is designed to simulate fluid flow and solute transport in fully-saturated porous media. Matrix assembly is performed in a horizontal slice-by-slice manner to improve efficiency. The model employs a combination of rectangular and triangular elements. Coupling of aquifer and aquitards is handled using a convolution integral to evaluate leakage fluxes and incorporate these fluxes into the matrix system. For aquifers comprised of several nodal sublayers, the matrix solution for each aquifer is performed using a two-stage algorithm, the ALternate sublayer And Line Sweep (ALALS) procedure.

Contact Address: GeoTrans, Inc., 46050 Manekin Plaza # 100, Sterling, VA 22170

IGWMC Key: 5732 Model Name: MASS Released: --
Authors: van Tonder, G., van Rensburg, H.J.

MASS is a two-dimensional triangular finite element model which solves the groundwater flow equation for a confined aquifer and the advective-dispersive solute transport equation for a conservative contaminant. It includes the program GEMASS, a simple mesh generator program for MASS.
Contact Address: van Rensburg, H.J., Dept. of Water Affairs, Private Bag X313, Pretoria, South Africa

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IGWMC Key: 5780 Model Name: POSSM/MCPOSSM Released: --
Authors: --

POSSM (PCB On-Site Spill Model) is a computer code representing the PCB Spill Exposure Assessment Methodology, a quantitative framework for estimating general public exposure levels associated with spills from electric utility equipment. POSSM is a chemical transport and fate model capable of considering such processes as volatilization, leaching to ground water and chemical washoff from a land surface due to runoff/erosion. On-site environmental concentrations can be estimated with POSSM; off-site concentrations with simple transport and fate models, PTDIS (for air), RIVLAK (for surface water) and GROUND (for ground water), all part of the methodology. MCPOSSM puts the POSSM model in a monte carlo framework to estimate uncertainties of chemical levels associated with spills.

Contact Address: Electric Power Research Inst., Off. of Commercial and Business Developm., P.O. Box 10412, Palo Alto, CA 94303

IGWMC Key: 5861 Model Name: TWODIMPL Released: 1988
Authors: Lindstrom, F.T., Boersma, L.

TWODIMPL is a linear, two-dimensional quasi-analytical model for advective-dispersive transport of reactive chemicals leaking into a rectangular-shaped confined aquifer from constant strength sources, emitting uniformly across the finite vertical aquifer thickness. Linear equilibrium rates are assumed to apply to reversible sorbing soil components made up of weakly sorbing and strongly sorbing fractions and organic matter. First- or zero-order loss rates due to microbial or other irreversible loss processes are included. Irregularly shaped sources are approximated by an assembly of maximum 25 constantly emitting rectangular source regions. The equation is solved using Green's function approach, resulting in a time convolution integral for the concentration distribution.

Contact Address: SEA, Inc., Corvallis, Oregon

IGWMC Key: 6354 Model Name: GWTR3D Released: 1989
Author: Walton, W.C.

GWT3D is a random walk model for simulation of contaminant transport in a heterogeneous, anisotropic confined, leaky-confined, or water-table aquifer. It uses a particle-in-a-cell method to solve for advective transport and the random walk technique for the dispersion mechanism. The model requires a pre-calculated or measured head distribution. It can handle linear adsorption and single-component radio-active decay. It allows for a wide variety of source types and source geometry.

Contact Address: Lewis Publishers, Inc. c/o CRC Publishers, Inc., 2000 Corporate Blvd. N.W., Boca Raton, FL 33431

IGWMC Key: 6603 Model Name: ASM Released: 1991
Authors: Kinzelbach, W., Rausch, R.

ASM (Aquifer Simulation Model) is a menu-driven numerical model for steady-state or transient groundwater flow and (uncoupled) solute transport. The two-dimensional block-centered finite difference equations for (leaky-)confined or unconfined flow are solved using either the IADI or PCG method. Pathlines and isochrones around pumping well are computed by point-tracking in the velocity filed using Euler integration. Solute transport is simulated by the random walk method based on the Ito-Fokker-Planck theory. The model can simulate variable well rates, constant flux and constant head boundaries, and constant or instantaneous contaminant sources. It includes various graphic display option to view the simulation results.

Contact Address: W. Kinzelbach, Gesamthochschule Kassel-Universitat, FB 14, Moritzstr. 21, D-3500 Kassel, Germany; or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 6770 Model Name: CUMOC/MIKERN Released: 1988
Authors: Illangasekare, T.H., Doll, P.

CUMOC/MIKERN is a two-dimensional solute transport model for water-table aquifers using a discrete kernel approach for flow and a method-of-characteristics approach for solute transport. The MOC method has been improved by using an influence area particle tracking scheme that avoids oscillations and step jumps of breakthrough curves. The transport model includes advection, dispersion, linear equilibrium sorption and the influence of immobile zones. The model is designed to simulate sources, sinks and the effects of varying saturated thickness. Biodegradation and radioactive decay are described as first-order reactions. The model handles sorption hysteresis and different rates for decay of solute and sorbed species.

Contact Address: T.H. Illangasekare, Dept. of Civil and Environm. Eng., Univ. of Colorado, Boulder, CO 80309

Appendix C.2: Solute Transport; Two-Dimensional Numerical Models For Saturated Zone, Part 2: Usability and Reliability

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
251	WTQUAL1	U	U	Y	Y	U	L	Y	U	L	U	U
588	SEFTRAN	Y	U	Y	Y	N	N	Y	U	L	L	F
680	GWSIM-II	N	N	Y	Y	N	N	Y	U	L	L	F
740	USGS-2D-TRANSPORT/ MOC/ KONBRED	Y	Y	Y	Y	N	Y	Y	Y	E	L	M
742	MOCDENSE	Y	N	Y	Y	N	L	Y	U	L	U	F
1010	GGWP	Y	Y	Y	Y	Y	L	Y	U	L	U	U
2120	PATHS	N	N	Y	Y	N	N	Y	U	L	N	M
2690	RANDOM WALK/ TRANS	Y	Y	Y	Y	N	L	Y	Y	E	L	M
3084	CHNTRNS	U	U	Y	Y	U	U	Y	U	U	U	U
3220	GEOFLOW	Y	Y	Y	Y	Y	U	Y	U	L	U	U
3233	PORFLOW-II	Y	Y	Y	Y	Y	Y	Y	U	E	L	M
3376	FEMA	N	N	Y	Y	N	L	Y	U	L	U	F
3378	AQUITRAN	N	N	Y	Y	N	L	Y	U	L	U	F
3610	CHEMTRN/ THCC	N	N	Y	Y	U	U	Y	U	U	U	U
3790	PORFLO	Y	Y	Y	Y	Y	L	Y	U	L	U	F
3831	SATRA-CHEM	N	N	Y	Y	N	L	Y	U	L	U	U
3868	MAST-2D	U	U	Y	Y	U	U	U	U	U	U	U
3940	RESSQ	Y	Y	Y	Y	N	L	Y	Y	L	N	M
4320	SOTRAN	U	U	Y	Y	N	N	Y	U	L	U	U

KEY: Y = YES N = NO L = LIMITED E = EXTENSIVE M = MANY F = FEW U = UNKNOWN

Appendix C.2, part 2 (continued)

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
4360	IONMIG	U	U	Y	Y	U	U	U	U	U	U	U
4450	TRANQL/ MICROQL	U	U	Y	Y	U	U	U	U	U	U	U
4694	SAFTMOD	Y	Y	Y	Y	Y	L	Y	U	L	U	U
4910	BIOPLUME II	Y	Y	Y	Y	N	L	Y	U	E	L	F
4911	OASIS	Y	Y	Y	Y	Y	L	Y	N	E	L	F
4930	TARGET-2DH	Y	Y	Y	Y	Y	Y	Y	N	L	U	M
4932	TARGET-2DM	Y	Y	Y	Y	Y	Y	Y	N	L	U	M
5018	AQUA	Y	Y	Y	Y	Y	Y	Y	U	L	U	M
5120	FEMSEEP	Y	Y	Y	Y	Y	Y	Y	U	L	U	U
5244	CFEMTRAN	U	U	Y	Y	U	U	Y	N	L	U	U
5270	MADPD	U	U	Y	Y	U	U	Y	U	L	U	U
5330	CANSAZ (EPA-CMS)	U	U	U	U	U	U	Y	U	U	U	U
5530	SANDWICH	U	U	Y	Y	N	N	Y	U	L	U	U
5732	MASS	U	U	Y	Y	Y	L	U	U	L	U	U
5780	POSSM/ MCPOSSM	U	U	Y	Y	U	U	Y	U	L	U	U
5861	TWODIMPL	U	U	Y	Y	U	U	Y	U	U	U	U
6354	GWTR3D	Y	Y	Y	Y	Y	L	Y	Y	L	L	M

KEY: Y = YES N = NO L = LIMITED E = EXTENSIVE M = MANY F = FEW U = UNKNOWN

Appendix C.2, part 2 (continued)

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
6603	ASM	Y	Y	Y	Y	Y	L	Y	N	L	U	M
6770	CUMOC/ MIKERN	U	U	Y	Y	U	U	Y	U	U	U	U

KEY: Y = YES N = NO L = LIMITED E = EXTENSIVE M = MANY F = FEW U = UNKNOWN

Appendix C.3: Solute Transport; Three-Dimensional Numerical Models for Saturated Zone, Part 1: Model Description

Note: Many three-dimensional models may also be used for simulation of one- and two-dimensional systems; most three-dimensional models for dual porosity media may also be used for simulation of regular porous media systems (see Appendix F); there are some three-dimensional variably saturated models which may also be used for simulation of systems with fully saturated conditions (see Appendix C.4).

IGWMC Key: 515 Model Name: PTC Released: 1986
Authors: Babu, D.K. , Pinder, G.F., Niemi, A., Ahlfield, D.P.

PTC (Princeton Transport Code) is a three-dimensional model for simulation of uncoupled transient flow and solute transport in confined or unconfined porous media. The model solves the advective-dispersive transport equation for reactive and non-reactive solutes using a hybrid finite element Galerkin technique coupled with a finite difference scheme. The FEM formulation is applied to the horizontal slices, and the FDM to the cross-sections.

Contact Address: G.F. Pinder, University of Vermont, 101 Votey Building, Burlington, Vermont 05405

IGWMC Key: 582 Model Name: GREASE Released: 1982
Author: Huyakorn, P.S.

GREASE 2 is a multi-purpose finite element model to simulate transient, multi-dimensional, saturated groundwater flow, solute and/or energy transport in fractured and non-fractured, anisotropic, heterogeneous, multilayered porous media. The analysis can be performed for confined, semiconfined, or unconfined groundwater reservoir systems. Fluid leakage or heat transfer between the aquifer and its confining layer can be taken into account. The model allows for analysis of areal flow, vertical cross-sectional flow or flow in an axisymmetric configuration. Coupled thermal fluid flow capability, and density dependent flow and solute transport capability area also available. Sorption and decay can be included in the solute transport analysis.

Contact Address: GeoTrans, Inc., 46050 Manekin Plaza, Suite 100, Sterling, VA 22170

IGWMC Key: 692 Model Name: SWIP/SWIPR/DWDM Released: 1985
Authors: INTERA Environm. Consult., Inc.

SWIP/SWIPR (Survey Waste Injection Program-Revised) or DWDM (Deep Well Disposal Model) is a finite difference model to simulate unsteady, coupled three-dimensional groundwater flow, heat transport and non-conservative contaminant transport in an anisotropic, heterogeneous aquifer. The model has been superseded by HST3D, SWENT, and the SWIFT series.

Contact Address: K. Kipp, U.S. Geological Survey, Box 25046, Mail Stop 411, Denver Federal Center, Lakewood, CO 80225

IGWMC Key: 697 Model Name: SWENT Released: 1983
Authors: Lantz, R.B., Pahwa, S.B., RamaRao, B.S.

SWENT (Simulator for Water, Energy, and Nuclide Transport) is a finite difference model for simulation of transient, multidimensional transport of fluid, energy, a single inert chemical species, and any number of radionuclides in straight or branched chains, through a heterogeneous, anisotropic confined aquifer. Flow and transport are coupled through density and viscosity. Salt dissolution and leaching can be simulated. Aquifer porosity is treated as function of pressure. Individual processes or a combination of the processes, including well bore flow, may be simulated using a number of boundary conditions. The model permits the choice of backward or central difference approximations and either direct or SOR iterative methods may be used for solving the matrix equations.

Contact Address: National Energy Software Center, Argonne National Laboratory, 9700 S. Cass Avenue, Argonne, IL 60439.

IGWMC Key: 2070 Model Name: CFEST Released: 1987
Authors: Gupta, S.K., Kincaid, C.T., Meyer, P.R., Cole, C.R.

CFEST (Coupled, Fluid, Energy and Solute Transport) is a three-dimensional finite element model for simulation of steady-state or transient, single-phase Darcian flow, and energy and solute transport in anisotropic, heterogeneous, multi-layered aquifers. The code has the capability to model discontinuous and continuous layering and time-dependent and constant sources/sinks. The partial differential equations for pressure, temperature, and solute concentration are coupled with fluid density and viscosity, and used in a Galerkin FEM (linear elements), sequential solution. The relationship between porosity and pore-pressure is also accounted for. The model comes with various programs for data input, gridding and post-processing including streamline generation and contouring. It has a restart option and data error checking.

CFEST has undergone extensive verification testing, among others, as part of the international HYDROCOIN project. Many of the test problems and the CFEST performance for the tests have been published.

Contact Address: Cole, C.R., Battelle Pacific NW Laboratories, P.O. Box 999, Richland, WA 99352

IGWMC Key: 2691 Model Name: RAND3D Released: 1990
Authors: Prickett, T.A., and D.H. Koch

RAND3D is an interactive three-dimensional solute transport model utilizing the random-walk algorithm. The model calculates horizontal advective transport based on a four point interpolation of the velocity vectors. Calculation of vertical transport is based on linear interpolation between the input vertical velocity vectors at the top and bottom of each layer. RAND3D includes first-order decay and linear, reversible adsorption (retardation). It calculates concentration distributions and solute concentration exiting the model at a sink. Transient flow simulations may be simulated by inputting a series of velocity files. A preprocessor, PREMOD3D, is available to use the output of MODFLOW as input and to create velocity vectors for the RAND3D model.

Contact Address: Koch and Assoc., 3458 Ellicott Center Drive, # 101, Ellicott City, MD 21043

IGWMC Key: 3840 Model Name: SWIFT Released: 1982
Authors: Dillon, R.T., Cranwell, R.M., Lantz, R.B., Pahwa, S.B.

SWIFT (Sandia Waste-Isolation Flow and Transport) is a three-dimensional finite difference model for

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SWIFT -- continued

simulation of coupled, transient, density-dependent flow and transport of heat, brine, tracers or radionuclides in heterogeneous, anisotropic, fractured, aquifers. Transport processes include advection, dispersion, diffusion, sorption, decay, and leaching. Two-line SOR iterative or direct-ordered solution methods may be utilized.

The SWIFT code has been based on the SWIP/SWIPR code developed in 1976 for the U.S. Geological Survey and modified in 1979. SWIFT has been superseded by SWIFT II from Sandia National Laboratories and by SWIFT III and SWIFT 386 from GeoTrans, Inc.

Contact Address: R.M. Cranwell, Sandia National Laboratories, Albuquerque, NM 87185, or National Energy Software Center, Argonne National Laboratory, 9700 S. Cass Avenue, Argonne, IL 60439.

IGWMC Key: 3841 Model Name: SWIFT II Released: 1987
Authors: Reeves, M., Ward, D.S., Johns, J.D., Cranwell, R.M.

SWIFT II is a three-dimensional finite difference model for simulation of steady-state or transient flow and transport of fluid, heat, brine, and radionuclide chains in confined or unconfined (fractured) porous media. The equations for fluid, heat, and brine are coupled by fluid density, fluid viscosity, and porosity. Both dual-porosity and discrete-fractures might be considered. Only one-dimensional migration is permitted in the rock matrix. The model includes a salt dissolution mechanism and a waste leaching algorithm. Moreover, SWIFT II has a well-bore submodel and handles both radial and cartesian coordinates. Among the many boundary conditions which can be used is a free phreatic surface condition.

In 1986, under contract to the U.S. Nuclear Regulatory Commission, GeoTrans, Inc. extended the SWIFT code of 1981 to include: fractured media, enhanced free water surface and extended boundary conditions. SWIFT II has been superseded by SWIFT III and SWIFT 386.

Contact Address: D.S. Ward, GeoTrans, Inc., 46050 Manekin Plaza, Suite 100, Sterling, VA 22170

IGWMC Key: 3842 Model Name: SWIFT III/SWIFT 386 Released: 1992
Author: Ward, D.S.

SWIFT/386 is a transient, fully three-dimensional model which simulates the flow and transport of fluid, heat (energy), brine, and radionuclide chains in porous and fractured geologic media. The primary equations for fluid, heat, and brine are coupled by fluid density, fluid viscosity, and porosity. Both Cartesian and cylindrical coordinate systems may be used. For the fracture zone the model allows both dual-porosity and discrete fractures. Migration within the rock matrix is characterized as a one-dimensional process. Aquifer hydraulic characteristics may be heterogeneous and anisotropic under confined or unconfined conditions. The model includes linear and nonlinear (Freundlich) isothermal equilibrium adsorption, hydrodynamic dispersion, and diffusion.

Discretization is performed by the finite-difference method using centered or backward weighing in the time and space domains. Matrix solution is performed either by Gaussian elimination or by two-line successive over-relaxation. SWIFT/386 incorporates a run-time monitor to display the actions and numerical behavior of on-going transport simulations. The IBM PC version handles between 10,000 and 30,000 finite difference blocks.

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SWIFT III/386 -- continued

SWIFT III/386 handles a variety of boundary conditions and source terms for both the porous and fractured media including prescribed pressure (head), temperature, and brine concentration; prescribed flux of fluid (water), heat, brine, or (nuclide) mass; wellbore injection/production submodel subject to pumping constraints; aquifer influence function (i.e. Carter-Tracy infinite reservoir); waste leach radionuclide submodel for waste repository nuclides and heat; and free (phreatic) surface with recharge.

SWIFT III/SWIFT 386 is an extension of SWIFT II (IGWMC Key # 3842), which in turn is an update and extension of SWIFT (Sandia Waste-Isolation Flow and Transport; IGWMC Key # 3841), released in 1981. Originally, refinements in user options, mapping facilities and auxiliary files were included. A postprocessing program UNSWIFT allows direct interfacing with the SURFER contouring package.

Contact Address: D.S. Ward, GeoTrans, Inc., 46050 Manekin Plaza, Suite 100, Sterling, VA 22170

IGWMC Key: 4610 Model Name: HST3D Released: 1991
Author: Kipp, Jr., K.L.

The Heat- and Solute-Transport Program HST3D simulates ground-water flow and associated heat and solute transport in three dimensions. The three governing equations are coupled through the interstitial pore velocity, the dependence of the fluid density on pressure, temperature, and solute mass fraction. The solute-transport equation is for only a single, solute species with possible linear-equilibrium sorption and linear decay. The finite difference model handles a variety of boundary conditions for confined and unconfined aquifer conditions including an approximate free surface. The matrix equations are solved by either direct (Gaussian) elimination or by an iterative solver, using two-line successive overrelaxation.

Two techniques are available for solution of the finite-difference matrix equations in HST3D. One technique is a direct-elimination solver, using equations reordered by alternating diagonal planes. The other is an iterative solver, using two-line successive overrelaxation. A re-start option is available for storing intermediate results and restarting the simulation at an intermediate time with modified boundary conditions. Data input and output in HST3D may be in metric (SI) units or inch-pound units. Output may include tables of dependent variables and parameters, zoned-contour maps, and plots of the dependent variables versus time. HST3D is a descendent of the Survey Waste Injection Program (SWIP) of the U.S. Geological Survey.

Contact Address: K.L. Kipp, Jr., U.S. Geological Survey, MS 413, Box 25046, Denver Federal Center, Denver, CO 80225; Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401; or Scientific Software Group, Washington, D.C.

IGWMC Key: 4631 Model Name: SWICHA Released: 1991
Authors: Huyakorn, P.S., Andersen, P.F., Mercer, J.W., White Jr., H.O.

SWICHA is a three-dimensional finite element model for analyzing seawater intrusion in coastal aquifers. The model is designed to simulate coupled variable density fluid flow and solute transport in fully-saturated porous media. The model which can also handle quasi-three-dimensional conditions and axisymmetric geometries, includes linear equilibrium adsorption and first-order decay. Matrix assembly is performed in a vertical slice-by-slice manner and solved with a SSOR scheme. The model computes spatial and temporal variations of piezometric head, groundwater flow pattern, and flow rates across specified boundaries. It also

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SWICHA -- continued

computes concentration distributions and velocities and includes a full fluid flow and solute transport mass balance scheme.

Contact Address: GeoTrans, Inc., 46050 Manekin Plaza, Suite 100, Sterling, VA 22170, or Internat. Ground Water Modeling Ctr., Colorado School of Mines, Golden, CO 80401.

IGWMC Key: 4700 Model Name: DSTRAM Current Released: 1988
Author: Huyakorn, P.S.

DSTRAM (Density-dependent Subsurface TRansport Analysis Model) is a three-dimensional finite-element model that simulates coupled, density-dependent single-phase fluid flow and solute or energy transport in saturated porous media. This model can perform steady-state or transient simulations in a cross-section, an axisymmetric configuration, or a fully-3D model. The contaminant transport equation includes advection, hydrodynamic dispersion, linear equilibrium adsorption, and first-order degradation. For heat transport simulation, additional processes of heat conduction and storage in the fluid and rock matrix can also be included. Nonlinearity resulting from density differences is handled via a Picard algorithm. The transport equation is solved using upstream weighted residual. A separate mesh generator MESHGN is available.

Boundary conditions in DSTRAM include prescribed nodal values of the equivalent fresh-water head or prescribed integrated nodal values of fluid volumetric fluxes. Boundary conditions for solute transport include prescribed nodal values of solute mass fluxes. Boundary conditions for heat transport include prescribed temperature and prescribed integrated nodal values of heat fluxes. Output include nodal values for hydraulic head, Darcy velocities and flow rates, and nodal concentrations and temperatures.

Contact Address: HydroGeologic, Inc., 1165 Herndon Parkway, Suite 100, Herndon, VA 22070

IGWMC Key: 4933 Model Name: TARGET-3DS Released: 1985
Authors: Moreno, J.L., Asgian, M.I., Lympany, S.D., Pralong, P-J. et al.

TARGET-3DS is one of five models of the TARGET series (Transient Analyzer of Reacting Groundwater and Effluent Transport). It simulates three-dimensional, saturated, density-coupled, transient groundwater flow and solute transport using a hybrid (integrated) finite difference method. The transport is based on the solution of the advective-dispersive transport equation for a single non-conservative contaminant with linear equilibrium adsorption (retardation). The solution method used is based on an iterative alternating direction implicit method. It includes an internal routine for selecting backward, forward, or central differencing schemes, based on the value of the local Peclet number and direction of flow.

Contact Address: Dames & Moore, 1125 17th. Str., #1200, Denver, Colorado 80202

IGWMC Key: 4941 Model Name: DYNTRACK Released: 1992
Authors: Riordan, P.J., Schroeder, D.J., Harley, B.M.

DYNTRACK is a computer program for simulation of three-dimensional transport. It uses the heads computed with the companion code DYNFLOW. DYNTRACK uses the same finite element grid representation of aquifer geometry, flow field, and stratigraphy used for a particular application for the

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DYNTRACK -- continued

DYNFLOW model. DYNTRACK can perform either simple particle tracking or can model three-dimensional advective dispersive transport of non-conservative contaminants. The contaminant transport is based on the random walk method for a statistically significant number of particles, each particle having an associated weight, decay rate, and retardation rate. Dispersion is simulated by imparting a random deflection to each particle in each time step and can be scale-dependent. DYNTRACK includes the option to use backtracking for source identification.

Contact Address: B.M. Harley, Camp Dresser & McKee Inc., One Cambridge Center, Cambridge, MA 02142

IGWMC Key: 4970 Model Name: MT3D Released: 1992
Author: Zheng, C.

MT3D (Modular Transport in 3 Dimensions) is a three-dimensional contaminant transport model using a hybrid method of characteristics. Two numerical techniques are provided for the solution of the advective-dispersive reactive solute transport equation: the method of characteristics (MOC) and the modified method of characteristics (MMOC). The MMOC method overcomes many of the traditional problems with MOC, especially in 3D simulations, by directly tracking nodal points backwards in time and by using interpolation techniques. MT3D selectively uses the MOC or the MMOC technique dependent on the problem at hand. The transport model is so structured that it can be used in conjunction with any block-centered finite difference flow model such as the USGS' MODFLOW model.

The MT3D code is distributed together with a version of the USGS flow model MODFLOW, including the PCG2 solver.

Contact Address: C. Zheng, S.S. Papadopulos & Assoc., Inc., 7944 Wisconsin Avenue, Bethesda, Maryland 20814, USA.

IGWMC Key: 5161 Model Name: INTERTRANS Released: --
Author: Voorhees, M.

INTERTRANS is an interactive three-dimensional solute transport model for calculation of travel times, pathlines and concentration distribution in heterogeneous, anisotropic groundwater systems. The transport model is based on the random-walk method, incorporating three-dimensional scale-dependent dispersion. The model includes an option for three-dimensional reverse pathline tracking. It requires a known flow field, either measured, generated with the model INTERSAT by the same author, or by MODFLOW. INTERTRANS includes on-line plan view and cross-sectional mapping and contouring of results, and real time particle movement.

Contact Address: ESE/Hydrosoft, Inc., 63 Sarasota Center Boulevard, #107, Sarasota, FL 34240

IGWMC Key: 5520 Model Name: FTWORK Released: 19909
Authors: Faust, C.R., Sims, P.N., Spalding, C.P., Andersen, P.F.

FTWORK is a three-dimensional, block-centered finite difference model for simulation of steady-state or

(continued.....)

FTWORK -- continued

transient, non-coupled groundwater flow and solute transport in fully saturated, multi-layered, confined or unconfined, porous hydrogeologic systems. Transport mechanisms include advection, hydrodynamic dispersion, linear equilibrium isotherm adsorption, and radioactive decay. It provides for parameter estimation of the steady state flow applications using a least-squares procedure. The model allows variable grid spacing and approximation of layers that have irregular thickness and/or are not horizontal by using deformed coordinate approximations. Boundary conditions include prescribed head and flux, and head-dependent flux. The model provides a cumulative mass balance.

The major limitations of the FTWORK code are: 1) water density is independent of concentration, thus seawater intrusion and brines cannot be simulated; 2) for water-table conditions, the free surface must not be steep and resaturation of dry grid blocks cannot occur; and 3) treatment of dispersive processes is based on uniform longitudinal and transverse dispersivity concepts. The program includes a subroutine which allows linkage with the particle tracking program MODPATH.

Contact Address: GeoTrans, Inc., 46050 Manekin Plaza, #100, Sterling, VA 22170, or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 5650 Model Name: 3D-MADPD Released: 1989
Authors: Koussis, A.D., Syriopoulou, D., Ramanujam, G.

3D-MADPD is a suite of PC and mainframe models for simulating 2-D, 2 1/2D (quasi-3D) and 3D solute transport in a steady flow field. The Principal Directions (PD) of the transport form of the mass balance equation is discretized by finite difference approximations along the curvilinear PD coordinates. The integration in each direction is carried out by a Locally One Dimensional (LOD) scheme during each step of the fractional time stepping. Longitudinal transport is computed by the Matched Artificial Dispersivity (MAD) method, limiting the integration to the area of actual plume extent. Grid design requires simultaneous selection of Courant and grid Peclet numbers to meet accuracy constraints. The model has been compared with the chloride plume observed at the Borden landfill, Ottawa, Canada.

Contact Address: A.D. Koussis, Dept. of Civil and Env. Eng., Vanderbilt Univ., Nashville, TN 37235

IGWMC Key: 5800 Model Name: MODMOC-3D Released: 1992
Authors: Williams, P.M.

MODMOC-3D adds a three-dimensional reactive, advective-dispersive solute transport module to the USGS finite difference flow model MODFLOW. The solute transport module is based on the method of characteristics and is compatible with a slightly modified version of the 3D multi-layered version of MODFLOW. MODMOC-3D can be run in 2D or 3D as a flow model, a flow and solute transport model, or as a solute transport model only. When run as a solute transport model, MODMOC-3D uses the starting water levels and aquifer parameter data from the flow model input file to calculate velocities. The model handles decay, linear, Freundlich or Langmuir sorption, monovalent or divalent exchange. It supports solute transport subgrids. Output includes velocities, dispersion coefficients, and concentration distribution.

