GROUNDWATER FLOW MODELS

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1.0 INTRODUCTION

The use of groundwater models is prevalent in the field of environmental science. Models have been applied to investigate a wide variety of hydrogeologic conditions. More recently, groundwater models are being applied to predict the transport of contaminants for risk evaluation.

In general, models are conceptual descriptions or approximations that describe physical systems using mathematical equations; they are not exact descriptions of physical systems or processes. By mathematically representing a simplified version of a hydrogeological system, reasonable alternative scenarios can be predicted, tested, and compared. The applicability or usefulness of a model depends on how closely the mathematical equations approximate the physical system being modeled. In order to evaluate the applicability or usefulness of a model, it is necessary to have a thorough understanding of the physical system and the assumptions embedded in the derivation of the mathematical equations.

Groundwater models describe the groundwater flow and transport processes using mathematical equations based on certain simplifying assumptions. These assumptions typically involve the direction of flow, geometry of the aquifer, the heterogeneity or anisotropy of sediments or bedrock within the aquifer, the contaminant transport mechanisms and chemical reactions. Because of the simplifying assumptions embedded in the mathematical equations and the many uncertainties in the values of data required by the model, a model must be viewed as an approximation and not an exact duplication of field conditions. Groundwater models, however, even as approximations, are a useful investigation tool that groundwater hydrologists may use for a number of applications.

Application of existing groundwater models include water balance (in terms of water quantity), gaining knowledge about the quantitative aspects of the unsaturated zone, simulating of water flow and chemical migration in the saturated zone including river-groundwater relations, assessing the impact of changes of the groundwater regime on the environment, setting up/optimising monitoring networks, and setting up groundwater protection zones.

The modelling studies in India have so far been confined to academic and research organisations. The practising professionals mostly still prefer to employ lumped models for planning of groundwater development and recharge. Such models completely ignore the distributed character of the groundwater regime. Thus, they are based upon rather conservative concepts like safe yields and are incapable of accounting for the stream-aquifer interaction and the dependence of lateral recharge on the water table pattern. Consequently, permissible mining (i.e. withdrawals in excess of vertical recharge) and perennial yield can not be arrived at. The objectives of modelling studies in India have been mainly (i) groundwater recharge, (ii) dynamic behaviour of the water table, (iii) stream-aquifer interaction, and (iv) sea-water intrusion etc.

It is important to understand general aspects of both groundwater flow and transport models so that application or evaluation of these models may be performed correctly.

2.0 MODEL DEVELOPMENT

A groundwater model application can be considered to be two distinct processes (Figure 1). The first process is model development resulting in a software product, and the second process is application of that product for a specific purpose. Groundwater models are most efficiently developed in a logical sequence.

2.1 Model Objectives

Model objectives should be defined which explain the purpose of using a groundwater model. The modelling objectives will profoundly impact the modelling effort required.

2.2 Hydrogeological Characterization

Proper characterization of the hydrogeological conditions at a site is necessary in order to understand the importance of relevant flow or solute transport processes. Without proper site characterization, it is not possible to select an appropriate model or develop a reliably calibrated model.

2.3 Model Conceptualization

Model conceptualization is the process in which data describing field conditions are assembled in a systematic way to describe groundwater flow and contaminant transport processes at a site. The model conceptualization aids in determining the modelling approach and which model software to use.

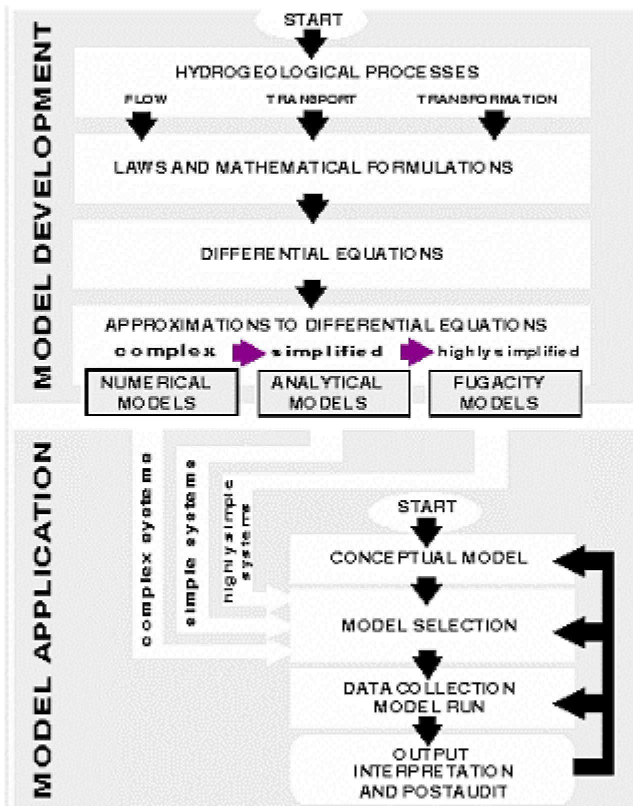

Figure 1: Development Process of a Model

2.4 Modelling Software Selection

After hydrogeological characterization of the site has been completed and the conceptual model developed, a computer model software is selected. The selected model should be capable of simulating conditions encountered at a site. For example, analytical models can be used where field data show that groundwater flow or transport processes are relatively simple. Similarly, one-dimensional/ two-dimensional/ three-dimensional groundwater flow and transport models should be selected based upon the hydrogeological characterization and model conceptualization.

2.5 Model Design (Input Parameters)

Model design includes all parameters that are used to develop a calibrated model. The input parameters include model grid size and spacing, layer elevations, boundary conditions, hydraulic conductivity/transmissivity, recharge, any additional model input, transient or steady state modelling, dispersion coefficients, degradation rate coefficients etc.

2.6 Model Calibration

Model calibration consists of changing values of model input parameters in an attempt to match field conditions within some acceptable criteria. Model calibration requires that field conditions at a site be properly characterized. Lack of proper site characterization may result in a model calibrated to a set of conditions that are not representative of actual field conditions.

2.7 Sensitivity Analysis

A sensitivity analysis is the process of varying model input parameters over a reasonable range (range of uncertainty in value of model parameter) and observing the relative change in model response. Typically, the observed change in hydraulic head, flow rate or contaminant transport are noted. Data for which the model is relatively sensitive would require future characterization, as opposed to data for which the model is relatively insensitive.

