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COMPUTER SIMULATION MODELS RELEVANT
TO GROUND WATER CONTAMINATION FROM EOR
OR OTHER FLUIDS—STATE-OF-THE-ART

Topical Report

By
Marshall B. Kayser
A. Gene Collins

March 1986

Work Performed Under Contract No. FC22-83FE60149

National Institute for Petroleum and Energy Research
Bartlesville, Oklahoma

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Bartlesville Project Office
U. S. DEPARTMENT OF ENERGY
Bartlesville, Oklahoma

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A. Gene Collins**

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**Prepared for
U.S. Department of Energy
Assistant Secretary for Fossil Energy**

**J. Keith Westhusing, Project Manager
Bartlesville Project Office
Virginia & Cudahy
Bartlesville, OK 74005**

**Prepared by
National Institute for Petroleum and Energy Research
A Division of IIT Research Institute
P.O. Box 2128
Bartlesville, OK 74005**

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TABLE OF CONTENTS

	<u>PAGE</u>
Abstract.....	ii
Introduction.....	1
Contamination from EOR Chemicals.....	3
Reservoir Simulation.....	4
Overview.....	4
Other Models--Petroleum Industry.....	11
Ground Water Modeling.....	13
Overview of Modeling Processes.....	13
Types of Models.....	14
Purposes of Models.....	14
Model Development.....	16
Recent Developments and Ongoing Work.....	21
Summary and Sampling of USGS Modeling Efforts.....	21
Profile Models.....	29
Advection and Dispersion in Modeling Concepts.....	31
Stochastic Modeling.....	33
Modeling Flow in Fractured Porous Media.....	34
Thermal Processes.....	36
Partially Saturated (Unsaturated) Fractured Media.....	40
Unsaturated Zone - Porous Media.....	40
Other Recent Developments.....	47
Ground Water Flow Models.....	47
Transport Models.....	50
Thermal Processes and Transport Models.....	52
Modeling Using Personal Computers.....	54
Techniques of Model Development.....	56
Summary and Conclusions.....	63
References.....	65

ABSTRACT

Ground water contamination is a serious national problem. The use of computers to simulate the behavior of fluids in the subsurface has proliferated extensively over the last decade. Numerical models are being used to solve water supply problems, various kinds of energy production problems, and ground water contamination problems. Modeling techniques have progressed to the point that their accuracy is only limited by the modeller's ability to describe the reservoir in question and the heterogeneities therein. Pursuant to the Task and Milestone Update of Project BE3A, this report summarizes the state of the art of computer simulation models relevant to contamination of ground water by enhanced oil recovery (EOR) chemicals and/or waste fluids.

INTRODUCTION

During the last decade great strides occurred in the numerical simulation of fluid flow in underground reservoirs. The anticipated rewards of increased oil production via EOR led to the development of very sophisticated computer models simulating reservoirs and EOR processes. Recognition of contamination of fresh ground water as a serious problem stimulated efforts by industry and federal and state agencies to numerically simulate the flow and mixing of ground water and contaminants.

Modeling techniques developed by researchers, when combined with EOR chemical degradation data, should make possible accurate predictions of the fate of contaminants. This report summarizes the state of the art of computer simulation models relevant to ground water contamination from EOR chemicals and other waste fluids. The Safe Drinking Water Act of 1974 requires development of minimum requirements to assist in the establishment of effective programs to protect underground sources of drinking water from contamination resulting from the subsurface emplacement of fluids through well injection. Additionally, the Safe Drinking Act states that these requirements not impede the reinjection of brine or other fluids resulting from oil and natural gas production or the injection of fluids used in secondary or tertiary recovery unless drinking water sources would be endangered (148).^{1/}

Title 40 CFR Parts 122, 123, 124, and 146, (the UIC Program) were enacted under the authority of PL 93-523 (147). Title 40 CFR Part 122 defines the regulatory framework of EPA-administered permit programs; title 40 CFR Part 123 describes the elements of an approved state program and criteria for EPA approval of that program; title 40 CFR Part 124 describes the procedures the agency will use for issuing permits under covered programs; and title 40 CFR Part 146 sets forth technical criteria and standards for the UIC (148 149)

Underground injection is defined as the subsurface emplacement of fluids through a well (Title 40, Part 146.03). For purposes of the UIC program, injection wells are classified into five categories based on the nature of the fluids injected. In general they are as follows:

^{1/} Underlined numbers in parentheses refer to items listed in the reference at the end of this report

- Class I - includes industrial and municipal waste disposal wells, other than Class IV wells;
- Class II - wells which involve the underground injection of brine and other fluids brought to the surface in connection with conventional oil or gas production and which may be commingled with hazardous wastes from gas plants which are an integral part of production operations; injection of fluids for enhanced recovery operations, and injection for storage of hydrocarbons which are liquid at standard temperatures and pressure;
- Class III - wells which are used to inject fluids for the extraction of minerals including sulfur, uranium, potash, and salts;
- Class IV - wells used to dispose of hazardous or radioactive wastes into or above a formation which, within one-quarter mile of the well, contain an underground source of drinking water;
- Class V - wells that are used for any other type of injection.

