WORKSHOP

ON

MODELLING OF HYDROLOGIC SYSTEMS

4-8 September, 2000

Modelling of Groundwater Flow

by
B. Chakravorty

Organised by

Hard Rock Regional Centre
National Institute of Hydrology
Belgaum-590 001 (Karnataka)

MODELING OF GROUNDWATER FLOW

Biswajit Chakravorty
Scientist 'C'
Ganga Plain North Regional Centre
National Institute of Hydrology
Patna- 801 505 (Bihar)

1.0 What is an Aquifer Model?

Mathematical model of an aquifer is an *evaluation and prediction tool* which integrates all information about a ground water system, checks assumptions postulated throughout the exploration, quantifies various parameters and processes, and simulates future development scenarios under modified conditions of recharge and discharge. A mathematical model of groundwater simulates groundwater flow indirectly by means of governing equations thought to represent the physical processes that occur in the system together with equations that describe heads or flows along the boundaries of the model (boundary conditions).

2.0 How a Model is Created?

First, the continuous aquifer system parameters are replaced by an equivalent set of discrete elements. Second, the equations governing the flow of groundwater in the discretized model are written in finite-difference form (or finite element). Both the space and time are treated as discrete parameters. Finally, the set of finite-difference equations are solved numerically.

3.0 How Good is a Model?

Any model is good if the database used in its construction are good. Thus, the computer and computer programs for running a model, are only necessary prerequisites or tools in modeling. The database is the essence of a model. Sufficient data, both in quantity and quality, is normally the bottleneck of a model.

4.0 Prerequisites for Constructing a Model

i. The modeler must have a basic understanding of hydrogeology of the model area, and importance of processes involved in order to select a proper modeling code or program.

ii. Basic hydrogeological parameters, such as effective porosity, transmissivity, leakage if any, hydraulic conductivity, must be known to some extent, or at least their ranges of variation should be known with certain accuracy.

iii. The behaviour of water table over the model area must be known at sufficient number of points and over considerably long time period, which must not be less than one full year.

iv. Distribution of abstraction points, the volumes of pumping over the same past time in which water levels are being monitored.

v. The boundaries of the system must be fully understood. The hydrologic and meteorologic input parameters, such as rainfall, river flow, etc. must be quantified with sufficient accuracy.

Hydraulic boundaries (static and dynamic) such as sea levels and/or river, must be known.

Many things can be done with a ground water model, but model's value is *limited* where the aquifer and the overall groundwater system is poorly understood. The model demands that the aquifer characteristics be as well known as possible, the water table has been carefully monitored, rainfall figures are reliable and the recharge mechanism is carefully considered.

5.0 Equations

The three dimensional unsteady movement of groundwater of constant density through porous earth material in a heterogenous anisotropic medium can be described by the following partial differential equation:

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

Where,

K_{xx}, K_{yy}, K_{zz}	:	hydraulic conductivity along major axes $[LT^{-1}]$,
h	:	potentiometric head [L],
W	:	volumetric flux per unit volume and represents sources and/or sinks of water $[T^{-1}]$,
S_s	:	specific storage of the porous material $[L^{-1}]$ and,
t	:	time [T].

Possible Source and/or Sink terms (W) are:

- Recharge from rainfall.
- Artificial recharge through wells.
- Pumping through wells.
- Evapotranspiration loss.
- Recharge from river/canal cells.
- Outflow into a river/canal cell.
- Inflow/Outflow across a boundary cell.
- Outflow through drains.
- Spring flow.
- etc.

In general, S_s, K_{xx}, K_{yy} and K_{zz} are function of space, for example; $S_s = S_s(x,y,z)$, $K_{xx} = K_{xx}(x,y,z)$, etc. whereas W and h are functions of space and time i.e $W = W(x,y,z,t)$ and $h = h(x,y,z,t)$. Equation (1) together with specification of flow conditions at the boundaries of an aquifer system and specification of initial head conditions, constitutes a mathematical model of ground water flow.

Except for very simple systems, analytical solutions of equation (1) are rarely possible. So, various numerical methods are employed to obtain an approximate solution of the above equation. One such approach is the *finite-difference* method. The continuous system described by equation (1) is replaced by a finite set of discrete elements in space and time, and the set of finite difference equations are solved numerically which yields *values of head* at specific points and times. These values constitute an approximation to the time-varying head distribution that would be given by an analytical solution of the flow equation.