2.8 Model Verification

A calibrated model uses selected values of hydrogeologic parameters, sources and sinks and boundary conditions to match historical field conditions. The process of model verification may result in further calibration or refinement of the model. After the model has successfully reproduced measured changes in field conditions, it is ready for predictive simulations.

2.9 Predictive Simulations

A model may be used to predict some future groundwater flow or contaminant transport condition. The model may also be used to evaluate different remediation alternatives. However, errors and uncertainties in a groundwater flow analysis and solute transport analysis make any model prediction no better than an approximation. For this reason, all model predictions should be expressed as a range of possible outcomes that reflect the assumptions involved and uncertainty in model input data and parameter values.

2.10 Performance Monitoring Plan

Groundwater models are used to predict the migration pathway and concentrations of contaminants in groundwater. Errors in the predictive model, even though small, can result in gross errors in solutions projected forwarded in time. Performance monitoring is required to compare future field conditions with model predictions.

3.0 MODELLING OF GROUNDWATER FLOW AND MASS TRANSPORT

Groundwater modelling begins with a conceptual understanding of the physical problem. The next step in modelling is translating the physical system into mathematical terms. In general, the results are the familiar groundwater flow equation and transport equations. The governing flow equation for three-dimensional saturated flow in saturated porous media is:

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right)-Q=S_s\frac{\partial h}{\partial t} \qquad \ldots (1)$$

where,

K_{xx}, K_{yy}, K_{zz}	=	hydraulic conductivity along the x,y,z axes which are assumed to be parallel to the major axes of hydraulic conductivity;
h	=	piezometric head;
Q	=	volumetric flux per unit volume representing source/sink terms;
S_s	=	specific storage coefficient defined as the volume of water released from storage per unit change in head per unit volume of porous material.

The transport of solutes in the saturated zone is governed by the advection-dispersion equation which for a porous medium with uniform porosity distribution is formulated as follows:

$$\frac{\partial c}{\partial t}=-\frac{\partial}{\partial x_i}(cv_i)+\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial c}{\partial x_j}\right)+R_c \qquad i, j = 1,2,3 \qquad \ldots (2)$$

where,

c	=	concentration of the solute;
R_c	=	sources or sinks;
D_{ij}	=	dispersion coefficient tensor;
v_i	=	velocity tensor.

An understanding of these equations and their associated boundary and initial conditions is necessary before a modelling problem can be formulated. Basic processes, that are considered, include groundwater flow, solute transport and heat transport. Most groundwater modelling studies are conducted using either deterministic models, based on precise description of cause-and-effect or input-response relationships or stochastic models reflecting the probabilistic nature of a groundwater system.

The governing equations for groundwater systems are usually solved either analytically or numerically. Analytical models contain analytical solution of the field equations, continuously in space and time. 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. Various numerical solution techniques are used in groundwater models. Among the most used approaches in groundwater modelling, three techniques can be distinguished: Finite Difference Method, Finite Element Method, and Analytical Element Method. All techniques have their own advantages and disadvantages with respect to availability, costs, user friendliness, applicability, and required knowledge of the user.

4.0 GROUNDWATER FLOW MODELS

Salient features of the frequently used groundwater models have been presented below. The most widely used numerical groundwater flow model is MODFLOW which is a three-dimensional model, originally developed by the U.S. Geological Survey (McDonald and Harbaugh, 1988). It uses block-centred finite difference scheme for saturated zone. The advantages of MODFLOW include numerous facilities for data preparation, easy exchange of data in standard form, extended worldwide experience, continuous development, availability of source code, and relatively low price. However, surface runoff and unsaturated flow are not included, hence in case of transient problems, MODFLOW can not be applied if the flux at the groundwater table depends on the calculated head and the function is not known in advance.

1. 3DFEMFAT

(3-D Finite-Element Model of Flow and Transport through Saturated-Unsaturated Media)

3DFEMFAT is a 3-Dimensional Finite-Element Model of Flow And Transport through Saturated-Unsaturated Media. Typical applications are infiltration, wellhead protection, agriculture pesticides, sanitary landfill, radionuclide disposal sites, hazardous waste disposal sites, density-induced flow and transport, saltwater intrusion, etc. 3DFEMFAT can do simulations of flow only, transport only, combined sequential flow and transport, or coupled density-dependent flow and transport. In comparison to conventional finite-element or finite-difference models, the transport module of 3DFEMFAT offers several advantages: (1) it completely eliminates numerical oscillation due to advection terms, (2) it can be applied to mesh Peclet numbers ranging from 0 to infinity, (3) it can use a very large time step size to greatly reduce numerical diffusion, and (4) the hybrid Lagrangian-Eulerian finite-element approach is always superior to and will never be worse than its corresponding upstream finite-element or finite-difference method. Because of these advantages, 3DFEMFAT is suitable for applications to large field problems. It is flexibile and versatile in modeling a wide range of real-world problems.

2. AQUA3D

(3-D Groundwater Flow and Contaminant Transport Model)

AQUA3D is a program developed to solve three-dimensional groundwater flow and transport problems using the Galerkin finite-element method. AQUA3D solves transient groundwater flow with inhomogeneous and anisotropic flow conditions. Boundary conditions may be prescribed nodal head and prescribed flow as a function of time or head-dependent flow. AQUA3D also solves transient transport of contaminants and heat with convection, decay, adsorption and velocity-dependent dispersion. Boundary conditions may be either prescribed nodal concentration (temperature) or prescribed dispersive mass (heat) flux.

3. AT123D

(Analytical Groundwater Transport Model for Long-Term Pollutant Fate and Migration)

AT123D, analytical, transient One-, Two-, and Three-Dimensional Model, is an analytical groundwater transport model. AT123D computes the spatial-temporal concentration distribution of wastes in the aquifer system and predicts the transient spread of a contaminant plume through a groundwater aquifer. The fate and transport processes accounted for in AT123D are advection, dispersion, adsorption, and decay. AT123D estimates all the above components on a monthly basis for up to 99 years of simulation time. AT123D can be used as an assessment tool to help the user estimate the dissolved concentration of a chemical in three dimensions in groundwater resulting from a mass release over a source area. AT123D can handle: two kinds of source releases – instantaneous, continuous with a constant loading or time-varying releases; three types of waste–radioactive, chemicals, heat; four types of source configurations–a point source, a line source parallel to the x-, y-, z-axis, an area source perpendicular to the z-axis, a volume source; four variations of the aquifer dimensions–finite depth and finite width, finite depth and infinite width, infinite depth and finite width, infinite depth and infinite width.