Public Law 98-616 was signed November 8, 1984. It addressed, among other things, the underground injection of hazardous wastes into areas above underground sources of drinking water. In essence it states that the disposal of hazardous waste by underground injection into or above any formation which contains a potential underground source of drinking water (within one-quarter mile of injection well) is banned. Because drinking or potable water can be found in aquifers more than 3000 feet below the land surface in certain geographical areas, detailed geological knowledge is necessary before injecting hazardous wastes.

Major environmental impacts associated with EOR are possible contamination of surface and groundwater, and possible contamination of land. Because many liquid wastes are injected into subsurface reservoirs, they also are considered in this report.

Underground injection of chemical compounds for EOR has been challenged by environmental groups on the grounds that it may cause groundwater pollution if proper precautions are not taken. This means that environmental activists may slow the development and employment of certain EOR technologies if they cannot be defended. Consequently, research must be conducted to develop a better understanding of interactions and compatibilities of reservoir fluids with

injected EOR chemicals and other waste fluids, and the long term fate of these injected fluids.

It is imperative that every possible precaution be taken to protect the purity of groundwater. Current estimates are that: (1) 50 percent of the nation's drinking water comes from groundwater, (2) 75 percent of our cities obtain all or part of their supplies from groundwater, and (3) rural areas are 95 percent dependent upon groundwater. America places tremendous symbolic value on groundwater: "because it comes from a well therefore it must be pure." Unfortunately this no longer is true. The EOR industry also has an economic incentive to prevent groundwater contamination because EOR chemicals that might be lost during injection are costly.

An interesting point is that during 1983 deep well injection accounted for about 80 percent of all wastes disposed, about 5 percent were disposed in landfills, and the remaining 15 percent by other methods. These figures serve to indicate that deep well injection must receive adequate and knowledgeable research to ensure that regulations be realistic.

The major disposal practices utilized at the present time are these:

- o Deep well injection
- o Landfarming
- o Surface impoundment
- o Landfill
- o Solidification

CONTAMINATION FROM EOR CHEMICALS

Royce, et al, (1) developed a method for modeling the transport of EOR chemicals accidentally released into fresh water aquifers. Examples involving hypothetical releases of EOR chemicals at surrogate aquifer sites, based on characteristics of actual aquifers where chemical flooding is done, were used to demonstrate application of this method. They used three examples involving polyacrylamide releases and three involving petroleum sulfonate releases.

They postulated that the injection well passes through a fresh water formation directly above the oil reservoir, wherein the well tubing develops a crack, and a small percentage of the injected fluid leaks undetected directly

into the overlying aquifer for a short period of time. When a leak was discovered, injection was discontinued until the well was repaired. Each example was treated as a slug release by the model.

Five models (2-6) were selected and evaluated and the Random-Walk model developed by Prickett, et al, was chosen because of its ease of application to a wide variety of ground water contamination problems (6). It is written in generalized form and has many subroutine options. An advantage of this is that subroutines can be altered without significant effort, and new subroutines easily added to test different theories of solute transport and behavior.

According to Prickett (6), the Random-Walk model can simulate one- or two-dimensional, steady/non-steady flow and solute transport problems in homogeneous or heterogeneous aquifers. Also, the model can evaluate the impact of time and takes into account advection, dispersion, and chemical reactions. A report is available which provides good documentation and a listing of the code.

Royce, et al (1) concluded that the use of numerical models to simulate groundwater contamination from EOR is possible, however application is highly site specific. Further, these models usually imply simplifications (e.g., constant head; uniform flow; homogeneous, isotropic groundwater flow) which may seriously affect their results. The report stressed the importance of the significant amount of data required to model groundwater systems adequately.

RESERVOIR SIMULATION

OVERVIEW

Few models are available to specifically simulate ground water contamination from EOR chemicals (7). Nevertheless, the need to evaluate production potentials of EOR candidate reservoirs spawned development of sophisticated computer modeling techniques in the petroleum engineering field. Initially, computer reservoir simulation was a major technological advancement because it allowed solution of large sets of finite difference equations describing two- and three-dimensional (2- and 3-D) transient, multiphase flow in a heterogeneous reservoir (8). At first, efforts were largely devoted to two-phase gas/water and three-phase gas/oil/water reservoir problems. The EOR scene of the '70's brought forth the need to characterize

oil displacement as influenced by temperature, reaction kinetics, chemical adsorption and degradation, interfacial tension, and other complex equilibrium phase behavior.