Contact Address: P.M. Williams, Aquifer Simulation Inc., 102 Chester Road, Fremont, NH 03044

IGWMC Key: 5822 Model Name: SAFTAP Released: 1991

Authors: Huyakorn, P.S., Blandford, T.N.

SAFTAP (SAturated Flow and Transport And Particle tracking) simulates saturated groundwater flow and solute transport in 3D. It is composed of two separate modules: the flow and transport module FTM, and the particle tracking module PTM. FTM is a finite element code for multi-aquifer systems with a wide range of aquifer conditions (e.g., confined, unconfined or partially confined with storage conversion). It analyses 3D unconfined flow using a saturated-pseudo unsaturated modeling approach, allowing the prediction of the water table and flow rates without characterization of the unsaturated zone. Many types of steady-state or time-dependent boundary conditions can be used. Transport mechanisms considered include advection, dispersion, molecular diffusion, adsorption, and first-order degradation.

FTM includes various matrix solvers: direct banded, layer successive over-relaxation, preconditioned-conjugate gradient, and ORTHOMIN accelerated conjugate gradient solver. The most efficient solver is automatically selected dependent on the dimensionality of the problem. The transport equation is approximated using the upstream-weighted residual finite element method. Various types of time-varying sources and observation points may be introduced.

PTM performs 1-D solute transport analysis along a pathline defined through input of head distribution and interpolation of velocities. It uses the 1D upstream-weighted finite element method and include advection, longitudinal dispersion, retardation and first-order degradation. PTM's output can be used by various post-processing software, such as the GRAF module of the WHPA code for pathline generation..

Contact Address: HydroGeologic, Inc., 1165 Herndon Parkway, Suite 900, Herndon, VA 22070

Appendix C.3: *Solute Transport; Three-Dimensional Numerical Models for Saturated Zone, Part 2:* Usability and Reliability

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
515	PTC	Y	U	Y	Y	Y	L	Y	U	L	L	M
582	GREASE	U	U	Y	Y	N	L	Y	U	L	L	F
692	SWIP/SWIPR/ DWDM	N	N	Y	Y	N	N	Y	U	L	L	M
697	SWENT	N	N	Y	Y	N	N	Y	U	L	L	F
2070	CFEST	Y	Y	Y	Y	Y	Y	Y	U	E	E	M
2691	RAND3D	Y	Y	Y	Y	Y	L	U	U	L	U	F
3840	SWIFT	N	N	Y	Y	N	N	Y	Y	E	E	M
3841	SWIFT II	Y	N	Y	Y	N	N	Y	Y	E	E	M
3842	SWIFT III/ SWIFT-386	Y	Y	Y	Y	Y	L	Y	U	E	E	M
4610	HST3D	Y	Y	Y	Y	N	L	Y	U	L	U	M
4631	SWICHA	Y	Y	Y	Y	Y	Y	Y	U	L	U	F
4700	DSTRAM	Y	Y	Y	Y	Y	Y	Y	U	L	U	U
4933	TARGET-3DS	Y	Y	Y	Y	Y	Y	Y	U	L	U	U
4941	DYNTRACK	Y	Y	Y	Y	Y	Y	Y	U	L	U	M
4970	MT3D	Y	Y	Y	Y	Y	Y	Y	U	L	L	M
5161	INTERTRANS	Y	Y	Y	Y	Y	Y	U	U	U	U	U
5520	FTWORK	N	N	Y	Y	N	L	Y	N	L	L	F
5650	3D-MADPD	U	U	Y	Y	U	U	Y	U	L	U	U
5800	MODMOC-3D	Y	Y	Y	Y	Y	Y	U	U	L	U	U
5822	SAFTAP	Y	Y	Y	Y	Y	Y	Y	U	L	L	U

KEY: Y = YES N = NO L = LIMITED E = EXTENSIVE M = MANY F = FEW U = UNKNOWN

Appendix C.4: Solute Transport; Models for Unsaturated Zone, Part 1: Model Description

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IGWMC Key: 583 Model Name: SATURN Released: 1985
Authors: Huyakorn, P.S., S.D. Thomas, J.W. Mercer, and B.H. Lester

SATURN (SATurated-Unsaturated flow and RadioNuclide transport) is a two-dimensional finite element model to simulate transient, single phase fluid flow and advective-dispersive transport of radionuclides and other contaminants in fully or partially saturated, anisotropic, heterogeneous porous media. The flow problem is solved using the Galerkin method to approximate the governing equation, and either the Picard or Newton-Raphson iterative techniques to treat material nonlinearities. It uses the upstream-weighted residual method to treat the transport equation.

Contact Address: D.S. Ward, GeoTrans, Inc., 46050 Manekin Plaza, Suite 100, Sterling, VA 22170

IGWMC Key: 2891 Model Name: GS2 Released: 1985
Authors: Davis, L.A., and G. Segol

GS2 is a two-dimensional Galerkin finite element code for the analysis of flow and contaminant transport in partially saturated media. Either vertical or horizontal plane simulation is possible. Mass transport analysis includes convection, dispersion, radioactive decay and adsorption.

Contact Address: L.A. Davis, Water, Waste and Land, Inc., 1311 S. College Avenue, Fort Collins, CO 80524

IGWMC Key: 2892 Model Name: GS3 Released: 1985
Authors: Davis, L.A., and G. Segol

GS3 is a three-dimensional Galerkin finite element code for analysis of fluid flow and contaminant transport in partially saturated media. The code is particularly useful for simulation of anisotropic systems with strata of varying thickness and continuity. This code contains many of the same features as UNSAT2 (IGWMC Key # 0021) such as the ability to simulate mixed Dirichlet and Neuman boundary conditions for flow and mass transport (concentration of waste leaving the system through evaporated water is zero) by specifying minimum surface pressure and maximum infiltration rate, and seepage faces. However, it will not simulate evapotranspiration by defining a root zone and corresponding plant species data. Unsaturated hydraulic properties are input in table form. There is no restart feature.

Contact Address: L.A. Davis, Water, Waste and Land, Inc., 1311 S. College Avenue, Fort Collins, CO 80524

IGWMC Key: 3234 Model Name: VADOSE Released: 1982
Author: Sagar, B.

VADOSE is an integrated finite difference model for analysis of steady or transient, two-dimensional areal, cross-sectional or radial simulation of coupled density-dependent transport of moisture, heat and solutes in variably-saturated, heterogeneous, anisotropic porous media.

Contact Address: B. Sagar, Southwest Research Inst., Div. 20, 6220 Culebra Road, P.O. Drawer 0510, San Antonio, TX 38510

IGWMC Key: 3235 Model Name: FLOTRA Released: 1982
Author: Sagar, B.

FLOTRA is an integrated finite difference model for simulation of steady or transient, two-dimensional areal, cross-sectional or radial, density- dependent flow, heat and mass transport in variably saturated, anisotropic, heterogeneous, deformable porous media.

Contact Address: B. Sagar, Southwest Research Inst., Div. 20, 6220 Culebra Road, P.O. Drawer 0510, San Antonio, TX 38510

IGWMC Key: 3238 Model Name: PORFLOW-3D Released: 1992
Author: Runchal, A.K.

PORFLOW-3D is an integrated finite difference model to simulate coupled transient or steady-state, multiphase, fluid flow, and heat, salinity, or chemical species transport in variably saturated porous or fractured, anisotropic and heterogeneous media. The program facilitates arbitrary sources or sinks in three-dimensional cartesian or axisymmetric (cylindrical) geometry. The user interface is based on the FREEFORM language using simple English-like commands. The software includes the ARCPLOT graphic post processor.

Contact Address: A. Runchal, 1931 Stradella Road, Bel Air, CA 90077

IGWMC Key: 3371 Model Name: FEMWASTE/FECWASTE Released: 1987
Authors: Yeh, G.T., and D.S. Ward

FEMWASTE/FECWASTE are two-dimensional finite element models for transient simulation of areal or cross-sectional transport of dissolved non-conservative constituents for a given velocity field in an anisotropic, heterogeneous saturated or unsaturated porous medium. The velocity field is generated by the accompanying FEMWATER/FECWATER two-dimensional flow models.

Contact Address: G.T. Yeh, Penn State Univ., Dept. of Civil Eng., 225 Sackett Bldg, University Park, PA 16802

IGWMC Key: 3411 Model Name: LEACHMP Released: 1992
Authors: Wagenet, R.J., and J.L. Hutson

LEACHMP Leaching Estimation And CHemistry Model - Pesticides) simulates transport and fate of non-volatile pesticides in the unsaturated zone. Finite difference techniques are used to calculate water and solute movement. It models a multilayered soil profile under transient conditions and can incorporate linear equilibrium adsorption and degradation of pesticides and plant uptake of water and pesticides. The model can address multiple rainfall and evaporation cycles including ponding conditions. Pesticides can be applied in wet or dry form to the soil surface. The program allows for oxidation and hydrolysis reactions of pesticides, such as Aldicarb.

Contact Address: R.J. Wagenet, Dept. of Soil, Crop and Atmospheric Sc., Cornell Univ., Ithica, New York 14853

IGWMC Key: 3432 Model Name: CXTFIT Released: 1985
Authors: Parker, J.C., M.Th. Van Genuchten

The purpose of CXTFIT is to determine values for one-dimensional analytical solute transport parameters using a nonlinear least-squares inversion method. The analytical model includes advection, dispersion, diffusion, first-order decay and zero-order production.

Contact Address: J.C. Parker, Virginia Polytechnical Institute, Dept. Soil & Environmental Science, Blacksburg, VA 24061; or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 3450/3451 Model Name: DISPEQ/DISPER/PISTON Released: 1983
Authors: Fluhler, H., and W.A. Jury

DISPEQ/DISPER/PISTON is a series of three finite difference research models to simulate one-dimensional transport of reactive solute species through soil columns, including dispersion, instantaneous equilibrium adsorption (DISPEQ) and rate dependent adsorption (DISPER). PISTON is based on piston type flow without dispersion.

Contact Address: H.U. Fluhler, 240 Nick Davis Road, Madison, AL 35758

IGWMC Key: 3540 Model Name: CREAMS Released: 1982
Author: Knisel, W.G.

CREAMS (A field scale model for Chemicals, Runoff, and Erosion from Agricultural Management Systems) is a general watershed model designed to evaluate non-point source pollution from alternate management practices for field-size areas. It consists of three main components: hydrology, erosion/sedimentation and chemistry. The hydrology model handles storm runoff, infiltration, soil water movement (providing amount of seepage beneath root zone and initial soil water content before a storm), and soil/plant evapotranspiration between storms. The chemistry model includes a nutrient (nitrogen and phosphorus) submodel and a pesticide submodel. CREAMS was developed for evaluation of agricultural management systems and their effects on non-point pollution potential. CREAMS is the predecessor of GLEAMS.

Contact Address: W.G. Knisel, USDA Agricultural Research Service, Southeast Watershed Research Laboratory, P.O. Box 946, Tifton, GA 31793

IGWMC Key: 3541 Model Name: GLEAMS Released: 1990
Authors: Leonard, R.A., W.G. Knisel, and F.M. Davis

GLEAMS (Groundwater Loading Effects on Agricultural Management Systems) was developed as an extension of an earlier USDA model, CREAMS. Both models simulate soil water balance and surface transport of sediments and chemicals from agricultural field management units. GLEAMS, in addition, simulates chemical transport in and through the plant root zone. Several other features were added such as irrigation/chemigation options, pesticide metabolite tracking, and software to facilitate model implementation and output data analysis. Input requirements for the model include daily rainfall volumes, crop and management parameters; soil and physical parameters; pesticide property data such as solubility, and expected half-life in soil and/or foliage.

Contact Address: USDA-ARS, P.O. Box 946, Tifton, GA 31793

IGWMC Key: 3830 Model Name: SUTRA Released: 1990
Author: Voss, C.I.

SUTRA (Saturated-Unsaturated TRAnsport) simulates transient or steady-state, two-dimensional, variably saturated, fluid density dependent ground water flow with transport of energy or chemically reactive species solute transport. The model employs a hybrid finite-element and integrated-finite-difference method to approximate the coupled equations. Solute transport include advection, dispersion, diffusion, equilibrium adsorption on the porous matrix, and both first-order and zero-order decay or production. Energy transport may take place in both the solid matrix and the liquid phase. SUTRA may be employed in both areal (horizontal) and cross-sectional mode for saturated systems or in cross-sectional mode only for unsaturated systems.

SUTRA provides, as preliminary calculated results, fluid pressures and either solute concentrations or temperatures. Mesh construction is flexible for arbitrary geometries employing quadrilateral finite elements in Cartesian or radial-cylindrical coordinates. The mesh might be coarsened through the use of pinch nodes. Boundary conditions, sources and sinks may be time dependent. The model has a rest art option. Options are also available to print fluid velocities, and fluid mass, and solute mass or energy budgets for the system. SUTRA's numerical algorithms are not specifically applicable to non-linearities of unsaturated flow. Therefor SUTRA, as distributed by the USGS, requires fine spatial and temporal discretization for unsaturated flow. The user can replace the included function for unsaturated flow by others, and recompile the code.

Contact Address: Voss, C.I., U.S. Geological Survey, 431 National Center, Reston, VA 22092; Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401; or Scientific Software, Washington, D.C.

IGWMC Key: 4081 Model Name: TRIPM Released: 1983
Author: Gureghian, A.B.

TRIPM is a two-dimensional finite element model to predict the transport of radionuclides decay chain into and in a phreatic aquifer. It simulates the simultaneous cross-sectional flow water and the transport of reacting solutes through saturated and unsaturated porous media. The influence of soil-water pH on the distribution coefficient is included. Boundary conditions include seepage faces.

Contact Address: Performance Assessment Dept., Office of Nuclear Waste Isolation, Battelle Project Management Division, 505 King Avenue, Columbus, OH 43201

IGWMC Key: 4140 Model Name: MLSOIL/DFSOIL Released: 1984
Authors: Sjoreen, A.L., D.C. Kocher, G.G. Killough, and C.W. Miller.

MLSOIL (Multi-Layer SOIL model) calculates an effective ground surface concentration to be used in computations of external doses. The program implements a five compartment linear-transfer model to calculate the concentrations of radionuclides in the soil following deposition on the ground surface from the atmosphere. The model considers leaching through the soil as well as radioactive decay and buildup. DFSOIL calculates the dose in air per unit concentration at 1m above the ground from each of the five soil layers used in MLSOIL and the dose per unit concentration from an infinite plane source. MLSOIL and DFSOIL are part of the Computerized Radiological Risk Investigation System (CRRIS).

Contact Address: A.L. Sjoreen, Oak Ridge Nat. Lab., Health and Safety Research Div., Oak Ridge, Tennessee 37831

IGWMC Key: 4270 Model Name: TRACR3D Released: 1984
Author: Travis, B.J.

TRACR3D is a three-dimensional finite difference model for simulation of transient two-phase flow of water and air and transport of non-conservative multi-component transport in deformable, heterogeneous, water-saturated or variably-saturated, reactive porous and/or fractured media.

Contact Address: Travis, B.J., Los Alamos National Laboratory, MS-F665, Los Alamos, NM 87545

IGWMC Key: 4290 Model Name: CADIL/AGTEHM Released: 1984
Authors: Emerson, C.J., B. Thomas, R.J. Luxmoore, and D.M. Hetrick

CADIL (Chemical Adsorption and Degradation In Land) is a moisture and chemical species mass balance model which simulates chemical transport through soils. It includes the processes of deposition, infiltration, adsorption (Freundlich isotherm) and first-order (bio-)chemical degradation of chemicals. It also simulates the effect of soil temperature on chemical degradation. Chemical transport in soil water may be either vertical or lateral. Both macropore and matrix flows of chemicals in soil water are modeled. CADIL couples to AGTEHM, which in turn calculates soil water transport through the bulk matrix and soil macro-pores. AGTEHM simulates interception, throughfall, infiltration, soil evaporation, plant transpiration, and surface runoff.

Contact Address: Emerson, C.J., Oak Ridge National Laboratory, Computer Sciences Department, Oak Ridge, TN 37831

IGWMC Key: 4350 Model Name: FEMTRAN Released: 1984
Author: Martinez, M.J.

FEMTRAN is a two-dimensional finite element model to simulate cross-sectional advective radionuclide transport in saturated/unsaturated porous media. The model considers chain-decay of the radionuclides. It requires user prescribed heads.

Contact Address: M. Martinez, Sandia National Laboratories, Fluid Mechanics and Heat Transfer Div., Albuquerque, NM 87185

IGWMC Key: 4391 Model Name: SBIR Released: 1987
Author: Li, R-M.

SBIR is a three-dimensional finite difference model for simulation of flow and mass transport in a variable saturated porous medium. A vector processor is used in the solution. Benchmark tests indicated the relatively high efficiency of the code.

Contact Address: Li, Ruh-Ming, 3901 Westerly Place, Suite 101, Newport Beach, CA 92660

IGWMC Key: 4570 Model Name: VS2D/VS2DT Released: 1990
Authors: Lappala, E.G., R.W. Healy, and E.P. Weeks

VS2D is a two-dimensional finite difference simulator for cross-sectional or cylindrical variably saturated flow in porous media. The model allows consideration of non-linear storage, conductance, and sink terms and boundary conditions. Processes included are infiltration, evaporation and plant root uptake. The program also handles seepage faces. VS2DT is a solute transport module to be used with VS2D. It is based on a

(continued.....)

VS2D/VS2DT -- continued

finite difference approximation of the advection-dispersion equation for a single species. Program options include first-order decay, equilibrium adsorption described by Freundlich or Langmuir isotherms, and ion-exchange. Nonlinear storage terms are linearized by an implicit Newton-Raphson method.

Nonlinear conductance terms, boundary conditions, and sink terms are linearized implicitly. Relative hydraulic conductivity is evaluated at cell boundaries by using full upstream weighting, the arithmetic mean, or the geometric mean of values of adjacent cells. Saturated hydraulic conductivities are evaluated at cell boundaries by using distance weighted harmonic means. The linearized matrix equations are solved using the strongly implicit method. Nonlinear conductance and storage coefficients are represented by closed-form algebraic equations or interpolated from tables.

Nonlinear boundary conditions treated by the code include infiltration, evaporation, and seepage faces. Extraction by plant roots is included as a nonlinear sink term. Initial conditions may be input as moisture content or pressure head by blocks defined by row and column, or in a formatted file by cell. An equilibrium profile may be specified above a user defined free water surface. Infiltration may be simulated by specified flux nodes, specified pressure nodes, or a ponding function where the user specifies rainfall rate and ponding height. Evaporation is simulated by a user defined potential evapotranspiration, pressure potential of the atmosphere, and surface resistance. Evapotranspiration is simulated through the use of user defined potential evapotranspiration, minimum root pressure, depth of rooting, and root activity at the bottom of the root zone and land surface. Seepage faces may also be simulated.

Contact Address: Weeks, E.P., U.S. Geological Survey, Box 25046, M.S. 413, Denver Federal Center, Denver, CO 80225; or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 4630 Model Name: FLAMINCO Released: 1985
Author: Huyakorn, P.S.

FLAMINCO is a three-dimensional upstream weighted finite element model to simulate transient water flow and solute transport processes in fully- and variably saturated porous media. Transport processes included are advection, hydrodynamic dispersion, linear equilibrium adsorption and first-order decay. Nonlinearities due to unsaturated soil properties and atmospheric boundary conditions are treated using Picard iterations. The model uses a Slice Successive Over Relaxation (SSOR) matrix solution scheme.

Contact Address: D.S. Ward, GeoTrans, Inc., 46050 Manekin Plaza, Suite 100, Sterling, VA 22170

IGWMC Key: 4690 Model Name: VAM2D Released: 1988
Author: Huyakorn, P.S.

VAM2D (Variably saturated Analysis Model in 2 Dimensions) is a two-dimensional Galerkin finite element model to simulate flow and contaminant transport in variably saturated porous media. The code can perform simulations in an areal plane, a cross-section, or an axisymmetric configuration. The highly nonlinear soil moisture relations can be treated using Picard or Newton-Raphson iterations. The model uses the upstream weighted residual method to treat the advective-dispersive transport equation with linear or non-linear equilibrium sorption, and first-order degradation. Cross-sectional unconfined flow problems can be analyzed using a rigorous unsaturated-saturated modeling approach or an approximate saturated-pseudo unsaturated modeling approach that does not require user-supplied soil moisture relations.

Contact Address: HydroGeologic, Inc., 1165 Herndon Parkway, Suite 100, Herndon, VA 22070

IGWMC Key: 4691 Model Name: VAM3D Released: 1988
Author: Huyakorn, P.S.

VAM3D (Variably saturated Analysis Model in 3 Dimensions) is a three-dimensional finite-element model for simulation of flow and contaminant transport in variably saturated porous media. It is capable of steady-state and transient simulations in an areal plane, a cross-section, an axisymmetric configuration, or a fully three-dimensional mode using rectangular and triangular prisms. Nonlinearities in the unsaturated flow equation is solved using Picard iteration. The matrix equations are solved using a slice-successive over-relaxation scheme or conjugate gradient algorithms. The advective-dispersive transport equation is solved using upstream weighted procedure. Transport includes linear and Freundlich adsorption isotherms and first-order degradation. An element mesh generator is available.

Contact Address: HydroGeologic, Inc., 1165 Herndon Parkway, Suite 100, Herndon, VA 22070

IGWMC Key: 4693 Model Name: VADOFT Released: 1988
Authors: Huyakorn, P.S., T.D. Wadsworth, H.O. White Jr., and J.E. Buckley

VADOFT is a one-dimensional finite element code that solves the Richard's equation for flows in the unsaturated zone. The user may make use of constitutive relationships between pressure, water content, and hydraulic conductivity to solve the flow equations. VADOFT also simulates the fate and transport of two parent and two daughter products.

Contact Address: Hydrogeologic, Inc., 1165 Herndon Parkway, #900, Herndon, VA 22070

IGWMC Key: 4720 Model Name: PRZM Released: 1984
Authors: Carsel, R.F., C.N. Smith, L.A. Mulkey, and J.D. Dean

PRZM (Pesticide Root Zone Model) simulates the vertical one-dimensional movement of pesticides in the unsaturated zone within and below the root zone. The model consists of hydrologic (flow) and chemical transport components to simulate runoff, erosion, plant uptake, leaching, decay, foliar washoff, and volatilization. Pesticide transport and fate processes include advection, dispersion, molecular diffusion, and soil sorption. The model includes soil temperature effects, volatilization and vapor phase transport in soils, irrigation simulation and a method of characteristics algorithm to eliminate numerical dispersion. PRZM is capable of simulating fate and transport of the parent and up to two daughter species. Predictions can be made for daily, monthly or annual output. A finite difference numerical solution, using a backwards difference implicit scheme, is employed. PRZM allows the user to perform dynamic simulations considering pulse loads, predicting peak events, and estimating time-varying emission or concentration profiles in layered soils. PRZM, VADOFT and SAFTMOD are part of RUSTIC. RUSTIC (MARS Key # 4721) links these models in order to predict the fate and transport of chemicals to drinking water wells. The codes are linked together with the aid of a flexible execution supervisor (software user interface) that allows the user to build models that fit site-specific situations.

Contact Address: R.F. Carsel, U.S. Environm. Prot. Agency, Environm. Res. Lab., Athens, GA 30613

IGWMC Key: 4721 Model Name: RUSTIC Released: 1989
Authors: Dean, J.D., P.S. Huyakorn, A.S. Donigan, Jr., K.A. Voos, R.W. Schanz, Y.J. Meeks, and R.F. Carsel

RUSTIC is a coupled root zone (PRZM), unsaturated zone (VADOFT), and saturated zone (SAFTMOD) modeling package. RUSTIC links these models in order to predict the fate and transport of chemicals to drinking water wells. The codes are linked together with the aid of a flexible execution supervisor (software interface) that allows the user to build models that fit site-specific situations. For exposure assessments, the code is equipped with a Monte Carlo pre- and post-processor.

Contact Address: R.F. Carsel, U.S. EPA, Environm. Res. Lab., Athens, GA 30613

IGWMC Key: 4931 Model Name: TARGET-2DU Released: 1985
Authors: Moreno, J.L., M.I. Asgian, S.D. Lympany, and P-J. Pralong.

TARGET-2DU is one of five models of the TARGET series (Transient Analyzer of Reacting Groundwater and Effluent Transport). It simulates two-dimensional, variably saturated, density coupled, transient groundwater flow and solute transport using a hybrid finite difference method. The transport is based on the solution of the advective-dispersive transport equation for a single non-conservative contaminant with linear equilibrium adsorption (retardation). The solution method used is based on an iterative alternating direction implicit method.

Contact Address: Dames & Moore, 1125 17th Str., #1200, Denver, Colorado 80202

IGWMC Key: 4934 Model Name: TARGET-3DU Released: 1985
Authors: Moreno, J.L., M.I. Asgian, S.D. Lympany, and P-J. Pralong

TARGET-3DU is one of five models of the TARGET series (Transient Analyzer of Reacting Groundwater and Effluent Transport). It simulates three-dimensional, variably-saturated, density-coupled, transient groundwater flow and solute transport using a hybrid finite difference method. The transport is based on the solution of the advective-dispersive transport equation for a single non-conservative contaminant with linear equilibrium adsorption (retardation). The solution method used is based on an iterative alternating direction implicit method.

Contact Address: Dames & Moore, 1125 17th. Str., #1200, Denver, Colorado 80202

IGWMC Key: 5021 Model Name: BIOSOIL Released: 1986
Author: Baek, N.H.

The system modeled by BIOSOIL consists of four components: 1) soil water flow to transport a limiting substrate and a recalcitrant chemical; 2) chemical persistence mitigated by an ultimate removal mechanism of biodegradation; 3) soil microbial growth enriched by exogenous supply of a limiting substrate; and 4) substrate availability to support soil microbial growth for the enhancement of chemical removal. Variable-step and variable order Gear's method is employed as a numerical approximation to solve the set of four ODE's which result from the transformation of four PDE's via the finite difference method. The response of the system to different values for such model inputs as substrate concentration, application rate, and application cycle can be studied.

Contact Address: N.H. Baek, Occidental Chemical Corporation, Technology Center, 2801 Long Road, Grand Island, NY 14072

IGWMC Key: 5028 Model Name: GTC (Group Transfer Concentration) Released: 1985
Authors: Yu, C., W.A. Jester, and A.R. Jarrett

GTC is a general purpose finite difference solute transport model developed to simulate solute movement in both homogeneous and non-homogeneous media. It splits up the modeled area in zones of constant properties, including dispersion coefficient, retardation factor, and degradation rate. Mass transfer between the solid phase and the liquid phase is proportional to the concentration gradient. The GTC model can be used for both saturated and unsaturated conditions. It covers the conventional advection-dispersion model, the mobile-immobile pore model, the nonequilibrium adsorption-desorption model and the jointed porous rock model.

Contact Address: C. Yu, Argonne National Laboratory, 9700 S. Cass Avenue, Argonne, IL 60439

IGWMC Key: 5031 Model Name: CTSPAC Released: 1988
Authors: Lindstrom, F.T., D.E. Cawlfield, and L. Boersma

CTSPAC is an one-dimensional numerical model that couples the flow of water and the transport of heat and solutes in layered soils with the uptake and transport of water and solutes in plants. Initial root distribution is specified. The rate of uptake is a function of the environmental conditions that determine the plant's transpiration rate. Water transport in the plant is based on water potential and pressure gradients according to Munch pressure flow hypothesis. The model was developed for assessing risks involved in the use of xenobiotic chemicals. It allows an evaluation of the rate of uptake of such chemicals from the soil solution and the accumulation in the various plant parts.

Contact Address: L. Boersma, Dept. of Soil Science, Oregon State University, Corvallis, OR 97331

IGWMC Key: 5039 Model Name: SESOIL (Seasonal Soil Compartment Model) Released: 1987
Author: Bonazountas, M.