4. BIOF&T 2-D/3-D

(Biodegradation, Flow and Transport in the Saturated/Unsaturated Zones)

BIOF&T 3-D models biodegradation, flow and transport in the saturated and unsaturated zones in two or three dimensions in heterogeneous, anisotropic porous media or fractured media. BIOF&T allows real world modeling not available in similar packages. Model convection, dispersion, diffusion, adsorption, desorption, and microbial processes based on oxygen-limited, anaerobic, first-order, or Monod-type biodegradation kinetics as well as anaerobic or first-order sequential degradation involving multiple daughter species.

5. Chemflo

(Simulates Water and Chemical Movement in Unsaturated Soils)

Chemflo is an interactive software system for simulating one-dimensional water and chemical movement in unsaturated soils. Chemflo was developed to enable decision-makers, regulators, policy-makers, scientists, consultants, and students to simulate the movement of water and chemicals in unsaturated soils. Water movement is modeled using 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 Chemflo can be displayed in the form of graphs and tables.

6. ChemFlux

(Finite Element Mass Transport Model)

ChemFlux is a stable finite element contaminant transport modeling software. It is a finite element software package characterized by automatic mesh generation, automatic mesh refinement and automatic time-step refinement. The solver offers speed and reduction in convergence problems. Results of benchmark tests run against MT3D confirm the effectiveness of the solver. ChemFlux is able to provide the same level of accuracy as MT3D in solutions dominated by advection while implementing the irregular geometry benefits of the finite element method. ChemFlux can also import groundwater gradients from the SVFlux groundwater modeling package. Predicting the movement of contaminant plumes through the processes of advection, diffusion, adsorption and decay is possible. The ChemFlux design module provides an elegant and simple user interface. Problem geometry and groundwater gradients may be imported from the SVFlux software.

7. FEFLOW

(Finite Element Subsurface Flow System)

FEFLOW is a finite-element package for simulating 3D and 2D fluid density-coupled flow, contaminant mass (salinity) and heat transport in the subsurface. It is capable of computing:

- Groundwater systems with and without free surfaces (phreatic aquifers, perched water tables, moving meshes);
- Problems in saturated-unsaturated zones;
- Both salinity-dependent and temperature-dependent transport phenomena (thermohaline flows);
- Complex geometric and parametric situations.

The package is fully graphics-based and interactive. Pre-, main- and post-processing are integrated. There is a data interface to GIS (Geographic Information System) and a programming interface. The implemented numerical features allow the solution of large problems. Adaptive techniques are incorporated.

8. FLONET/TRANS

(2-D cross-sectional groundwater flow and contaminant transport modeling)

FLONET/TRANS is a software package for 2-D cross-sectional groundwater flow and contaminant transport modeling. The modeling environment offers all the advantages of finite-element modeling (numerical stability and flexible geometry) together with a logical and intuitive graphical interface that makes finite-element modeling fast and easy. It uses the dual formulation of hydraulic potentials and streamlines to solve the saturated groundwater flow equation and create accurate flownet diagrams for any two-dimensional, saturated groundwater flow system. In addition, it also simulates advective-dispersive contaminant transport problems with spatially-variable retardation and multiple source terms.

9. FLOWPATH

(2-D Groundwater Flow, Remediation, and Wellhead Protection Model)

FLOWPATH for Windows is a popular model for groundwater flow, remediation, and wellhead protection. It is a comprehensive modeling environment specifically designed for simulating 2-D groundwater flow and contaminant transport in unconfined, confined and leaky aquifers with heterogeneous properties, multiple pumping wells and complex boundary conditions. Some typical applications of FLOWPATH include:

- Determining remediation well capture zones
- Delineating wellhead protection areas
- Designing and optimizing pumping well locations for dewatering projects
- Determining contaminant fate and exposure pathways for risk assessment

10. GFLOW

(Analytic Element Model with Conjunctive Surface Water and Groundwater Flow and a MODFLOW Model Extract Feature)

GFLOW is an efficient stepwise groundwater flow modeling system. It is a Windows 95/98/NT program based on the analytic element method. It models steady-state flow in a single heterogeneous aquifer using the Dupuit-Forchheimer assumption. While GFLOW supports some local transient and three-dimensional flow modeling, it is particularly suitable for modeling regional horizontal flow. To facilitate detailed local flow modeling, it supports a MODFLOW-extract option to automatically generate MODFLOW files in a user-defined area with aquifer properties and boundary conditions provided by the GFLOW analytic element model. GFLOW also supports conjunctive surface water and groundwater modeling using stream networks with calculated baseflow.

11. GMS

(Groundwater Modeling Environment for MODFLOW, MODPATH, MT3D, RT3D, FEMWATER, SEAM3D, SEEP2D, PEST, UTCHEM, and UCODE)

GMS is a sophisticated and comprehensive groundwater modeling software. It provides tools for every phase of a groundwater simulation including site characterization, model development, calibration, post-processing, and visualization. GMS supports both finite-difference and finite-element models in 2D and 3D including MODFLOW 2000, MODPATH, MT3DMS/RT3D, SEAM3D, ART3D, UTCHEM, FEMWATER and SEEP2D. The program's modular design enables the user to select modules in custom combinations, allowing the user to choose only those groundwater modeling capabilities that are required.

12. Groundwater Vistas

(Model Design and Analysis for MODFLOW, MODPATH, MT3D, RT3D, PEST and UCODE)

Groundwater Vistas (GV) is a sophisticated windows graphical user interface for 3-D groundwater flow and transport modeling. It couples a model design system with comprehensive graphical analysis tools. GV is a model-independent graphical design system for MODFLOW MODPATH (both steady-state and transient versions), MT3DMS, MODFLOWT, MODFLOW-

SURFACT, MODFLOW2000, GFLOW, RT3D, PATH3D, SEAWAT and PEST, the model-independent calibration software. The combination of PEST and GV's automatic sensitivity analysis make GV a good calibration tool. The advanced version of Groundwater Vistas provides the ideal groundwater risk assessment tool. Groundwater Vistas is a modeling environment for the MODFLOW family of models that allows for the quantification of uncertainty. Stochastic (Advanced) Groundwater Vistas includes, Monte Carlo versions of MODFLOW, MODPATH and MT3D, Geostatistical Simulators SWIFT support advanced output options and more. GV displays the model design in both plan and cross-sectional views using a split window (both views are visible at the same time). Model results are presented using contours, shaded contours, velocity vectors, and detailed analysis of mass balance.