In 1982, Coats (8) described the state of the art of reservoir simulation:

"A simulation model is a set of partial-difference equations requiring numerical solution as opposed to a set of partial differential equations amenable to analytical solution. The reasons for this are: (1) reservoir heterogeneity - variable permeability and porosity and irregular geometry, (2) nonlinearity of relative permeability and capillary pressure vs. saturation relationship; and (3) nonlinearity of fluid PVT properties as functions of pressure, composition, and temperature. The models require high-speed digital computers because of the amount of arithmetic associated with the solutions.

"A simulation model requires three types of input data. First, reservoir description data include (1) overall geometry, (2) grid size specification, (3) permeability, porosity, and elevation for each grid block, and (4) relative permeability and capillary pressure vs. saturation functions or tables. Geological and petrophysical work involving logs and core analyses is necessary for items 1 and 3. Laboratory tests on core samples yield estimates of relative permeability and capillary pressure relationships. Second, fluid PVT properties, such as formation volume factors, solution gas, and viscosities are obtained by laboratory tests. Finally, well locations, perforated intervals, productivity indices (PI's), and rate schedules must be specified.

"Model output or calculated results include spatial fluid pressure and saturation distributions, and producing gas-oil ratio (GOR) and water-oil ratio (WOR) and injection/production rate (for wells on injectivity/productivity) for each well at the end of each time step of the computations. Internal manipulation of these results gives average reservoir pressure and instantaneous rates and cumulative injection/production of oil, gas, and water by well and total field vs. time."

Odeh (9) describes the conceptual simplicity of a simulation model, illustrating the subdivision of a reservoir into a 2- or 3-D network of grid blocks. Basically, the volumetric material balance equation, commonly used in reservoir engineering, is written for each phase in each grid block, forming the model.

Reservoir properties such as permeability and porosity, and fluid properties such as pressure, temperature, and composition, are assumed uniform throughout a given grid block. However, reservoir and fluid properties vary from one block to another; fluid properties for each grid block also vary with time during the simulation period (8).

Different types of models are used to describe different oil recovery mechanisms. According to Coats, the most widely used types are black oil, compositional, thermal, and chemical flood. The four basic recovery mechanisms for recovering oil from reservoirs are: fluid expansion, displacement, gravity drainage, and capillary imbibition, with a fifth mechanism, "oil mobilization," being added to encompass various phenomena that essentially release previously trapped oil.

Coates says: "The black oil model accounts for the four basic mechanisms in simulation of oil recovery by natural depletion or pressure maintenance (e.g., waterflooding). This isothermal model applies to reservoirs containing immiscible water, oil, and gas phases with a simple pressure-dependent solubility of gas in the oil phase. This two-component representation of the hydrocarbon content presumes constant (pressure-independent) oil and gas phase compositions, no volatility of oil in the gas phase, and zero solubility of gas and oil in the water."

Compositional models are used to simulate recovery processes for which the black oil assumption of constant-composition, immiscible gas and oil phases is invalid, as in CO₂ or miscible gas flooding. The compositional model describes reservoir hydrocarbon content as an N-component mixture. Gas/oil phase properties and equilibrium (K-values) are calculated from pressure- and composition-dependent correlations or, more recently, from equations of state (8).

Thermal simulators are used in analyzing steam or *in situ* combustion processes, and include PVT correlations to describe N-component oil and gas

phase properties as functions of pressure, temperature, and composition. Chemical flood simulators, used in polymer, micellar, and alkaline flooding, involve additional complexities associated with partitioning of chemical phases in reservoir fluids.

Although the development of many models for various EOR processes has been fairly successful, Coats asserts that current research points toward the desirable goal of a generalized model applicable to all or most recovery processes (8):

"The general model is a set of N partial difference equations written for each grid block comprising the reservoir. Each equation is simply a mathematical statement of conservation of mass of a specified substance or of conservation of energy. Each substance or component may be present in all phases, distributed according to K -values or distribution coefficients obtained from correlations or an equation of state. With allowance for rock adsorption isotherms, chemical reactions, temperature-, pressure-, and composition-dependence of viscosity, relative permeabilities, and capillary pressure, each of the previously described model types is a subset of a single, general model.

"Note that components (and energy), not phases, are the conserved substances requiring equations in the simulation model. Thus, the number of phases is unrelated to the number of model equations.