SESOIL is a user-friendly finite-difference soil compartment model designed for long-term hydrologic, sediment, and pollutant fate simulations. The model distinguishes three major components, the hydrological cycle, the sediment cycle and pollutant transport and fate. Elements of the hydrologic cycle included are rainfall, soil moisture variations, infiltration, exfiltration, surface runoff, evapotranspiration, and groundwater runoff; simulation of the sediment cycle include sediment washload from storms and sediment resuspension due to wind; the pollutant fate cycle simulated takes into account advection, diffusion, volatilization, adsorption and desorption, chemical degradation or decay, biological transformations, hydrolysis, complexation, and ion exchange.

Contact Address: D. Hetrick, 8417 Mecklenburg Court, Knoxville, TN 37923

IGWMC Key: 5186 Model Name: NITRO Released: --
Authors: Kaluarachchi, J.J., and J.C. Parker

NITRO is a 2-dimensional vertical section or radially symmetric finite element program for simulation of steady-state and transient uncoupled flow and transport in the unsaturated zone. The nonlinearity is handled by Picard iteration. Soil hydraulic properties are described by the Brooks-Corey or van Genuchten model with hysteresis. The model handles transport of up to two species with linear or Freundlich equilibrium adsorption and zero and first order transformations. It facilitates atmospheric and seepage boundaries as well as first-type and second-type (flux) boundary conditions.

Contact Address: J.C. Parker, Environmental Systems & Technologies, Inc., P.O. Box 10457, Blacksburg, VA 24062-0457

IGWMC Key: 5213 Model Name: TDFD1O Released: --
Author: Slotta, L.S.

TDFD1O (Two-Dimensional Finite Difference 1st Order sorption) is a two-dimensional model for simultaneous simulation of movement of moisture, transport of heat, and transport and fate of a contaminant in a shallow unconfined aquifer. The porous medium may be heterogeneous. The coupled system of non-linear unsaturated/saturated moisture flow and heat and chemical transport are solved using a finite difference approximation. The porous medium is partitioned in three fractions: sand, clay, and organic material, with for each fraction first-order sorption kinetics included. Time integration is performed using the backward Euler method. Dynamic boundary conditions at the air-porous medium interface are included. A variety of first- and second-type boundary conditions are included.

Contact Address: J. Heydarpour, Slotta Engineering Assoc., Inc., P.O. Box 1376, Corvallis, OR 97339

IGWMC Key: 5220 Model Name: VSAFT2 Released: 1990
Authors: Yeh, T.C.J.

VSAFT2 (Variably SAturated Flow and Transport in 2 dimensions) is a program for simulating two-dimensional steady or transient, variably saturated flow and convective-dispersive transport of a conservative solute, using a finite element method with the Newton-Raphson or Picard iteration scheme. For the linear equation solution a preconditioned conjugate gradient method is used. Solute transport is handled by an upstream weighting scheme. The model uses rectangular and/or triangular finite elements and a banded matrix solver. The two-dimensional flow can be either in a horizontal or in a vertical plane. Furthermore, the model can handle radial symmetric simulations. The code contains a restart feature for changing boundary conditions.

Evapotranspiration is simulated in VSAFT2 by a user specified root zone consisting of one or more plant species. User supplied information on the root zone includes wilting pressure, maximum transpiration rate, root effectiveness function, and root zone geometric data. Evaporation \ Infiltration is simulated through user defined maximum evaporation or infiltration rates, minimum soil surface pressure head, and soil surface geometric data. Analytical functions must be used for relative hydraulic conductivity relationships and moisture characteristic curve functions. The user is given the choice of the van Genuchten model, exponential model, Gardener-Russo model, or a user specified function for which a subroutine must be written.

Contact Address: T.C.J. Yeh, Dept. of Hydrology and Water Resources, Univ. of Arizona, Tuscon, AZ 85721

IGWMC Key: 5310 Model Name: PRZMAL Released: 1986
Authors: Wagner, J., and C. Ruiz-Calzada

PRZMAL is an aquifer linkage model for US EPA's Pesticide Root Zone Model (PRZM). It connects PRZM with the analytical three-dimensional transport model PLUME 3D developed at Oklahoma State University. This linkage allows the user to predict contaminant movement from the point of application, in a continuous manner, into and within the aquifer.

Contact Address: J. Wagner, Oklahoma State Univ., School of Chem. Eng., Stillwater, OK 74074

IGWMC Key: 5500 Model Name: BIO1D Released: 1989
Authors: Srinivasan, P., and J.W. Mercer

BIO1D is a one-dimensional finite difference model for simulation of biodegradation and sorption in reactive contaminant transport in a uniform flow field. Advective and dispersive transport of a substrate and an electron acceptor are considered. The reactions may include aerobic (Monod function) and anaerobic (Michaelis- Menten kinetics) degradation, and/or adsorption described by a linear, Freundlich or Langmuir equilibrium isotherm. Dirichlet, Neumann, or Cauchy boundary conditions are allowed. The resulting nonlinear problem is solved using a Newton-Raphson itrtive technique. The program includes an user-friendly preprocessor and post simulation display graphics. The program assumes flow velocities known.

Contact Address: GeoTrans, Inc., 46050 Manekin Plaza, Suite 100, Sterling, VA 22170

IGWMC Key: 5630 Model Name: MULTIMED Released: --
Authors: --

MULTIMED is a multimedia transport model that simulates the movement of contaminants leaching from a waste disposal facility. The model includes two options or simulating leachate flux. Either the infiltration rate to the unsaturated or saturated zone can be specified directly or a landfill module can be used to estimate the infiltration rate. The landfill module is one-dimensional and steady-state, and simulates the effect of precipitation, runoff, infiltration, evapotranspiration, barrier layers (which can include flexible membrane liners), and lateral drainage. A steady-state, one-dimensional, semi-analytical module simulates flow in the unsaturated zone. The output from this module, water saturation as function of depth, is used as input to the unsaturated transport module.

The unsaturated transport module simulates transient, one-dimensional (vertical) transport and includes the effects of longitudinal dispersion, linear adsorption, and first-order decay. Output from this module -i.e. steady-state or time-varying concentrations at the water table- is used to couple the unsaturated zone transport module with a steady-state or transient, semi-analytical saturated zone transport module. The saturated zone transport model of MULTIMED includes one-dimensional uniform flow, three-dimensional dispersion, linear adsorption (retardation), first-order decay, and dilution due to direct infiltration into the ground water plume. Contamination of a surface stream due to the complete interception of a steady-state saturated zone plume is simulated by the surface water module. Finally, the air emissions and the atmosphere dispersion modules simulate the movement of chemicals into the atmosphere. The module includes option for Monte Carlo simulations.

Contact Address: U.S. EPA, Environm. Res. Lab., Athens, GA 30613

IGWMC Key: 5661 Model Name: FLAME Released: 1992
Authors: Baca, R.G., and S.O. Magnuson

FLAME is a finite element code designed to simulate two-dimensional, cross-sectional subsurface transport of low-concentration contaminants in either time-dependent or steady-state, known flow field in a highly heterogeneous variably-saturated porous media with complex stratigraphy. The code can be applied to two-dimensional transport in an arid vadose zone or in an unconfined aquifer. FLAME handles advective-dispersive transport, equilibrium sorption using a linear isotherm, first-order decay, and a complex source/sink term. It accommodates advection-dominated mass transport. In addition, the code has the capability to describe transport processes in a porous media with discrete fractures. It describes the mass transfer between the porous media and discrete fractures.

(continued.....)

FLAME -- continued

FLAME can handle both Dirichlet and Neumann transport boundary conditions. The code can model transport of contaminants in a single phase, being either liquid, gaseous (e.g. organic vapors), or colloidal. The modified equation approach of Fletcher with a build-in dissipation mechanism is used to dampen oscillations in a convection dominated transport system. The resulting finite element matrix equations are solved by a Gaussian elimination procedure without pivoting. Two solvers are used: 1) standard band solver utilizing a skyline storage scheme, and 2) frontal method.

Contact Address: Baca, R.G., Idaho Nat. Eng. Lab., EG&G Idaho, Inc., P.O. Box 1625, Idaho Falls, Idaho 83415

IGWMC Key: 5681 Model Name: VIP Released: 1991
Authors: Stevens, D.K., W.J. Grenney, and Z. Yan

VIP (Vadose zone Interactive Processes model) is an one-dimensional finite-difference solute transport and fate model for simulating the behavior of organic (oily) compounds in the vadose zone as part of a land treatment system. The model uses advection and dispersion in the water and air phases as the dominant transport mechanism for contaminant and oxygen. Monthly values for recharge rate and soil moisture conditions are used to calculate an effective water velocity. The model includes first-order degradation of a contaminant in water, air and soil, and of oxygen. It uses an implicit technique to calculate the degradation of the contaminant in the oil phase as well as the oil phase itself, and related oxygen changes.

VIP uses partition coefficients and rate constants to calculate contaminant concentration in each medium. The model has various output options including echo of input data, (graphic) profile of initial condition (constituent concentration in water, oil, air, and soil phases), and the initial fractions as well as initial oxygen concentration. Other output options include (graphic) depth-concentration profiles and data versus time tables. Input preparation facilitates exchange of Lotus 123 and wordprocessed ASCII files.

Contact Address: D.K. Stevens, Civil and Environm. Eng. Dept., Utah State Univ., UMC 4110, Logan, Utah 84321; or Center for Subsurface Modeling Support (CSMOS), R.S. Kerr Environm. Res. Lab., U.S. EPA, P.O. Box 1198, Ada, OK 74820

IGWMC Key: 5690 Model Name: VLEACH Released: 1990
Author: J. Turin

VLEACH (Vadose Zone LEACHing Model) is a relatively simple one-dimensional finite difference model designed to simulate leaching of a volatile, adsorbed contaminant through the vadose zone. It can be used to simulate the transport of any non-reactive chemical that displays linear partitioning behavior. In particular, VLEACH simulates downward liquid-phase advection, solid-phase sorption, gas diffusion in the vapor phase, and three-phase equilibrium. The contaminant mass within each model cell is partitioned among liquid (dissolved in water), vapor, and solid phases. The model assumes a homogeneous porous medium with steady flow and no dispersion. There is no in-situ degradation or production, and free product is not present. Input data for VLEACH consists of: organic carbon coefficient (Koc), Henry's Law constant (Kh), the aqueous solubility and the free air diffusion coefficient. The input soil properties are dry bulk density, total porosity, volumetric water content and organic carbon fraction, and site-specific input parameters such as recharge rate and depth to groundwater.

Contact Address: Center for Subsurface Modeling Support (CSMOS), R.S. Kerr Environm. Res. Lab., U.S. EPA, P.O. Box 1198, Ada, OK 74820; or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401

IGWMC Key: 5850 Model Name: RZWQM Released: 1990
Authors: DeCoursey, D.G., K.W. Rojas, and L.R. Ahuja

RZWQM (Root Zone Water Quality Model) is a physically based model simulating the movement of water, nutrients, and pesticides over and through the root zone at a representative point in a field. The physical processes included are soil matrix infiltration, macropore flow, surface runoff, heat flow, potential evaporation, and transpiration, soil-water redistribution and chemical transport. Root water uptake, actual evaporation and transpiration, are calculated in the crop growth section in conjunction with water redistribution and plant growth. Soil chemical processes include bicarbonate buffering, dissolution and precipitation of calcium carbonate, gypsum, and aluminum hydroxide, ion exchange involving bases and aluminum, and solution chemistry of aluminum hydroxide. RZWQM also includes various nutrient processes such as decomposition of organic matter, mineralization, immobilization and demineralization of appropriate nitrogen and phosphorus species, and adsorption/desorption of both species. Pesticide processes the model can handle include computation of the amount of pesticides reaching the soil surface, and the amounts absorbed and moving through each soil layer. Dissipation via volatilization, photolysis, hydrolysis, biodegradation, oxidation, and complexation are simulated. These processes may be lumped in a single process. Other pesticide related processes simulated in RZWQM are dissipation by formulation of metabolites (tracked throughout their life time). Either equilibrium isotherms or kinetic adsorption/desorption processes may be simulated. The model allows to include certain management practices such as effects of tillage practices on chemical distribution, soil density, and macro- and microporosity; fertilizer and pesticide applications; planting densities; and irrigation and drainage practices.

Contact Address: L.R. Ahuja, USDA Agric. Res. Service, P.O. Box E, Fort Collins, CO 80522

IGWMC Key: 5860 Model Name: NEWTMC Released: 1985
Authors: Lindstrom, F.T., and F.T. Piver

NEWTMC is an one-dimensional mass balance model for simulating the transport and fate of nonionizable organic compounds in unsaturated/saturated porous media. Using the principles of water mass, momentum, heat energy and chemical mass balance, the model solves simultaneously for moisture, temperature and liquid phase chemical concentration. The model uses a dynamic free boundary to represent the air-soil interface and a prescribed water table height as lower boundary. The model allows for elaborate simulation of air conditions at the air-soil interface, allowing the boundary conditions to be dependent on the air conditions. Chemicals may be introduced via incoming air (vapor phase), rain water, inflow from the water table, or initially distributed within the soil column.

Contact Address: Lindstrom, F.T., Dept. of Mathematics, Oregon State Univ., Corvallis, OR 97331

IGWMC Key: 6130 Model Name: PESTAN Released: 1990
Authors: Enfield, C.G., R.F. Carsel, S.Z. Cohen, and T. Phan

PESTAN (PESticide Analytical Model) is an interactive analytical model, used for estimating organic chemical movement in the unsaturated zone. The model is based on an analytical solution of the convective dispersive solute transport equation for single layer homogeneous soils. It calculates vertical convective movement of chemicals with linear equilibrium sorption and first-order (bio-) chemical decay. Hydrologic loading is based on annual water balance. The primary application has been for pesticide screening.

Contact Address: Center for Subsurface Modeling Support (CSMOS), R.S. Kerr Environm. Res. Lab., U.S. EPA, P.O. Box 1198, Ada, OK 74820; or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 6225 Model Name: CHAIN Released: 1985
Author: van Genuchten, M. A.

The CHAIN model simulates multi-ion transport across the unsaturated zone using an analytical procedure. The model includes longitudinal dispersion and first-order decay. It calculates the time history of chemical concentration exiting the unsaturated zone.

Contact Address: M.Th. van Genuchten, U.S. Salinity Lab., Agricultural Res. Service, 4500 Glenwood Drive, Riverside, CA 92501

IGWMC Key: 6229 Model Name: HYDRUS/WORM Released: 1992
Authors: Kool, J.B., M.Th. van Genuchten

HYDRUS is a Galerkin linear finite element program for simulation of transient one-dimensional flow and solute transport in variably saturated porous media. The solution of the flow problem considers the effects of root uptake and hysteresis in the soil hydraulic properties. The solute transport equation incorporates the processes of ionic or molecular diffusion, hydrodynamic dispersion, linear or nonlinear equilibrium adsorption, and first-order decay. Boundary conditions for the flow and transport may be constant or time-varying. For flow boundary conditions, HYDRUS can solve the steady-state flow equation in a single step without the need of performing time-marching. The HYDRUS program is a modification of the WORM program developed at the U.S. Salinity Laboratory.

The solution of the flow equation in HYDRUS requires specification of the initial condition in terms of pressure head or water content. Either first- or second-type boundary conditions can be imposed at the soil surface. Alternatively, the upper boundary condition may be specified in terms of total amount of surface applied water, combining both types of boundary conditions. The auxiliary condition at the lower boundary is given in terms of imposed pressure head, zero head gradient, or imposed net drainage flux. Type of boundary condition might change in time.

Soil hydraulic properties in HYDRUS can be described by the parametric functions of Van Genuchten (1978). Uptake of water by plant roots includes evapotranspiration, a normalized root uptake distribution function, and a pressure-salinity stress response function. HYDRUS uses the fully-implicit scheme to solve the set of matrix equations for flow and transport. Nonlinearities in the flow equations are treated using Picard iteration with under-relaxation. For solute transport, corrections are applied to the dispersion coefficient to reduce numerical problems.

Contact Address: M.Th. van Genuchten, U.S. Salinity Lab., Agricultural Res. Service, 4500 Glenwood Drive, Riverside, CA 92501

IGWMC Key: 6390 Model Name: MOUSE Released: 1984
Authors: Pacenka, S., and T. Steenhuis

MOUSE (Method Of Underground Solute Evaluation) is developed for classroom and Cooperative Extension Service educational purposes. The model tracks soluble chemical movement in both the saturated and the unsaturated zone by coupling 1D vertical flow and transport in three-layer soils with 2D cross-sectional flow and transport in an anisotropic, heterogeneous aquifer. Surface runoff is calculated using the USDA Soil Conservation Service curve number equation. Active evapotranspiration occurs in the top layer of the soil. The finite difference model includes first-order degradation, dispersion, diffusion and convective mass movement. Furthermore, the model can handle linear equilibrium adsorption/desorption isotherms.

Contact Address: T. Steenhuis, Cornell Univ., Agricult. Eng. Dept., Ithaca, New York 14853

IGWMC Key: 6620 Model Name: RITZ Released: 1988
Authors: Nofziger, D.L., J.R. Williams, and T.E. Short

RITZ (Regulatory and Investigative Treatment Zone model) is an interactive program for simulation of the movement and fate of hazardous chemicals during land treatment of oily wastes. The model considers a constant water flux and downward movement of the pollutant with the soil solution (leaching), volatilization and loss to the atmosphere, and (bio-)chemical degradation. The treatment site modeled consists of a plow zone and a treatment zone. The model incorporates the influence of oil upon the transport and fate of the pollutant. As input the model requires the properties of the chemicals and oil in the waste material, the soil properties of the treatment site, the management practices, and the parameters relevant to the environment of the site.

Contact Address: J.R. Williams, R.S. Kerr Environm. Res., U.S. EPA, P.O. Box 1198, Ada, OK 74820

IGWMC Key: 6640 Model Name: CHEMRANK Released: 1988
Authors: Nofziger, D.L., P.S.C. Rao, and A.G. Hornsby

CHEMRANK is an interactive package which utilizes four ranking schemes for screening organic chemicals relative to their potential to leach into groundwater systems. The schemes are based on rates of chemical movement or relative rates of mobility and degradation of the chemicals within the vadose zone. Two schemes use steady state groundwater recharge rates and the other two require daily rainfall and evaporation data. The latter two schemes rank chemical mobility by travel time in the vadose zone or mass emission of selected chemicals at some specified depth in the vadose zone.

Contact Address: Inst. of Food and Agricultural Sciences, University of Florida, Gainesville, FL 32611

IGWMC Key: 6710 Model Name: CMIS (Chemical Movement in Soil) Released: 1986
Authors: Nofziger, D.L., and A.G. Hornsby

CMIS is a management/educational computer program that provides qualitative predictions of pesticide fate as function of key soil, chemical, and climatic variables. Model assumptions limit it to nonpolar pesticides (and other xenobiotics) moving in sandy soils. Linear adsorption/desorption isotherms are used to describe chemical affinity to the soil matrix.

Contact Address: Inst. of Food and Agric. Sciences, IFAS, University of Florida, Building 664, Gainesville, FL 32611

IGWMC Key: 6711 Model Name: CMLS (Chemical Movement in Layered Soils) Released: 1988
Authors: Nofziger, D.L., and A.G. Hornsby

CMLS is an interactive microcomputer model to be used as management tool and a decision aid in the application of organic chemicals to soils. The model estimates the location of the peak concentration of non-polar organic chemicals as they move through a soil in response to the downward movement of water. The model also estimates the relative amount of each chemical still in the soil at any time. The model can deal with soils with up to 20 layers or horizons, each having its own partition coefficient and degradation half-life of the chemical of interest.

Contact Address: Inst. of Food and Agric. Sciences IFAS, University of Florida, Building 664, Gainesville, FL 32611

IGWMC Key: 6712 Model Name: CHEMFLO Released: 1989
Authors: Nofziger, D.L., K.Rajender, S.K. Nayudu, and P-Y. Su.

CHEMFLO is an interactive program for simulating water and chemical movement in unsaturated soils. Water movement is modeled using the Richards equation. Chemical transport is modeled by means of the convection-dispersion equation. These equations are solved numerically for one-dimensional flow and transport using finite differences. Results of the flow model can be displayed in the form of graphs of water content, matric potential, driving force, conductivity, and flux density of water versus distance or time. Graphs of concentration, and flux density of chemical as function of distance or time can also be displayed. CHEMFLO is an expansion and update of the water movement model WATERFLO by Nofziger (1985).

CHEMFLO is an extension and update of WATERFLO by Nofziger (1985; see IGWMC key # 6630). Soil and chemical parameters required by the model include: soil bulk density, water-soil partition coefficient, diffusion coefficient of chemical in water, dispersivity, first-order degradation rates for contaminant in the water and the solid phases, and a zero order rate constant for the liquid. Other parameters required for solving the Richards equation are the function relationships for soil-water retention and unsaturated hydraulic conductivity.

Contact Address: J.R. Williams, R.S. Kerr Environm. Res. Lab., U.S. EPA, Ada, Oklahoma 74820

Appendix C.4: Solute Transport; Models for Unsaturated Zone, Part 2: Usability and Reliability

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
583	SATURN	N	N	Y	Y	N	N	Y	U	L	L	F
2891	GS2	U	U	Y	Y	N	N	Y	U	L	L	F
2892	GS3	U	U	Y	Y	N	N	Y	U	L	L	F
3234	VADOSE	Y	Y	Y	Y	Y	Y	Y	U	L	L	F
3235	FLOTRA	Y	Y	Y	Y	Y	Y	Y	U	L	L	F
3238	PORFLOW-3D	Y	Y	Y	Y	Y	Y	Y	U	E	L	F
3371	FEMWASTE/ FECWASTE	N	N	Y	Y	N	Y	Y	U	E	L	M
3411	LEACHM(-P)	Y	Y	Y	Y	Y	L	Y	U	E	L	M
3432	CXTFIT	Y	Y	Y	Y	Y	Y	Y	U	L	U	M
3450/ 3451	DISPEQ/ DISPER/PISTON	N	N	Y	Y	N	N	Y	U	L	U	F
3540	CREAMS	Y	Y	Y	Y	N	L	Y	U	E	L	M
3541	GLEAMS	Y	Y	Y	Y	N	L	Y	U	E	L	M
3830	SUTRA	Y	Y	Y	Y	N	L	Y	U	L	L	M
4081	TRIPM	U	U	Y	Y	N	N	Y	U	L	U	F
4140	MLSOIL/DFSOIL	U	U	Y	Y	U	U	Y	U	U	U	U
4270	TRACR3D	U	U	Y	Y	U	U	Y	U	L	U	U
4290	CADIL/AGTEHM	U	U	Y	Y	U	U	Y	N	L	U	U
4350	FEMTRAN	U	U	Y	Y	U	U	Y	U	L	U	U
4391	SBIR	U	U	Y	Y	U	U	Y	U	E	U	U
4570	VS2D/VS2DT	Y	Y	Y	Y	N	L	Y	U	L	L	M

KEY: Y = YES N = NO L = LIMITED E = EXTENSIVE M = MANY F = FEW U = UNKNOWN

Appendix C.4, part 2 (continued)

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
4630	FLAMINCO	N	N	Y	Y	N	N	Y	U	E	L	F
4690	VAM2D	Y	Y	Y	Y	N	L	Y	U	E	L	F
4691	VAM3D	Y	Y	Y	Y	N	L	Y	U	E	L	F
4693	VADOFT	U	U	Y	Y	N	L	Y	U	E	L	F
4720	PRZM	Y	Y	Y	Y	Y	L	Y	U	E	L	M
4721	RUSTIC	U	U	Y	Y	U	U	Y	U	L	U	U
4931	TARGET-2DU	Y	Y	Y	Y	Y	Y	Y	U	L	U	U
4934	TARGET-3DU	Y	Y	Y	Y	Y	Y	Y	U	L	U	U
5021	BIOSOIL	N	N	Y	Y	N	N	Y	U	L	U	F
5028	GTC	U	U	Y	Y	U	U	Y	N	L	U	U
5031	CTSPAC	U	U	Y	Y	U	U	Y	U	L	U	U
5039	SESOIL	Y	Y	Y	Y	Y	Y	Y	U	L	L	M
5186	NITRO	Y	Y	Y	Y	Y	Y	Y	U	L	U	U
5213	TDF1O	U	U	Y	Y	Y	L	Y	U	L	U	U
5220	VSAFT2	Y	Y	Y	Y	Y	L	Y	U	L	U	U
5310	PRZMAL	Y	Y	Y	Y	Y	L	Y	U	L	U	F
5500	BIO1D	Y	Y	Y	Y	Y	L	Y	U	L	L	F

KEY: Y = YES N = NO L = LIMITED E = EXTENSIVE M = MANY F = FEW U = UNKNOWN

Appendix C.4, part 2 (continued)

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
5630	MULTIMED	Y	Y	Y	Y	Y	L	Y	U	L	U	M
5661	FLAME	N	N	Y	Y	U	U	Y	U	E	U	U
5681	VIP	Y	Y	Y	Y	Y	Y	Y	U	L	U	F
5690	VLEACH	N	N	Y	Y	Y	L	Y	U	L	U	U
5850	RZWQM	Y	Y	Y	Y	Y	Y	Y	U	E	L	F
5860	NEWTMC	N	N	Y	Y	N	N	Y	N	L	N	F
6130	PESTAN	Y	N	Y	Y	N	L	Y	U	L	L	M
6225	CHAIN	N	N	Y	Y	N	N	Y	U	L	U	U
6229	HYDRUS/WORM	Y	Y	Y	Y	Y	Y	Y	U	L	U	F
6390	MOUSE	Y	Y	Y	Y	Y	Y	Y	U	L	U	U
6620	RITZ	Y	Y	Y	Y	Y	Y	Y	U	L	U	M
6640	CHEMRANK	Y	Y	Y	Y	Y	Y	Y	U	L	U	M
6710	CMIS	Y	Y	Y	Y	Y	Y	Y	U	L	U	M
6711	CMLS	Y	Y	Y	Y	Y	Y	Y	U	L	U	M
6712	CHEMFLO	Y	Y	Y	Y	Y	Y	Y	U	L	U	M

KEY: Y = YES N = NO L = LIMITED E = EXTENSIVE M = MANY F = FEW U = UNKNOWN

Appendix D: Heat Transport Models, Part 1: Model Description

IGWMC Key: 0100 Model Name: PT/CCC Released: 1981
Authors: M.J. Lippmann, T.N. Narasimhan, D.C. Mangold and G.S. Bodvarsson

PT/CCC is a integrated finite difference method to calculate steady and unsteady temperature and pressure distributions, and vertical compaction in multidimensional heterogeneous systems with complex geometry and a single phase, non-isothermal liquid.

Contact address: Nat. Energy Software Center, Argonne Nat. Lab., 9700 South Cass Avenue, Argonne, IL 60439

IGWMC Key: 0160 Model Name: SCHAFF Released: 1976
Authors: M.L. Sorey and M.J. Lippmann

SCHAFF is a three-dimensional finite difference model to simulate coupled unsteady heat transport and fluid flow in slightly compressible heterogeneous porous media.

Contact address: Nat. Energy Software Center, Argonne Nat. Lab., 9700 South Cass Avenue, Argonne, IL 60439

IGWMC Key: 0513 Model Name: GAFETTA Released: 1980
Authors: G.F. Pinder, P.E. Kinnmark and C.I. Voss

GAFETTA is a two-dimensional finite element model intended to simulate thermal energy transport in confined and unconfined aquifers with horizontal non-density dependent ground water flow. The model computes the distribution of hydraulic head and temperature in an anisotropic, heterogeneous aquifer and allows analysis of temperature changes in over- and underlying layers due to pumping or injection wells, artificial or natural infiltration of hot or cold water, steady leakage of hot or cold water from adjacent aquifers, connection with lakes and rivers, and changing air temperature.

Contact address: C.I. Voss, U.S. Geological Survey, Water Resources Division, 431 National Center, Reston, VA 22092

IGWMC Key: 0581 Model Name: FTRANS Released: 1982
Author: P.S. Huyakorn

FTRANS is a 2-D finite-element model to simulate transient, saturated single phase ground water flow, heat transport, and chemical or radionuclide transport in fractured or unfractured, anisotropic, heterogeneous, multilayered porous media. For any type of fractured system, the flow and transport analysis are performed taking into account interaction between the porous matrix and the fractures. The analyses are made in the main areal flow plane, in a vertical cross-section, or in an axisymmetric configuration. The code fully accounts for fluid leakages, hydrodynamic dispersion, sorption, first-order decay, chain reactions, and solute diffusion and heat conduction in the porous matrix, coupled thermal fluid capability and density-dependent flow and solute transport.