13. HST3D

(3-D Heat and Solute Transport Model)

HST3D is a powerful user-friendly interface for HST3D integrated within the Argus Open Numerical Environments (Argus ONE) modeling environment. HST3D allows the user to enter all spatial data, graphically run HST3D, and visualize the results. Argus ONE integrates CAD, GIS, Database, Conceptual Modeling, Geostatistics, Automatic Grid and Mesh Generation, and Scientific Visualization within one comprehensive graphical user interface (GUI). The Heat and Solute Transport Model HST3D simulates ground-water flow and associated heat and solute transport in three dimensions. The HST3D model may be used for analysis of problems such as those related to subsurface-waste injection, landfill leaching, saltwater intrusion, freshwater recharge and recovery, radioactive waste disposal, water geothermal systems, and subsurface energy storage. The Argus ONE GIS and Grid Modules are required to run HST3D.

14. MicroFEM

(Finite-Element Program for Multiple-Aquifer Steady-State and Transient Groundwater Flow Modeling)

The Windows version of MicroFEM is a new program, based on the DOS package Micro-Fem. It takes you through the whole process of ground-water modeling, from the generation of a finite-element grid through the stages of preprocessing, calculation, postprocessing, graphical interpretation and plotting. Confined, semi-confined, phreatic, stratified and leaky multi-aquifer systems can be simulated with a maximum of 20 aquifers. Irregular grids, as typically used by finite-element programs, have several advantages compared to the more or less regular grids used by finite-difference codes. A model with a well-designed irregular grid will show more accurate results with fewer nodes, so less computer memory is required while calculations are faster. MicroFEM offers extensive possibilities as to the ease of creating such irregular grids. Other MicroFEM features include the ease of data preparation and the presentation and analysis of modeling results. A flexible way of zone-selection and formula-assignment is used for all parameters: transmissivities, aquitard resistances, well discharges and boundary conditions for each layer. Depending on the type of model, this can be extended with layer thicknesses, storativities, spatially varying anisotropy, topsystem and user-defined parameters. To inspect and interpret model results, maps and profiles can be used to visualize contours, heads, 3D-flowlines, flow vectors, etc. Time-drawdown curves and water balances can be selected with just a few keystrokes or mouse clicks.

15. MOC

(2-D Solute Transport and Dispersion in Groundwater)

MOC simulates 2-D solute transport in flowing groundwater. MOC is both general and flexible in that it can be applied to a wide range of problem types. MOC is applicable for one- or two-dimensional problems involving steady-state or transient flow. MOC computes changes in concentration over time caused by the processes of convective transport, hydrodynamic dispersion, and mixing (or dilution) from fluid sources. MOC assumes that gradients of fluid density, viscosity and temperature do not affect the velocity distribution. However, the aquifer may be heterogeneous and/or anisotropic. MOC is based on a rectangular, block-centered, finite-difference grid. It allows the specification of injection or withdrawal wells and of spatially-varying diffuse recharge or discharge, saturated thickness, transmissivity, boundary conditions and initial heads and concentrations. MOC incorporates first-order irreversible rate-reaction; reversible equilibrium controlled sorption with linear, Freundlich, or Langmuir isotherms; and reversible equilibrium-controlled ion exchange for monovalent or divalent ions.

16. MOCDENSE

(Two-Constituent Solute Transport Model for Groundwater Having Variable Density)

MOCDENSE is a modified version of the ground-water flow and solute-transport model of Konikow and Bredehoeft which was designed to simulate the transport and dispersion of a single solute that does not affect the fluid density. This modified version of MOCDENSE simulates the flow in a cross-sectional plane rather than in an areal plane. Because the problem of interest involves variable density, the modified model solves for fluid pressure rather than hydraulic head in the flow equation; the solution to the flow equation is still obtained using a finite-difference method. Solute transport is simulated in MOCDENSE with the method of characteristics as in the original model. Density is considered to be a function of the concentration of one of the constituents.

17. MODFLOW

(Three-Dimensional Finite-Difference Ground-Water Flow Model)

MODFLOW is the name that has been given the USGS Modular Three-Dimensional Ground-Water Flow Model. Because of its ability to simulate a wide variety of systems, its extensive publicly available documentation, and its rigorous USGS peer review, MODFLOW has become the worldwide standard ground-water flow model. MODFLOW is used to simulate systems for water supply, containment remediation and mine dewatering. When properly applied, MODFLOW is the recognized standard model.

The main objectives in designing MODFLOW were to produce a program that can be readily modified, is simple to use and maintain, can be executed on a variety of computers with minimal changes, and has the ability to manage the large data sets required when running large problems. The MODFLOW report includes detailed explanations of physical and mathematical concepts on which the model is based and an explanation of how those concepts were incorporated in the modular structure of the computer program. The modular structure of MODFLOW consists of a Main Program and a series of highly-independent subroutines called modules. The modules are grouped in packages. Each package deals with a specific feature of the hydrologic system which is to be simulated such as flow from rivers or flow into drains or with a specific method of solving linear equations which describe the flow system such as the Strongly Implicit Procedure or Preconditioned Conjugate Gradient. The division of MODFLOW into modules permits the user to examine specific hydrologic features of the model independently. This also facilitates development of additional capabilities because new modules or packages can be added to the program without modifying the existing ones. The input/output system of MODFLOW was designed for optimal flexibility.

Ground-water flow within the aquifer is simulated in MODFLOW using a block-centered finite-difference approach. Layers can be simulated as confined, unconfined, or a combination of both. Flows from external stresses such as flow to wells, areal recharge, evapotranspiration, flow to drains, and flow through riverbeds can also be simulated.

18. MODFLOW SURFACT

(MODFLOW-Based Ground-Water Flow and Contaminant Transport Model)

A new flow and transport model, MODFLOW SURFACT, is based on the USGS MODFLOW code, the most widely-used ground-water flow code in the world. MODFLOW, however, has certain limitations in simulating complex field problems. Additional computational modules have been incorporated to enhance the simulation capabilities and robustness. MODFLOW SURFACT is a seamless integration of flow and transport modules.