"Until recently, simulation models made use of the common five-point difference scheme for area (x - y) interblock, Darcy flow terms in each of the conservation equations. A strong grid-orientation effect was reported by Todd, et al (10) for highly adverse mobility waterfloods and later observed by Coats, et al (11) for pattern steamfloods" (8).

This effect was reduced by the nine-point finite difference formulation of Yanosik and McCracken (12), which is now being utilized in steamflooding and CO_2 miscible flooding where adverse mobility ratios are encountered. A correct formulation for non-square grid networks was also developed (12). Current models generally employ the implicit pressure, explicit saturation

(IMPES) technique with options of increased stability provided by sequential and implicit formulations (8).

A leading example of reservoir simulators in use today is Scientific Software-Intercomp's "Chemflood" model. It is a 3-D, 3-phase chemical flood simulator which comes in two forms: one (CFTE) treats phase equilibria by means of ternary diagrams described in terms of phase envelopes and tie lines, the other (CFNC) by using equilibrium K-values representing the partitioning of a component between two equilibrium phases (13).

Additional program descriptive information is found in the user's manual: "The program provides for considerable flexibility in specifying reservoir geometry. Three coordinate options for use in the finite difference spatial discretization are:

- (1) Cartesian coordinates
- (2) a quarter five-spot conformal map coordinate system, and
- (3) any user specified curvilinear orthogonal coordinate system in the x-y plane.

By means of modification, data, arrays and data tables, permeability and porosity heterogeneities, variable grid block thickness, elevations, permeability barriers, etc., can be easily specified. Irregularly shaped reservoirs are modeled by deleting those finite difference grid blocks outside the reservoir boundaries. By storing quantities only for the remaining active grid blocks, a minimum of the computer storage resources are wasted.

There are two key assumptions involved in the program formulation. First, there is no volume change upon mixing; that is, the volume occupied by a component is the same regardless of the phase in which it is distributed. Second, the fluids and rock are incompressible.

The conservation equation for component i can then be written

$$\phi \frac{\partial N_i}{\partial t} + \nabla \cdot \left(\sum_p \vec{u}_p C_{p_i} - \sum_p \phi S_p K_p \nabla C_{p_i} \right) = q_i \quad (I-1)$$

where N_i is the total volume fraction of species i, C_{p_i} is the volume fraction of species i in phase p, $\vec{u}_p$, S_p , and K_p are velocity, saturation and total diffusivity (both molecular and velocity dispersion) of phase p.

Summing over all species and using the identities $\sum_i N_i = 1$ and $\sum_i C_{p_i} = 1$ results in the overall continuity equation

$$\nabla \cdot (\sum_p \vec{u}_p) = \sum_i q_i \quad (I-2)$$

CHEMFLOOD employs an IMPES solution procedure to solve (I-2) implicitly for pressure with saturations and concentrations dated at the old time level. Equation (I-1) is then solved explicitly to obtain the new total concentration N_i in each grid block. An equilibrium calculation performed for each grid block yields phase concentrations C_{p_i} and saturations S_p . Because of the incompressibility assumption, the pressure solution need be obtained only once per time step and is decoupled from the flash calculation. The explicit treatment of phase saturations and concentrations imposes the usual stability limitations in that grid block throughput per time step must be limited to about one-half grid block pore volume."

According to Fanchi, et al (14), the black oil simulator is the workhorse of modern reservoir engineering, probably the most routinely used of the technically sophisticated programs, yet until recently available only for a substantial fee. A significant achievement was the development of BOAST (14), a 3-D, 3-phase black oil simulator developed under a DOE contract and made available to the public through the DOE Bartlesville Project Office.

Fanchi states,

"The BOAST program simulates isothermal, darcy flow in three dimensions. It assumes reservoir fluids can be described by three fluid phases (oil, gas, and water) of constant composition with physical properties that depend on pressure only. These reservoir fluid approximations are acceptable for a large percentage of the world's oil and gas reservoirs. Consequently, BOAST should have a wide range of applicability. For example, BOAST can simulate oil and/or gas recovery by fluid expansion, displacement, gravity drainage, and capillary imbibition mechanisms. Some of the typical field production problems which can be handled by BOAST include: primary depletion studies, pressure maintenance by water

and/or gas injection, and evaluation of secondary recovery waterflooding and displacement operations.

"Technically, BOAST is a finite-difference, implicit pressure-explicit saturation (IMPES) numerical simulator. It contains both direct (BAND, D4) and iterative (LSOR) solution techniques for solving systems of algebraic equations. The well model in BOAST allows specification of rate or pressure constraints on well performance, and the user is free to add or recomplete wells during the simulation. Included in BOAST is a pressure initialization algorithm, a bubble point tracking scheme, an automatic time step control method, and a material balance check on solution stability. Many user-controlled output options are also available" (14).

