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**Ground-Water Modeling Issues in Ground-Water Development:
Types of Models/Choosing the Right Model**

by

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**UNCOVERING THE HIDDEN RESOURCE:
GROUND WATER LAW, HYDROLOGY, AND POLICY
IN THE 1990S**

June 15-17, 1992
Boulder, Colorado

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**TYPES OF MODELS (PROS AND CONS)/
CHOOSING THE RIGHT MODEL**

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The Model Application Process

Introduction

The effective application of computer simulation models to field problems is a qualitative procedure, a combination of science and art.

A successful model application requires knowledge of scientific principles, mathematical methods, and site characterization, paired with expert insight into the modeling process. These elements often are provided in a multidisciplinary team framework.

Modeling imposes discipline by forcing all concerned to be explicit on goals, criteria, constraints, relevant processes, and parameter values.

The preparation of an operational model of a groundwater system can be divided into three distinct stages:

- (1) model formulation and input preparation
- (2) model calibration and verification
- (3) problem solving or scenario analysis (sometimes called prediction stage)

Each stage consists of various steps; often, results from a certain step are used as feedback in previous steps, resulting in a rather iterative procedure.

Modeling Objectives

The modeling process is initiated with the formulation of the modeling objectives and modeling scenarios derived from an analysis of the management problem under study. Within this context, compilation, inspection, and interpretation of available data result in a first conceptualization of the system under study.

Often, the technical expert is charged with the task of making sense of an ill-posed problem with a large amount of mostly irrelevant data. It is his/her task to rationalize the ill-posed problem into an unambiguous question that, to be answered, utilizes a subset of the data available together with data specifically collected to solve the problem.

System Conceptualization

Conceptualization of a groundwater system consists of three elements:

- (1) identification of the state of the system;
- (2) determination of the system's active and passive controls;
- (3) analysis of the level of uncertainty in the system.

To identify the *state of the system*, its hydraulic, chemical, thermal, and hydrogeologic characteristics are defined, and conservation of mass, energy, and momentum are quantified.

The *active input* refers to such system controls and constraints as pumpage schedules, artificial recharge, development of new well fields, waste injection rates, and the construction of impermeable barriers, and clay caps and liners.

Passive or uncontrollable inputs include elements of the hydrologic cycle external to the system under study, such as natural recharge and evapotranspiration, subsidence, and natural water quality. Certain contamination sources such as leaching landfills, spills, and the leaching of agricultural chemicals present in soil might also be considered as passive controls. Other passive controls, such as water demand resulting from population growth, may be external management factors.

Many modeling studies found to be inadequate were hampered by deficiencies in the analysis of the problem to be modeled or in the conceptualization of the groundwater system.

Code Selection

Introduction

Based on the objectives of the study and the characteristics of the system, the need for and complexity level of the simulation model must be determined.

Selection of a computer code takes place; if the code is new to the technical staff, they need some time to become familiar with its operational characteristics.

In the model application process, code selection is critical in ensuring an optimal trade-off between effort and result. The result is generally expressed as the expected effectiveness of the modeling effort in terms of forecast accuracy. The effort is ultimately represented by the costs. Such costs should not be considered independently from those of field data acquisition. For a proper assessment of modeling cost, such measures as choice between the development of a new code or the acquisition of an existing code, the implementation, maintenance, and updating of the code, and the development and maintenance of databases, need to be considered. Additional information can be found in Simmons and Cole (1985), Boutwell et al. (1985), Hamilton (1982), Kincaid et al. (1984), and van der Heijde et al. (1988).

Code Selection Process

As code selection is in essence matching a detailed description of the modeling needs with well-defined characteristics of existing models, selecting an appropriate model requires analysis of both the modeling needs and the characteristics of existing models.

Major elements in evaluating modeling needs are:

- (1) formulation of the management objective to be addressed and the level of analysis sought (based among others on the sensitivity of the project for incorrect or imprecise answers or risk involved);
- (2) knowledge of the physical system under study;
- (3) analysis of the constraints in human and material resources available for the study.