19. MODFLOWT

(An Enhanced Version of MODFLOW for Simulating 3-D Contaminant Transport)

MODFLOWT is an enhanced version of the USGS MODFLOW model which includes packages to simulate advective-dispersive contaminant transport. Fully three-dimensional, MODFLOWT simulates transport of one or more miscible species subject to adsorption and decay through advection and dispersion. MODFLOWT performs groundwater simulations utilizing transient transport with steady-state flow, transient flow, or successive periods of steady-state flow. Groundwater flow data sets created for the original MODFLOW model function without alteration in MODFLOWT; thus extension of modeling projects to simulate contaminant transport is very easy using MODFLOWT. It is thoroughly tested and has been bench-marked against other transport codes including MT3D, SWIFT and FTWORK. A comprehensive and pragmatic approach to contaminant transport has been incorporated into MODFLOWT which allows for three distinct directional dispersivity values, multiple chemicals and a rigorous treatment of the hydrodynamic dispersion tensor.

20. MODFLOWwin32

(MODFLOW for Windows)

MODFLOWwin32 has all the features of other MODFLOW versions including the newest packages added over the years since MODFLOW's original release by the USGS. These new packages include the Stream Routing Package, Aquifer Compaction Package, Horizontal Flow Barrier Package, BCF2 and BCF3 Packages, and the new PCG2 solver. In addition, MODFLOWwin32 will create files for use with MODPATH (particle-tracking model for MODFLOW) and MT3D (solute transport model). MODFLOWwin32, as its name implies, is a 32-bit program designed to address all the memory available to Windows. MODFLOWwin32 will run in all versions of Windows including Version 3.1, 3.11, Windows 95, 98 and Windows NT.

21. MODPATH

(3-D Particle Tracking Program for MODFLOW)

MODPATH, "A Particle Tracking Post-Processing Package for MODFLOW, the USGS 3-D Finite-Difference Ground-Water Flow Model (MODFLOW)," is a widely-used particle-tracking program.

22. MOFAT

(Multiphase (Water, Oil, Gas) Flow and Multicomponent Transport Model)

MOFAT for Windows includes a graphical preprocessor, mesh editor and postprocessor with on-line help. Simulate multiphase (water, oil and gas) flow and transport of up to five non-inert chemical species in MOFAT. Model flow of light or dense organic liquids in three fluid phase systems. Simulate dynamic or passive gas as a full three-phase flow problem. Model water flow only, oil-water flow, or water-oil-gas flow in variably-saturated porous media. MOFAT achieves a high degree of computational efficiency by solving flow equations at each node (on the finite-element mesh) only for phases that are undergoing changes in pressures and saturations above specified tolerances using a new adaptive solution domain method. Therefore, if NAPL is absent or exists at a residual saturation, MOFAT will locally eliminate those flow equations. MOFAT analyzes convective-dispersive transport in water, NAPL, and gas phases by assuming local equilibrium or nonequilibrium partitioning among the fluid and solid phases. MOFAT considers interphase mass transfer and compositional dependence of phase densities. A concise but accurate description of soil capillary pressure relations is used which assures natural continuity between single-phase, two-phase and three-phase conditions.

23. MS-VMS

(MODFLOW-Based Visual Modeling System with Comprehensive Flow and Transport Capability)

MS-VMS is a comprehensive MODFLOW-based ground-water flow and contaminant transport modeling system. The USGS modular ground-water flow model, MODFLOW, is the most widely-used ground-water flow model in the world. But, in its original form, MODFLOW has certain limitations and cannot be used to simulate some complex problems encountered regularly by modelers, hydrogeologists, and engineers in the field. MS-VMS overcomes these limitations.

24. MT3D

(A Modular 3D Solute Transport Model)

MT3D is a comprehensive three-dimensional numerical model for simulating solute transport in complex hydrogeologic settings. MT3D has a modular design that permits simulation of transport processes independently or jointly. MT3D is capable of modeling advection in complex steady-state and transient flow fields, anisotropic dispersion, first-order decay and production reactions, and linear and nonlinear sorption. It can also handle bioplume-type reactions, monad reactions, and daughter products. This enables MT3D to do multi-species reactions and simulate or assess natural attenuation within a contaminant plume. MT3D is linked with the USGS groundwater flow simulator, MODFLOW, and is designed specifically to handle advectively-dominated transport problems without the need to construct refined models specifically for solute transport.

25. PEST

(Parameter Estimation for Any Model)

PEST is a nonlinear parameter estimation and optimization package. It can be used to estimate parameters for just about any existing model whether or not you have the model's source code. PEST is able to "take control" of a model, running it as many times as it needs while adjusting its parameters until the discrepancies between selected model outputs and a complementary set of field or laboratory measurements is reduced to a minimum in the weighted least-squares sense.

26. PESTAN

(Pesticide Transport Model)

PESTAN, Pesticide Transport, is a U.S. EPA program for evaluating the transport of organic solutes through the vadose zone to groundwater. PESTAN uses an analytical solution to calculate organic movement based on a linear isotherm, first-order degradation and hydrodynamic dispersion. Input data includes water solubility, infiltration rate, bulk density, sorption constant, degradation rates, saturated water content, characteristic curve coefficient, saturated hydraulic conductivity and dispersion coefficient.

27. Processing Modflow (PMWIN)

(Graphical Interface for MODFLOW, MODPATH, PMPATH, MT3D, PEST, and UCODE)

Processing MODFLOW for Windows (PMWIN) is a complete simulation system. It comes complete with a professional graphical preprocessor and postprocessor, the 3-D finite-difference ground-water models MODFLOW-88, MODFLOW-96, and MODFLOW 2000; the solute transport models MT3D, MT3DMS, RT3D and MOC3D; the particle tracking model PMPATH 99; and the inverse models UCODE and PEST-ASP for automatic calibration. A 3D visualization and animation package, 3D Groundwater Explorer, is also included.

28. POLLUTE

(Finite-Layer Contaminant Migration Model - Landfill Design)

POLLUTE can be used for fast, accurate, and comprehensive contaminant migration analysis. It implements a "1½-dimensional" solution to the advection-dispersion equation. Unlike finite-element and finite-difference formulations, POLLUTE does the numerical stability problems of alternate approaches. Landfill designs that can be considered range from simple systems on a natural clayey aquitard to composite liners with multiple barriers and multiple aquifers. In addition to advective-dispersive transport, POLLUTE can consider adsorption, radioactive and biological decay, phase changes, and transport through fractures. The Graphical User Interface makes the editing, execution, and printing of data easy and flexible. This interface also has options to quickly design landfills with primary composite barriers or primary and secondary composite barriers.