6.0 Basic Steps in Making a Model

- Develop a conceptual model of the system.
- Design a grid to represent the model area with as much detail as needed.
- Assign hydrologic properties to each grid cell.
- Select an appropriate time step for transient models.
- Set up boundary conditions.
- Select a solver.
- Run the model and compare with measured data to evaluate the effectiveness of the model.
- If necessary, revise the model.
- Plotting the data.
- Tracking down errors.

If groundwater modeling is part of some larger project, it is good to start the modeling effort at an early stage. Even a poorly calibrated model can provide insight into the system being modeled and may help in identifying deficiencies in the data which is collected.

7.0 Input to and Output from Model

The modeling process can be thought of an

INPUT + PROGRAM FOR SOLUTION $\Rightarrow$ OUTPUT

7.1 Input to the Model

- Boundary data.
- Geometry of aquifer.
- Permeability(ies).
- Effective porosity.
- Specific storage.
- Recharge data.
- Evapotranspiration data.
- Surface water – groundwater exchange.
- Pumping from/to aquifer.
- Artificial recharge.
- etc.

7.2 Program for Solution

- MODFLOW
- MOC3D

- MODFLOW-SURFACT
- MT3D
- MT3DMS
- MICRO-FEM
- MODFE
- MOCDENS and MOCDENS3D
- SUTRA
- **SHARP**
- MODFLOWP
- PMWIN 5.0
- Visual MODFLOW
- GMS
- Groundwater Vistas
- MS-VMS
- ASM (Aquifer Simulation Model and ASM for Windows)
- SEAWAT
- PEST (WinPEST and PEST98)
- VS2DT (infiltration modeling)

7.3 Output from the Model

- Water levels.
- Drawdowns.
- Water balance of the whole model domain and required sub-regions.
- Distribution of aquifer parameters.
- Distribution of evapotranspiration.
- Distribution of recharge.
- Outflow across model boundaries.
- etc.

8.0 Modeling Software Packages

8.1. MODFLOW

MODFLOW is a MODular 3-dimensional finite difference groundwater FLOW model developed by McDonald and Harbough of the USGS, USA in 1988. It simulates steady and non-steady flow in three dimensions for an irregularly shaped flow system in which aquifer layer can be confined, unconfined, or a combination of confined and unconfined. Flow from external sources, such as flow to wells, areal recharge, evapotranspiration, flow to drains, and flow through river, can be simulated

MODFLOW uses a modular structure wherein similar program functions are grouped together. The modular structure consists of a main program and a large number of independent subroutines called "modules". The modules, in turn, have been grouped into "packages". Each package deals with a specific aspect of the hydrological system to be simulated. For example, the option Well package simulates the effect of wells, the River package simulate the effect of river etc.

8.2. MOC3D

MOC3D is a three-dimensional method of characteristics groundwater flow and transport model. It simulates three-dimensional solute transport in flowing groundwater and computes changes in concentration of a single dissolved chemical constituent over time caused by advective transport, hydrodynamic dispersion (including both mechanical dispersion and diffusion), mixing (or dilution) from fluid sources and mathematically simple chemical reactions (including linear sorption, represented by a retardation factor and decay).

MOC3D is integrated with MODFLOW. It uses the method of characteristics to solve the transport equation on the basis of the hydraulic gradients computed with MODFLOW for a given time step. Particle tracking is used to represent advective transport and explicit finite-difference methods are used to calculate the effects of other processes.

8.3. MODFLOW-SURFACT

It is a comprehensive three-dimensional finite-difference flow and contaminant transport modeling code based on the USGS modular groundwater flow model, MODFLOW. Salient features of MODFLOW-SURFACT are:

i. It extends physical modeling capabilities of MODFLOW for subsurface flow calculations:

New flow package in MODFLOW-SURFACE handles complete drying and re-wetting of grid blocks including vertical flow components throughout the domain and delayed yield. It also provided with axi-symmetric simulation option for quick pump-test type analyses.

New fracture well package in this model provides automatic and physically consistent approportioning of a total well flow rate, to the respective nodes of a well open to multiple layers.