To select models efficiently management-oriented criteria need to be developed for evaluating and accepting models. Such a set of scientific and technical criteria should

include:

- Trade-offs between costs of running a model (including data acquisition for the required level of analyses) and accuracy
- A profile of model user and a definition of required user-friendliness
- Accessibility in terms of effort, cost, and restrictions
- Acceptable temporal and spatial scale and level of aggregation.

If different problems must be solved, more than one model might be needed or a model might be used in more than one capacity. In such cases, the model requirements for each of the problems posed have to be clearly defined at the outset of the selection process. To a certain extent this is also true for modeling the same system in different stages of the project. Often, a model is selected in an early stage of a project to assist in problem scoping and system conceptualization. Limitations in time and resources and in data availability might initially force the selection of a "simple" model. Growing understanding of the system and increasing data availability might lead to a need for a succession of models of increasing complexity. In such cases, flexibility of the candidate model or the availability of a set of integrated models of different levels of sophistication might become an important selection criterion.

The major model-oriented criteria in model selection are:

- (1) that the model is suitable for the intended use;
- (2) that the model is reliable;
- (3) that the model can be applied efficiently.

The reliability of a model is defined by the level of quality assurance applied during its development, its verification and field validation, and its acceptance by users. A model's efficiency is determined by the availability of its code and documentation, and its usability, portability, modifiability, and economy with respect to human and computer resources required.

As model credibility is a major problem in model use, special attention should be given in the selection process to ensure the use of qualified models that have undergone adequate review and testing. However, a standardized review and testing procedure has not yet been widely adopted, although various organizations have established their own procedures (e.g. ASTM, ASCE).

Finally, acceptance of a model for decision-support use should be based on technical and

scientific soundness, user friendliness, and legal and administrative considerations.

In selecting a code, its applicability to the management problem studied and its efficiency in solving these problems are important criteria. In evaluating a code's applicability to a problem, a good description of its operating characteristics should be accessible. For a large number of groundwater modeling codes, such information is obtainable from the International Ground Water Modeling Center (IGWMC), which operates a clearinghouse service for information and software pertinent to groundwater modeling.

Although adequate models are available for analysis of most flow-related problems, this is less the case for modeling contaminant transport and other complex processes in the subsurface. For example, computer codes are available for situations that do not require analysis of complex transport mechanisms or chemistry. The use of such programs for groundwater quality assessment is generally restricted to conceptual analysis of pollution problems, to feasibility studies in design and remedial action strategies, and to data acquisition guidance. It should be noted that, considering the uncertainties associated with the parameters of groundwater systems, much progress has been made in determining the probabilities of the arrival of a pollution front rather than the calculation of concentrations.

A perfect match rarely exists between desired characteristics and those of available models. Model selection is partly quantitative and partly qualitative. Many of the selection criteria are subjective or weakly justified, often because there are insufficient data in the selection stage of the project to establish the importance of certain characteristics of the system to be modeled. If a match is hard to obtain, reassessment of these criteria and their relative weight in the selection process is necessary. Hence, model selection is very much an iterative process.

Finally, as model selection is very closely related to system conceptualization and problem solving, "expert systems" systematically integrating system conceptualization and model selection on a problem-oriented basis promise to be valuable tools in the near future.

Code Selection Criteria

Acceptance of a model should be based on technical and scientific soundness, its efficiency, and legal and administrative considerations. A model's efficiency is determined by the availability of its code and documentation, access to user support, and by its usability, portability, modifiability, reliability, and economy. A brief discussion of some of these criteria is given below.

Availability

A model is defined as available if the program code associated with it can be obtained either as source code or as an executable, compiled version or if the program can be accessed easily by potential users. The two major categories of groundwater software are public domain and proprietary software. In the United States, most models developed by federal or state agencies or by universities through funding from such agencies are available without restrictions in their use and distribution, and are therefore considered to be in the public domain. In other countries the situation is often different, with most software having a proprietary status, even if developed with government support or its status is not well-defined. In this case the computer code can be obtained or accessed under certain restrictions of use, duplication, and distribution.