Contact address: Performance Assessment Dept., Office of Nuclear Waste Isolation, Battelle Project Management Division, 505 King Avenue Columbus, Ohio 43201

IGWMC Key: 0582 Model Name: GREASE Released: 1982
Author: P.S. Huyakorn

GREASE 2 is a multi-purpose finite element model to simulate transient, multi-dimensional, saturated groundwater flow, solute and/or energy transport in fractured and unfractured, anisotropic, heterogeneous, multilayered porous media. The analysis can be performed for confined, semiconfined, or unconfined groundwater reservoir systems. Fluid leakage or heat transfer between the aquifer and its confining layer can be taken into account. The model allows for analysis of areal flow, vertical cross-sectional flow or flow in an axisymmetric configuration. Coupled thermal fluid flow capability, and density dependent flow and solute transport capability area also available. Sorption and decay can be included in the solute transport analysis.

Contact address: GeoTrans, Inc., 46050 Manekin Plaza, Suite 100, Sterling, VA 22170

IGWMC Key: 0588 Model Name: SEFTRAN Released: 1986
Authors: P.S. Huyakorn, D.S. Ward, J.O. Rumbaugh III and R.W. Broome

SEFTRAN (Simple and Efficient Flow and TRANsport model) is a concise finite element model to simulate transient two-dimensional fluid flow and transport of non-conservative contaminants or heat in isotropic, heterogeneous aquifers. It can solve the flow and transport equations in an areal plane, a vertical cross-section, or an axisymmetric configuration. Line elements may be used to simulate discrete fractures or rivers.

Contact address: D.S. Ward, GeoTrans, Inc., 46050 Manekin Plaza, Suite 100, Sterling, VA 22170

IGWMC Key: 0612 Model Name: HOTWTR Released: --1985
Author: J.E. Reed

HOTWTR is a three-dimensional finite-difference model to simulate steady-state coupled water and heat flow in an isotropic, heterogeneous aquifer system with uniform thermal properties and viscosity dependent hydraulic conductivity.

Contact address: J.E. Reed, U.S. Geological Survey, P.O. Box 25046, MS 417, Federal Center, Denver, CO 80225

IGWMC Key: 0696 Model Name: BORHOL Released: 1984
Authors: L.D. Rickertsen, C.J. Noronha and M. Reeves

BORHOL is a finite difference model that treats the case of an open borehole through a salt formation connecting two aquifers, and determines the borehole radius as a function of depth and time. Within the borehole, the model treats the transient, one-dimensional coupled processes of flow, heat transport and volume modification subject to the mechanism of salt dissolution, precipitation and creep. Within the rock formation, the model simulates three-dimensional transport of heat from a nuclear waste repository since both creep and convective heat transfers to the fluid depends upon the rock temperature.

Contact address: Performance Assessment Department, Office of Nuclear Waste Isolation, Battelle Project Management Division, 505 King Avenue, Columbus, OH 43201

IGWMC Key: 0697 Model Name: SWENT Released: 1983
Authors: R.B. Lantz, S.B. Pahwa and B.S. RamaRao

SWENT (Simulator for Water, Energy, and Nuclide Transport) is a finite difference model for simulation of transient, multidimensional transport of fluid, energy, a single inert chemical species, and any number of radionuclides in straight or branched chains, through a heterogeneous, anisotropic geological medium. Flow and transport are coupled through density and viscosity. Aquifer porosity is treated as function of pressure. The code has options to simulate any one of the individual processes or a combination of the processes. It offers a wide choice of boundary conditions. The model permits the choice of backward or central difference approximations. Either direct or iterative methods may be used for solving the matrix equations.

Contact address: Performance Assessment Department, Office of Nuclear Waste Isolation, Battelle Project Management Division, 505 King Avenue, Columbus, OH 43201

IGWMC Key: 0730 Model Name: GEOTHER Released: 1983
Authors: C.R. Faust and J.W. Mercer

GEOTHER is a finite difference model for simulation of transient three-dimensional, single and two-phase heat transport in anisotropic, heterogeneous, porous media. It is based on the continuity equations for steam and water, which are reduced to two nonlinear partial differential equations in which the dependent variables are fluid pressure and enthalpy. The nonlinear coefficients in the equations are calculated using Newton-Raphson iterations, and an option is provided for using either upstream or midpoint weighing on the mobility terms. GEOTHER may be used to simulate the fluid-thermal interaction in rock that can be approximated by a porous media representation. It can simulate heat transport and flow of compressed water, two-phase mixtures, and super-heated steam.

Contact address: Performance Assessment Department, Office of Nuclear Waste Isolation, Battelle Project Management Division, 505 King Avenue, Columbus, Ohio 43201

IGWMC Key: 2034 Model Name: SHALT Released: 1980
Authors: J.F. Pickens and G.E. Grisak

SHALT is a finite element model that simulates heat and solute transport in a fractured, saturated or unsaturated, two-dimensional groundwater flow system. The model simulates density dependent compressible fluid flow; heat convection, conduction and dispersion; solute advection, dispersion and linear equilibrium adsorption; radioactive decay; and various first-order chemical reactions.

Contact address: Intera Technologies, Inc., 6850 Austin Center Blvd., Suite # 300, Austin, TX 78731

IGWMC Key: 2070 Model Name: CFEST Released: 1987
Authors: S.K. Gupta, C.T. Kincaid, P.R. Meyer and C.R. Cole

CFEST is a three-dimensional finite element model for simulation of steady-state or transient, single-phase Darcian flow, and energy and solute transport in anisotropic, heterogeneous, multi-layered aquifers. The code has the capability to model discontinuous and continuous layering and time-dependent and constant sources/sinks. The partial differential equations for pressure, temperature, and solute concentration are coupled with fluid properties of density and viscosity. The relationship between porosity and pore-pressure is also accounted for. The model comes with various programs for data input, gridding and post-processing including streamline generation and contouring. It has a restart option and data error checking.

Contact address: C. Cole, Battelle Pacific NW Lab., P.O. Box 999, Richland, WA 99352

IGWMC Key: 2580 Model Name: SHAFT Released: 1980
Authors: K. Pruess and R.C. Schroeder

SHAFT is a two-phase geothermal reservoir simulator. It uses the integrated finite difference technique for transient simulation of simultaneous three-dimensional heat and fluid transport in porous media. The model handles condensation, heat convection, heat conduction and phase changes.

Contact address: Nat. Energy Software Center, Argonne Nat. Lab., 9700 South Cass Avenue, Argonne, IL 60439

IGWMC Key: 2581 Model Name: MULKOM Released: 1985
Author: K. Pruess

MULKOM is an integrated finite difference model to simulate multi-component, multi-phase fluid and heat flow in porous or fractured media. The model incorporates convection, change of phase, dissolution and precipitation of silica, equilibration of noncondensible gases, transport of noncondensible gases and dissolved solids.

Contact address: K. Pruess, Lawrence Berkeley Lab., Earth Sciences Div., M.S. 50E LBL, Univ. of California, Berkeley, CA 94720

IGWMC Key: 2582 Model Name: TOUGH Released: 1987
Authors: K. Pruess, Y.W. Tsang and J.S.Y. Wang

TOUGH is a multi-dimensional integrated finite difference model for transient simulation of the coupled transport of water, air, vapor and heat transport in fractured unsaturated porous media. The model includes convection, condensation, capillary forces, evapotranspiration, heat conduction and diffusion, change of phase, adsorption, fluid compression, dissolution of air in liquid, and buoyancy.

Contact address: K. Pruess, Lawrence Berkeley Lab., Earth Science Div., M.S. 50E LBL, Univ. of California, Berkeley, CA 94720

IGWMC Key: 2620 Model Name: MARIAH Released: 1980
Authors: D.K. Gartling and C.E. Hickox

MARIAH is a finite element model to simulate steady or non-steady state two-dimensional fluid flow in saturated porous media including the effects of heat transfer. The specific types of flow problems for which MARIAH is suitable include isothermal flows, forced convection, free convection, and mixed convection. The porous matrix is considered homogeneous and rigid. For non-isothermal flows, the fluid and matrix are assumed to be in thermal equilibrium. Buoyancy driven flows are assumed to follow the Boussinesq approximation. MARIAH is a self-contained analysis program with its own mesh-generator, data analysis and plotting packages.

Contact address: D.K. Gartling, Sandia National Lab., Fluid Mechanics and Heat Transfer Division I, 5511, Albuquerque, NM 87185

Appendix D, table 1 (continued)

IGWMC Key: 2760 Model Name: MUSHRM Released: 1980
Author: J.W. Pritchett

MUSHRM is a hydrothermal finite difference reservoir model to simulate unsteady multi-phase fluid and heat flow in multi-dimensional geometries including 3-D. The program handles convection, conduction, change of phase and degassing phenomena.

Contact address: J.W. Pritchett, Systems, Science and Software, P.O. Box 1620, La Jolla, CA 92038

IGWMC Key: 2761 Model Name: CHARGR Released: 1980
Author: J.W. Pritchett

CHARGR is a three-dimensional multi-phase compressible liquid simulator for transient, multi-phase fluid flow with dissolved incondensable gases, and heat transport in anisotropic, heterogeneous deformable porous media. It uses the finite difference method to predict pressures and temperatures.

Contact address: J.W. Pritchett, Systems, Science and Software, P.O. Box 1620, La Jolla, CA 92038

IGWMC Key: 2830 Model Name: GWTHERM Released: 1979
Authors: A. Runchal, J. Treger, G. Segal

GWTHERM is a two-dimensional integrated finite difference model for cross-sectional or radial symmetric simulation of fluid flow, heat and solute transport in an anisotropic, heterogeneous, water table aquifer with density- and temperature-dependent fluid properties.

Contact address: Dames and Moore, Advanced Technology Group, 1100 Glendon Avenue - Suite 1000, Los Angeles, CA 90024

IGWMC Key: 2860 Model Name: UWIS-2D-TRANSPORT Released: 1980
Author: C.B. Andrews

UWIS-2D-TRANSPORT is a finite element model to simulate two-dimensional, areal or cross-sectional, steady or transient, single-phase heat flow or conservative mass transport in a confined or phreatic, anisotropic, heterogeneous aquifer.

Contact address: C. Andrews, S.S. Papadopulos & Assoc., 7944 Wisconsin Ave, Bethesda, MD 20814

IGWMC Key: 2950 Model Name: TRANS Released: 1981
Authors: W.R. Walker, J.D. Sabey and D.R. Hampton

TRANS is a finite element model for transient simulation of two-dimensional, horizontal, cross-sectional, or axial symmetric, coupled flow of heat and moisture in partially or fully saturated porous media, especially for assessment of buried thermal reservoirs and the heat exchange piping internal to the reservoirs.

Contact address: D. Hampton, Western Michigan Univ., Geology Dept., Kalamazoo, MI 49008

IGWMC Key: 3083 Model Name: ROCMAS-THM Released: --
Authors: J. Noorishad and P.A. Witherspoon

ROCMAS-THM is a two-dimensional model for coupled hydraulic-thermal-mechanical analysis of porous fractured rock.

Contact address: J. Noorishad, Lawrence Berkeley Labor., Earth Sciences Div., Univ. of Calif., Berkeley, CA 94720

IGWMC Key: 3084 Model Name: CHNTRNS Released: 1987
Authors: J. Noorishad, C.L. Carnahan and L.V. Benson

CHMTRNS is a temperature-dependent non-equilibrium reactive chemical transport code, based on the CHEMTRN code (Miller and Benson) developed in the early 1980's. Equations solved include mass balance, aqueous species transport, non-equilibrium reactions, transport of hydrogen and hydroxide ions, equilibrium complexation, dissolution and precipitation, ion exchange, redox reactions, and heat transport. The code is capable of simulating kinetic calcite and silicate dissolution, irreversible glass dissolution, oxidation and reduction, and stable carbon isotope fractionation during transport. The code can handle Neumann and Dirichlet boundary conditions and includes a mesh generation scheme. The 1-D transport equation is solved using a upstream weighted finite difference algorithm.

Contact address: J. Noorishad, Lawrence Berkeley Labor., Earth Sciences Div., Univ. of Calif., Berkeley, CA 94720

IGWMC Key: 3232 Model Name: FRACFLOW Released: 1981
Author: B. Sagar, B.

FRACFLOW is an integrated finite difference model for steady and nonsteady state analysis of coupled, density-dependent flow, heat and mass transport in fractured confined aquifers. The processes in the porous medium are simulated in two dimensions and in the fractures in one dimension. Fractures may have arbitrary orientations. Any number of fractures, each of different properties may be incorporated. The program includes first-order chemical reactions. A preprocessor and a number of graphic post-processing routines are available.

Contact address: Rockwell Hanford Oper., P.O. Box 800, Richland, WA 99352

IGWMC Key: 3233 Model Name: PORFLOW - II (2D) Released: 1988
Authors: A.K. Runchal

PORFLOW II (2D) is an integrated finite difference model for analysis of coupled, steady-state or transient, 2-dimensional horizontal, vertical or radial, density dependent flow and heat and/or mass transport in anisotropic, heterogeneous, non-deformable saturated porous media with time dependent aquifer and fluid properties. User interface is based on the FREEFORM language with simple English commands.

Contact address: Analytical & Computational Research, Inc., 1931 Stradella Road, Bel Air, CA 90077.

IGWMC Key: 3234 Model Name: VADOSE Released: -1982
Author: B. Sagar

VADOSE is an integrated finite difference model for analysis of steady or transient, two-dimensional areal, cross-sectional or radial simulation of coupled, density-dependent transport of moisture, heat and solutes in variably-saturated, heterogeneous, anisotropic porous media.

Contact address: Rockwell Hanford Operations, P.O. Box 800, Richland, WA 99352

IGWMC Key: 3235 Model Name: FLOTRA Released: 1982
Authors: B. Sagar

FLOTRA is an integrated finite difference model for simulation of steady or transient, two-dimensional areal, cross-sectional or radial, density- dependent flow, heat and mass transport in variably saturated, anisotropic, heterogeneous deformable porous media.

Contact address: Rockwell Hanford Operations, P.O. Box 800, Richland, WA 99352

IGWMC Key: 3236 Model Name: PORFREEZE Released: 1981
Author: A.K. Runchal

PORFREEZE simulates steady-state or transient two-dimensional density-dependent saturated flow and heat transport in freezing soils. The coupled equations are solved with the finite difference method and include time and temperature dependency of fluid and aquifer properties.

Contact address: Analytic & Computational Research, Inc., 1931 Stradella Road, Bel Air, CA 90077

IGWMC Key: 3238 Model Name: PORFLOW-3D Released: 1991
Author: A.K. Runchal

PORFLOW-3D is an integrated finite difference model to simulate coupled transient or steady-state, multiphase, fluid flow, and heat, salinity, or chemical species transport in variably saturated porous or fractured, anisotropic and heterogeneous media. The program facilitates arbitrary sources or sinks in three-dimensional cartesian or axisymmetric (cylindrical) geometry. The user interface is based on the FREEFORM language using simple English-like commands. The software includes the ARCPLOT graphic post processor.

Contact address: Analytic and Computational Research, Inc., 1931 Stradella Road, Bel Air, CA 90077

IGWMC Key: 3375 Model Name: MATTUM Released: 1983
Authors: G.T. Yeh and R.J. Luxmoore

MATTUM is a three-dimensional model for simulating moisture and thermal transport in unsaturated porous media. The model solves both the flow equation and the heat transport equation under unsaturated water conditions using the integrated compartment method. The entire unsaturated zone is divided in a number of compartment of different sizes and shapes. The Philip-de Vries equations governing moisture movement and heat transfer are integrated over each of the compartments to yield a system of nonlinear ordinary differential equations. There three optional time integration schemes: split explicit, implicit pointwise iteration, and matrix inversion iteration.

Contact address: Oak Ridge Nat. Lab., Environmental Sciences Div., Oak Ridge, TN 37830

IGWMC Key: 3590 Model Name: SPLASHWATER Released: 1983
Author: P.C.D. Milly

SPLASHWATER is a finite element model for simulation of coupled heat and moisture fields in the unsaturated zone. The model includes evapotranspiration, hysteresis, and heat convection and conduction.

Contact address: P.C.D. Milly, Princeton University, Dept. of Civil Engineering, Princeton, NJ 08544

IGWMC Key: 3790 Model Name: PORFLO Released: 1985
Authors: A.K. Runchal, B. Sagar, R.G. Baca and N.W. Kline

PORFLO is an integrated finite difference model for transient two-dimensional or axisymmetric simulation of coupled buoyancy driven groundwater flow, heat transfer and radionuclide transport in layered geologic systems. Heat transfer processes include storage, advection, conduction, dispersion and heat generation. Fluid flow processes include storage, inflows and outflows, pore pressure buildup, buoyancy driving force and temperature dependent hydraulic conductivity. Mass transport processes include storage, advection, dispersion and diffusion, retardation, decay and mass release.

Contact address: N.W. Kline, Boeing Computer Services Richland, P.O Box 300, Richland, WA 99352

IGWMC Key: 3830 Model Name: SUTRA Released: 1990
Author: C.I. Voss

SUTRA (Saturated-Unsaturated TRAnsport) simulates transient or steady-state, two-dimensional, variably saturated, fluid density dependent ground water flow with transport of energy or chemically reactive species solute transport. The model employs a hybrid finite-element and integrated-finite-difference method to approximate the coupled equations. Solute transport include advection, dispersion, diffusion, equilibrium adsorption on the porous matrix, and both first-order and zero-order decay or production. Energy transport may take place in both the solid matrix and the liquid phase. SUTRA may be employed in both areal (horizontal) and cross-sectional mode for saturated systems or in cross-sectional mode only for unsaturated systems.

Contact address: C.I. Voss, C.I., U.S. Geological Survey, 431 National Center, Reston, VA 22092; Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401, or Scientific Software, Washington, D.C.

IGWMC Key: 3840 Model Name: SWIFT Released: 1981
Authors: R.T. Dillon, R.M. Cranwell, R.B. Lantz and S.B. Pahwa

SWIFT (Sandia Waste-Isolation Flow and Transport) is a three-dimensional finite difference model for simulation of coupled, transient, density dependent flow and transport of heat, brine, tracers or radionuclides in heterogeneous, anisotropic, saturated porous media.

Contact address: R.M. Cranwell, Sandia National Laboratories, Albuquerque, NM 87185

IGWMC Key: 3841 Model Name: SWIFT II Released: 1987
Authors: M. Reeves, D.S. Ward, J.D. Johns and R.M. Cranwell

SWIFT II is a three-dimensional finite difference model for simulation of steady-state or transient flow and transport of fluid, heat, brine, and radionuclide chains in confined or unconfined (fractured) porous media.

continued.....

SWIFT II -- continued

The equations for fluid, heat, and brine are coupled by fluid density, fluid viscosity, and porosity. Both dual-porosity and discrete-fractures might be considered. Only one-dimensional migration is permitted in the rock matrix. The model includes a salt dissolution mechanism and a waste leaching algorithm. Moreover, SWIFT II has a well-bore submodel and handles both radial and cartesian coordinates. Among the many boundary conditions which can be used is a free phreatic surface condition.

Contact address: D.S. Ward, GeoTrans, Inc., 46050 Manekin Plaza, Suite 100, Sterling, VA 22170

IGWMC Key: 3842 Model Name: SWIFT III/386 Released: 1992
Authors: D.S. Ward

SWIFT III/386 is a fully transient, three-dimensional model which simulates the flow and transport of fluid, heat (energy), brine, and radionuclide chains in porous and fractured geologic media. The primary equations for fluid, heat, and brine are coupled by fluid density, fluid viscosity, and porosity. Both Cartesian and cylindrical coordinate systems may be used. For the fracture zone the model allows both dual-porosity and discrete fractures. Migration within the rock matrix is characterized as a one-dimensional process. Aquifer hydraulic characteristics may be heterogeneous and anisotropic under confined or unconfined conditions. The discretization is performed by the finite difference method using centered or backwards weighing in time and space.

Contact address: D.S. Ward, GeoTrans, Inc., 46050 Manekin Plaza, Suite 100, Sterling, VA 22170

IGWMC Key: 3860 Model Name: DFT/C-1D Released: 1984
Author: C.S. Desai

DFT/C-1D is a finite element model for one-dimensional analysis of linear stress-deformation (consolidation) and steady-state or transient fluid flow. The model calculates matrix displacement, fluid head, temperature and pore water pressure.

Contact address: C.S. Desai, Univ. of Arizona, Dept. of Civil Eng. and Mech. Eng., Tuscon, AZ 85721

IGWMC Key: 3861 Model Name: FIELD-2D Released: --
Author: C.S. Desai

FIELD-2D is a finite element model for analysis of linear steady state two-dimensional problems in torsion, potential flow, seepage and heat flow.

Contact address: C.S. Desai, Univ. of Arizona, Dept. of Civil Eng. and Mech. Eng., Tuscon, AZ 85721

IGWMC Key: 3890 Model Name: PT (Pressure-Temperature) Released: 1986
Author: G.S. Bodvarsson

PT is a three-dimensional integrated finite difference model for simulation of three-dimensional, transient, single phase fluid flow with simultaneous heat transport and one-dimensional subsidence in isotropic, heterogeneous porous media.

Contact address: G.S. Bodvarsson, Lawrence Berkeley Lab., Earth Sciences Div., Univ. of California, Berkeley, CA 94720

IGWMC Key: 3970 Model Name: TEXASHEAT Released: 1980
Authors: E.K. Grubaugh and D.L. Reddell

TEXASHEAT is a three-dimensional transient finite element model for solution of simultaneous flow and heat transport through anisotropic, heterogeneous porous media.

Contact address: D. Reddell, Texas Water Resources Inst., Texas A&M Univ., College Station, TX 77843

IGWMC Key: 4030 Model Name: TRUMP Released: 1980
Authors: A.L. Edwards, A. Rasmuson, I. Neretnicks and T.N. Narasimhan

TRUMP is a multi-dimensional model based on the integral finite difference method, to simulate coupled steady-state or transient ground water flow and heat or solute transport in (porous) fractured rock.

Contact address: A. Rasmuson, Royal Inst. of Technology, Dept. of Chem. Eng., S-100 44 Stockholm, Sweden

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IGWMC Key: 4550 Model Name: MOTIF Released: 1986
Author: V. Guvanasen

MOTIF is a finite element model to simulate one-, two-, and three-dimensional coupled processes of saturated or unsaturated fluid flow, conductive and convective heat transport, brine transport and single species radionuclide transport in a compressible rock of low permeability intersected with a few major fractures. The model includes diffusion into the rock matrix.

Contact address: Tin Chan, Atomic Energy of Canada, Ltd., Whiteshell Nuclear Research Estb., Pinawa, Manitoba, Canada R0E1l0

IGWMC Key: 4590 Model Name: MAGNUM-2D Released: 1985
Authors: R.L. England, N.W. Kline, K.J. Ekblad and R.G. Baca

MAGNUM-2D is a two-dimensional, cross-sectional or three-dimensional axi-symmetric finite element model for transient or steady-state analysis of coupled heat transfer and groundwater flow in an inhomogeneous, anisotropic, fractured porous medium. A set of support programs are available to generate, manipulate, and display the finite element grid; to compute and plot pathlines and traveltimes; and to plot contours, spatial cross-sections, and time histories for temperature and hydraulic head.

Contact address: R.G. Baca, Rockwell Hanford Operations, P.O. Box 800, Richland, WA 99352

IGWMC Key: 4600 Model Name: SANGRE Released: 1986
Author: C.A. Anderson

SANGRE is a finite element code for thermomechanical analysis of two-dimensional problems in structural geology. It allows simulation of convective heat transport, consolidation, and fluid migration. It includes modeling capabilities for highly deformable and deformed geologic media, large deformations, faults, overthrusts, etc. The model has a flexible, grid which can rotate and translate in time, following the displacements of the rock matrix.

Contact address: C.A. Anderson, Los Alamos Nat. Lab., Los Alamos, NM 87545

IGWMC Key: 4610 Model Name: HST3D Released: 1991
Author: K.L. Kipp, Jr.

The Heat- and Solute-Transport Program HST3D simulates ground-water flow and associated heat and solute transport in three dimensions. The three governing equations are coupled through the interstitial pore velocity, the dependence of the fluid density on pressure, temperature, and solute mass fraction. The solute-transport equation is for only a single, solute species with possible linear-equilibrium sorption and linear decay. The finite difference model handles a variety of boundary conditions for confined and unconfined aquifer conditions including an approximate free surface. The matrix equations are solved by either direct (Gaussian) elimination or by an iterative solver, using two-line successive overrelaxation.

Contact address: K.L. Kipp, U.S. Geol. Surv., Box 25046, Denver Fed. Ctr., Denver, CO 80225, or Internat. Ground Water Modeling Ctr., Col. Sch. of Mines, Golden, CO 80401.

IGWMC Key: 4700 Model Name: DSTRAM Released: 1988
Author: P.S. Huyakorn

DSTRAM is a 3-D finite-element model that simulates coupled, density-dependent single-phase fluid flow and solute or energy transport in saturated porous media. This model can perform steady-state or transient simulations in a cross-section, an axisymmetric configuration, or a fully-3D model. The contaminant transport equation includes advection, hydrodynamic dispersion, linear equilibrium adsorption, and first-order degradation. For heat transport simulation, additional processes of heat conduction and storage in the fluid and rock matrix can also be included. Nonlinearity resulting from density differences is handled via a Picard algorithm. The transport equation is solved using upstream weighted residual. A mesh generator is available.

Contact address: HydroGeologic, Inc., 1165 Herndon Parkway, Suite 100, Herndon, VA 22070

IGWMC Key: 5018 Model Name: AQUA Released: 1992
Authors: S.P. Kjaran, D. Egilson and S. Th. Sigurdson

AQUA is a program package developed for solving steady-state and transient two-dimensional ground-water flow and transport problems using the finite element method. The model can be applied to either confined or unconfined aquifers allowing for heterogeneity and anisotropy of aquifer hydraulic parameters and time-varying infiltration and pumping. Processes included in the simulation of transport of heat and dissolved chemicals are convection, decay, adsorption and velocity dependent dispersion. For heat transport conduction is included. The AQUA package includes various graphic pre- and post processors facilitating interactive grid design and data entry for areal and cross-sectional problems.

Contact address: S.P. Kjaran, Vatnaskil Consulting Engineers, Armuli 11, IS-108 Reykjavik, Iceland

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IGWMC Key: 5027 Model name: DIFFMOD Released: 1987
Authors: R.W. Healy, A.L. Ishii and R.G. Striegl

DIFFMOD is a modular computer code for the numerical solution of the linear diffusion equation (Fick's law) in one or two dimensions in Cartesian or cylindrical coordinates. Applications of this generalized code include molecular diffusion, heat conduction, and fluid flow in confined anisotropic, heterogeneous groundwater systems. The model is based on finite difference approximations of the governing equations and a preconditioned conjugate gradient method to solve the resulting set of algebraic equations.

Contact address: U.S. Geol. Survey, District Office, 4th floor, 102 East Main Str., Urbana, IL 61801

IGWMC Key: 5031 Model Name: CTSPAC Released: 1988
Authors: F.T. Lindstrom, D.E. Cawlfield and L. Boersma

CTSPAC is an one-dimensional numerical model that couples the flow of water and the transport of heat and solutes in layered soils with the uptake and transport of water and solutes in plants. Initial root distribution is specified. The rate of uptake is a function of the environmental conditions that determine the plant's transpiration rate. Water transport in the plant is based on water potential and pressure gradients according to Munch pressure flow hypothesis. The model was developed for assessing risks involved in the use of xenobiotic chemicals. It allows an evaluation of the rate of uptake of such chemicals from the soil solution and the accumulation in the various plant parts.

Contact address: L. Boersma, Dept. of Soil Science, Oregon State University, Corvallis, OR 97331

IGWMC Key: 5213 Model Name: TDFD1O Released: --
Authors: L.S. Slotta

TDFD1O is a two-dimensional model for simultaneous simulation of movement of moisture, transport of heat, and transport and fate of a contaminant in a shallow unconfined aquifer. The porous medium may be heterogeneous. The coupled system of non-linear unsaturated/saturated moisture flow and heat and chemical transport are solved using a finite difference approximation. The porous medium is partitioned in three fractions: sand, clay, and organic material, with for each fraction first-order sorption kinetics included. Time integration is performed using the backward Euler method. Dynamic boundary conditions at the air-porous medium interface are included. A variety of first- and second-type boundary conditions are included.