New recharge/seepage face package in this model provides capability for non-ponding or prescribed ponding conditions. Also handles seepage-face boundary conditions.

ii. Enhances robustness and efficiency of MODFLOW even for its existing capabilities.

New adaptive time stepping and output control package, ATO4, provides great robustness and efficiency in all flow simulations, cutting the time-step size when the simulation becomes difficult, and increasing it when the difficulty passes. Also provides improved organization and control of simulation output. New conjugate gradient solution package, PCG4, provides a robust alternative to the available solvers in MODFLOW.

MODFLOW's time stepping increases the step size in geometric progression indefinitely, sacrificing robustness, efficiency, and efficient control of simulation output. Solvers available in MODFLOW are efficient for small or easy problems, but become inefficient, or fail altogether, for large, complex problems.

iii. Integrates state-of-the-art, mass conservative, multi-component contaminant transport simulations capabilities.

- It has accurate, robust, and efficient mass-conservative transport solution schemes.
- Numerical schemes, data input/output, grid considerations, and simulation control fully compatible with all MODFLOW and MODFLOW-SURFACT flow options.
- Axi-symmetric option for quick analyses of slug tests or tracer tests.
- Accommodates up to five contaminant species in a single simulation including first-order chain reactions which may occur due to radioactive decay (species dependent), or biochemical transformation (species and soil/location dependent).
- Provides linear or non-linear (Freundlich) equilibrium adsorption options.
- Provides two, three, and four component dispersivity options for various anisotropic conditions. Under isotropic conditions, the three and four dispersivity formulations collapse to Scheidegger's two component (longitudinal and transverse) dispersivity equation.
- Consistent transport solution options - upstream, central, or mixed weighting for efficient solution, or Total Variation Diminishing (TVD) schemes for extremely accurate, physically correct solutions.

iv. Dynamic memory allocation advantages permits unlimited problem dimensions.

- Windows systems allocate available memory to all applications open on the computer. Efficient use of memory by MODFLOW- SURFACT maximizes available memory space for other user applications.
- Due to dynamic allocation of memory, simulation problem dimensions are limited only by available computer memory, or prohibitively long simulation times for large, complex problems.

v. Modular structure allows further development of additional simulation capabilities to provide a comprehensive, general purpose simulator within the MODFLOW framework.

8.4 MT3D (Modular three-dimensional transport model)

MT3D is a comprehensive three-dimensional solute transport model for simulation of advection, dispersion and chemical reactions of contaminants in groundwater systems. MT3D was first developed by Chunmiao Zheng in 1990 at S.S. Papadopulos & Associates, Inc. with partial support from the U.S. Environmental Protection Agency (USEPA).

MT3D is based on a modular structure to permit simulation of transport components independently or jointly. MT3D interfaces directly with the U.S. Geological Survey finite-difference groundwater flow model, MODFLOW, for the head solution, and supports all the hydrologic and discretization features of MODFLOW. MT3D has been widely accepted by practitioners and researchers alike and applied in numerous field-scale modeling studies in the United States and throughout the world.

The MT3D code has a comprehensive set of solution options, including the method of characteristics (MOC), the modified method of characteristics (MMOC), a hybrid of these two methods (HMOC), and the standard finite-difference method (FDM). The availability of these solution options in one program, and the continuing enhancement and expansion of its capabilities, makes MT3D uniquely suitable for handling a wide range of field problems of different natures.

8.4.1 MT3DMS

The new mass transport model referred to as MT3DMS, where MT3D stands for the Modular 3-Dimensional Transport model while MS denotes the Multi-Species structure for accommodating add-on reaction packages. MT3DMS has a comprehensive set of options and capabilities for simulating advection, dispersion/diffusion, and chemical reactions of contaminants in groundwater flow systems under general hydrogeologic conditions.

MT3DMS is unique in that it includes three major classes of transport solution techniques in a single code, i.e., the standard finite difference method; the particle-tracking-based Eulerian-Lagrangian methods; and the higher-order finite-volume TVD method. Since no single numerical technique has been shown to be effective for all transport conditions, the combination of these solution techniques, each having its own strengths and limitations, is believed to offer the best approach for solving the most wide-ranging transport problems with desired efficiency and accuracy.