Documentation provided includes the derivation of flow equations and their conversion to finite difference form, technical description of the model and the Fortran code, and a user's guide to implement the model in engineering situations.

Recently published (1984-85) is CHEM2D, a 2-D, 3-phase, nine component chemical flood simulator (15). The DOE sponsored the development of the simulator at the University of Texas (16,17), and the modification by Keplinger for public distribution (15). CHEM2D uses a finite-difference, IMPES technique. First, the pressure equation is solved. The new pressures are used to compute Darcy velocities for each phase. Concentrations of each component in each grid block are then computed. Finally, a "flash" calculation is performed to determine how much of each component partitions into each of the three phases. The procedure is repeated as long as the user specifies.

The model can simulate primary depletion, waterfloods, polymer floods, and micellar/polymer floods using heterogeneous linear, areal, or cross-sectional reservoir descriptions. The user may specify well performance as either pressure or rate constrained. Both a constant time step size and a variable time step size based on extrapolation of concentration changes are available as options. One injection well and up to four production wells may be used.

The major physical mechanisms that are modeled include adsorption, capillary trapping, cation exchange, dilution, dispersion, interfacial tension, binary or ternary phase behavior, non-Newtonian polymer rheology, and two phase or three-phase relative permeability. Typical components include water, oil, surfactant, polymer, and three ions (chloride, calcium, and sodium). Components may partition amongst the aqueous, oleic, and microemulsion phases.

It was pointed out that black oil simulation technology is more reliable than chemical flood simulation, thus CHEM2D uses concepts not yet proven by industry experience and may not correctly represent actual chemical flood performance.

OTHER MODELS - PETROLEUM INDUSTRY

Odeh (18) reported a reservoir simulation project, in which seven companies participated, to compare results obtained by black oil simulation technology. The participants, chosen to represent a cross section of solution methods in the industry, were to predict gas/oil production data for a given reservoir over an eight-year period. Since the models are not directly related to groundwater, their descriptions will not be given here. Yet, the reference is worth noting as a good summary of examples of reservoir engineering simulators.

Trimble and McDonald describe WELCOS, a 3-D, 3-phase well coning simulator that couples the well rate equation to the reservoir flow equations (150). The model may be used to obtain the maximum well productivity using a given set of physical conditions and regulatory restraints. It can function as a production or injection well and study any single well behavior. The authors state that it has seen extensive usage in their company and it can be handled relatively easily by inexperienced users to solve difficult problems.

Williamson and Chapplear describe the theoretical background of a well model, which is used by a reservoir simulation system to represent flow within a grid block as it enters or leaves a well (19). It frequently has been noted, they observed, that except in the case of a central well in a problem involving cylindrical coordinates, it is impractical to represent a well with an internal boundary. An alternative procedure which approximately replaces the well boundary by a source function was described. In a companion paper,

the authors describe the installation of a well model in a simulator, including potential problems encountered and possible remedies (20).

Coats (21) developed an implicit, 3-D formulation to simulate compositional-type reservoir problems. The model treats 3-phase flow in Cartesian or cylindrical (r - θ - z) geometries, and has applicability to problems such as depletion or cycling of volatile oil and gas condensate, or miscible flooding operations involving either outright or multi-contact miscibility.

According to Fussell (22), "Compositional reservoir models are a class of phase equilibria models. The equations of these models, and especially those incorporating the Redlich-Kwong equation of state, are highly nonlinear and must be solved by an iterative method. The method of successive substitution commonly is used. This method, however, demonstrates linear convergence and almost always diverges or, at best, demonstrates poor convergence, for conditions where phase equilibria calculations are required near the bubble point, dewpoint, or the critical point. This paper presents a new technique for solving the equations associated with compositional models. This technique incorporates the Redlich-Kwong equation of state and uses minimum variable Newton-Raphson methods to solve the equations. The formulation of the problem allows simultaneous solution of the phase-equilibria and flow equations. Application of this technique gives quadratic convergence near the solution and yields convergent solutions for near critical mixtures. Reordering of the equations minimizes computer storage and execution time."

A 3-D, highly implicit numerical model for simulating steamflooding with distillation or solution gas was discussed by Coats (23). The model uses direct solution to simultaneously solve three and four equations for the dead-oil and 2-component oil cases, respectively. It was believed to be superior to earlier published models with respect to stability and computing time in certain difficult problem areas.

Youngren presented a 3-D, 3-phase *in situ* combustion reservoir simulator that rigorously models fluid flow, heat transfer, and vaporization/condensation (24). The simulator has five components: water, oxygen, nonvolatile oil, and two arbitrary volatile components. It can be used to interpret laboratory results and predict effects of reservoir and operational characteristics on field performance.