Contact address: Slotta Engineering Associates, Inc., P.O. Box 1376, Corvallis, OR 97339

IGWMC Key: 6602 Model Name: ICE-1 Released: 1989
Author: A.I. El-Kadi

ICE-1 is a one-dimensional analytical solution for the analysis of heat, solute, and water transport in unsaturated, partially frozen soils. The program runs interactively and includes graphical representation of results.

Contact address: A.I. El-Kadi, Dept. of Geology & Geophysics, Univ. of Hawaii-Manoa, Honolulu, HI 96822, or Intern. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

Appendix D: Heat Transport, Part 2: Usability and Reliability

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
100	PT/CCC	N	N	Y	Y	N	L	Y	U	L	L	F
160	SCHAFF	N	N	Y	Y	N	U	Y	U	L	U	F
513	GAFETTA	N	N	Y	Y	N	U	Y	U	L	U	U
581	FTRANS	N	N	Y	Y	N	N	Y	U	L	L	F
582	GREASE	U	U	Y	Y	N	N	Y	U	L	L	F
588	SEFTRAN	Y	Y	Y	Y	Y	N	Y	U	E	L	M
612	HOTWTR	U	U	Y	Y	N	L	Y	U	L	U	F
696	BORHOL	N	N	Y	Y	N	U	U	U	L	U	U
697	SWENT	U	U	Y	Y	N	L	Y	U	E	L	M
730	GEOTHER	N	N	Y	Y	N	L	Y	U	L	L	M
2034	SHALT	N	N	Y	Y	N	U	Y	U	L	U	F
2070	CFEST	Y	Y	Y	Y	N	L	Y	U	E	L	M
2580	SHAFT	U	U	Y	Y	N	L	Y	U	L	U	F
2581	MULKOM	U	U	Y	Y	N	L	Y	U	L	U	F
2582	TOUGH	U	U	Y	Y	N	L	Y	U	L	U	F
2620	MARIAH	U	U	Y	Y	U	U	Y	U	L	U	F
2760	MUSHRM	U	U	Y	Y	U	U	Y	U	L	U	U
2761	CHARGR	U	U	Y	Y	U	U	Y	U	L	U	U
2830	GWTHERM	U	U	Y	Y	U	U	U	U	U	U	U
2860	UWIS-2D-TRANSPORT	N	N	Y	U	U	U	Y	U	U	U	U

KEY: Y = YES N = NO L = LIMITED E = EXTENSIVE M = MANY F = FEW U = UNKNOWN

Appendix D, part 2 (continued)

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
2950	TRANS	N	N	Y	U	U	U	U	U	U	U	U
3083	ROCMAS-THM	U	U	Y	Y	U	U	Y	U	L	U	U
3084	CHNTRNS	U	U	Y	Y	U	U	Y	U	L	U	U
3232	FRACFLOW	Y	Y	Y	Y	Y	L	Y	Y	L	U	F
3233	PORFLOW-II	Y	Y	Y	Y	Y	L	Y	Y	E	L	M
3234	VADOSE	Y	Y	Y	Y	Y	L	Y	U	L	U	U
3235	FLOTRA	Y	Y	Y	Y	Y	L	Y	U	L	U	U
3236	PORFREEZE	Y	Y	Y	Y	Y	L	Y	U	L	U	F
3238	PORFLOW-3D	Y	Y	Y	Y	Y	L	Y	U	E	L	M
3375	MATTUM	N	N	Y	Y	N	U	Y	U	L	U	U
3590	SPLASHWATER	N	N	Y	Y	N	N	Y	U	L	U	U
3790	PORFLO	Y	Y	Y	Y	Y	L	Y	Y	E	L	M
3830	SUTRA	Y	Y	Y	Y	Y	Y	Y	U	E	L	M
3840	SWIFT	N	N	Y	Y	N	N	Y	U	E	L	M
3841	SWIFT II	U	U	Y	Y	N	N	Y	U	E	L	M
3842	SWIFT III/386	Y	Y	Y	Y	Y	L	Y	U	E	L	M
3860	DFT/C-1D	U	U	Y	Y	U	U	Y	U	U	U	U

KEY: Y = YES N = NO L = LIMITED E = EXTENSIVE M = MANY F = FEW U = UNKNOWN

Appendix D, part 2 (continued)

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
3861	FIELD-2D	N	N	Y	Y	U	U	Y	U	U	U	U
3890	PT	N	N	Y	Y	N	L	Y	U	L	U	F
3970	TEXASHEAT	N	N	Y	Y	N	N	Y	U	L	U	F
4030	TRUMP	N	N	Y	Y	N	L	Y	U	L	L	F
4550	MOTIF	N	N	Y	Y	N	U	Y	U	U	U	U
4590	MAGNUM-2D	N	N	Y	Y	N	L	Y	N	L	U	F
4600	SANGRE	N	N	Y	Y	N	L	Y	U	L	U	F
4610	HST3D	Y	Y	Y	Y	Y	L	Y	U	E	L	M
4700	DSTRAM	U	U	Y	Y	Y	L	Y	U	E	L	F
5018	AQUA	Y	Y	Y	Y	Y	Y	Y	U	E	L	M
5027	DIFFMOD	U	U	Y	Y	N	L	Y	U	L	U	F
5031	CTSPAC	U	U	Y	Y	U	U	Y	U	L	U	U
5213	TDFD10	U	U	Y	Y	U	U	Y	U	U	U	U
6602	ICE-1	Y	Y	Y	Y	Y	L	Y	U	L	N	F

KEY: Y = YES N = NO L = LIMITED E = EXTENSIVE M = MANY F = FEW U = UNKNOWN

Appendix E: Gas Flow and Vapor Transport, Part 1: Model Description

IGWMC Key: 5180 Model Name: MOFAT Released: 1990
Authors: Kaluarachchi, J.J , Parker, J.C.

MOFAT is an upstream-weighted finite element model to simulate coupled flow of water, nonaqueous phase liquid (NAPL) and air, and multicomponent transport of up to five non-inert species in a two-dimensional vertical section through saturated and unsaturated zones in Cartesian or radial coordinates. The flow module can be used to simulate 2- or 3-phase system with gas phase treated dynamically or assumed at constant pressure. Convective-dispersive transport in water, NAPL and gas phase is analyzed assuming local equilibrium partitioning among phases and with the solid phase. MOFAT comes with pre- and post-processing capabilities. Only rectangular elements with sides parallel to the principle flow axes are permitted.

Contact Address: Environm. Systems and Technologies, Inc., P.O. Box 10457, Blacksburg, VA 24062

IGWMC Key: 5182 Model Name: VENTING Released: 1990
Authors: P.C. Johnson, M.W. Kemblowski, and J.D. Colthart (Shell Development, Houston, Texas)

VENTING is a practical program which consists of two semi-analytical models used as screening tools in determining viability of in-situ soil venting at a given soil site. The two-dimensional (radial gas flow) models are an equilibrium-based venting model and a vapor-phase diffusion-limited model. Ideal gas behavior is assumed and no chemical/biological degradation is considered. They have been used to illustrate that the three factors that most significantly influence the performance of a venting operation are: vapor flow rate; contaminant composition; and vapor flow path relative to the contaminant location. They relate the applied vacuum, soil permeability, and spill composition to the vapor flow rates, velocities, mass removal rates, and residual composition changes with time.

Contact Address: Environm. Systems and Technologies, Inc., P.O. Box 10457, Blacksburg, VA 24062

IGWMC Key: 5185 Model Name: MOTRANS Released: 1992
Authors: Katyal, A.K. , Parker, J.C.

MOTRANS is a 2-dimensional vertical section or radially symmetric upstream-weighted finite element program for flow of air, light or dense organic liquid and water, and coupled transport of up to 5 partionable species. The program, which uses linear rectangular elements, allows inclusion or elimination of flow equations for selected phases to achieve maximum flexibility and efficiency. Soil hydraulic properties are described by the multi-phase van Genuchten model with NAPL entrapment. The nonlinearity in the equations is handled by Newton-Raphson iteration. Multispecies transport is simulated assuming local equilibrium or kinetically controlled interphase mass transfer. Pre- and postprocessing modules are available.

Contact Address: Environm. Systems and Technologies, Inc., P.O. Box 10457, Blacksburg, VA 24062

IGWMC Key: 5390 Model Name: CSUGAS Released: 1991
Authors: G.P. Sabadell, J.J. Eisenbeis, and D.K. Sunada

A finite-difference model for simulating one-, two-, or three-dimensional compressible gas flow in a porous medium. It can model steady-state and transient conditions and computes soil gas pressure distribution due to hydrologic or artificial influence.

Contact address: D.K. Sunada, Dept. Civil Eng., Colorado State Univ., Fort Collins, CO 80523.

IGWMC Key: 5400 Model Name: -- Released: 1991
Author: Jong Soo Cho

A steady-state model based on point-source, line source, point dipole, line dipole and panel dipole solutions of the soil air pressure distribution equation. The model can handle various boundary conditions by superposition of the line and panel dipoles on the boundaries.

Contact address: Jong Soo Cho, U.S. EPA, R.S. Kerr Env. Res. Lab, Ada, OK 74820.

IGWMC Key: 5401 Model Name: -- Released: 1991
Author: Jong Soo Cho

Based on a finite difference solution of the three-dimensional steady-state soil air flow and transient contaminant transport equations together with a mass balance equation for residual hydrocarbon inside soil matrices. Includes interfacial mass transfer between air and residual hydrocarbon contacting the air. The air flow equations are solved with a point Jacobi iterative method; an explicit method is used to solve the convective diffusion equations.

Contact address: Jong Soo Cho, U.S. EPA, R.S. Kerr Env. Res. Lab, Ada, OK 74820.

IGWMC Key: 5410 Model Name: -- Released: 1987
Authors: D.E. Metcalfe and G.J. Farquhar

A finite-element model for simulation of two-dimensional gas migration through the unsaturated zone. It includes advection and transient gas phase flow. The model accounts for gas migration due to gas pressure, concentration (diffusion), and velocity gradients. It is based on the continuum approach presented by Bear (1972) for contaminant transport in groundwater. This research model successfully reproduced observed gas pressure and concentration data at landfill sites.

Contact address: CANVIRO Consultants, Ltd., 178 Loisa Str., Kitchener, Ontario, Canada N2H 5M5.

IGWMC Key: 5411 Model Name: -- Released: 1980
Authors: M.F.N. Mohsen, G.J. Farquhar, and N. Kouwen

A finite-element model for transient simulation of three-dimensional (axisymmetric) gas migration through various soil strata. The model uses quadratic triangular elements to solve the diffusion-convection equation of a binary mixture of gases. It handles soil stratification with varying properties, inhomogeneous fluid, a combination of Dirichlet, Neumann, and flux type boundary conditions, and time-varying boundary conditions. This research model compares favorably with an analytical solution of the diffusion-convection equation for simple situations and with observed field measurements.

Contact address: G.J. Farquhar, Dept. of Civil Eng., Univ. of Waterloo, Waterloo, Ontario, Canada N2L 3G1.

IGWMC Key: 3432 Model Name: CXTFIT Released: 1985
Authors: Parker, J.C., M.Th. Van Genuchten

The purpose of CXTFIT is to determine values for one-dimensional analytical solute transport parameters using a nonlinear least-squares inversion method. The analytical model includes advection, dispersion, diffusion, first-order decay and zero-order production.

Contact Address: J.C. Parker, Virginia Polytechnical Institute, Dept. Soil & Environmental Science, Blacksburg, VA 24061; or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 3450/3451 Model Name: DISPEQ/DISPER/PISTON Released: 1983
Authors: Fluhler, H., and W.A. Jury

DISPEQ/DISPER/PISTON is a series of three finite difference research models to simulate one-dimensional transport of reactive solute species through soil columns, including dispersion, instantaneous equilibrium adsorption (DISPEQ) and rate dependent adsorption (DISPER). PISTON is based on piston type flow without dispersion.

Contact Address: H.U. Fluhler, 240 Nick Davis Road, Madison, AL 35758

IGWMC Key: 3540 Model Name: CREAMS Released: 1982
Author: Knisel, W.G.

CREAMS (A field scale model for Chemicals, Runoff, and Erosion from Agricultural Management Systems) is a general watershed model designed to evaluate non-point source pollution from alternate management practices for field-size areas. It consists of three main components: hydrology, erosion/sedimentation and chemistry. The hydrology model handles storm runoff, infiltration, soil water movement (providing amount of seepage beneath root zone and initial soil water content before a storm), and soil/plant evapotranspiration between storms. The chemistry model includes a nutrient (nitrogen and phosphorus) submodel and a pesticide submodel. CREAMS was developed for evaluation of agricultural management systems and their effects on non-point pollution potential. CREAMS is the predecessor of GLEAMS.

Contact Address: W.G. Knisel, USDA Agricultural Research Service, Southeast Watershed Research Laboratory, P.O. Box 946, Tifton, GA 31793

IGWMC Key: 3541 Model Name: GLEAMS Released: 1990
Authors: Leonard, R.A., W.G. Knisel, and F.M. Davis

GLEAMS (Groundwater Loading Effects on Agricultural Management Systems) was developed as an extension of an earlier USDA model, CREAMS. Both models simulate soil water balance and surface transport of sediments and chemicals from agricultural field management units. GLEAMS, in addition, simulates chemical transport in and through the plant root zone. Several other features were added such as irrigation/chemigation options, pesticide metabolite tracking, and software to facilitate model implementation and output data analysis. Input requirements for the model include daily rainfall volumes, crop and management parameters; soil and physical parameters; pesticide property data such as solubility, and expected half-life in soil and/or foliage.

Contact Address: USDA-ARS, P.O. Box 946, Tifton, GA 31793

IGWMC Key: 3830 Model Name: SUTRA Released: 1990
Author: Voss, C.I.

SUTRA (Saturated-Unsaturated TRAnsport) simulates transient or steady-state, two-dimensional, variably saturated, fluid density dependent ground water flow with transport of energy or chemically reactive species solute transport. The model employs a hybrid finite-element and integrated-finite-difference method to approximate the coupled equations. Solute transport include advection, dispersion, diffusion, equilibrium adsorption on the porous matrix, and both first-order and zero-order decay or production. Energy transport may take place in both the solid matrix and the liquid phase. SUTRA may be employed in both areal (horizontal) and cross-sectional mode for saturated systems or in cross-sectional mode only for unsaturated systems.

SUTRA provides, as preliminary calculated results, fluid pressures and either solute concentrations or temperatures. Mesh construction is flexible for arbitrary geometries employing quadrilateral finite elements in Cartesian or radial-cylindrical coordinates. The mesh might be coarsened through the use of pinch nodes. Boundary conditions, sources and sinks may be time dependent. The model has a rest art option. Options are also available to print fluid velocities, and fluid mass, and solute mass or energy budgets for the system. SUTRA's numerical algorithms are not specifically applicable to non-linearities of unsaturated flow. Therefor SUTRA, as distributed by the USGS, requires fine spatial and temporal discretization for unsaturated flow. The user can replace the included function for unsaturated flow by others, and recompile the code.

Contact Address: Voss, C.I., U.S. Geological Survey, 431 National Center, Reston, VA 22092; Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401; or Scientific Software, Washington, D.C.

IGWMC Key: 4081 Model Name: TRIPM Released: 1983
Author: Gureghian, A.B.

TRIPM is a two-dimensional finite element model to predict the transport of radionuclides decay chain into and in a phreatic aquifer. It simulates the simultaneous cross-sectional flow water and the transport of reacting solutes through saturated and unsaturated porous media. The influence of soil-water pH on the distribution coefficient is included. Boundary conditions include seepage faces.

Contact Address: Performance Assessment Dept., Office of Nuclear Waste Isolation, Battelle Project Management Division, 505 King Avenue, Columbus, OH 43201

IGWMC Key: 4140 Model Name: MLSOIL/DFSOIL Released: 1984
Authors: Sjoreen, A.L., D.C. Kocher, G.G. Killough, and C.W. Miller.

MLSOIL (Multi-Layer SOIL model) calculates an effective ground surface concentration to be used in computations of external doses. The program implements a five compartment linear-transfer model to calculate the concentrations of radionuclides in the soil following deposition on the ground surface from the atmosphere. The model considers leaching through the soil as well as radioactive decay and buildup. DFSOIL calculates the dose in air per unit concentration at 1m above the ground from each of the five soil layers used in MLSOIL and the dose per unit concentration from an infinite plane source. MLSOIL and DFSOIL are part of the Computerized Radiological Risk Investigation System (CRRIS).

Contact Address: A.L. Sjoreen, Oak Ridge Nat. Lab., Health and Safety Research Div., Oak Ridge, Tennessee 37831

MAGICS - continued

curbs numerical oscillations. Direct banded matrix solvers are used to solve the matrix systems of 2-D problems. A block-iterative ORTHOMIN solver is used to solve 3-D problems. All boundary conditions can be chosen constant in time or variable in time with either continuous or stepwise changes. MAGICS has been verified for a variety of problems by comparison of its numerical solutions with available analytical solutions and documented numerical results from several other codes including HYDRUS, VAM2D, VAM3D, SWANFLOW, and NAPL3D. MAGICS is a robust code designed to solve highly nonlinear field problems involving large contrasts in soil properties and highly nonlinear situations involving sharp saturation fronts, and to provide accurate mass balance calculations.

Contact address: HydroGeologic, Inc., 1165 Herndon Parkway, suite 900, Herndon, VA 22070

IGWMC Key: 5940 Model Name: HYPERVENTILATE Released: 1992
Author: Johnson, P.

HYPERVENTILATE is an user-friendly vapor flow screening model for feasibility studies. It operates as a decision tree for investigating the potential implementation of soil-vapor extraction at a site. The program is based on the use of hypercard/hypertext using multiple card files, addressing such topics as air permeability testing, aquifer characterization and system design. It requires the following input: flow rate, site dimension, porosity, temperature, sorption isotherms, boiling point data on spill components. It estimates flow rates, removal rates, residual concentrations, and the number of wells required.

Contact address: Johnson, P., Shell Development, Westhollow Research Center, Houston, Texas

IGWMC Key: 5950 Model Name: SVE COLUMN Released: 1991
Author: Wilson, D.J.

SVE Column is a model for simulation of soil vapor stripping, either for use as a lab column model using experimental data to obtain the effective Henry's constant, or as a filed model assuming axial symmetry. The models are used to examine the effects of well depth, well spacing, the use of impermeable caps, passive vent wells, soil pneumatic permeability, and recontamination from underlying NAPL. The models are either solved analytically, or using an over-relaxation finite difference technique.

Contact address: Wilson, D.J., Vanderbilt Univ., Dept. of Chemistry, Box 1822, Sta. B., Nashville, TN 37235.

IGWMC Key: 6605 Model Name: AIR Released: 1990
Authors: C. Lin and W. Kinzelbach

A user-friendly PC implementation of a three-dimensional finite difference model of one-phase, steady-state gas flow in the unsaturated zone. It facilitates alternatively the computation of compressible or incompressible gas flow. The model assumes that the soil moisture distribution is constant in time and that the free ground-water surface is an impervious boundary for gas and its location known and fixed in space. The finite difference equations are solved using a preconditioned conjugate gradient method. Pathlines are computed using particle tracking in the velocity field and Euler integration. The software includes graphic display of results.

Contact address: W. Kinzelbach, Gesamthochschule Kassel-Universitat, FB-14, D-3500 Kassel, Germany.

Appendix E: Gas Flow and Vapor Transport, Part 2: Usability and Reliability

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
5180	MOFAT	Y	Y	Y	Y	Y	Y	Y	U	L	U	F
5182	VENTING	Y	Y	Y	Y	Y	Y	Y	U	L	L	M
5185	MOTRANS	Y	Y	Y	Y	Y	Y	Y	U	L	U	F
5390	CSUGAS	U	U	Y	Y	U	U	Y	U	L	L	F
5400	---	Y	Y	Y	Y	Y	L	Y	N	Y	L	U
5401	---	N	N	Y	Y	N	N	Y	Y	Y	L	F
5410	---	U	U	Y	U	U	U	Y	U	L	U	U
5411	---	U	U	Y	U	U	U	Y	U	L	U	U
5420	---	U	U	Y	U	U	U	Y	U	L	U	U
5430	---	U	U	Y	U	U	U	Y	U	L	U	U
5440	---	U	U	Y	U	U	U	Y	U	L	U	U
5441	---	U	U	Y	U	U	U	Y	U	L	U	U
5450	---	U	U	Y	U	U	U	Y	U	L	U	U
5490	PETROS	U	U	Y	U	U	U	Y	U	L	U	U
5821	MAGICS	Y	Y	Y	Y	Y	Y	Y	U	E	L	F
5940	HYPER-VENTILATE	Y	Y	Y	Y	Y	Y	Y	U	E	L	M
5950	SVE COLUMN	U	U	Y	U	U	U	Y	U	L	U	U
6605	AIR	Y	Y	Y	Y	Y	Y	Y	U	E	L	M

KEY: Y = YES N = NO L = LIMITED E = EXTENSIVE M = MANY F = FEW U = UNKNOWN

Note: Most codes listed are research codes and not designed as general-use codes. Most of the general-use codes have user-friendly data entry and postprocessing options.

Appendix F: Flow and Transport in Fractured Rock, Part 1: Model Description

Note: Many of the models for flow and transport in fractured rock are research codes.

IGWMC Key: 581 Model Name: FTRANS Released: 1982
Authors: Huyakorn, P.S., et al.

FTRANS (fracture Flow, Thermal and RAdioNuclide Solute transport)is a 2D finite-element model to simulate transient, saturated single phase flow, heat transport, and chemical or radionuclide transport in fractured or unfractured, anisotropic, heterogeneous, confined or semi-confined multilayered porous media. For any type of fractured system, the flow and transport analysis are performed taking into account interaction between the porous matrix and the fractures. The analyses are made in the main areal flow plane, in a vertical cross-section, or in an axisymmetric configuration. The code fully accounts for fluid leakages, advection, dispersion, sorption, first-order decay, chain reactions, and solute diffusion and heat conduction in the porous matrix, coupled thermal fluid capability and density-dependent flow and solute transport.

Contact Address: Performance Assessment Dept., Office of Nuclear Waste Isolation, Battelle Project Management Division, 505 King Avenue Columbus, Ohio 43201

IGWMC Key: 582 Model Name: GREASE Released: 1982
Author: Huyakorn, P.S., et al.

GREASE 2 is a multi-purpose finite element model to simulate transient, multi-dimensional, saturated groundwater flow, solute and/or energy transport in fractured and non-fractured, anisotropic, heterogeneous, multilayered porous media. The analysis can be performed for confined, semiconfined, or unconfined groundwater reservoir systems. Fluid leakage or heat transfer between the aquifer and its confining layer can be taken into account. The model allows for analysis of areal flow, vertical cross-sectional flow or flow in an axisymmetric configuration. Coupled thermal fluid flow capability, and density dependent flow and solute transport capability area also available. Sorption and decay can be included in the solute transport analysis.

Contact Address: GeoTrans, Inc., 46050 Manekin Plaza, Suite 100, Sterling, VA 22170

IGWMC Key: 584 Model Name: STAFAN Released: 1982
Author: Huyakorn, P.S., et al.

STAFAN (STress And Flow ANalysis) is a two-dimensional finite element model for simulation of transient fluid flow and the interaction of fluid pressure and mechanical stresses in deformable fractured and unfractured porous media. The model takes into account the flow behavior of a deformable fractured system with fracture-porous matrix interactions, the coupling effects of fluid pressure and mechanical stresses in a medium containing discrete joints, and inelastic response of the individual joints of the rock mass subject to the combined fluid pressure and mechanical loading.

Contact Address: Office of Nuclear Waste Isolation, Battelle Project Management Division, 505 King Avenue, Columbus, Ohio 43201

IGWMC Key: 588 Model Name: SEFTRAN Released: 1986
Authors: Huyakorn, P.S., Ward, D.S.3, Rumbaugh, J.O., Broome, R.W.

SEFTRAN (Simple and Efficient Flow and TRANsport model) is a concise finite element model to simulate transient two-dimensional fluid flow and transport of non-conservative contaminants or heat in isotropic, heterogeneous aquifers. It can solve the flow and transport equations in an areal plane, a vertical cross-section, or an axisymmetric configuration. Line elements may be used to simulate discrete fractures or rivers.

Contact Address GeoTrans, Inc., 46050 Manekin Plaza, Suite 100, Sterling, VA 22170

IGWMC Key: 589 Model Name: TRAFRAP Released: 1987
Authors: Huyakorn, P.S., White, Jr., H.O., Guvanasen, V.M., Lester, B.H.

TRAFRAP-WT is a two dimensional finite element code which simulates transient groundwater flow and transport of a non-conservative contaminant or a radionuclide in fractured or unfractured porous media. Fracture systems may be modeled using either the dual porosity approach or the discrete fracture approach. TRAFRAP-WT can be used for both confined and unconfined aquifer systems. Model processes include fluid interactions between fractures and porous matrix blocks, advective-dispersive transport in fractures and diffusion in the porous matrix blocks, and chain reactions of radionuclides.

Contact Address: Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401

IGWMC Key: 695 Model Name: NETFLO (Network Flow) Released: 1982
Authors: Pahwa, S.B., Rama Rao, B.S.

NETFLO is a finite element model to simulate steady-state saturated flow in a fractured medium by an equivalent three-dimensional network of in-series and parallel flow members. The algorithm is based on the application of Darcy's law along each member and conservation of mass in each node. The boundary conditions may be either prescribed head or a sink/source at each node. The code output pressures at each node and velocities, fluxes and travel times in each member. It also provides all possible flow paths between a source node (e.g. a repository) and a specified discharge node, the path lengths and the pertinent mean interstitial velocity and travel time along each path for use in a one-dimensional transport code such as GETOUT. The nodal equations are solved using Gaussian elimination.

Contact Address: Performance Assessment Department, Office of Nuclear Waste Isolation, Battelle Project Management Division, 505 King Avenue, Columbus, Ohio 43201

IGWMC Key: 2034 Model Name: SHALT Released: 1979
Authors: Pickens, J.F., Grisak, G.E.

SHALT is a finite element model that simulates heat and solute transport in a fractured, anisotropic, heterogeneous, saturated or unsaturated, confined or unconfined, two-dimensional groundwater flow system. The Galerkin finite element method uses triangular elements and a sequential solution technique. The model simulates density dependent compressible fluid flow; heat convection, conduction and dispersion; solute advection, dispersion and linear equilibrium adsorption; radioactive decay; ion exchange; diffusion; sorption; and various first-order chemical reactions.

Contact Address: Pickens, J.F., Intera Technologies, Inc., 6850 Austin Center Blvd., Suite # 300, Austin, TX 78731

IGWMC Key: 2581 Model Name: MULKOM Released: 1985
Author: Pruess, K.

MULKOM is an integrated finite difference model to simulate multi-component, multi-phase fluid and heat flow in porous or fractured media. The model incorporates convection, change of phase, dissolution and precipitation of silica, equilibration of noncondensible gases, transport of noncondensible gases and dissolved solids.

Contact Address: Pruess, K.,Lawrence Berkeley Lab., Univ. of California, Berkeley, CA 94720

IGWMC Key: 2582 Model Name: TOUGH Released: 1987
Authors: Pruess, K., Tsang, Y.W., Wang, J.S.Y.

TOUGH (Transport of Unsaturated Groundwater and Heat) is a multi-dimensional integrated finite difference model for transient simulation of the strongly coupled transport of water, air, vapor and heat transport in fractured unsaturated porous media. The model includes convection, condensation, capillary forces, evapotranspiration, heat conduction and diffusion, change of phase, adsorption, fluid compression, dissolution of air in liquid, and buoyancy. The gas and liquid phase flow of air and water, and heat transport are solved in a fully coupled manner. Time is discretized fully implicitly. The TOUGH code includes a library of commonly used functions for the capillary pressure-relative permeability relationships (does not allow for hysteresis). The model handles a variety of boundary conditions.

Contact Address: Pruess, K., Lawrence Berkeley Lab., Earth Science Div., Univ. of California, Berkeley, CA 94720

IGWMC Key: 3083 Model Name: ROCMAS-THM Released: --
Authors: Noorishad, J., Witherspoon, P.A.

ROCMAS-THM is a two-dimensional research model for coupled hydraulic-thermal-mechanical analysis of porous fractured rock.