29. PRINCE

(7 Mass Transport and 3 Flow Models)

PRINCE is a well-known software package of ten analytical groundwater models originally developed as part of an EPA 208 study. There are seven one-, two- and three-dimensional mass transport models and three two-dimensional flow models in PRINCE. These groundwater models have been rewritten from the original mainframe FORTRAN codes in graphics-rich and PC-friendly C. Two popular analytical models have been added to the original collection, and the ability to import digitized or AutoCAD-produced DXF site map files has been added. The result is a widely acclaimed, user-friendly, menu-driven package with built-in high resolution graphics for X-Y, 2-D contour and 3-D surface plots.

30. PRZM3

(Pesticide Transport Model - Exposure Assessments)

PRZM3 links two models, PRZM and VADOFT to predict pesticide transport and transformation down through the crop root and vadose (unsaturated) zone to the water table. PRZM3 incorporates soil temperature simulation, volatilization and vapor phase transport in soils, irrigation simulation, and microbial transformation. PRZM is a one-dimensional finite-difference model which uses a method of characteristics (MOC) algorithm to eliminate numerical dispersion. VADOFT is a one-dimensional finite-element code that solves Richards' equation for flow in the unsaturated zone. The user may make use of constituting relationships between pressure, water content, and hydraulic conductivity to solve the flow equation. PRZM3 is capable of simulating multiple pesticides or parent-daughter relationships. PRZM3 is also capable of estimating probabilities of concentrations or fluxes in or from various media for the purpose of performing exposure assessments. PRZM and VADOFT are linked together with the aid of a flexible execution supervisor that allows the user to build models that are tailored to site-specific situations. Monte Carlo pre and postprocessors are provided in order to perform probability-based exposure assessments.

31. RBCA Tier 2 Analyzer

(2D Groundwater Flow and Biodegradation Model)

The RBCA Tier 2 Analyzer is a two-dimensional groundwater model with a comprehensive selection of contaminant transport simulation capabilities including single or multiple species sequential decay reactions such as reductive dechlorination of PCE instantaneous or kinetic-limited BTEX biodegradation with single or multiple electron acceptors and equilibrium or non-equilibrium sorption.

32. SEAWAT

(Three-Dimensional Variable-Density Ground-Water Flow)

The SEAWAT program was developed to simulate three-dimensional, variable-density, transient ground-water flow in porous media. The source code for SEAWAT was developed by combining MODFLOW and MT3DMS into a single program that solves the coupled flow and solute-transport equations. The SEAWAT code follows a modular structure, and thus, new capabilities can be added with only minor modifications to the main program. SEAWAT reads and writes standard MODFLOW and MT3DMS data sets, although some extra input may be required for some SEAWAT simulations. This means that many of the existing pre- and post-processors can be used to create input data sets and analyze simulation results. Users familiar with MODFLOW and MT3DMS should have little difficulty applying SEAWAT to problems of variable-density ground-water flow.

33. SESOIL

(Long-Term Pollutant Fate and Migration in the Unsaturated Zone)

SESOIL is a seasonal compartment model which simulates long-term pollutant fate and migration in the unsaturated soil zone. SESOIL describes the following components of a user-specified soil column which extends from the ground surface to the ground-water table.

- Hydrologic cycle of the unsaturated soil zone.
- Pollutant concentrations and masses in water, soil, and air phases.
- Pollutant migration to groundwater.
- Pollutant volatilization at the ground surface.
- Pollutant transport in washload due to surface runoff and erosion at the ground surface.

SESOIL estimates all of the above components on a monthly basis for up to 999 years of simulation time. It can be used to estimate the average concentrations in groundwater. The soil column may be composed of up to four layers, each layer having different soil properties which affect the pollutant fate. In addition, each soil layer may be subdivided into a maximum of 10 sublayers in order to provide enhanced resolution of pollutant fate and migration in the soil column. The following pollutant fate processes are accounted for: Volatilization, Adsorption, Cation Exchange, Biodegradation, Hydrolysis and Complexation.

34. SLAEM / MLAEM

(Analytic Element Models - Model Regional Groundwater Flow in Systems of Confined Aquifers, Unconfined Aquifers and Leaky Aquifers)

The AEM family of computer programs, SLAEM, MLAEM/2, and MLAEM, are based on the Analytic Element Method developed by Dr. O.D.L. Strack. The computer programs are intended for modeling regional groundwater flow in systems of confined, unconfined, and leaky aquifers. SLAEM (Single Layer Analytic Element Model) is the single-layer version of the program. MLAEM/2 (Multi Layer Analytic Element Model) can access two layers while the number of layers supported by MLAEM is limited only by hardware. All programs run under Microsoft Windows 95, 98 and NT. The programs are native windows applications and are accessed via a modern and flexible Graphical User Interface (GUI), as well as via a command-line interface. The latter capability makes it easy to drive the program from other programs such as Arc-View, ARC/INFO, and PEST. The programs create files from data entered graphically via the GUI; these files can be read in later. The programs read DXF-files and produce BNA files that may be read by other programs such as SURFER.

35. SOLUTRANS

(3-D Analytic Solute Transport Model)

SOLUTRANS is a 32-bit Windows program for modeling three-dimensional solute transport based on the solutions presented by Leij et al. for both equilibrium and non-equilbrium transport. The interface and input requirements are so simple that it only takes a few minutes to develop models and build insight about complex solute transport problems. With SOLUTRANS you can, in a matter of minutes, model solute transport from a variety of source configurations and build important insights about key processes. SOLUTRANS offers a quick and simple alternative to complex, time-consuming 3-D numerical flow and transport models.

36. SUTRA

(2-D Saturated/Unsaturated Transport Model)

SUTRA is a 2D groundwater saturated-unsaturated transport model, a complete saltwater intrusion and energy transport model. SUTRA simulates fluid movement and transport of either energy or dissolved substances in a subsurface environment. SUTRA employs a two-dimensional hybrid finite-element and integrated finite-difference method to approximate the governing equations that describe the two interdependent processes that are simulated: (1) fluid density-dependent saturated or unsaturated groundwater flow and either (2a) transport of a solute in the groundwater, in which the solute may be subject to equilibrium adsorption on the porous matrix and both first-order and zero-order production or decay, or (2b) transport of thermal energy in the groundwater and solid matrix of the aquifer. A 3-D version of SUTRA has been recently released.