Models developed by consultants and private industry are often proprietary. This may also be true of software developed by some universities and private research institutions. Proprietary codes are in general protected by copyright law. Although the source codes of some models have appeared in publications such as textbooks, and are available on tape or diskette from the publisher, their use and distribution might be restricted by the publication's copyright.

Further restrictions occur when a code includes proprietary third-party software, such as mathematical or graphic subroutines. For public domain codes, such routines are often external and their presence on the host-computer is required to run the program successfully.

Between public domain and proprietary software is a grey area of so-called freeware or user-supported software. Freeware can be copied and distributed freely, but users are encouraged to support this type of software development with a voluntary contribution.

For some codes developed with public funding, distribution restrictions are in force, as might be the case if the software is exported, or when an extensive maintenance and support facility has been created. In the latter case, restrictions are in force to avoid use of non-quality-assured versions, to prevent non-endorsed modification of source code, and to facilitate efficient code update support to a controlled user group.

User Support

If a model user has decided to apply a particular model to a problem, he may encounter technical problems in running the model code on the available computer system. Such a difficulty may result from (1) compatibility problems between the computer on which the model was developed and the model user's computer; (2) coding errors in the original model; and (3) user errors in data input and model operation.

User-related errors can be reduced by becoming more familiar with the model. Here the user benefits from good documentation. If, after careful selection of the model, problems

in implementation or execution of the model occur and the documentation does not provide a solution, the user needs help from someone who knows the code. Such assistance, called model support, cannot replace the need for proper training in model use; requests for support by model developers may assume such extensive proportions that model support becomes a consulting service or an on-the-job training activity. This potentiality is generally recognized by model developers, but not always by model users.

Usability

Various problems can be encountered when a simulation code is implemented on the user's computer system. Such difficulties may arise from hardware incompatibilities or coding of user errors in code installation, data input, or program execution. Programs that facilitate rapid understanding and knowledge of their operational characteristics and which are easy to use are called user-friendly and are defined by their usability. In such programs, emphasis is generally placed on extensive, well-edited documentation, easy input preparation and execution, and on well-structured, informative output. Adequate code support and maintenance also enhance the code's usability.

Portability

Programs that can be easily transferred from one execution environment to another are called portable. To evaluate a program's portability both software and hardware dependency need to be considered. If the program needs to be altered to run in a new computer environment, its modifiability is important.

Modifiability

In the course of a computer program's useful life, the user's experiences and changing management requirements often lead to changes in functional specifications for the software. In addition, scientific developments, changing computing environments, and the persistence of errors make it necessary to modify the program. If software is to be used over a period of time, it must be designed so that it can be continually modified to keep pace with such events. A code that is difficult to modify is called fragile and lacks maintainability. Such difficulties may arise from global, program-wide implications of local changes.

Reliability

A major issue in model use is credibility. A model's credibility is based on its proven reliability and the extent of its use. Model users and managers often have the greatest

confidence in those models most frequently applied. This notion is reinforced if successful applications are peer-reviewed and published. As reliability of a program is related to the localized or terminal failures that can occur because of software errors, it is assumed that most such errors originally present in a widely used program have been detected and corrected. Yet no program is without programming errors, even after a long history of use and updating. Some errors will never be detected and do not or only slightly influence the program's utility. Other errors show up only under exceptional circumstances. Decisions based on the outcome of simulations will be viable only if the models have undergone adequate review and testing. However, relying too much on comprehensive field validation (if present), extensive field testing or frequency of model application may exclude certain well-designed and documented models, even those most efficient for solving the problem at hand.

Extent of Model Use

A model used by a large number of people demonstrates significant user confidence. Extensive use often reflects the model's applicability to different types of groundwater systems and to various management questions. It might also imply that the model is relatively easy to use. Finally, if a model has a large user base, many opportunities exist to discuss particular applications with knowledgeable colleagues.