Contact Address: Noorishad, J., Lawrence Berkeley Lab., Earth Science Div., Univ. of California, Berkeley, CA 94720

IGWMC Key: 3232 Model Name: FRACFLOW Released: 1981
Author: Sagar, B.

FRACFLOW is an integrated finite difference model for steady and nonsteady state analysis of coupled, density-dependent flow, heat and mass transport in fractured confined aquifers. The processes in the porous medium are simulated in two dimensions and in the fractures in one dimension. Fractures may have arbitrary orientations. Any number of fractures, each of different properties may be incorporated. The program includes first-order chemical reactions. A preprocessor and a number of graphic post-processing routines are available.

Contact Address: B. Sagar, Southwest Research Inst., P.O.Box 0510, Div. 20, San Antonio, TX 28510

IGWMC Key: 3238 Model Name: PORFLOW-3D Released: 1992
Author: Runchal, A.K.

PORFLOW-3D is an integrated finite difference model to simulate coupled transient or steady-state, multiphase, fluid flow, and heat, salinity, or chemical species transport in variably saturated porous or fractured, anisotropic and heterogeneous media. The program facilitates arbitrary sources or sinks in three-dimensional cartesian or axisymmetric (cylindrical) geometry. The user interface is based on the FREEFORM language using simple English-like commands. The software includes the ARCPLOT graphic post processor.

Contact Address: A. Runchal, 1931 Stradella Road, Bel Air, CA 90077

IGWMC Key: 3374 Model Name: FRACPORT Released: 1985
Authors: Deangelis, D.L., Yeh, G.T., Huff, D.D.

FRACPORT (FRACtured PORous medium Transport) is an integrated compartmental model for describing the advective-dispersive transport of a non-conservative solute in a three-dimensional fractured saturated porous medium. The model assumes a known velocity field. It solves the transport equation on two different time scales: one related to rapid transport of solute along fractures and the other related to slower transport through the porous matrix. A governing equation is developed for each interior compartment. The equation are assembled in matrix form and solved in two steps, first using a direct method or an iterative method, followed by an iteration procedure over all boundary connectors. The model handles Dirichlet, Neumann, Cauchy, and variable boundary conditions.

Contact Address: DeAngelis, D.L., Oak Ridge Nat. Lab., Environm. Sc. Div., Oak Ridge, TN 37830

IGWMC Key: 3790 Model Name: PORFLO Released: 1985
Authors: Runchal, A.K., Sagar, B., Baca, R.G., Kline, N.W.

PORFLO is an integrated finite difference model for transient two-dimensional or axisymmetric simulation of coupled buoyancy driven groundwater flow, heat transfer and radionuclide transport in layered geologic systems. Heat transfer processes include storage, advection, conduction, dispersion and heat generation. Fluid flow processes include storage, inflows and outflows, pore pressure buildup, buoyancy driving force and temperature dependent hydraulic conductivity. Density is a function of concentration. Mass transport processes can handle multi-phase conditions and include storage, advection, dispersion, diffusion, sorption, retardation, dissolution, decay, and mass release.

Contact Address: N.W. Kline, Boeing Computer Services, P.O Box 300, Richland, WA 99352

IGWMC Key: 3842 Model Name: SWIFT III/SWIFT 386 Released: 1992
Author: Ward, D.S.

SWIFTIII/386 is a transient, fully three-dimensional model which simulates the flow and transport of fluid, heat (energy), brine, and radionuclide chains in porous and fractured geologic media. The primary equations for fluid, heat, and brine are coupled by fluid density, fluid viscosity, and porosity. Both Cartesian and cylindrical coordinate systems may be used. For the fracture zone the model allows both dual-porosity and discrete fractures. Migration within the rock matrix is characterized as a one-dimensional process.

continued.....

SWIFT III/386 -- *continued*

Aquifer hydraulic characteristics may be heterogeneous and anisotropic under confined or unconfined conditions. The model includes linear and nonlinear (Freundlich) isothermal equilibrium adsorption, hydrodynamic dispersion, and diffusion.

Discretization is performed by the finite-difference method using centered or backward weighing in the time and space domains. Matrix solution is performed either by Gaussian elimination or by two-line successive over-relaxation. SWIFT/386 incorporates a run-time monitor to display the actions and numerical behavior of on-going transport simulations. The IBM PC version handles between 10,000 and 30,000 finite difference blocks.

SWIFT III/386 handles a variety of boundary conditions and source terms for both the porous and fractured media including prescribed pressure (head), temperature, and brine concentration; prescribed flux of fluid (water), heat, brine, or (nuclide) mass; wellbore injection/production submodel subject to pumping constraints; aquifer influence function (i.e. Carter-Tracy infinite reservoir); waste leach radionuclide submodel for waste repository nuclides and heat; and free (phreatic) surface with recharge.

SWIFT III/SWIFT 386 is an extension of SWIFT II (IGWMC Key # 3842), which in turn is an update and extension of SWIFT (Sandia Waste-Isolation Flow and Transport; IGWMC Key # 3841), released in 1981. Originally, refinements in user options, mapping facilities and auxiliary files were included. A postprocessing program UNSWIFT allows direct interfacing with the SURFER contouring package.

Contact Address: D.S. Ward, GeoTrans, Inc., 46050 Manekin Plaza, Suite 100, Sterling, VA 22170

IGWMC Key: 4031 Model Name: TRUCHN/ZONE Released: 1984
Authors: Rasmuson, A., Neretnieks, I.

TRUCHN/ZONE is an integrated finite difference model for simulation of advective-dispersive transport of radionuclides in strongly fissured zones including diffusion into the rock matrix. The model may handle instantaneous sorption in a portion of the rock (surface sorption) and sorption on the micropore surface. The prescribed water velocity may vary strongly along a flow path, especially if the flow paths enters a strongly fissured zone. The model, which uses an axi-symmetric coordinate system, can handle varying matrix block sizes and shapes using an improved MINC concept (Multiple INter-acting Continua).

Contact Address: Rasmuson, A., Royal Institute of Technology, Department of Chemical Engineering, S-100 44 Stockholm, Sweden

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IGWMC Key: 4270 Model Name: TRACR3D Released: 1984
Author: Travis, B.J.

TRACR3D is a three-dimensional implicit (for flow)/semi-implicit (for transport) finite difference model for simulation of transient two-phase flow of water and air and of non-conservative multi-component transport in deformable, heterogeneous, water-saturated or variably-saturated, reactive porous and/or fractured media. Transport processes include advection, dispersion, sorption, and decay. The code has been applied to study the hydrology and transport of colloids with radioactive materials at a low-level radioactive waste disposal site.

Contact Address: Travis, B.J., Los Alamos Nat. Lab., Los Alamos, NM 87545

IGWMC Key: 4470 Model Name: FRACTEST Released: 1986
Author: Karasaki, K.

FRACTEST simulates three-dimensional flow in unconfined non-porous rock with discrete fractures. The model has been developed to support well test analysis in fractured systems. The model includes a mesh generator to produce a representative fracture system, and a finite element simulator for calculation of transient hydraulic heads using a parallel processor.

Contact Address: Lawrence Berkeley Lab., Earth Sc. Div., Univ. of Calif., Berkeley, CA 94720

IGWMC Key: 4550 Model Name: MOTIF released: 1984
Authors: Guvanasen, V.

MOTIF (Model of Transport in Fractured/Porous Media) is a finite element model to simulate one-, two-, and three-dimensional coupled processes of saturated or unsaturated fluid flow, conductive and convective heat transport, brine transport and single species radionuclide transport in a compressible rock of low permeability intersected with a few major fractures. The model includes diffusion into the rock matrix.

Contact Address: T. Chan, Atomic Energy of Canada, Ltd., Whiteshell Nuclear Research Estb., Pinawa, Manitoba, Canada R0E1l0

IGWMC Key: 4590 Model Name: MAGNUM-2D Released: 1985
Authors: England, R.L., Kline, N.W., Ekblad, K.J., Baca, R.G.

MAGNUM-2D is a two-dimensional, cross-sectional or three-dimensional axi-symmetric finite element model for transient or steady-state analysis of coupled heat transfer and groundwater flow in an inhomogeneous, anisotropic, fractured porous medium. Transport processes include advection, dispersion, diffusion, sorption and decay for multiple species. A set of support programs are available to generate, manipulate, and display the finite element grid; to compute and plot pathlines and traveltimes; and to plot contours, spatial cross-sections, and time histories for temperature and hydraulic head. The program can be linked with a radionuclide-chain transport code CHAINT (IGWMC Key 3791).

Contact Address: Rockwell Hanford Operations, P.O. Box 800, Richland, WA 99352

IGWMC Key: 4600 Model Name: SANGRE Released: 1986
Author: Anderson, C.A.

SANGRE is a finite element code for thermomechanical analysis of two-dimensional problems in structural geology. It allows simulation of convective heat transport, consolidation, and fluid migration. It includes modeling capabilities for highly deformable and deformed geologic media, large deformations, faults, overthrusts, etc. The model has a flexible, grid which can rotate and translate in time, following the displacements of the rock matrix.

Contact Address: C.A. Anderson, Los Alamos Nat. Lab., Los Alamos, NM 87545

IGWMC Key: 4710 Model Name: STAFF2D Released: 1988
Authors: Huyakorn, P.S., et al.

STAFF2D (Solute Transport And Fracture Flow in 2 Dimensions) is a 2 dimensional finite element model that simulates groundwater flow and solute transport in fractured or granular porous media under confined or unconfined conditions. The code performs steady-state and transient simulations in a cross-section, an areal plane, or an axisymmetric configuration. Contaminant transport accounts for advection, dispersion, linear equilibrium sorption and first-order degradation. Fractured porous media are represented using discrete fracture and dual porosity approaches. Spatial discretization is performed using a combination of linear and rectangular elements. The transport equation is solved using upstream weighing. STAFF2D also provides an option to use orthogonal curvilinear elements for single or double well analysis.

Contact Address: Hydrogeologic, Inc., 1165 Herndon Parkway, #900, Herndon, VA 22070

IGWMC Key: 5003 Model Name: MLU Released: 1986
Author: Hemker, C.J.

MLU (Multi-Layer Unsteady-state model) is a program for drawdown calculations and inverse modeling (aquifer tests) of transient flow in layered (up to 9 aquifers) and fissured (double porosity aquifer systems of (semi-)confined and unconfined conditions. The model is based on a series of analytical solutions.

Contact Address: Hemker, C.J., Elandsgracht 83, 1016TR Amsterdam, The Netherlands

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IGWMC Key: 5022 Model Name: 3-D FE DUAL POROSITY FLOW AND TRANSPORT MODEL
Author: Glover, K.C. Released: 1987

This model simulates three-dimensional groundwater flow and advective-dispersive solute transport in oil shale and associated hydrogeologic units. The model treats oil shale as a dual porosity medium by simulating flow and transport in parallel fractures separated by a matrix (blocks) of high porosity, low permeability material using the upstream finite element method. Diffusion of the solute between fractures and the essentially static water of the shale matrix is simulated including an analytical solution that acts as a source-sink term to the differential equation of solute transport. The resulting equations are solved using a Gauss elimination scheme.

Contact Address: U.S. Geological Survey, P.O. Box 1125, Cheyenne, WY 82003

IGWMC Key: 5025 Model Name: NEFTRAN/NWFT/DVM Released: 1987
Authors: Longsine, D.E., Bonano, E.J., Harlan, C.P.

NEFTRAN (NEtwork Flow and TRANsport) is a discrete finite difference model for groundwater flow and radionuclide transport in high-level radioactive waste repositories in deep saturated and fractured basalt formations. It handles a generalized flow network, matrix diffusion, leg transfer, mixing cell and multiple radionuclide decay chains. The underlying assumption is that all significant flow and radionuclide transport take place along one-dimensional discrete 'legs' or paths. These legs are assembled into a multi-dimensional network. A particle tracking model is used to define the trajectory a particle follows from a given point until it crosses a boundary. The resulting information is used to construct the network and define the boundary conditions.

Contact Address: Sandia National Laboratories, Albuquerque, New Mexico 87185

IGWMC Key: 5320 Model Name: 3D FRACTURE GENERATOR Released: 1984
Authors: Huang, C., Evans, D.D.

This code is based on a 3-dimensional fracture generating scheme which can be used to simulate water flow and contaminant transport through fractured rock. It is limited to saturated conditions, zero rock matrix permeability, and steady state flow. The scheme creates finite planar plates of uniform thickness which represent fractures in 3-dimensional space. A given fracture is defined by its center location, orientation, shape, areal extent, and aperture. Individual fractures are generated to form an assemblage of a certain fracture density. Flow through the fractures is two-dimensional and laminar and is described by Poiseuille's law. The flow solution provides head, velocities, fluxes, and traveltimes. Transport is advective and piston-type, solved explicitly.

Contact Address: D.D. Evans, Dept. of Hydrology and Water Resources, University of Arizona, Tuscon, AZ 85721

IGWMC Key: 5640 Model Name: NETFLO/NETRANS Released: 1988
Author: Rouleau, A.

This stochastic discrete fracture (SDF) modeling package simulates groundwater flow and mass transport in fracture systems. It contains 4 programs: (1) NETWRK generates two-dimensional fracture networks using a monte carlo method based on the statistics of field data on fracture geometry; (2) APEGEN generates supplementary aperture distributions; (3) the NETFLO finite element code computes the steady-state fluid flow through the fracture network generated by NETWRK and APEGEN, and computes the statistics of selected parameters in every ten-degree range of direction, including the total length of fracture segments, total flow velocity, and total flow rate; and (4) NETRANS computes the transit time of particles over an arbitrary distance using a second-level stochastic process.

Contact Address: Rouleau, A., Dept. de Sciences Appliquees, Universite du Quebec a Chitoutimi, 555 Boulevard de l'Universite, Chicoutimi, Quebec G7H 2B1, Canada

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IGWMC Key: 5660 Model Name: FLASH Released: 1992
Authors: Baca, R.G., Magnuson, S.O.

FLASH is a finite element model for simulation of two-dimensional, cross-sectional, variably saturated fluid flow in fractured porous media at an arid site, together with two-dimensional, horizontal, saturated flow in an underlying unconfined aquifer. In addition, the code has the capability to simulate heat conduction in the vadose zone. The Richard's equation for variably saturated flow is solved iteratively using a Picard or Newton iteration technique, the unconfined flow equation is solved using Newton-Raphson iteration. The variably saturated module handles 1st, 2nd and 3rd type b.c.'s, the saturated module only 1st and 2nd type b.c.'s. The FLASH code can be interfaced with the FLAME code to simulate contaminant transport in the subsurface.

Contact Address: Baca, R.G., Idaho National Eng. Lab., Subsurface and Environm. Modeling Unit, Geoscience Group, EG&G, Inc, P.O. Box 1625, Idaho Falls, Idaho 83415.

IGWMC Key: 5980 Model Name: FRANET Released: 1987
Authors: Kanehiro, B.Y., Lai, C.H., Stow, S.H.

The discrete fracture code FRANET is based on a Galerkin finite element formulation for steady state and transient fluid flow in an arbitrary fracture network. It considers isothermal flow of a slightly compressible fluid in the laminar regime and assumes that fracture aperture or equivalent fracture hydraulic conductivity is a function of fluid pressure. The model solves the governing equation for fluid flow in a local one-dimensional coordinate system for each fracture of the network subject to the continuity of hydraulic head at fracture intersections. The model might be coupled with a fracture network mesh generator representing the statistical distribution of the fracture parameters.

Contact Address: Kanehiro, B.Y., Berkeley Hydrotechnique, Inc., 2030 Addison St., Suite 500, Berkeley, CA 94704

IGWMC key: 6660 Model Name: CRACK Released: 1988
Author: Sudicky, E.A.

The CRACK microcomputer software package contains four analytical models for mass transport in fractured porous media. The following models are included: transport in a single fracture including matrix diffusion with and without dispersion along fracture axis (models CRACKD and CRACKD0, respectively); transport in a system of parallel fractures including matrix diffusion with no dispersion along fracture axis (PCRACK0); and transport in a single fracture with matrix diffusion and radial diverging flow (RCRACK). The package includes a plotting routine for concentration vs. time at different locations or concentration vs. position for different times (PLOTC).

Contact Address: Waterloo Centre for Groundwater Research, Dept. of Earth Sciences, University of Waterloo, Waterloo, Ontario N21 3G1, Canada

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IGWMC Key: 6810 Model Name: BIM/BIM2D/BIM3D/FRACGEN Released: 1989
Authors: Rasmussen, T.C., Evans, D.D.

BIM/FRACGEN is simulates flow and (advective)solute transport in unsaturated, fractured, porous or non-porous media. It solves the boundary value problem within intersecting fracture planes using the boundary integral method applied to two and three-dimensional formulations for flow using a constant capillary head within individual fractures. The transport problem is solved through calculating travel times and breakthrough curves by integrating the inverse velocity over a streamline, and then summing over all streamlines. The transport equation includes linear equilibrium reversible sorption (retardation) and diffusion from fractures into the rock matrix and v.v. FRACGEN generates synthetic fracture networks for sensitivity analysis with respect to fracture network parameters.

Contact Address: D.D. Evans, Dept. of Hydrology and Water Resources, Univ. of Arizona, Tuscon, AZ 85721

Appendix F: Flow and Transport in Fractured Rock, Part 2: Usability and Reliability

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
581	FTRANS	N	N	Y	Y	N	N	Y	Y	L	N	F
582	GREASE	N	N	Y	Y	N	N	Y	U	L	L	F
584	STAFAN	N	N	Y	Y	N	N	Y	Y	L	L	F
588	SEFTRAN	Y	Y	Y	Y	Y	N	Y	U	L	L	M
589	TRAFRAP	N	N	Y	Y	N	N	Y	N	L	N	F
695	NETFLO	N	N	Y	Y	N	N	Y	U	L	U	F
2034	SHALT	U	U	Y	Y	U	U	Y	U	L	U	U
2581	MULKOM	U	U	Y	Y	N	L	Y	U	L	U	F
2582	TOUGH	U	U	Y	Y	N	L	Y	U	L	U	F
3083	ROCMAS-THM	U	U	Y	Y	N	U	Y	U	L	U	U
3232	FRACFLOW	Y	Y	Y	Y	Y	Y	Y	U	E	L	F
3238	PORFLOW-3D	Y	Y	Y	Y	Y	Y	Y	U	E	L	M
3374	FRACPORT	U	U	Y	Y	N	U	Y	U	L	U	U
3790	PORFLO	Y	Y	Y	Y	Y	Y	Y	U	L	L	F
3842	SWIFT III/386	Y	Y	Y	Y	Y	Y	Y	U	E	L	M
4031	TRUCHN/ZONE	U	U	Y	Y	N	L	Y	U	L	L	F
4270	TRACR3D	U	U	Y	Y	N	L	Y	U	L	U	U
4470	FRACTEST	U	U	Y	Y	U	U	Y	U	U	U	U
4550	MOTIF	U	U	Y	Y	N	L	Y	U	E	L	F
4590	MAGNUM-2D	U	U	Y	Y	N	U	Y	U	L	L	F

KEY: Y = YES N = NO L = LIMITED E = EXTENSIVE M = MANY F = FEW U = UNKNOWN

Appendix F, part 2 (continued)

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
4600	SANGRE	U	U	Y	Y	U	U	Y	U	L	U	F
4710	STAFF2D	Y	Y	Y	Y	Y	L	Y	U	L	L	F
5003	MLU	Y	Y	Y	Y	Y	L	Y	U	L	U	F
5022	3-D FE DUAL POROSITY	U	U	Y	Y	U	U	Y	U	L	U	U
5025	NEFTRAN	N	N	Y	Y	N	N	Y	U	L	L	U
5320	3D FRACTURE GENERATOR	N	N	Y	Y	N	N	Y	N	L	N	U
5640	NETFLO/ NETRANS	U	U	Y	Y	U	U	Y	U	U	U	U
5660	FLASH	N	N	Y	Y	N	L	Y	U	L	L	F
5680	FRANET	N	N	Y	Y	N	N	Y	U	L	U	U
6660	CRACK	Y	Y	Y	Y	Y	Y	Y	U	L	L	M
6810	BIM/FRACGEN	U	U	Y	Y	U	U	Y	U	L	U	U

KEY: Y = YES N = NO L = LIMITED E = EXTENSIVE M = MANY F = FEW U = UNKNOWN

Appendix G: Hydrogeochemical Models, Part 1: Model Description

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IGWMC Key: 124 Model Name: DYNAMIX Released: 1988
Authors: Narasimhan, T.N., Liu, C.W.

DYNAMIX is a redox-controlled multi-species, multidimensional reactive chemical transport model. It couples the chemical speciation code PHREEQE with the transport code TRUMP. The program includes acid-base reactions, aqueous complexation, redox reactions, precipitation-dissolution reactions and kinetic mineral dissolution. A search routine based on minimizing Gibbs free energy is used to identify the correct mineral assemblage during the equilibrium calculation. The transport equations of each chemical component are solved using the integral finite difference method. DYNAMIX uses a two-step dynamic mixing approach to solve the equations of chemical transport and chemical equilibrium.

Contact Address: T.N. Narasimhan, Dept. of Materials Sc. and Mineral Eng., Univ. of Calif., Berkeley, CA 94720

IGWMC Key: 2610 Model Name: PHREEQE Released: 1992
Authors: Parkhurst, D.L., Thorstenson, D.C., Plummer, L. N.

PHREEQE is an equilibrium geochemical speciation and reaction path model that calculates mass transfer as a function of stepwise temperature change or dissolution. Based on an ion-pairing aqueous model, PHREEQE can calculate Ph, redox potential, and mass transfer as a function of reaction progress. The original version included redox reactions and ion exchange for 19 elements, 120 aqueous species, 3 gases, 21 minerals. A series of coupled chemical equations are solved iteratively to yield the following: Ph, Eh, total concentration of elements, amount of minerals (or other phases) transferred into or out of the aqueous phase, distribution of aqueous species, and the saturation state of the aqueous phase with respect to specified mineral phases.

Contact Address: U.S. Geol. Survey, Water Resources Div., Nat. Center, Reston, VA 22092; or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 2611 Model Name: PHRQPITZ Released: 1988
Authors: Plummer, L.N., Parkhurst, D.L., Fleming, G.W., Dunkle, S.A.

PHRQPITZ is a code capable of making geochemical calculations in brines and other electrolyte solutions to high concentrations using Pitzer virial coefficient approach for activity-coefficient corrections. Reaction-modeling capabilities include calculation of 1) aqueous speciation and mineral saturation index, 2) mineral solubility, 3) mixing and titration of aqueous solutions, 4) irreversible reactions and mineral-water mass transfer, and 5) reaction path. The computed results for each aqueous solution include the osmotic coefficient, water activity, mineral saturation indices, mean and total activity coefficients, and scale-dependent values of pH, individual-ion activities, and individual-ion activity coefficients. It includes a data-base of Pitzer interaction parameters.

Contact Address: Water Resources Div., U.S. Geol. Survey, 432 National Ctr., Reston, VA 22092; or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 3084 Model Name: CHNTRNS Released: 1987
Authors: Noorishad, J., Carnahan, C.L., Benson, L.V.

CHMTRNS is a temperature-dependent non-equilibrium reactive chemical transport code, based on the CHEMTRN code (Miller and Benson) developed in the early 1980's. Equations solved include mass balance, aqueous species transport, non-equilibrium reactions, transport of hydrogen and hydroxide ions, equilibrium complexation, dissolution and precipitation, ion exchange, redox reactions, and heat transport. The code is capable of simulating kinetic calcite and silicate dissolution, irreversible glass dissolution, oxidation and reduction, and stable carbon isotope fractionation during transport. The code can handle Neumann and Dirichlet boundary conditions and includes a mesh generation scheme. The 1-D transport equation is solved using a upstream weighted finite difference algorithm.

Contact Address: Lawrence Berkeley Lab., Earth Sciences Div., Univ. of Calif., Berkeley, CA 94720

IGWMC Key: 3400 Model Name: BALANCE Released: 1992
Authors: Parkhurst, D.L., Plummer, L.N., Thorstenson, D.C.

BALANCE is a reaction model designed to define and quantify chemical reactions between groundwater and minerals. It uses the chemical composition of water samples from two points along a flow path and a set of mineral phases (minerals, organic substances, or gases) hypothesized to be the reactive constituents in the system to calculate the mass transfer necessary to account for the observed changes in composition between the two water samples. Additional constraints can be included in the problem formulation to account for mixing of two end-member waters, redox reactions, and, in a simplified form, isotropic composition. BALANCE solves any set of linear equations formulated by the user and is not constrained by thermodynamic criteria.

Contact Address: U.S. Geol. Survey, Water Resources Div., Federal Center, Lakewood, CO 80225; or
Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 3611 Model Name: CHMTRNS Released: 1987
Authors: Noorishad, J., Carnahan, C.L., Benson, V.

CHMTRNS is a one-dimensional hydrochemical model that uses 2-step coupling between chemical relations and transport equations. It includes kinetics and carbon-13 fractionation in addition to equilibrium calculations. The model handles precipitation and dissolution. Sorption is modeled by ion exchange and surface complexation. Activity coefficient is calculated by Davies equation.

Contact Address: Lawrence Berkeley Lab., Earth Sc. Div., Univ of Calif., Berkeley, CA 94720

IGWMC Key: 3620 Model Name: WATEQF Released: 1984
Authors: Plummer, L.N., Jones, B.F., Truesdell, A.H.

WATEQF is a program to model the thermodynamic speciation of inorganic ions and complex species in solution for given water analysis. Processes included are mass balances and redox reactions. (see also WATEQ2/WATEQ4F

Contact Address: U.S. Geol. Survey, Water Resources Div., Nat. Center, Reston, VA 22092

IGWMC Key: 3621 Model Name: NETPATH Released: 1992
Authors: Plummer, L.N., Prestemon, E.C., Parkhurst, D.L.

NETPATH is an interactive program for the interpretation of net geochemical mass-balance reactions between an initial and final water along a hydrologic flow path. Alternatively, NETPATH computes the mixing proportion of a final water. The program utilizes previously defined chemical and isotopic data for waters from a hydrochemical system. Every possible geochemical mass balance reaction model is examined between selected evolutionary waters for a set of chemical and isotopic constraints, and a set of plausible phases in the system. The calculations are of use in interpreting geochemical reactions, mixing proportions, evaporation and (or) dilution of waters, and mineral mass transfer in the chemical and isotopic evolution of natural and environmental waters.

Contact Address: Nat. Water Inform. System, U.S. Geol. Survey, 437 Nat. Ctr., Reston, VA 22092; or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 4450 Model Name: TRANQL/MICROQL Released: 1985
Authors: Cederberg, G.A., Street, R.L., Leckie, J.O.

TRANQL is a finite element transport model for simulation of multi-component solute transport with equilibrium interaction chemistry coupled with 1-D advective-dispersive finite element transport. Significant equilibrium reaction such as complexation, ion exchange, competitive adsorption, and dissociation of water may be included. It includes to models for ion-exchange, the constant capacity model and the triple-layer model. The model has been applied to cadmium, chloride, and bromide transport in a 1-D column.

Contact Address: G.A. Cederberg, 2305 A 37th Street, Los Alamos, NM 87544

IGWMC Key: 4810 Model Name: EQ3/EQ6 Released: 1988
Author: Wolery, T.J.

EQ3 is a geochemical aqueous speciation/solubility program that can be used alone or in conjunction with EQ6, which performs reaction-path calculations. EQ3 calculates the distribution of chemical species (ions, neutral species, ion-pairs, and complexes). The program EQ3/EQ6 accommodates 47 elements, 686 aqueous species, 15 gases, over 16 redox elements, and 716 minerals. The code embodies a ion-association conceptual model of solution behavior and simulates geochemical reactions using Newton-Raphson solution method. The code requires geochemical data for each solid, gaseous or dissolved chemical species being modeled. The data bases accompanying the code are for testing purposes only. A separate precipitation kinetics option has been added.

Contact Address: K.J. Jackson, Lawrence Livermore Lab., Livermore, CA 94550

IGWMC Key: 4820 Model Name: EQUILIB Released: 1981
Authors: Morrey, J.R., Shannon, D.W.

EQUILIB models chemical equilibria in geothermal brines at various elevated temperatures (0 - 300 degrees C). Its data base contains 26 elements, 200 aqueous species, 7 gases, 186 minerals, and it includes 9 redox reactions. The code uses ligand projection method of solution, and the activity coefficient is provided by the extended Debye-Huckel equation. It has been verified and partially validated by comparing it to four other geochemical codes and to five laboratory experiments. EQUILIB has been applied to studying mineral formation and corrosion in geothermal brines.