In addition to the explicit formulation of the original MT3D code, MT3DMS includes an implicit formulation that is solved with an efficient and versatile solver. The iterative solver is based on generalized conjugate gradient (GCG) methods. If the GCG solver is selected, dispersion, sink/source, and reaction terms are solved implicitly without any stability constraints. For the advection term, the user has the option to select any of the solution schemes available, including the standard finite-difference method, the particle tracking based Eulerian-Lagrangian methods, and the third-order TVD method. If the GCG solver is not selected, the explicit formulation is automatically used in MT3DMS with the usual stability constraints. The explicit formulation is efficient for solving advection-dominated problems in which the transport step sizes are restricted by accuracy considerations. It is also useful when the implicit solver requires a large number of iterations to converge or when the computer system does not have enough memory to use the implicit solver.

MT3DMS is implemented with an optional, dual-domain formulation for modeling mass transport. With this formulation, the porous medium is regarded as consisting of two distinct domains, a mobile domain where transport is predominately by advection and an immobile domain where transport is predominately by molecular diffusion.

MT3DMS retains the same modular structure of the original MT3D code, similar to that implemented in the U.S. Geological Survey modular three-dimensional finite-difference groundwater flow model, MODFLOW. The modular structure of the transport model makes it possible to simulate advection, dispersion/diffusion, source/sink mixing, and chemical reactions separately without reserving computer memory space for unused options. Furthermore new packages involving other transport processes and reactions can be added to the model readily without having to modify the existing code.

8.5 MICRO-FEM

MICRO-FEM is a large capacity finite-element microcomputer package for multi-aquifer steady-state and transient groundwater flow modeling, with a maximum of 16 aquifers and 12,500 nodes per aquifer. The actual capacity of the program depends on the available computer memory. Confined, leaky, unconfined and anisotropic aquifers can be modeled. Full graphical control makes the otherwise time-consuming and error-prone process of grid generation and data input easier.

8.6 MODFE

MODFE - Modular finite-element model for areal and axi-symmetric groundwater flow problems. It provides solutions to groundwater flow problems based on governing equations that describe two-dimensional and axi-symmetric radial flow in porous media.

Simulation capabilities and uses of MODFE are : transient or steady-state conditions; nonhomogeneous and anisotropic flow where directions of anisotropy change within the model region; vertical leakage from a semiconfining layer that contains laterally nonhomogeneous properties and elastic storage effects; point and areally distributed sources and sinks, specified head (Dirichlet); specified flow (Neumann); and head-dependent (Cauchy-type) boundary conditions; vertical cross-section and axisymmetric cylindrical flow; confined and unconfined (water-table) conditions; partial drying and resaturation of a water-table aquifer; conversion between confined- and unconfined-aquifer conditions; and nonlinear head-dependent fluxes (for simulating line, point, or areally distributed sources and sinks).

Software for Modeling Density Controlled Flow

8.7 MOCDENSE and MOCDENS3D

MOCDENSE - A two-constituent solute transport model for ground water having variable density. It was documented by Sanford and Konikow (1985). This model simulates solute transport in flowing ground water. It is applicable to two-dimensional, cross-sectional problems involving ground water with constant or variable density. The model computes changes in concentration over time caused by the processes of advective transport, hydrodynamic dispersion, mixing or dilution from fluid sources. The concentrations of two independent solutes can be modeled simultaneously. Temperature is assumed to be constant, but fluid density and viscosity are assumed to be a linear function of the first specified solute. If a second solute is specified, it is assumed to be of a trace amount such that it does not affect the fluid density or viscosity. The aquifer may be heterogeneous and anisotropic. The model has been used mostly in studies of either saltwater intrusion or dense contaminant plumes.

The model couples the ground-water flow equation with the solute-transport equation. It uses an iterative strongly-implicit procedure to solve a finite-difference approximation to the groundwater flow equation and the method of characteristics to solve the solute-transport equation. This incorporates a particle-tracking procedure to represent advective transport and a two-step explicit finite-difference procedure to solve equations that describe the effects of hydrodynamic dispersion and fluid sources. This explicit procedure has several stability criteria associated with it, but the consequent time-step limitations are automatically determined by the program.