MODEL CLASSIFICATION

There are various kinds of ground-water models, designed to simulate different types of ground-water systems, and able to compute different variables. To be able to identify the main attributes of a particular model a classification system is needed using standardized, well-defined descriptors. An early effort to classify ground-water models was published by Bachmat et al (1978). This classification approach has been used, modified and expanded by various researchers (Mercer and Faust 1981, Simmons and Cole 1985, van der Heijde et al. 1988, NRC 1990). The classification system presented here has been developed to enable the International Ground Water Modeling Center to systematically describe ground-water models in its computerized information system (see Table 1).

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

Objective-Oriented Classification

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

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

A classification system based on management objectives should include such aspects as

level of resolution required, accuracy accepted, and other technical, scientific, social, and economic objectives. However, in general, it is not practical to develop a classification system based on such management objectives, as these are more easily taken into account in the code selection process than in model characterization.

Another objective-based approach is to analyze the development objectives for the simulation code. One can distinguish between three major development objectives:

- (1) to develop an educational tool (educational code),
- (2) to study quantitatively the fundamental nature of a ground-water system (research codes)
- (3) to develop a code that can be applied routinely to various site-specific problems (general-use code).

Finally, an objective-based classification approach may be based on the variables which can be computed with the model. In this case, the major model types are:

- (1) prediction models designed to predict the system responses, assuming the system parameters and system stresses are known;
- (2) backtracking models, determining system stresses when system parameters are known and the system responses are either known or bounded;
- (3) inverse or parameter estimation models for the evaluation of system parameters when a history of stresses and responses are known.

The most common variables computed by prediction models are hydraulic head, drawdown, pressure, velocity (vector), fluid flux (vector), stream- or pathlines, isochrones, contaminant fronts, contaminant concentration (in both liquid and solid phase), solute flux (vector), temperature, enthalpy, heat flux (vector), optimum location of sources and sinks, location of (saltwater/freshwater) interface, water balance, and chemical mass balance. Backtracking models are used specifically to determine system stresses and boundary conditions (e.g, location and duration of contaminant source release, well-field pumping history, aquifer recharge rates). Inverse models are designed to determine the most likely distribution of system and process parameters (transmissivity, dispersivity, retardation coefficient).

Classification Based on the Nature of the Ground-Water System

The nature of the ground-water system is characterized by the system's hydrogeological framework (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) hydrogeological framework 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. Among others, distinction may be made between various kinds of hydrogeologic conceptualizations or zoning, e.g. saturated zone versus unsaturated zone, a single aquifer system versus a multilayered system of aquifers and aquitards (see Table 1). Another distinction may be 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. 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 multifluid flow occurs when layers of water of distinct density are separated by a relatively small transition zone, a situation often encountered when sea water intrusion occurs. Most flow models are based on a mathematical formulation which considers the hydraulic system parameters as independent field information and hydraulic head and flux as dependent variables. They are used to calculate steady-state distribution or changes in time in the distribution of hydraulic head or fluid pressure, drawdown, rate and direction of flow (e.g., determination of streamlines, particle pathways, velocities, and fluxes), travel times, and the position of interfaces between immiscible fluids (Mercer and Faust 1981, Wang and Anderson 1982, Kinzelbach 1986, Bear and Verruijt 1987). Inverse flow models simulate the flow field to calculate the spatial distribution of unknown system parameters using field information on the dependent variables such as hydraulic head and flux.

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

Hydrogeochemical speciation models represent the first type, as they consist solely of a mathematical description of equilibrium reactions or reaction kinetics (Jenne 1981, Rice

1986). These models, which are general in nature and are used for both ground water and surface water, simulate chemical processes in the liquid phase and sometimes between the liquid and solid phase (precipitation-dissolution; sorption) that regulate the concentration of dissolved constituents. They can be used to identify the effects of temperature, speciation, sorption, and solubility on the concentrations of dissolved constituents (Jenne 1981).