Contact Address: Electric Power Research Inst., P.O.Box 10412, Palo Alto, CA 94303

IGWMC Key: 4830 Model Name: GEOCHEM Released: 1980
Authors: Sposito, G., Mattigod, S.V.

GEOCHEM is a program for predicting the equilibrium distribution of chemical species in soil solution and other natural water systems. The programs data base includes 45 elements, 1853 aqueous species, 889 organic ligands, 3 gases, and 250 minerals and solids. It includes a mass balance for each species and can handle 7 redox reactions and cation adsorption and exchange. The Newton-Raphson solution method is used, and a Davies equation provides the activity coefficient. Sorption is handled by a surface complexation model.

Contact Address: G. Sposito, Dept. of Soil and Environm. Sc., Univ. of California, Riverside, CA 92521

IGWMC Key: 4840 Model Name: MINEQL2 Released: 1980
Authors: Westall, J.C., Zachary, J.L., Morel, F.M.M.

MINEQL2 is a program for the calculation of chemical equilibria in aqueous systems. It includes mass balance calculations for each component, redox reactions, and surface adsorption.

Contact Address: F.M.M. Morel, Massachusetts Inst. of Technology, Dept. of Civil Eng., Cambridge, MA 02139

IGWMC Key: 4850 Model Name: MINTEQ/MINTEQ2/MINTEQA2 Released: 1987
Authors: Felmy, A.R., Girvin, D.C., Jenne, E.A.

MINTEQ is a user-friendly program for calculation of the equilibrium behavior of various metals. It includes a complex series of reactions among solution species, gases, solids, and sorbed phases, including ion speciation/solubility, adsorption, gas phase equilibria, and precipitation/dissolution of solid phases. The thermodynamic data in MINTEQ was taken from the WATEQ3 data base and has been further expanded and updated using published critical reviews. Originally, MINTEQ included 31 elements, 373 aqueous species, 3 gases, and 328 solids. Its data base is being updated on a regular basis. The program calculates mass balance for each component, and includes redox reactions, ion exchange and six surface complexation models.

Contact Address: E.A. Jenne, Battelle Pacific NW Laboratory, P.O. Box 999, Richland, WA 99352; or CEAM, Environm. Res. Lab., US EPA, Athens, GA 30613-0801.

IGWMC Key: 4851 Model Name: MININR/MINICUP Released: 1983
Authors: Felmy, A.R., Reisenauer, A.E., Zachora, J.M., Gee, G.W.

MININR is a reduced form of the computer program MINTEQ which calculates equilibrium precipitation/dissolution of solid phases, aqueous speciation, adsorption, and gas phase equilibrium. The user-oriented features in MINTEQ were removed to reduce the size and increase the computational speed. MININR closely resembles the MINEQL program, their main differences being modifications to accept an initial starting mass of solid and necessary changes for linking with a water flow model. The thermochemical data are passed to MININR by a run from MINTEQB. MININR has been linked with the one-dimensional SATCOL saturated flow model in a code called MINICUP.

Contact Address: Battelle Pacific Northwest Lab., Environm. Res. Group, Richland, WA 99352

IGWMC Key: 4860 Model Name: PROTOCOL Released: 1984
Authors: Pickrell, G., Jackson, D.D.

PROTOCOL (PROgram TO COrrelate Leaching data) is a coupled kinetic/equilibrium program for calculating dissolution reactions of inorganic solids in aqueous solution, with specific application to corrosion of vitrified nuclear waste by groundwater. PROTOCOL was designed to function as a generic simulator without specific rate expressions or leaching mechanisms. Such functions may be input to the program as submodels. Initially three submodels have been incorporated. The program incorporates equilibrium routines from the program MINEQL and includes an extensive thermodynamic data base.

Contact Address: D.D. Jackson, Lawrence Livermore Lab., Univ. of Calif., L-329, Livermore, CA 94550

IGWMC Key: 4870 Model Name: REDEQL-EPA Released: 1978
Authors: Ingle, S.E., Schuldt, M.D., Schults, D.W.

REDEQL.EPA is a program to compute aqueous equilibria for up to 20 metals and 30 ligands in a system. It includes 46 elements, 94 aqueous species, 2 gases, and 13 minerals/solids. It calculates mass balances, and handles precipitation, redox reactions, complexation and pH-dependent phenomena.

Contact Address: D.W. Schults, Hatfield Marine Sciences Center, US EPA, Newport, OR 97365

IGWMC Key: 4871 Model Name: REDEQL-UMD Released: 1984
Authors: Harriss, D.K., Ingle, S.E., Taylor, D.K., Magnuson, V.R.

REDEQL-UMD is a program to compute equilibrium distributions of species concentrations in aqueous systems. The basic equilibria which may be treated include complexation, precipitation, oxidation-reduction, and adsorption. The standard version allows simultaneous consideration of reactions involving 20 metals and 30 ligands. Similarly, up to 20 redox reactions can be handled. The accompanying data base includes relevant data on the metals and ligands, thermodynamic stability constants for complexes, mixed complexes, redox reactions, solids, and mixed solids, and includes 53 elements, 109 aqueous species, and 158 minerals. It calculates the mass balance of each species.

Contact Address: V.R. Magnuson, Dept. of Chemistry, Univ. of Minnesota, Duluth, MN 55812

IGWMC Key: 4880 Model Name: SOLMNEQ/SOLMNEQF Released: 1988
Authors: Kharaka, Y.K., Barnes, I.

SOLMNEQ is a program, originally written in PL/1, for computing the equilibrium distribution of species in aqueous solution over a temperature range of 0 to 350 degrees C. The program includes 26 elements, 162 aqueous species, and 158 minerals. It calculates the mass balance of each element and includes redox reactions. The logic of the program has been developed in part following the logic of WATCHEM and WATEQF. A FORTRAN version was published in 1988 as SOLMNEQF. SOLMNEQF calculates the equilibrium distribution of 236 species including uranium, vanadium, and 18 organic species of acetate, oxalate, and succinate, as well as the saturation states of 196 minerals (see remarks)

Contact Address: Y.K. Kharaka, U.S. Geol. Survey, 345 Middlefield Road, Menlo Park, CA 94025

IGWMC Key: 4881 Model Name: SOLMNQ Released: 1983
Authors: Goodwin, B.W., Munday, M.

SOLMNQ is an interactive chemical speciation program that calculates equilibrium distributions for inorganic aqueous species often found in groundwater. The program is based on the SOLMNEQ program published in 1973. It includes 28 elements, 239 aqueous species and 181 solids. The program calculates the mass balance for each species of uranium and plutonium and handles redox reactions.

Contact Address: Atomic Energy of Can., Whiteshell Nucl. Res. Establ., Pinawa, Manitoba ROE 1LO, Canada

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IGWMC Key: 4882 Model Name: SOLMINEQ.88 Released: 1988
Authors: Kharaka, Y.K., Gunter, W.D., Aggarwal, P.K., Perkins, E.H., et Al.

SOLMINEQ.88 is an updated version of SOLMNEQ, first published in 1973, SOLMNEQF (1986), and several unpublished versions of the code. The computer program can be used to model speciation, saturation, dissolution/precipitation, ion exchange/adsorption, mixing, boiling, and gas partitioning between water, oil, and gas phases. The program is especially useful for modeling water-rock interactions in sedimentary basins where high temperatures, pressures, salinities, and dissolved organic species prevail. SOLMINEQ.88 has a database of 260 inorganic and 80 organic aqueous species and 220 minerals. It computes the activity coefficients in brines using Pitzer equations, and computes pH and mineral solubilities at subsurface temperatures and pressures.

Contact Address: U.S. Geol. Survey, 345 Middlefield Road, Menlo Park, CA 94025

IGWMC Key: 4890 Model Name: WATEQ2/WATEQ4F Released: 1991
Authors: Ball, J.W., Jenne, E.A., Nordstrom, D.K.

WATEQ2, written in PL/1, is a chemical equilibrium model for calculating aqueous speciation of major and minor elements among naturally occurring ligands. It uses field measurements of temperature, pH, Eh, dissolved oxygen and alkalinity, and the chemical analysis of a water sample as input and calculates and calculates the distribution of aqueous species, ion activities, and mineral saturation indices that indicate the tendency of a water to dissolve or precipitate a set of minerals. The program solves a set of nonlinear mass action and mass balance equations using the continued fraction method. WATEQ2 is a modified version of WATEQ (1974) and WATEQF (1976). WATEQ4F is an updated version, written in FORTRAN 77.

Contact Address: U.S. Geol. Survey, 345 Middlefield Road, Menlo Park, CA 94025; or Internat. Ground Water Modeling Ctr., Colorado Sch. of Mines, Golden, CO 80401.

IGWMC Key: 4891 Model Name: WATEQ3 Released: 1982
Authors: Ball, J.W., Jenne, E.A., Cantrall, M.W.

WATEQ3 is a chemical equilibrium model for calculating aqueous speciation of major and minor elements among naturally occurring ligands, including uranium species. The program, which is based on WATEQ2, calculates the mass balance of the species and handles redox reactions and gases. The Newton-Raphson solution technique is used to solve for 30 elements, 227 aqueous species, 12 organic ligands, and 309 precipitation/dissolution minerals. The activity coefficient is calculated by the Debye-Huckel equation. The thermodynamic data base of the code is probably the most thoroughly documented and evaluated of any available. WATEQ3 has been used extensively in field ground water investigations of the USGS.

Contact Address: U.S. Geol. Survey, 345 Middlefield Road, Menlo Park, CA 94025

IGWMC Key: 4990 Model Name: SENECA Released: 1981
Authors: Ma, Y.H., Shipman, C.W.

SENECA computes equilibrium compositions in a two-step process. The first step uses the free-energy minimization procedure to obtain an approximate composition of the system. The second step uses this approximate composition as an initial estimate for solving a set of mass-balance and mass-action equations by the Newton-Raphson method. Version 2 includes a permanent arrangement for an aqueous phase, a gas phase, and multiple solid phases; an activity coefficient calculation for aqueous species; oxidation-reduction reactions; and a thermodynamic data base for 70 complexes, gases and solids.

Contact Address: J.F. Kerrisk, Los Alamos Nat. Lab., P.O. Box 1663, Los Alamos, NM 87545

IGWMC Key: 5033 Model Name: FOWL Released: 1992
Authors: Hostetler, C.J., Erikson, R.L., Rai, D.

The FOWL (FOssil fuel combustion WasteLeaching) computer code allows the user to calculate the chemical composition, quantity, and release duration of leachates of fossil fuel combustion byproducts disposed of in ponds and landfills. The basis of FOWL is formed by precipitation-dissolution reactions at equilibrium with a given solid phase and solubility relationships based on laboratory and field data. The model assumes that these solid phases do not change rapidly and that thermodynamic equilibrium applies throughout the leaching time period. The FOWL code uses geochemical and water balance methods to calculate leachate composition and quantity over time. The model output provides the source term for subsequent transport and fate modeling.

Contact Address: Electric Power Research Inst., Box 10412, Palo Alto, CA 94303

IGWMC Key: 5840 Model Name: FASTCHEM Released: 1988
Authors: --

FASTCHEM (Fly Ash and Scrubber sludge Transport and geoCHEmistry Model) simulates hydrologic and geochemical processes of inorganics in saturated and unsaturated media.

Contact Address: Electric Power Research Inst., P.O. Box 10412, Palo Alto, CA 94303-9743

IGWMC Key: 6701 Model Name: CHROMAT Released: 1991
Authors: --

CHROMAT (CHROMium ATenuation evaluation model) calculates Cr concentration and attenuation as Cr-based leachate migrates through porous soils.

Contact Address: Electric Power Research Inst., P.O. Box 10412, Palo Alto, CA 94303-9743

Appendix G: Hydrogeochemical Models, Part 2: Usability and Reliability

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
124	DYNAMIX	N	N	Y	Y	N	L	Y	U	L	U	U
2610	PHREEQE	Y	Y	Y	Y	N	L	Y	U	L	U	M
2611	PHRQPITZ	N	N	Y	Y	N	L	Y	U	L	U	F
3084	CHNTRNS	U	U	Y	Y	N	U	Y	U	L	U	U
3400	BALANCE	Y	Y	Y	Y	N	L	Y	U	L	U	M
3611	CHMTRNS	U	U	Y	Y	N	U	Y	U	L	U	U
3620	WATEQF	N	N	Y	Y	N	N	Y	U	L	U	M
3621	NETPATH	Y	Y	Y	Y	N	L	Y	U	L	U	F
4450	TRANQL/ MICROQL	U	U	Y	Y	U	U	Y	U	U	U	U
4810	EQ3/EQ6	Y	Y	Y	Y	N	L	Y	U	L	U	M
4820	EQUILIB	U	U	Y	Y	U	U	Y	U	U	U	U
4830	GEOCHEM	U	U	Y	Y	U	U	Y	U	U	U	U
4840	MINEQL2	U	U	Y	Y	U	U	Y	U	U	U	U
4850	MINTEQ/ MINTEQ2/ MINTEQA2	Y	Y	Y	Y	Y	Y	Y	U	L	L	M
4851	MININR/ MINICUP	U	U	Y	Y	U	U	Y	U	U	U	U
4860	PROTOCOL	U	U	Y	Y	U	U	Y	U	U	U	U
4870	REDEQL-EPA	U	U	Y	Y	U	U	Y	U	U	U	U
4871	REDEQL-UMD	U	U	Y	Y	U	U	Y	U	U	U	U
4880	SOLMNEQ/ SOLMNEQF	U	U	Y	Y	N	L	Y	U	L	U	F
4881	SOLMNQ	U	U	Y	Y	N	U	Y	U	U	U	U

KEY: Y = YES N = NO L = LIMITED E = EXTENSIVE M = MANY F = FEW U = UNKNOWN

Appendix G, part 2 (continued)

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
4882	SOMINEQ.88	Y	Y	Y	Y	Y	L	Y	U	L	U	F
4890	WATEQ2/ WATEQ4F	Y	Y	Y	Y	Y	L	Y	U	E	L	M
4891	WATEQ3	U	U	Y	Y	N	N	Y	U	L	U	F
4990	SENECA	U	U	Y	Y	U	U	Y	U	U	U	U
5033	FOWL	Y	Y	Y	Y	Y	Y	Y	U	L	L	F
5840	FASTCHEM	Y	Y	Y	Y	Y	Y	Y	N	L	L	F
6701	CHROMAT	U	U	Y	Y	U	U	Y	U	U	U	U

KEY: Y = YES N = NO L = LIMITED E = EXTENSIVE M = MANY F = FEW U = UNKNOWN

Appendix H: Optimization Model for Ground-water Management, Part 1: Model Description

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IGWMC Key: 260 Model Name: DELTA Released: 1981
Authors: Morel-Seytoux, H.J., Rodriquez, C., Daly, C.

DELTA is a conjunctive use stream-aquifer model. It simulates two-dimensional transient areal groundwater flow in a confined or unconfined heterogeneous, isotropic aquifer and the quasi one-dimensional flow in a connected river. It calculates aquifer drawdown, river stage and aquifer return flow with the finite difference method. The model uses stream-aquifer response coefficients (discrete kernels) and mathematical programming for optimization. The decision variables are pumping rates, upstream river inflows, initial drawdown and recharge rates.

Contact Address: H.J. Morel-Seytoux, Colorado State Univ., Engineering Research Center, Fort Collins, CO 80523

IGWMC Key: 2060 Model Name: DELTIS Released: 1981
Authors: Morel-Seytoux, H.J., Illangasekare, T.

DELTIS is a stream-aquifer discrete kernel generator for horizontal confined or unconfined, transient ground water flow in isotropic, heterogeneous aquifers using the finite element technique. It can be used together with a mathematical programming package to determine optimal conjunctive use of surface water and groundwater resources.

Contact Address: H.J. Morel-Seytoux, Engineering Research Center, Colorado State University, Fort Collins, CO 80523

IGWMC Key: 2061 Model Name: DELPET - Discrete Kernel Generator Released: 1977
Authors: Morel-Seytoux, H.J., Daly, C.J., Peters, G.

DELPET is a discrete kernel generator for transient horizontal flow in an isotropic, heterogeneous, confined or unconfined aquifer to simulate drawdowns and return flows using the finite difference technique. It can be linked to a mathematical program package to optimize the location and pumping rates of wells.

Contact Address: H.J. Morel-Seytoux, Colorado State Univ., Engineering Research Center, Fort Collins, CO 80523

IGWMC Key: 3092 Model Name: AQMAN (AQuifer MANagement) Released: 1986
Authors: Gorelick, S.M., Lefkoff, L.J.

Used in conjunction with a mathematical programming code (e.g. MPS), AQMAN identifies the pumping or recharge strategy that achieves a user's management objective while maintaining groundwater hydraulic conditions within desired limits. The objective may be linear or quadratic, and may involve the minimization of pumping and recharge rates or of variable pumping costs. The problem may contain constraints on groundwater heads, gradients, and velocities for a complex, transient hydrologic system. A unit stress is applied at each decision point well and transient responses are computed using a modified two-dimensional finite difference flow model of the USGS. The program is based on the use of the response matrix optimization method.

Contact Address: WATSTORE Program Office, U.S. Geol. Surv., 437 Nat. Center, Reston, VA 22092

IGWMC Key: 3190 Model Name: GRNDFLO Released: 1978
Authors: Loganathan, G.V., Delleur, J.W., Tavalage, J.

GRNDFLO is a steady-state finite element model for simulation of ground-water flow in a confined, anisotropic, heterogeneous aquifer. It uses linear triangular elements and has an automatic mesh generating scheme. Boundary conditions include prescribed head and prescribed flow. GRNDFLO and the water demand model LANDUSE are included in the management model WATSUP, which uses a mixed integer programming formulation for the optimization of the water distribution system.
Contact Address: Delleur, J.W., Purdue University, School of Civil Engineering, West Lafayette, Indiana, 47907

IGWMC Key: 3191 Model Name: WATSUP Released: 1978
Authors: Logannathan, G.V.,Delleur, J.W., Tavalage, J.J.

The purpose of WATSUP is to determine optimal location of water wells and of distribution reservoirs along with optimal flow values and pipe sizes in an urban growth area.

Contact Address: Delleur, J.W., Purdue Univ., School of Civil Eng., West Lafayette, Indiana, 47907

IGWMC Key: 3983 Model Name: MODMAN (MODflow MANagement) Released: 1990
Authors: --

Contact Address: GeoTrans, Inc., 46050 Manekin Plaza, #100, Sterling, VA 22170

MODMAN is a program developed to add management capability to the USGS modular 3-D flow model MODFLOW. MODMAN in conjunction with optimization software, provide optimal locations of pumping and injection wells and optimal pumping or recharge rates for these well. The optimal solution maximizes or minimizes a user-defined objective function, such as maximizing total pumping rate from all wells, and satisfies all user-defined constraints, such as upper and lower limits on heads, gradients, and pumping rates. MODMAN utilizes the response matrix technique to transform the groundwater management problem into a linear or mixed-integer program. MODFLOW is called repeatedly as a subroutine. The program requires an external optimization program not included in MODMAN.

IGWMC Key: 4070 Model Name: GWUSER/CONJUN Released: 1983
Author: Kolterman, C.R.

GWUSER/CONJUN is a combined simulation-optimization model to determine optimal pumping locations and pumping rates for a confined aquifer with or without artificial recharge (GWUSER) or to determine the optimal conjunctive use of an aquifer-stream system (CONJUN). The simulation model is based on a finite difference approximation of transient groundwater flow and linear programming solution of the optimalization problem.

Contact Address: C.R. Kolterman, Desert Research Institute, Reno, Nevada

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Appendix H: Optimization Models for Ground-water Management, Part 2: Usability and Reliability

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
260	DELTA	N	N	Y	Y	N	N	Y	U	L	U	F
2060	DELTIS	N	N	Y	Y	N	N	Y	U	L	U	F
2061	DELPET	N	N	Y	Y	N	N	Y	U	L	U	F
3092	AQMAN	N	N	Y	Y	N	L	Y	U	L	U	F
3190	GRNDFLO	N	N	Y	Y	N	U	Y	U	U	U	U
3191	WATSUP	N	N	Y	Y	N	U	Y	U	U	U	U
3983	MODMAN	N	N	Y	Y	N	L	Y	U	L	U	F
4070	GWUSER/ CONJUN	N	N	Y	Y	N	L	Y	U	L	U	U
4480	GWMAN	U	U	Y	Y	U	U	Y	U	U	U	U
6703	OPTIC	Y	Y	Y	Y	Y	Y	Y	U	L	U	U

KEY: Y = YES N = NO L = LIMITED E = EXTENSIVE M = MANY F = FEW U = UNKNOWN

IGWMC Key: 4480 Model Name: GWMAN Released: 1984
Authors: Wanakule, N., Mays, N.W., Lasdon, L.S.

GWMAN is a computer program for determining optimal pumping and recharge of large scale artesian and/or non-artesian aquifers by coupling non-linear optimization with an existing finite difference simulator for transient horizontal flow in anisotropic, heterogeneous aquifers. The state variables which represent the heads, and the control variables which represent pumpages, are implicitly related through the groundwater simulator. The simulator equations are used to express the system states in terms of the controls, yielding so-called reduced problem functions. The reduced problem is solved by combining augmented Lagrangian and reduced gradient procedures. Both steady-state and transient type dewatering problems are solved.

Contact Address: N.W. Mays, Center for Research in Water Resources, Univ. of Texas at Austin, Austin, TX 78712

IGWMC Key: 6703 Model Name: OPTIC Released: 1992
Authors: --

OPTIC (Optimal Pumping To Immobilize Contaminants) calculates optimum pumping rate to hydraulically contain a contaminated ground water plume.

Contact Address: Electric Power Research Institute, P.O. Box 10412, Palo Alto, CA 94303-9743

Note: Only few models have been designed as general-use models. Often, they require the user to have access to a mathematical optimization package on their computer system. Many research models have been discussed in the literature; for most of them no code is available.

Appendix I: Multiphase Flow, Part 1: Model Description

IGWMC Key: 4420 Model Name: GASOLINE Released: 1984
Author: Baehr, A.L.

GASOLINE is a one-dimensional finite difference research model to solve a system of equations defining the transport of an immiscible contaminant immobilized in the unsaturated zone, with and without biodegradation. The program handles capillary forces, advection, dispersion, diffusion, linear adsorption, redox reactions, and biological activity.

Contact Address: Baehr, A.L., U.S. Geological Survey, Water Resources Div., Trenton, NJ 08628

IGWMC Key: 4650 Model Name: SWANFLOW Released: 1992
Authors: Faust, C.R., Rumbaugh, J.D.

SWANFLOW is a public domain, multi-dimensional finite difference model for simulation of simultaneous flow of water, air and immiscible non-aqueous phase liquids (NAPL's) within and below the vadose zone. The conservation equations for mass and momentum of water, gas (air), and a NAPL are simplified to yield two strongly coupled nonlinear partial differential equations. Pressure gradients in the air phase are considered negligible; air pressure is assumed to be constant and equal to atmospheric pressure. The model determines the spatial and temporal distribution of NAPL pressure and water saturation. Acceptable boundary conditions are: specified flux, fluid potential and fluid potential-dependent flux. There are three primary limitations to the code: 1) the air phase is considered to be at constant atmospheric pressure, thus flow of air is not modeled; 2) mass transfer between phases is not considered, i.e. NAPL cannot dissolve in water or evaporate; 3) practical application of the code to field problems can be complicated by lack of site-specific capillary pressure and relative permeability. A user-friendly, proprietary two-dimensional version is also available.

Contact Address: GeoTrans, Inc., 46050 Manekin Plaza, Suite #100, Sterling, VA 22170; for 3-D version also Internat. Ground Water Modeling Center, Colorado School of Mines, Golden, Co 80401.

IGWMC Key: 5180 Model Name: MOFAT Released: 1990
Authors: Kaluarachchi, J.J., Parker, J.C.

MOFAT is an upstream-weighted finite element model to simulate coupled flow of water, nonaqueous phase liquid (NAPL) and air, and multicomponent transport of up to five non-inert species in a two-dimensional vertical section through saturated and unsaturated zones in Cartesian or radial coordinates. The flow module can be used to simulate 2- or 3-phase system with gas phase treated dynamically or assumed at constant pressure. Convective-dispersive transport in water, NAPL and gas phase is analyzed assuming local equilibrium partitioning among phases and with the solid phase. MOFAT comes with pre- and post-processing capabilities. Only rectangular elements with sides parallel to the principle flow axes are permitted.

All flow simulations in MOFAT can be performed using either van Genuchten or Brooks-Corey soil properties. The program is dimensioned to handle 1500 nodes with 10 different material properties, 50 type-1 boundary nodes and 100 flux-type boundary elements, and 25 boundary condition cycles with 4 subcycles per cycle. A maximum of two seepage faces are allowed with a maximum of 50 nodes along any seepage face for a given phase. To run MOFAT the following data is required: mesh geometry, boundary condition parameters,

continued.....

MOFAT -- continued

simulation control parameters, initial distribution of heads, porosity, van Genuchten's n, van Genuchten's alpha, residual water saturation, scaling parameter for air-NAPL interfacial tension, NAPL-water interfacial tension, ratio of NAPL to water density, ratio of NAPL to water viscosity, maximum NAPL residual saturation, saturated hydraulic conductivity, dispersivity, and equilibrium coefficients for NAPL/water, air/water, and soil/water. Other required input for MOFAT includes first-order decay coefficients for each species in water, NAPL, air, and soil phases; diffusion constants in water, NAPL and air; and liquid density of the pure species.

Contact Address: Environmental Systems and Technologies Inc., P.O. 10457, Blacksburg, VA 24062-0457; or Internat. Ground Water Modeling Center, Colorado School of Mines, Golden, CO 80401.

IGWMC Key: 5181 Model Name: SPILLVOL Released: 1990
Authors: Parker, J.C., Lenhard, R.J.

SPILLVOL is an interactive menu-driven program to estimate areal hydrocarbon distributions and integrated volumes from well fluid level data. The program can be used to determine: 1) current volume of "free" hydrocarbon in the soil; 2) the current residual product volume associated with historical fluid level variations; and 3) the volume of hydrocarbon which can be recovered by skimming either without water pumping or for a specified final water table configuration. Calculations are based on a physically-based model for vertical equilibrium three phase fluid distributions which includes effects of oil entrapment in the saturated zone and non-drainable residual oil in the unsaturated zone.

Soil properties are described in SPILLVOL using the van Genuchten capillary pressure model, the parameters of which may be estimated by the program from grain size distribution data. The user also supplies data from a network of observation wells on current depth to oil and depth to water, historical minimum depth to oil and maximum depth to water, and anticipated future water table elevations. Furthermore, the program gives information on areal distribution of uncertainty in volume estimates due to uncertainty in soil properties, fluid properties and interpolation error.

Contact Address: Environmental Systems and Technologies Inc., P.O. 10457, Blacksburg, VA 24062-0457; Internat. Ground Water Modeling Center, Colorado School of Mines, Golden, CO 80401; or Scientific Software Group, Washington, D.C.

IGWMC Key: 5184 Model Name: ARMOS Released: 1992
Authors: Kaluarachchi, J., Parker, J.C., Zhu, J.L., Katyal, A.K.

ARMOS (Areal Multiphase Organic Simulator) is a numerical model to simulate areal flow of water and separate phase light hydrocarbon in unconfined aquifers under natural gradients or forced gradients associated with well or trench free product recovery systems. The model assumes vertical equilibrium pressure distributions of water and hydrocarbon phases with consideration of residual hydrocarbon in the saturated and unsaturated zones associated with water imbibition and oil drainage. The nonlinear governing equations are solved using an upstream weighted finite element scheme with linear rectangular elements. Nonlinearity is handled by Picard iteration. The model handles multiple recovery wells with water and hydrocarbon pumping. Properties are based on van Genuchten model with hysteresis due to residual oil.

ARMOS is based on vertical integration of the governing flow equations under the assumption of near-equilibrium conditions in the vertical direction with zero gas pressure gradients. The new version uses

continued.....

ARMOS -- continued

a serial solution procedure for water and oil flow equations. Other options include simulation of hydrocarbon flow only assuming steady-state water flow, or to model water flow only to facilitate calibration.

