INTRODUCTION TO GROUNDWATER MODELLING

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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.

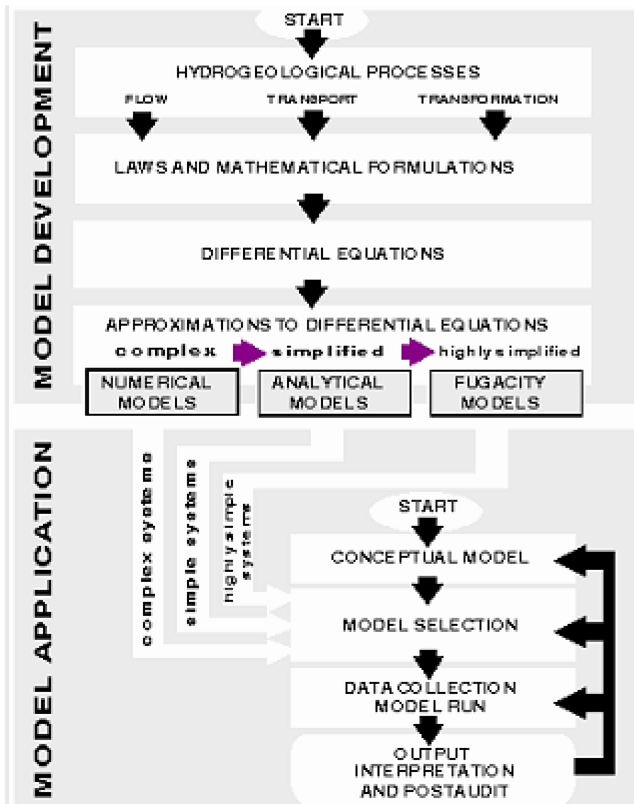

Figure 1: Development Process of a Model

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 GROUNDWATER FLOW EQUATION

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:

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

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. 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.

2. 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.

3. 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.

4. 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.

5. 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.

6. 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.

7. 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.

8. 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.

9. 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

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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