Another thermal recovery process simulator was prepared by Crookston, et al (25), to be rigorous but general in nature. Conservation balance equations are employed for oxygen, water, coke, inert gases, light, and heavy hydrocarbon pseudocomponents, and energy.

Coats extended the generality of the previous two models while preserving or reducing the amount of computer time required (26). His simulator for wet or dry, forward or reverse combustion in one, two, or three dimensions allows any number of identities of components. It is implicit in nature and allows any number of chemical reactions and reaction products, with no assumptions regarding degree of oxygen consumption. The generality of the model is evidenced in its range of applicability, from single-component geothermal problems to multicomponent steamflood and *in situ* combustion problems. Myhill (27) modified this simulator, and checked it against laboratory steamflood experimental results. A close match was obtained.

Mayer and Breit reported the use of a caustic flooding simulator in conjunction with the Ranger VII pilot study, Wilmington field, California (28). The simulator, developed to model the alkaline flooding process, can account for injection/production and reservoir flow of up to six different active agents in the aqueous phase. The simulator was based on a general 3-D, 3-phase black oil model developed by Breit (29).

A water and polymer flooding predictive model for use in screening studies and feasibility analysis was developed by Jones, et al (30). Using only a fraction of the computing time of numerical simulators, the model fills the gap between the limited simplified predictive methods and the numerical simulators with their large input requirements and operating expense. To accomplish this, a 2-D cross-sectional model using vertical equilibrium was combined with areal sweep correlations and injectivity functions to give results (oil rate vs. time) suitable for economic analysis. The model still includes most of the factors affecting flood performance, and was validated against simulator, analytical, and field results.

GROUNDWATER MODELING

OVERVIEW OF MODELING PROCESSES

In 1981, Mercer and Faust published Groundwater Modeling, to fill the gap between those who develop models, and those such as managers and hydrologists who have little modeling experience but need to apply the technology to solve groundwater problems (31). The basic concepts of groundwater modeling are shown along with how the various model types can be effectively applied.

A mathematical model of a groundwater system is a set of equations which, subject to certain assumptions, describes the physical processes active in the aquifer. The model may be analytical, in which equations are simplified so that solutions can be obtained analytically; or numerical, in which equations are approximated numerically, resulting in a matrix equation that can be solved on a computer. This is done using finite-difference or finite-element techniques, in which continuous variables are replaced with discrete variables defined at grid blocks or nodes. A continuous differential equation is thus replaced by a number of algebraic equations and generally solved by matrix techniques.

Types of Models

The authors list four general types of groundwater models. Water supply problems are usually described by one equation, usually in terms of hydraulic head. The groundwater flow model handles this type of problem, along with others, such as regional aquifer analyses, near-well performance, and groundwater/surface water interactions. When contamination is involved, one or more additional equations for concentration of chemical species are added, giving a solute transport model. Problems involving waste injection, seawater intrusion, radioactive waste, and groundwater pollution, etc. are solved using this type of model. Heat transport models use similar equations, in terms of temperature, and are used in geothermal, thermal pollution, etc. problems. In cases where land subsidence is involved, a deformation model, combining a groundwater flow model with equations describing deformation, is used. Table 1 summarizes major processes, along with dependent variables and application dependent variations in model development.

Purposes of Models

Purposes for groundwater modeling are many and varied and include the prediction of rates of movement and chemical fates of hazardous or other wastes originating from waste injection or petroleum wells, landfills, or underground repositories; the encroachment rate of salt water in coastal regions due to fresh water withdrawal; geothermal reservoir behavior; aquifer performance due to artificial or natural recharge, leaky confining beds, boundary condition effects, well location and spacing effects and effects of various injection/withdrawal rates; aquifer behavior during sensitivity analysis to determine effects of various interactions or mechanisms proposed to explain observed behavior.

TABLE 1. Major processes with dependent variables and application variations (31)

Major process	Dependent Variable	Application Dependent Variations
Fluid Flow	fluid pressure, hydraulic head, hydraulic potential or drawdown	Porous Media Doubly Porous Media Discrete Fractured Media Single-phase Fluid Two-phase Fluid
Heat Transport	temperature enthalpy or internal energy	Same as for fluid flow plus Convection Conduction Radiation
Solute Transport	concentration	Same as for fluid flow plus Convection Dispersion Chemical Source Terms Nuclide Decay & Daughter Products Adsorption & Desorption Precipitation & Dissolution Complexing
Deformation	strain or strain rate	Elastic Media Plastic Media Visco - Elastic Media Visco - Plastic Media Discrete Fractured Media

Model Development

Continuing (31), data preparation for the groundwater model first involves determining the boundaries of the region to be modeled. The region is then subdivided into a grid, and aquifer parameters and initial data are specified.