Input data for ARMOS include initial conditions prescribed as elevations of air-oil and oil-water fluid tables, prescribed boundary conditions, soil properties, fluid properties and run-time parameters such as mesh data, time increments and convergence criteria. Fluid properties required by ARMOS are viscosity, density and surface tension of the hydrocarbon. Soil properties include the saturated hydraulic conductivity and parameters defining the saturation-capillary pressure-relative permeability relations. Soil properties can vary spatially. Initial conditions in ARMOS are specified by giving fluid level data from a set of observation wells that are interpolated internally to define nodal air-oil and oil-water elevations. Boundary conditions can be stipulated as prescribed fluid table elevations or fluid fluxes. Multiple recovery wells for free product skimming with or without water pumping may be modeled.

The main output from ARMOS are predicted fluid table elevations and the total, free and residual oil volume per unit area. For recovery well locations, water and oil pumping rates, cumulative recovery water and hydrocarbon pumpage and well fluid levels are output. For each output time, the cumulative change in oil volume, area of soil with free oil present and area of soil with residual or free oil present are given.

Contact Address: Environmental Systems and Technologies Inc., P.O. 10457, Blacksburg, VA 24062-0457; Internat. Ground Water Modeling Center, Colorado School of Mines, Golden, CO 80401; or Scientific Software Group, Washington, D.C.

IGWMC 5185 Model Name: MOTRANS Released: 1992
Authors: Katyal, A.K., Parker, J.C.

MOTRANS is a 2-dimensional vertical section or radially symmetric upstream-weighted finite element program for flow of air, light or dense organic liquid and water, and coupled transport of up to 5 partionable species. The program, which uses linear rectangular elements, allows inclusion or elimination of flow equations for selected phases to achieve maximum flexibility and efficiency. Soil hydraulic properties are described by the multi-phase van Genuchten model with NAPL entrapment. The nonlinearity in the equations is handled by Newton-Raphson iteration. Multispecies transport is simulated assuming local equilibrium or kinetically controlled interphase mass transfer. Pre- and postprocessing modules are available.

The flow module of MOTRANS can be used to analyze two-phase flow of water and NAPL in a system with gas present but at constant pressure, or explicit three-phase flow of water, NAPL and gas at variable pressure. Systems with no NAPL present or with immobile NAPL at a residual saturation may also be modeled. The transport module can handle up-to five components that partition among water, NAPL, gas and solid phases assuming either local equilibrium interphase mass transfer or first-order kinetically controlled mass transfer. MOTRANS requires specification of parameters defining the air-water capillary retention function, NAPL surface tension and interfacial tension with water, NAPL viscosity, NAPL density, maximum residual NAPL saturation and soil hydraulic conductivity. The latter may be anisotropic and soil properties may vary spatially. For transport analyses, additional data input include porous media dispersivities, initial water phase concentrations, equilibrium partition coefficients, component densities, diffusion coefficients, and first-order decay coefficients. Additional transport input data for MOTRANS: mass transfer coefficients (for nonequilibrium analyses) and boundary condition data. Time dependent boundary conditions for the flow analysis may involve user-specified phase heads at nodes or phase fluxes along a

continued.....

MOTRANS -- continued

boundary segment with zero flux as the default condition. For transport analysis, time-dependent boundary conditions include equilibrium water phase concentrations or prescribed fluxes defined in terms of a specified concentration in the influent liquid. If not specified, the b.c. is a zero dispersive flux. MOTRANS calculates pressure heads, saturations and velocities for each phase at every node for specified output intervals. In addition, the total volume of mass of each phase, time-step size and number of iterations are given. For transport analysis, the phase concentrations at each node are computed. The program has a restart option.

Contact Address: Environmental Systems and Technologies Inc., P.O. 10457, Blacksburg, VA 24062-0457; or Internat. Ground Water Modeling Center, Colorado School of Mines, Golden, CO 80401.

IGWMC Key: 5189 Model Name: SPILLCAD Released: 1992
Authors: --

SPILLCAD is a program for determining hydrocarbon spill volume. First, total petroleum hydrocarbon (TPH) data from soil samples can be integrated directly to estimate total (residual and free) product within the sampled zone. Also, the volume of free product floating on the water table can also be determined. This latter is accomplished by determining the vertical distribution of hydrocarbon in the soil in equilibrium with well fluid levels based on a theoretically rigorous treatment of the three phase saturation-capillary pressure relations for the soil. Soil and fluid properties required to carry out the calculations can be estimated by the program using a number of options. Finally, SPILLCAD enables the user to evaluate various free product control and recovery options.

Procedures developed for estimation of hydrocarbon spill volume include interpolation and spatial integration of TPH measurements from soil cores, and spatial integration of hydrocarbon volume per area computed from monitoring well fluid levels. The first method involves vertical integration of TPH measurements to yield oil volume per unit area followed by kriging and areal integration to estimate the volume within the measurement zone. This method is especially well suited to determine the volume of residual product in the unsaturated zone.~The second method involves kriging of well fluid levels, calculation of free oil volume per area using a physically-based model for hydrostatic three-phase fluid distributions, followed by areal integration to estimate the volume of free product floating on the water table. An analytical procedure was developed to evaluate effects of steady-state water pumping from multiple point sources on the oil flow gradients to enable hydraulic control of plume spreading. Estimates of residual oil in the unsaturated and saturated zone are made from the hysteric three-phase capillary pressure-saturation relations and from initial oil thickness distributions and computed water table drawdown, which enable determination of the recoverable spill volume for alternative well configurations.~The PC implementation of SPILLCAD operates within a graphical windowed environment. It is highly interactive and includes a graphical data base system for management of spatial data.

Contact Address: Environmental Systems and Technologies Inc., P.O. 10457, Blacksburg, VA 24062-0457; or Internat. Ground Water Modeling Center, Colorado School of Mines, Golden, CO 80401.

IGWMC Key: 5280 Model Name: KOPT Released: 1989
Authors: Charbenau, C.J., Weaver, J.W., Smith, V.J.

KOPT (Kinematic Oily Pollutant Transport model) is a oily pollutant transport model, based on the kinematic theory of one-dimensional multiphase flow. The model assumes steady infiltration of water. It is intended to be a screening tool for hydrocarbon spills or near-surface releases. It addresses the questions of how far an oil release might go into the soil and how soon it might get there. The solution is obtained by solving an approximate governing equation for the water by the method of characteristics (MOC). With the proper constitutive relationships for two-phase flow, the water solution is analytic. For the oily phase, a semi-analytic solution has been developed. The model is based on advective transport and includes (bio-)transformations, linear equilibrium sorption, and volatilization.

Contact Address: R.J. Charbenau, Univ. of Texas, Water Resources Research Center, Dept. of Civil Eng., Austin, TX 78712

IGWMC Key: 5281 Model Name: KROPT Released: 1989
Authors: Charbenau, R.J., Weaver, J.W., Smith, V.J.

KROPT (Kinematic Rainfall and Oily Pollutant Transport model) is an oily pollutant transport model, based on the kinematic theory for one-dimensional multi-phase flow. The model includes transient hydrologic phenomena such as evaporation and infiltration, along with a model of stochastic generation of rainfall. The model handles multiple loadings or releases of oily wastes at or near ground surface, multiple rainfall events, potential oil migration, linear equilibrium sorption, volatilization, and biodegradation. The solution is obtained by solving an approximate governing equation for the water by the method of characteristics (MOC). With the proper constitutive relationships for two-phase flow, the water solution is analytic. For the oily phase, a semi-analytic solution has been developed.

Contact Address: R.J. Charbenau, Univ. of Texas, Dept. of Civil Eng., Austin, TX 78712

IGWMC Key: 5681 Model Name: VIP Released: 1991
Authors: Stevens, D.K., Grenney, W.J., Yan, Z.

VIP (Vadose zone Interactive Processes model) is an one-dimensional finite-difference solute transport and fate model for simulating the behavior of organic compounds in the vadose zone as part of a land treatment system. The model uses advection and dispersion in the water and air phases as the dominant transport mechanism for contaminant and oxygen. Monthly values for recharge rate and soil moisture conditions are used to calculate an effective water velocity. Volatilization is represented by mass flux into the air phase and subsequent advection and dispersion. The model includes first-order degradation of a contaminant in water, air and soil, and of oxygen. It uses an implicit technique to calculate the degradation of the contaminant in the oil phase as well as the oil phase itself, and related oxygen changes.

VIP uses partition coefficients and rate constants to calculate contaminant concentration in each medium. The model has various output options including echo of input data, (graphic) profile of initial condition (constituent concentration in water, oil, air, and soil phases), and the initial fractions as well as initial oxygen concentration. Other output options include (graphic) depth-concentration profiles and data versus time tables. Input preparation facilitates exchange of Lotus 123 and word processed ASCII files. The pore velocity in water is calculated by dividing the average infiltration rate by the water content of the soil as estimated by the procedure of Clapp and Hornberger.

Contact Address: D.K. Stevens, Civil and Environm. Eng. Dept., Utah State Univ., UMC 4110, Logan, UT 84321; or EPA/CSMoS, RSKERL, P.O. Box 1198, Ada, OK 74820

IGWMC Key: 5820 Model Name: MAGNAS Released: 1992
Authors: Huyakorn, P.S., Kool, J.

MAGNAS is a finite element model for simulation of 3D and 2D flow of water, NAPL (light or dense), and air in heterogeneous and anisotropic porous media. Transport calculations include advection, dispersion in all fluid phases, sorption, volatilization, dissolution, precipitation and degradation. Alternative pseudo 3-phase and sharp interface formulations are available. The model can handle large contrasts in soil properties and highly nonlinear constitutive relationships. The model converges well and provides an accurate mass balance.

Contact Address: HydroGeologic Inc., 1165 Herndon Parkway, # 900, Herndon, VA 22070

IGWMC Key: 5821 Model Name: MAGICS Released: 1992
Authors: Huyakorn, P.S., et al.

MAGICS (Multiphase model for Air, Ground-water, Immiscible Contaminant and Solute transport) is a Galerkin finite element model for simulation of the flow of water, nonaqueous phase liquid, and air through porous media in two or three dimensions. MAGICS may be used to simulate the flow of air as a fully active phase. The solute transport simulation accounts for advection and hydrodynamic dispersion in all fluid phases, equilibrium sorption, volatilization, dissolution, precipitation and first-order degradation. As subsets of the most general fully three-phase modeling approach, a variety of simpler flow formulations may be simulated using the code. The fluid flow and solute transport simulations are performed sequentially.

Subsets of the full three-phase model in MAGICS includes pseudo-three-phase (with passive air phase), two-phase and single phase flow. Additionally, a sharp-interface areal simulation option is provided to handle situations where capillary pressure and relative permeability data is unavailable or a 3-D simulation unwarranted. A wide range of boundary conditions can be treated including those involving influx and afflux boundaries, water-table conditions, infiltration or recharge, and wells. The solution procedure for MAGICS incorporates upstream weighing of nodal values of phase mobilities and storage matrix lumping for linear rectangular elements. Element matrices are evaluated using enhanced influence-coefficient algorithms that avoid numerical integration and take advantage of nodal connectivities. These algorithms produce 5-point (finite difference) and 9-point (finite element) lattice in 2-D, and an 11-point (hybrid) lattice in 3-D.

Use of the hybrid approximation in MAGICS combines the advantages of the FD and FE techniques (e.g. positive transmissivity and insensitivity of the numerical solution to grid orientation) for 3-D problems. Nonlinearities are treated using a modified Newton-Raphson procedure with automatic under-relaxation and aggressive time-stepping. A Picard scheme and single-step steady-state analysis are provided as options in the single-phase flow formulations. For solute transport simulations, an upstream-weighted residual FE procedure is used for the phase-summed equation. ~The upstream weighing scheme for the solute transport curbs numerical oscillations. Direct banded matrix solvers are used to solve the matrix systems of 2-D problems. A block-iterative ORTHOMIN solver is used to solve 3-D problems. All boundary conditions can be chosen constant in time or variable in time with either continuous or stepwise changes.

MAGICS has been verified for a variety of problems by comparison of its numerical solutions with available analytical solutions and documented numerical results from several other codes including HYDRUS, VAM2D, VAM3D, SWANFLOW, and NAPL3D. MAGICS is a robust code designed to solve highly nonlinear field problems involving large contrasts in soil properties and highly nonlinear situations involving sharp saturation fronts, and to provide accurate mass balance calculations.

Contact Address: HydroGeologic Inc., 1165 Herndon Parkway, # 900, Herndon, VA 22070

Appendix I: Models for Multiphase Flow, Part 2: Usability and Reliability

IGWMC Key	Model	Usability						Reliability				
		Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users
4420	GASOLINE	N	N	Y	Y	N	N	Y	U	L	U	U
4650	SWANFLOW	Y	Y	Y	Y	Y	Y	Y	U	L	U	F
5180	MOFAT	U	U	Y	Y	Y	Y	Y	U	L	U	F
5181	SPILLVOL	Y	Y	Y	Y	Y	Y	Y	U	L	U	M
5184	ARMOS	Y	Y	Y	Y	Y	Y	Y	U	L	U	M
5185	MOTRANS	Y	Y	Y	Y	Y	Y	Y	U	L	U	M
5189	SPILLCAD	Y	Y	Y	Y	Y	Y	Y	U	L	U	M
5280	KOPT	U	U	Y	Y	U	U	Y	U	U	U	U
5281	KROPT	U	U	Y	Y	U	U	Y	U	U	U	U
5681	VIP	Y	Y	Y	Y	Y	Y	Y	U	L	U	F
5820	MAGNAS	U	U	Y	Y	U	U	Y	U	U	U	U
5821	MAGICS	Y	Y	Y	Y	Y	Y	Y	U	L	U	U

KEY: Y = YES N = NO L = LIMITED E = EXTENSIVE M = MANY F = FEW U = UNKNOWN

Appendix J: Cross-Reference Table for Appendices A through I

Model	IGWMC Key	Appendix /page
—	5400	E-1-2
—	5401	E-1-2
—	5410	E-1-2
—	5411	E-1-2
—	5420	E-1-3
—	5430	E-1-3
—	5440	E-1-3
—	5441	E-1-3
—	5450	E-1-4
2-D Finite Element Galerkin Model	3881	A.2-1-7
2-D Steady State FE Model	5810	A.2-1-14
3-D Free Surface FE Model	5560	A.3-1-4
3-D FE DUAL POROSITY	5022	F-1-7
3-D FRACTURE GENERATOR	5320	F-1-8
3D-MADPD	5650	C.3-1-7
3DFEMWATER	3377	B.1-1-4
AIR	6605	E-1-5
ANALYTICAL MODELS	5100	A.1-1-4
AQ/BASIC GWF	6030	A.2-1-14
AQ series	4752/54	A.6-1-4
AQ-AT	4751	A.4-1-1
AQ-EF	4754	A.2-1-9
AQ-FEM	4753	A.2-1-9
AQMAN	3092	H-1-1
AQMODEL	5710	A.1-1-7
AQTESOLV	6670	A.4-1-7
AQU-1	1230	A.2-1-2
AQUA	5018	D-1-11
AQUA	5018	C.2-1-8
AQUAMOD	5730	A.2-1-13
AQUIFEM	514	A.2-1-1
AQUIFEM-1/AQUIFEM-N	2630	A.2-1-4
AQUIFER	5110	A.2-1-11
AQUIFLOW	3372	A.2-1-6
AQUITRAN	3378	C.2-1-4
AQUIX	6681	A.1-1-10
AQUIX-T/AQUIX-4	6681	A.4-1-7
ARMOS	5184	I-1-2
ASM	6603	A.6-1-7
ASM	6603	C.2-1-11
AT123D	6120	C.1-1-8
BALANCE	3400	G-1-2
BEAVERSOFT	6590	C.1-1-10
BEAVERSOFT	6590	A.1-1-9

Appendix J (continued)

Model	IGWMC Key	Appendix /page
BEAVERSOFT	6590	A.6-1-7
BIM/FRACGEN	6810	F-1-9
BIO1D	5500	C.4-1-11
BIOPLUME II	4910	C.2-1-7
BIOSOIL	5021	C.4-1-8
BLOB3D	5242	C.1-1-5
BORHOL	696	D-1-2
CADIL/AGTEHM	4290	C.4-1-5
CANSAZ (EPA-CMS)	5330	C.2-1-9
CATTI	6600	C.1-1-10
CFEMTRAN	5244	C.2-1-9
CFEST	2070	C.3-1-2
CFEST	2070	D-1-3
CFITIM	6227	C.1-1-8
CGAQUFEM	5240	A.2-1-12
CHAIN	6225	C.4-1-14
CHARGR	2761	D-1-5
CHEMFLO	6712	C.4-1-16
CHEMRANK	6640	C.4-1-15
CHEMTRN/THCC	3610	C.2-1-4
CHMTRNS	3611	G-1-2
CHNTRNS	3084	G-1-2
CHNTRNS	3084	D-1-6
CHNTRNS	3084	C.2-1-3
CHROMAT	6701	G-1-7
CMIS	6710	C.4-1-15
CMLS	6711	C.4-1-15
CONFLOW	2770	A.1-1-2
CONFLOW	2770	A.6-1-2
CRACK	6660	F-1-9
CRACK	6660	C.1-1-11
CRAFLUSH	5243	C.1-1-5
CREAMS	3540	C.4-1-3
CRREL	2791	A.1-1-2
CSUFDM	5392	A.2-1-12
CSUGAS	5390	E-1-1
CSUPAW	5391	A.1-1-6
CTRAN/W	5340	A.6-1-6
CTSPAC	5031	D-1-12
CTSPAC	5031	C.4-1-9
CUMOC/MIKERN	6770	C.2-1-11
CXPMPM	5211	C.1-1-4
CXTFIT	3432	C.1-1-2
CXTFIT	3432	C.4-1-3
DELPET	2061	H-1-1

Appendix J (continued)

Model	IGWMC Key	Appendix /page
DELTA	260	H-1-1
DELTIS	2060	H-1-1
DFT/C-1D	3860	D-1-9
DIFFMOD	5027	D-1-11
DISIFLAQ	2870	A.2-1-5
DISPEQ/DISPER/PISTON	3450/ 3451	C.4-1-3
DREAM	4670	A.1-1-3
DSTRAM	4700	D-1-11
DSTRAM	4700	C.3-1-5
DYNAMIX	124	G-1-1
DYNFLOW	4990	A.3-1-4
DYNTRACK	4941	C.3-1-5
EPA-VHS	6601	C.1-1-11
EQ3/EQ6	4810	G-1-3
EQUILIB	4820	G-1-3
FASTCHEM	5840	G-1-7
FE3DGW	2072	A.3-1-1
FE3DGW	2072	A.6-1-2
FEM301	3450	A.3-1-3
FEMA	3376	C.2-1-4
FEMSAT	3350	A.2-1-6
FEMSEEP	5120	C.2-1-8
FEMTRAN	4350	C.4-1-5
FEMWASTE/FECWASTE	3371	C.4-1-2
FEMWATER/FECWATER	3370	B.1-1-4
FEWA	3373	A.2-1-7
FIELD-2D	3861	D-1-9
FINITE	5130	A.1-1-4
FLAME	5661	C.4-1-11
FLAMINCO	4630	C.4-1-6
FLASH	5660	F-1-8
FLO	1092	B.1-1-2
FLOFIT	5187	B.2-1-1
FLONET	4922	A.6-1-5
FLONETS	5241	A.2-1-12
FLOP series	1820	A.6-1-1
FLOP/FLOP-LIESTE/FLOP-Z1/FLOP-ZN	1820	A.1-1-1
FLOSA	4660	A.6-1-4
FLOSA	4660	A.3-1-4
FLOTRA	3235	C.4-1-2
FLOTRA	3235	D-1-7
FLOWNET	5001	A.2-1-10
FLOWNET	5001	A.6-1-5
FLOWNS	5200	A.6-1-6
FLOWNS	5200	A.2-1-11

Appendix J (continued)

Model	IGWMC Key	Appendix /page
FLOWPATH	4920	A.6-1-5
FLOWPATH	4920	A.2-1-10
FLOWVEC	4390	B.1-1-5
FLSTAT	5570	A.1-1-6
FLUMP	122	B.1-1-2
FOWL	5033	G-1-7
FP	6170	B.2-1-2
FRACFLOW	3232	F-1-3
FRACFLOW	3232	D-1-6
FRACPORT	3374	F-1-4
FRACQUAL	5174	C.1-1-4
FRACSOL	2037	C.1-1-1
FRACTEST	4470	F-1-6
FRANET	5680	F-1-9
FRESAL	5540	A.2-1-13
FRONT	1822	A.1-1-1
FRONT	1822	A.6-1-1
FTRANS	581	F-1-1
FTRANS	581	D-1-1
FTWORK	5520	C.3-1-6
GAFETTA	513	D-1-1
GASOLINE	4420	I-1-1
GEOCHEM	4830	G-1-4
GEOFLOW	3220	C.2-1-3
GEOFLOW	5230	A.2-1-12
GEOTHER	730	D-1-3
GEOTRACK	5501	A.6-1-6
GETOUT	2080	C.1-1-1
GGWP	1010	C.2-1-2
GLEAMS	3541	C.4-1-3
GLOVER	5140	A.1-1-5
GM5	3240	A.2-1-6
GRDFLX	3380	C.1-1-1
GREASE	582	C.3-1-1
GREASE	582	D-1-2
GREASE	582	F-1-1
GRNDFLO	3190	H-1-2
GROUND	6100	C.1-1-7
GROUND WATER DISCHARGE TESTS	5460	A.4-1-5
GRWATER	3660	B.1-1-5
GS2	2891	C.4-1-1
GS3	2892	C.4-1-1
GTC	5028	C.4-1-9
GW-UN/DTCD	4730	A.1-1-3
GWAP	5040	A.4-1-2

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Model	IGWMC Key	Appendix /page
GWFL3D	6353	A.2-1-15
GWFLOW/GWMESH/GWPLOT	3101	A.2-1-5
GWFLOW	6023	A.1-1-8
GWHEAD	2880	A.3-1-2
GWMAN	4480	H-1-3
GWPATH	6650	A.6-1-8
GWPATH	6650	A.2-1-15
GWPT	6352	A.1-1-8
GWSIM	681	A.2-1-1
GWSIM-II	680	C.2-1-1
GWTHERM	2830	D-1-5
GWTR3D	6354	C.2-1-11
GWUSER/CONJUN	4070	H-1-2
HJ-MATCH	5050	A.4-1-2
HOTWTR	612	D-1-2
HPATCH3D	5245	C.1-1-5
HSSWDS	4410	B.1-1-6
HST3D	4610	C.3-1-4
HST3D	4610	D-1-11
HVRLV 1	3150	A.4-1-1
HWELL	6383	A.1-1-9
HYDROPAL	5150	A.1-1-5
HYDRUS/WORM	6229	C.4-1-14
HYPER-VENTILATE	5940	E-1-5
ICE-1	6602	D-1-12
IMAGEW-1	683	A.1-1-1
INFGR	4380	B.1-1-5
INFIL	3570	B.1-1-4
INTERFACE	2720	A.2-1-4
INTERSAT	5160	A.2-1-11
INTERTRANS	5161	C.3-1-6
IONMIG	4360	C.2-1-6
ISOQUAD	510	A.3-1-1
JDB2D/3D	5720	A.2-1-13
KOPT	5280	I-1-5
KROPT	5281	I-1-5
LANDFIL	4400	B.1-1-5
LAYFLO	4082	C.1-1-2
LEACHM(-P)	3411	C.4-1-2
LEAKY	5131	A.1-1-4
LINE2D	5246	C.1-1-6
LTIRD	6310	C.1-1-9
MADPD	5270	C.2-1-9
MAF	5790	A.1-1-7
MAGICS	5821	E-1-4

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Model	IGWMC Key	Appendix /page
MAGICS	5821	I-1-6
MAGNAS	5820	I-1-6
MAGNUM-2D	4590	D-1-10
MAGNUM-2D	4590	F-1-6
MAGNUM-3D	4591	A.6-1-4
MAQWF	4530	A.2-1-8
MARIAH	2620	D-1-4
MASCOT	4620	C.1-1-2
MASS	5732	C.2-1-10
MAST-2D	3868	C.2-1-5
MATE	5002	A.4-1-1
MATTUM	3375	D-1-7
MFLOP	5004	A.6-1-5
MFLOP	5004	A.1-1-4
MICROFEM	5000	A.2-1-10
MINEQL2	4840	G-1-4
MININR/MINICUP	4851	G-1-4
MINTEQ/MINTEQ2/MINTEQA2	4850	G-1-4
MLSOIL/DFSOIL	4140	C.4-1-4
MLU	5003	A.4-1-2
MLU	5003	A.1-1-3
MLU	5003	F-1-7
MOCDENSE	742	C.2-1-2
MODFE	4100	A.2-1-8
MODFLOW	3980	A.3-1-3
MODFLOWP	3987	A.5-1-1
MODINV	3981	A.5-1-1
MODMAN	3983	H-1-2
MODMOC-3D	5800	C.3-1-7
MODPATH	3984	A.6-1-3
MOFAT	5180	E-1-1
MOFAT	5180	I-1-1
MOTIF	4550	D-1-10
MOTIF	4550	F-1-6
MOTRANS	5185	I-1-3
MOTRANS	5185	E-1-1
MOUSE	6390	C.4-1-14
MT3D	4970	C.3-1-6
MULKOM	2581	D-1-4
MULKOM	2581	F-1-3
MULTIMED	5630	C.4-1-11
MUSHRM	2760	D-1-5
MUST	1771	B.1-1-2
MYGRT	6700	C.1-1-11
NEFTRAN	5025	F-1-7

Appendix J (continued)

Model	IGWMC Key	Appendix /page
NETFLO	695	F-1-2
NETFLO/ NETRANS	5640	F-1-8
NETPATH	3621	G-1-3
NEWTMC	5860	C.4-1-13
NITRO	5186	C.4-1-9
NMFD-3D	2740	A.3-1-2
NON-LINEAR FE/FD REGRESSION	195	A.5-1-1
NUSEEP	5030	A.2-1-11
OASIS	4911	C.1-1-3
OASIS	4911	C.2-1-7
ODAST	6312	C.1-1-9
ONE-D	6220	C.1-1-8
ONESTEP	3433	B.2-1-1
OPTIC	6703	H-1-3
OPTP/PTEST	6570	A.1-1-9
PAPADOP	5051	A.4-1-2
PAT	6604	A.1-1-9
PAT	6604	A.6-1-8
PATCH3D	5247	C.1-1-6
PATH3D	3982	A.3-1-3
PATH3D	3982	A.6-1-3
PATHRAE	5024	C.1-1-3
PATHS	2120	C.2-1-2
PATHS	2120	A.1-1-2
PATHS	2120	A.6-1-2
PC-SEEP	4980	B.1-1-6
PESTAN	6130	C.4-1-13
PETROS	5490	E-1-4
PHREEQE	2610	G-1-1
PHRQPITZ	2611	G-1-1
PLASM	322	A.2-1-1
PLUME	5055	C.1-1-3
PLUME	6020	C.1-1-7
PLUME2D	6024	C.1-1-7
POLLUT	5175	C.1-1-4
PORFLO	3790	C.2-1-5
PORFLO	3790	D-1-8
PORFLO	3790	F-1-4
PORFLOW-3D	3238	D-1-7
PORFLOW-3D	3238	F-1-4
PORFLOW-3D	3238	C.4-1-2
PORFLOW-II	3233	C.2-1-4
PORFLOW-II	3233	D-1-6
PORFREEZE	3236	D-1-7
PORSTAT/ PORMC	3237	A.2-1-5

Model	IGWMC Key	Appendix /page
POSSM/MCPOSSM	5780	C.2-1-10
PROTOCOL	4860	G-1-5
PRZM	4720	C.4-1-7
PRZMAL	5310	C.4-1-10
PRZMAL	5310	C.1-1-6
PT/CCC	100	D-1-1
PT	3890	D-1-9
PTC	515	C.3-1-1
PTDPS II	5061	A.4-1-3
PTDPS III	5062	A.4-1-4
PTDPS I	5060	A.4-1-3
PULSE	5210	C.1-1-4
PUMP	5080	A.4-1-4
PUMPING TEST PACKAGE	5190	A.4-1-5
PUMPING TEST PROGRAM	5070	A.4-1-4
PUMPTEST	6382	A.4-1-6
Quasi-3-D Multiaquifer Model	2510	A.2-1-3
QUICKFLOW	5300	A.1-1-6
QUICKFLOW	5300	A.6-1-6
RAND3D	2691	C.3-1-2
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