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

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

The inclusion of geochemistry in solute transport models is often based on the assumption that the reaction proceeds instantaneously to equilibrium. Recently, various researchers have become interested in the kinetic approach that incorporates chemical reactions in the transport model. Initially, this inclusion of geochemistry has focused on single reaction such as ion-exchange or sorption for a small number of reacting solutes (Valocchi et al. 1981, Charbeneau 1981).

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

There are three major types of heat transport models in the subsurface: (1) transport through the fluid phase only, (2) transport through the solid phase only, and (3) transport through both the fluid and solid phase of the subsurface. In ground-water modeling we deal primarily with model types 1 and 3. Within each of these two latter groups of models one may distinguish four more types of models: (1) low temperature, single phase heat transport without phase change (e.g. to evaluate heat-pump efficiencies), (2) low temperature, dual phase heat transport with two fluids (water and vapor, e.g. in soils), (3)

low temperature, dual phase heat transport with phase change (freezing/thawing, e.g. for studying frost front propagation in soils), and (4) high-temperature, multi phase (liquid/vapor) heat transport with phase change (steam/water; e.g. for evaluation of geothermal exploration potential). Typical processes incorporated include convection, dispersion, conduction, radiation, evaporation/condensation, and freezing/thawing.

Table 2 lists the most important processes encountered in ground-water systems.

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

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

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

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

Recently, increased interest in such multi-system modeling has been motivated by the need to simulate the flow and chemical transport in systems with complex interaction between the surface water and subsurface water, specifically in wetland systems, in watersheds subject to nonpoint pollution from the use of agricultural chemicals, and in

regional systems where local soil and ground-water pollution contribute to the quality of surface water bodies. To model this type of problem, transport and fate processes are added to the multi-system flow models.

The flow and solute transport models may be embedded in a management model. The hydrologic system is described in terms of objective function(s) and constraints. For ground-water hydraulic management problems, e.g., the objective function is aimed at managing ground-water stresses such as pumping and recharge and the discretized ground-water flow equations are treated as part of the constraint set. The resulting equations are solved through an optimization technique such as linear and quadratic programming (Gorelick 1983, Gorelick et al. 1983, Kaunas and Haines 1985, Wagner and Gorelick 1987).

Classification Based on Mathematical Approaches

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

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

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

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

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

In numerical models, a discrete solution is obtained in both the space and time domains by using numerical approximations of the governing partial differential equation. As a result of these approximations the conservation of mass is not always assured (because of truncation and round off errors) and thus needs to be verified for each application. Spatial and temporal resolution in applying such models is a function of study objectives and availability of data. If the governing equations are nonlinear, linearization often precedes the matrix solution (Remson et al. 1971, Huyakorn and Pinder 1983). Sometimes, solution of nonlinear equations is achieved using nonlinear matrix methods such as predictor-corrector or Gauss-Newton (Gorelick 1985).

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

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

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

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

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GROUND-WATER MODEL CATEGORIES.

1. Objective-based model categories

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

2. Processed-based model categories

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

3. Physical-system-characteristics-based model categories

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

more.....

Table 1 - continued

4. Mathematics

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

TABLE 2. IMPORTANT PROCESSES IN GROUND-WATER MODELING

Flow:

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

Fate:

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

Transport:

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

Phase Transfers:

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

Phase Changes:

- freezing/thawing
- vaporization (evaporation)/condensation

IGWMC CLEARINGHOUSE as a MODEL INFORMATION RESOURCE

IGWMC Mission: Acquire, evaluate store, and transfer ground water modeling information to:

- **ground water modelers and/or hydrologists**
- **federal, state and local agencies and their staff**
- **consultants**
- **researchers**
- **academia**
- **industry**

This Mission is a Response to the:

- **increasing detection of contaminated groundwater systems**
- **increasing scientific knowledge related to the physical, biological and chemical processes occurring in ground water systems**
- **rapid advancements in modeling software, other software, and computer hardware**

IGWMC Clearinghouse Tasks:

- **acquire model information, documentation and code**
- **review and describe each model**
- **enter the information into databases**
- **test models**
- **distribute models**