Initial estimating of aquifer parameters constitutes the first step in a trial and error procedure known as model calibration or history matching. When the output from the model can satisfactorily match the observed history of the system under study, the model can predict future performance also. Table 2 lists data requirements to be considered for a predictive model (32).

TABLE 2. (32)

I. Physical Framework

A. Groundwater Flow

1. Hydrogeologic map showing areal extent, boundaries, and boundary conditions of all aquifers.
2. Topographic map showing surface-water bodies.
3. Water-table, bedrock-configuration, and saturated-thickness maps.
4. Transmissivity map showing aquifer and boundaries
5. Transmissivity and specific storage map of confining bed
6. Map showing variation in storage coefficient of aquifer
7. Relation of saturated thickness to transmissivity
8. Relation of stream and aquifer (hydraulic connection)

B. Solute Transport (in addition to above)

9. Estimates of the parameters that comprise hydrodynamic dispersion
10. Effective porosity distribution
11. Background information on natural concentration distribution (water quality) in aquifer.
12. Estimates of fluid density variations and relationship of density to concentration.
13. Hydraulic head distributions (used to determine ground-water velocities).
14. Boundary conditions for concentrations.

C. Heat Transport (in addition to above)

15. Estimates of thermal conductivities and specific heats of rock and water.
16. Background information on natural temperature distribution in aquifer, including heat flow measurements.
17. Estimates of fluid density variations and relationships of density and viscosity to temperature.
18. Boundary conditions for temperature.

TABLE 2. (cont'd)

II. Stresses on System

A. Ground-Water Flow

1. Type and extent of recharge areas (irrigated areas, recharge basins, recharge wells, etc.)
2. Surface-water diversions.
3. Ground-water pumpage (distributed in time and space).
4. Stream flow (distributed in time and space).
5. Precipitation

B. Solute Transport (in addition to above)

6. Areal and temporal distribution of water quality in aquifer.
7. Stream flow quality (distribution in time and space).
8. Sources and strengths of pollution.

C. Heat Transport (in addition to above)

9. Areal and temporal distribution of temperature in aquifer.
10. Strengths of heat-sources.

III. Other Factors

Ground-Water Flow and Transport

1. Economic information of water supply.
2. Legal and administrative rules.
3. Environmental factors.
4. Planned changes in water and land use.

In addition, to have confidence in results obtained from simulation work, the correct model must be properly applied to the specific problem at hand. Requirements are: (1) a thorough understanding of model limitations, (2) the accuracy of the match with observed behavior, and (3) knowledge of data reliability and aquifer characteristics.

The major numerical techniques used in groundwater modeling are finite difference (FDM) and finite element methods (FEM). Table 3 summarizes their advantages and disadvantages (31).

In the FDM a partial differential equation is replaced by its finite difference equivalent, derived by making a truncated Taylor series expansion of the function at a given point and solving for the required derivative. A map of the region of interest is divided into a grid. The grid may be mesh-centered or block-centered. Associated with the grids are node points that represent the position at which the solution of the unknown values is obtained. Boundary conditions often determine the type of grid used. The block-centered grid is advantageous in problems where flux is specified across

TABLE 3. Brief summary of important advantages and disadvantages of FDM and FEM (as they are commonly used) (31)

Advantages	Disadvantages
FINITE DIFFERENCE METHOD	
Intuitive basis. Easy data input. Program changes easy.	Low accuracy for some problems. Regular grids.
FINITE-ELEMENT METHOD	
Flexible geometry. High accuracy easily included. Evaluates cross-product terms better.	Mathematical basis is advanced. Difficult data input. Difficult programming.

a boundary; the mesh-centered grid is convenient when head is specified.

The time domain is also discretized into a number of steps to model changes that occur in the aquifer as time passes (33). During each time step, the problem is solved to obtain new values of the dependent parameter. Proceeding from prior time levels to new time levels may be done in two ways. In the explicit scheme, the new values are calculated one at a time by sequential solution of one equation with one unknown. The implicit method calculates all the new values simultaneously by solving an $N \times N$ system of simultaneous linear equations (33). Explicit methods are not generally used in reservoir simulation because of the usually severe restrictions on the time step size. Also, the running time (and expense) is quite substantial, however, the programming effort required to build a simulator in this manner is much less than any other.

Alternatively, a more intuitive approach than the Taylor series technique can be used to obtain the final equations needed. This method considers the fluxes into and out of a finite difference block (34), and is akin to the integrated FDM which utilizes an arbitrary grid dividing the region of interest into smaller 'nodal areas' (35). Regardless of the approach, the result is an algebraic equation for each node in the grid system (31).

