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Robert S. Kerr
Environmental Research Laboratory
Ada, OK 74820

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Project Summary

Compilation of Ground-Water Models

Paul K.M. van der Heijde and Osman A. Elnawawy

The full report presents an overview of currently available computer-based simulation models for ground-water flow, solute and heat transport, and hydrogeochemistry in both porous media and fractured rock. Separate sections address multiphase flow and related chemical species transport, and ground-water management models. The study reflects the on-going ground-water modeling information collection and processing activities at the International Ground Water Modeling Center (IGWMC). The full report includes a section that defines ground-water modeling, presents the classification approach taken by the IGWMC and discusses different types of models and the mathematical approaches invoked for developing the models. Separate sections discuss and review the different categories of ground-water models: flow models, transport models, chemical reaction models, stochastic models, models for fractured rock and ground-water management models. The appendices include a listing and description from the IGWM Model Annotation Search and Retrieval System (MARS) database of selected models from each category.

This Project Summary was developed by EPA's Robert S. Kerr Environmental Research Laboratory, Ada, OK, to announce key findings of the research report that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

The full report contains the results of research and information processing activities performed by the IGWMC under a research and technology transfer cooperative agreement with the U.S. Environmental Protection Agency, initiated in 1988. The report, together with the reports on management models and multiphase flow and transport, provides an overview of the status of major types of ground-water models. These reports present an update of Chapter 5 and the appendices of the report, "Groundwater Modeling: An Overview and Status Report," (EPA/600/2-89/028) prepared in 1988 under a previous cooperative agreement with the US EPA.

The review of models has been based on information gathered by the IGWMC through research and interviews on an on-going basis since 1978. To manage the rapidly growing amount of information, IGWMC maintains a descriptive model information system, MARS. Currently, this database is installed on a microcomputer operating under MS-DOS. Detailed information on the reviewed models is presented in a series of tables, preceded by an introduction on model classification and principal characteristics of the described models.

Discussion

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

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

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

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

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

- Determining or evaluating the need for regulation of specific waste disposal, agricultural, and industrial practices
- Analyzing policy impacts, as in evaluating the consequences of setting regulatory standards and rules
- Assessing exposure, hazard, damage, and health risks
- Evaluating reliability, technical feasibility and effectiveness, cost, operation and maintenance, and other aspects of waste disposal facility designs and of alternative remedial actions
- Providing guidance in siting new facilities and in permit issuance and petitioning
- Developing aquifer or well head protection zones
- Assessing liabilities such as post-closure liability for waste disposal sites.

Computer-based ground-water modeling began in the mid 1960's and has gradually grown into a widely accepted and applied decision-support tool. In the last few years, modeling has been made easier, faster, and "flashier" by rapidly evolving computer hardware and software technologies. The widespread availability of powerful desktop microcomputers and user-oriented software interfaces has made running ground-water computer codes a rather mundane task in hydrogeological assessments. The mechanics of entering data, running simulations, and creating high-quality graphics have become less time-consuming and less complex due to the availability of various, extensively supported window environments and expanded functionality, easy-to-debug, programming languages. These high-powered software development systems integrate editing, compiling, and debugging functions with additional programming tools and libraries allowing efficient development of flexible, menu-driven software while facilitating achievement of high quality-assurance goals. Increased portability of the software due to the development of multi-platform operating systems such as UNIX, and standardization of high-level programming languages (e.g., FORTRAN 90) and the subsequent release of new compilers, makes it possible for software development groups to continue to improve the simulation components of the software. Furthermore, the use of object-oriented programming holds the promise of more flexibility regarding post-development expansion and maintenance, and in overall reliability and portability of the software.

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

However, the reduction in time and effort in modeling due to new software developments does not mean that modeling has become a simple task; in fact, modeling is becoming more challenging as ground-water specialists are able to deal with increasingly complex mathematical descriptions of natural systems and resource management problems. In addition, these problems can be studied in much more detail by using high-order spatial and temporal resolution. In-depth treatment of the theoretical basis of ground-water models can be found in NRC (1990), among others. Extensive discussion on modeling methodology is given in van der Heijde *et al.* (1988) and NRC (1990).

Classification of the Ground-Water System

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

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

A classification based on processes distinguishes between flow, transport (solute and heat), fate of chemical compounds, phase transfers and other processes (Table 1 lists important processes encountered in ground-water systems). Flow models simulate the movement of one or more fluids in porous or fractured rock. One such fluid is water; the others, if present, can be air, methane, or other vapors (in soil) or immiscible nonaqueous phase liquids (NAPLs) sometimes having a density distinct from water (LNAPLs, DNAPLs). A special case of multi-fluid flow occurs when layers of water of distinct density are separated by a relatively small transition zone, a situation often encountered when sea water intrusion occurs. Most flow models are based on a mathematical formulation which considers the hydraulic system parameters as independent field information, and hydraulic head and flux as dependent variables. They are used to calculate steady-state distribution or changes in time in the distribution of hydraulic head or fluid pressure, drawdown, rate and direction of flow (*e.g.,* determination of streamlines, particle pathways, velocities, and fluxes), travel times, and the position of interfaces between immiscible fluids. Inverse flow models simulate the flow field to calculate the spatial distribution of unknown system parameters using field information on the dependent variables such as hydraulic head and flux.

Table 1. *Important Processes in Ground-Water Modeling*

Flow:

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

Transport

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

Fate:

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

Phase Transfers:

- *solid↔gas:*
  - *(vapor) sorption*
- *solid↔liquid:*
  - *sorption*
  - *ion exchange*
- *liquid↔gas:*
  - *volatilization*
  - *condensation*
  - *sublimation*

Phase Changes:

- *freezing/thawing*
- *vaporization (evaporation)/condensation*

Two types of models can be used to evaluate the chemical quality of groundwater: (1) pollutant transformation and degradation models, where the chemical and microbial processes are posed independent of the movement of the pollutants; and (2) solute transport models simulating displacement of the pollutants only (conservative transport), or including the effects of phase transfers, (bio-chemical transformation and degradation processes (transport and fate; non-conservative transport). In fact, one may argue a third type exists, where a conservative solute transport model is coupled with a hydrogeochemical speciation model.

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

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

The nonconservative solute transport models include some type of solute transformation, primarily adsorption, radioactive decay, and simple (bio-)chemical transformations and decay.

The inclusion of geochemistry in solute transport models is often based on the assumption that the reaction proceeds instantaneously to equilibrium. Recently, various researchers have become interested in the kinetic approach that incorporates chemical reactions in transport model. This inclusion of geochemistry has focused on a single reaction such as ion-exchange or sorption for a small number of reacting solutes.

Conclusions

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

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

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

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

Finally, developments most promising for practical application may be found in the area of parameter estimation. Various geostatistic and stochastic approaches have become available together with new or updated parameter estimation models and are increasingly used in the field, specifically in determining the distribution of hydraulic parameters.

References

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P. K.M. van der Heijde is with the Colorado School of Mines, Golden, CO 80401, and Osman A. Elnawawy is with the Indiana University/Purdue University at Indianapolis, Indianapolis, IN 46204.

***Joseph R. Williams** is the EPA Project Officer (see below).*

The complete report, entitled "Compilation of Ground-Water Models," (Order No. PB93-209401; Cost: $44.50, subject to change) will be available only from

National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
Telephone: 703-487-4650

The EPA Project Officer can be contacted at

Robert S. Kerr Environmental Research Laboratory
U.S. Environmental Protection Agency
Ada, OK 74820

United States
Environmental Protection Agency
Center for Environmental Research Information
Cincinnati, OH 45268