37. SVFlux 2D

(Saturated/Unsaturated Automated 2D/3D Seepage Modeling Software)

SVFlux 2D represents the next level in seepage analysis software. Designed to be simple and effective, the software offers features designed to allow the user to focus on seepage solutions, not convergence problems or difficult mesh creation. Great care has been taken to model geometry CAD-style input after the popular AutoCAD(TM) software. Freeform boundary equations and an optional soil database of over 6,000 soils to choose from further simplify model design. The finite element solution makes use of fully automatic mesh generation and mesh refinement to solve the problem quickly as well as indicating zones of critical gradient.

38. SWIFT

(3-D Model to Simulate Groundwater Flow, Heat, Brine and Radionuclide Transport)

SWIFT is a fully-transient, three-dimensional model to simulate groundwater flow, heat (energy), brine and radionuclide transport in porous and fractured geologic media. The primary equations for fluid (flow), heat and brine are coupled by fluid density, viscosity and porosity. In addition to transient analysis, SWIFT offers a steady-state option for coupled flow and brine. The equations are solved using central or backward spatial and time weighting approximations by the finite-difference method. In addition to Cartesian, cylindrical grids may be used. Contaminant transport includes advection, dispersion, sorption and decay, including chains of constituents. Both dual-porosity and discrete-fracture representations along with rock matrix interactions may be simulated. The nonlinearities resulting from water table and variable density are solved iteratively.

39. SWIMv1/SWIMv2

(Soil water infiltration and movement model - simulate soil water balances)

SWIMv1 (Soil Water Infiltration and Movement model version 1) is a software package for simulating water infiltration and movement in soils. SWIMv1 consists of a menu-driven suite of three programs that allow the user to simulate soil water balances using numerical solutions of the basic soil water flow equations. As in the real world, SWIMv1 allows addition of water to the system as precipitation and removal by runoff, drainage, evaporation from the soil surface and transpiration by vegetation. SWIMv1 helps researchers and consultants understand the soil water balance so they can assess possible effects of such practices as tree clearing, strip mining and irrigation management. SWIMv1 is valuable for scientists and consultants involved in land planning and land management. For example, if a development is being considered which involves tree clearing, SWIMv1 can be used to indicate salinity or surface runoff problems that could result from a change in the soil water balance associated with the removal of the trees.

SWIMv2 (Soil Water Infiltration and Movement model version 2) is a mechanistically-based model designed to address soil water and solute balance issues associated with both production and the environmental consequences of production. SWIMv2 employs fast, numerically-efficient techniques for solving Richards' equation for water flow and the convection-dispersion equation for solute transport and is suitable for personal computer applications. The model deals with a one-dimensional vertical soil profile which may be vertically inhomogeneous but is assumed to be horizontally uniform. It can be used to simulate runoff, infiltration, redistribution, solute transport and redistribution of solutes, plant uptake and transpiration, evaporation, deep drainage and leaching.

40. TWODAN

(2-D Analytic Ground-Water Flow Model)

TWODAN is a popular and versatile analytic ground-water flow model for Windows. TWODAN has a suite of advanced analytic modeling features that allow you to model everything from a single well in a uniform flow field to complex remediation schemes with numerous wells, barriers, surface waters, and heterogeneities. TWODAN has many capabilities: heterogeneities, impermeable barriers, resistant barriers, and transient solutions, to name a few. The analytic method of TWODAN demands minimal input, and the new seamless Windows interface can be quickly mastered. TWODAN can be used for modeling remedial design alternatives, wellhead capture zones, and regional aquifer flow. TWODAN combines advanced analytic elements with a user interface. Compare It is a good tool for most remediation design, capture zone analysis, and regional modeling problems.

41. VAM2D

(2-D Variably-Saturated Groundwater Analysis Model)

VAM2D (Variably Saturated Analysis Model in Two (2) Dimensions) is a two-dimensional finite-element groundwater model that simulates transient or steady-state groundwater flow and contaminant transport in porous media. VAM2D analyzes unconfined flow problems using a rigorous saturated-unsaturated modeling approach using efficient numerical techniques. Accurate mass balance is maintained in VAM2D even when simulating highly nonlinear soil moisture relations. Hysteresis effects in the water retention curve can also be simulated. A wide range of boundary conditions can be treated in VAM2D including seepage faces, water-table conditions, recharge, infiltration, evapotranspiration, and pumping and injection wells. The contaminant transport option can account for advection, hydrodynamic dispersion, equilibrium sorption, and first-order degradation. Transport of a single species or multiple parent-daughter components of a decay chain can be simulated. The VAM2D code can perform simulations using an areal plane, cross section, or axisymmetric configuration.

42. Visual Groundwater

(3-D Visualization and Animation of Site Data and Modeling Results)

Visual Groundwater is a 3-D visualization software package which can be used to deliver high-quality, three-dimensional presentations of subsurface characterization data and groundwater modeling results. Visual Groundwater combines state-of-the-art graphical tools for 3-D visualization and animation with a data management system specifically designed for borehole investigation data. Visual Groundwater also comes with a data conversion utility to create 3-D data files using random X, Y, Z data, and gridded data sets. Three-dimensional images of complex site characterization data and modeling results can be easily created.

43. VISUAL HELP

(Modeling Environment for the U.S. EPA HELP Model for Evaluating and Optimizing Landfill Designs)

Visual HELP for Windows 95/98/2000/NT is an advanced hydrological modeling environment available for designing landfills, predicting leachate mounding and evaluating potential leachate contamination. Visual HELP combines the latest version of the HELP model with an easy-to user interface and powerful graphical features for designing the model and evaluating the modeling results. Visual HELP's user-friendly interface and flexible data handling procedures provides convenient access to both the basic and advanced features of the HELP model. This completely-integrated modeling HELP environment allows the user to graphically create several profiles representing different parts of a landfill; automatically generate statistically-reliable weather data (or create your own); run complex model simulations; visualize full-color, high-resolution results; and prepare graphical and document materials for your report.