8.8 SUTRA

SUTRA - Saturated and (or) unsaturated, constant or variable-density fluid flow, and solute or energy transport (2-dimensional finite-element code). SUTRA is a finite-element simulation model for saturated-unsaturated, fluid-density-dependent ground-water flow with energy transport or chemically-reactive single-species solute transport. SUTRA may be employed for areal and cross-sectional modeling of saturated groundwater flow systems, and for cross-sectional modeling of unsaturated zone flow. Solute transport simulation using SUTRA may be employed to model natural or man-induced chemical species transport including processes of solute sorption, production and decay, and may be applied to analyze groundwater contaminant transport problems and aquifer restoration designs. In addition, solute transport simulation with SUTRA may be used for modeling of variable density leachate movement, and for cross-sectional modeling of saltwater intrusion in aquifers in near-well or regional scales, with either dispersed or relatively sharp transition zones between freshwater and saltwater. SUTRA energy transport simulation may be employed to model thermal regimes in aquifers, subsurface heat conduction, aquifer thermal energy storage systems, geothermal reservoirs, thermal pollution of aquifers, and natural hydrogeologic convection systems.

8.9 SHARP

SHARP - A quasi-three-dimensional, numerical finite-difference model to simulate freshwater and saltwater flow separated by a sharp interface in layered coastal aquifer systems

SHARP is a quasi-three-dimensional, numerical model that solves finite-difference approximations of the equations for coupled freshwater and saltwater flow separated by a sharp interface in layered coastal aquifer systems. The model is quasi-three dimensional because each aquifer is represented by a layer in which flow is assumed to be horizontal.

An implicit finite-difference discretization scheme that is central in space and backward in time is used to solve the freshwater and saltwater flow equations for each model layer. In the central difference approximations for the space derivatives, the thicknesses at the grid block boundaries are linearly interpolated, and the conductivity terms are estimated using the harmonic mean of nodal values. At blocks containing pumped wells, the amount of freshwater and saltwater extracted depends on the position of the interface relative to the elevation of the screened interval of the well. The rate of freshwater and (or) saltwater extraction from a block, relative to the total fluid extraction rate, is determined linearly on the basis of the proportion of screen penetrating the freshwater and saltwater zones relative to the total open interval of the well.

The interface elevation in each finite-difference block is calculated using the numerically-determined freshwater and saltwater head distributions. The shape of the interface can be obtained by connecting the discretized interface elevations.

SHARP requires all of the input parameters typically required by a finite-difference ground-water flow model (initial conditions, boundary conditions, aquifer properties). However, because it solves both freshwater and saltwater flow equations, it has additional input requirements. The fresh and saltwater specific gravities and dynamic viscosities must be specified. Freshwater hydraulic conductivities are specified and saltwater hydraulic conductivities are calculated in the model. Fresh and saltwater specific storages, effective porosity and confining layer leakance values must be specified.

Parameter Estimation Software

8.10 MODFLOWP

MODFLOWP - Parameter-estimation version of the modular model. This program is a new version of the U.S. Geological Survey modular, three-dimensional, finite-difference, ground-water flow model MODFLOW, which, with the new Parameter-Estimation Package, can be used to estimate parameters by nonlinear regression. The new version of MODFLOW is called MODFLOWP (pronounced MOD-FLOW-P) and functions nearly identically to MODFLOW when the Parameter-Estimation Package is not used. Parameters used to compute the MODFLOW model inputs can be estimated. Data used to estimate parameters can include existing independent estimates of parameter values, observed hydraulic heads or temporal changes in hydraulic heads, and observed gains and losses along head-dependent boundaries (such as streams). Model output includes statistics for analyzing the parameter estimates and the model; these statistics can be used to quantify the reliability of the resulting model, to suggest changes in model construction, and to compare results of models constructed in different ways.

Pre- and Post-processing Modeling Software

8.11 Processing Modflow for Windows (PMWIN 5.0)

PMWIN 5.0 is one of the most complete groundwater simulation systems in the world. It comes with a professional graphical user interface and full versions of groundwater flow models (MODFLOW-88, MODFLOW-96), solute transport models (MT3D, MT3DMS, MOC3D), particle tracking model (PMPATH for Windows), inverse models (PESTLITE, UCODE) and lots of modeling tools including Field Interpolator and Field Generator.

8.12 Visual Modflow

8.13 GMS

8.14 Groundwater Vistas

8.15 MS-VMS