44. Visual MODFLOW

(Integrated Modeling Environment for MODFLOW, MODPATH, MT3D)

Visual MODFLOW provides professional 3D groundwater flow and contaminant transport modeling using MODFLOW-2000, MODPATH, MT3DMS and RT3D. Visual MODFLOW Pro seamlessly combines the standard Visual MODFLOW package with WinPEST and the Visual MODFLOW 3D-Explorer to give the most complete and powerful graphical modeling environment available. This fully-integrated groundwater modeling environment allows to:

- Graphically design the model grid, properties and boundary conditions,
- Visualize the model input parameters in two or three dimensions,
- Run the groundwater flow, pathline and contaminant transport simulations,
- Automatically calibrate the model using WinPEST or manual methods, and
- Display and interpret the modeling results in three-dimensional space using the Visual MODFLOW 3D-Explorer

45. VISUAL PEST

(Graphical Model-Independent Parameter Estimation and Optimization)

Visual PEST combines the powerful parameter estimation capabilities of PEST2000 with the graphical processing and display features of WinPEST. PEST2000 is the latest version of PEST, the pioneer in model-independent parameter estimation. Since it was first released over six years ago, PEST has gained extensive use all over the world in many different fields. During this time it has undergone continued development with the addition of many new features that have improved its performance and utility to a level that makes it uniquely applicable in just about any modeling environment. PEST is now used extensively for automated model calibration and data interpretation in groundwater and surface-water hydrology, geophysics, geotechnical, mechanical and mining engineering as well as many other fields.

46. VLEACH

(One-Dimensional Finite-Difference Vadose Zone Leaching Model)

VLEACH, a One-Dimensional Finite-Difference Vadose Zone Leaching Model, is a U.S. EPA program which describes the movement of an organic contaminant within and between three phases: (1) as a solute dissolved in water, (2) as a gas in the vapor phase, and (3) as an adsorbed compound in the solid phase. The leaching is simulated in a number of distinct, user-defined polygons vertically divided into a series of user-defined cells. At the end of the simulation, the results from each polygon are used to determine an area-weighted ground-water impact for the modeled area. VLEACH is a computer program for estimating the impact due to the mobilization and migration of a sorbed organic contaminant located in the vadose zone on the underlying groundwater resource. A graphical user interface for VLEACH is now available in the WHI UnSat Suite.

47. VS2DT

(Flow and Solute Transport in Variably-Saturated, Single-Phase Flow in Porous Media)

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

48. WHI UnSat Suite

(A Compilation of the Most Popular Unsaturated Zone Models)

The WHI UnSat Suite Plus combines SESOIL, VLEACH, PESTAN, VS2DT and HELP in a revolutionary graphical environment specifically designed for simulating one-dimensional groundwater flow and contaminant transport through the unsaturated zone. All five of these models are compiled and optimized to run as native Windows applications and are seamlessly integrated within the WHI UnSat Suite modeling environment. Professional Applications of the WHI UnSat Suite Plus

- Simulate long-term pollutant fate and transport (VOCs, PAHs, pesticides and heavy metals) in the unsaturated zone under seasonally variable conditions using SESOIL.
- Predict vertical migration of volatile hydrocarbons through the vadose zone using VLEACH.

- Estimate agricultural pesticide migration through the unsaturated zone using PESTAN.
- Simulate groundwater flow and transport processes through heterogeneous, unsaturated soil using VS2DT.
- Predict seasonal recharge rates through heterogeneous soil conditions under variable weather conditions using the HELP model.
- Generate up to 100 years of statistically reliable climatalogical data for virtually any location in the world using the WHI Weather Generator.

49. WinFlow

(Analytical Steady-State and Transient Groundwater Flow Model)

WinFlow is a powerful yet easy-to-use groundwater flow model. WinFlow is similar to Geraghty & Miller's popular QuickFlow model which was developed by one of the authors of QuickFlow. WinFlow is a true Windows program incorporating a multiple document interface (MDI). WinFlow is an interactive analytical model that simulates two-dimensional steady-state and transient groundwater flow. The steady-state module in WinFlow simulates groundwater flow in a horizontal plane using analytical functions developed by Strack. The transient module uses equations developed by Theis and by Hantush and Jacob for confined and leaky aquifers, respectively. Each module uses the principle of superposition to evaluate the effects from multiple analytical functions (wells, etc.) in a uniform regional flow field.

50. WinTran

(Groundwater Flow and Finite-Element Contaminant Transport Model)

WinTran couples the steady-state groundwater flow model from WinFlow with a contaminant transport model. The transport model has the feel of an analytic model but is actually an embedded finite-element simulator. The finite-element transport model is constructed automatically by WinTran but displays numerical criteria (Peclet and Courant numbers) to allow the user to avoid numerical or mass balance problems. Contaminant mass may be injected or extracted using any of the analytic elements including wells, ponds, and linesinks. In addition, constant concentration elements have been added. WinTran displays both head and concentration contours, and concentration may be plotted versus time at selected monitoring locations. The transport model includes the effects of dispersion, linear sorption (retardation), and first-order decay. WinTran aids in risk assessment calculations by displaying the concentration over time at receptor or observation locations. WinTran will display the breakthrough curves after the simulation is finished.

Considering the large variability and the quick development of groundwater models, a new, more sophisticated model can often replace a previously applied model.

Additionally, the reconsideration of the conceptual model and the regeneration of the mesh may need a new allocation of the parameters. Therefore, it is important that model data (information) are stored independently from a given model, with a preference for GIS-based databases. Considerable development in the field of user-friendly GIS and data base servers makes the set-up and the modification of models easier and more time-effective. One such model is FEFLOW which incorporates mathematical modelling with GIS-based data exchange interfaces.

The input data for a groundwater model include natural and artificial stress, and parameters, dimensions, and physico-chemical properties of all aquifers considered in the model. A finer level of detail of the numerical approximation (solution) greatly increases the data requirements. Input data for aquifers are common values such as transmissivities, aquitard resistances, abstraction rates, groundwater recharges, surface water levels etc. The most common output data are groundwater levels, fluxes, velocities and changes in these parameters due to stress put into the model.

5.0 CONCLUDING REMARKS

Mathematical models are tools, which are frequently used in studying groundwater systems. In general, mathematical models are used to simulate (or to predict) the groundwater flow and in some cases the solute and/or heat transport. Predictive simulations must be viewed as estimates, dependent upon the quality and uncertainty of the input data. Models may be used as predictive tools, however field monitoring must be incorporated to verify model predictions. The best method of eliminating or reducing modelling errors is to apply good hydrogeological judgement and to question the model simulation results. If the results do not make physical sense, find out why.

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