According to Mercer and Faust (31), the FEM approximates differential equations by an integral approach. The region is divided into elements, whose shapes are determined by nodes.

The first step in applying the method is to derive an integral representation of the partial differential equation. Two of the more popular ways to do this are (1) the method of weighted residuals, in which one works directly with the differential equation and boundary conditions, and (2) the variational method, where a functional (function of a function) related to the differential equation and boundary conditions is used.

"The next step is to approximate the dependent variables (head, concentration or temperature) in terms of interpolation functions. The interpolation functions are called basis functions, and are chosen to satisfy certain mathematical requirements and for ease of computation. Although any system of independent functions can be chosen as the basis function, piecewise-continuous polynomial sets are often preferred because they are both easily integrated and differentiated. Since the element is usually small, the interpolation function can be sufficiently approximated by a low-order polynomial, for example, linear, quadratic, or cubic.

"Once the basis functions are specified and the grid designed, the integral relationship must be expressed for each element as a function of the coordinates of all node points of the element. Next the values of the integrals are calculated for each element. The values for all elements are combined, including boundary conditions, to yield a system of first-order linear differential equations in time. As previously mentioned, this is approximated using finite-difference techniques to produce a set of algebraic equations. As with finite-difference equations, matrix methods are required for solution (31)."

In general, matrix equations are numerically solved by direct or iterative methods. Direct methods involve a sequence of operations performed only once, providing an exact solution. Iterative methods use successive approximation to improve upon an initial guess at the solution. Convergence and convergence rate are important in these techniques. Table 4 summarizes the methods' advantages and disadvantages (31).

TABLE 4. Advantages and disadvantages of direct and iterative methods (31)

Advantages	Disadvantages
DIRECT METHODS	
Sequence of operations performed only once.	May be inefficient in terms of storage and computation time for large problems.
No initial estimates required.	Can have round-off errors.
No iteration parameters required.	
No tolerance required.	
ITERATIVE METHODS	
Efficient in terms of storage and computation time for large problems.	Requires initial estimates.
	Requires iteration parameters.
	Requires tolerance.
	Matrix must be well conditions.

Serious numerical difficulties may at times be encountered in certain applications. For example, convective-dominated transport problems can sometimes yield unrealistic results, and some nonlinear problems can cause no results at all to be forth coming. Some special techniques have been devised to deal with these situations and are mentioned briefly here. Numerical dispersion (answers that are "smeared out") or oscillartory solutions (e.g. large negative concentrations) can happen in convection-dominated problems. The method of characteristics (36,5) has been used in groundwater applications to solve the solute transport equation and overcome these problems (31). Problems arise from nonlinear differential equations in which there are products and/or derivatives of dependent variables. In unconfined flow problems, the transmissivity is a function of saturated thickness, and consequently, of head. In transport problems, equations are nonlinear when changes in pressure, concentration, or temperature cause changes in density, viscosity or porosity. This causes the matrix equation in the simulator to have a coefficient matrix that is a function of the unknown values, requiring an iterative type procedure. Normally, an initial estimate of the unknowns is made, coefficients calculated, and the matrix equation solved for the unknowns. The solution then becomes the new estimate and the procedure is repeated until the computed values of the unknowns do not change (or change slightly). In situations of severe nonlinearity (unsaturated flow problems

and very thin unconfined aquifers) lack of convergence is a problem. Peaceman (37) discusses techniques to use in these cases.

RECENT DEVELOPMENTS AND ONGOING WORK

SUMMARY AND SAMPLING OF USGS MODELING EFFORTS

The last decade has seen major strides in numerical model development. The remainder of this paper describes these developments, centering on the most recent work. As a backdrop, the following table is excerpted from USGS Circular 737, 1976, which summarizes the status of groundwater modeling in the U.S. Geological Survey (38).

In 1977, Konikow demonstrated the application of a numerical solute transport model to a complex field problem involving contaminant movement in an alluvial aquifer (40). Liquid waste by products from pesticide and chemical warfare manufacture at the Rocky Mountain Arsenal had damaged groundwater and irrigated crops near the South Platte River. The wastes, containing chloride concentrations of several thousand mg/l, originated from disposal into unlined ponds from 1943-1956. The problem was simulated for a 30-year period, 1943-1972, and later during the years 1972-80. A history match based on observed chloride concentrations was developed so that conditions of the aquifer in the 1980's could be predicted. The model used a coupled finite difference solution to the groundwater flow equation with the method-of-characteristics solution to the solute-transport equation. The area modeled was approximately 34 mi², and was subdivided into a grid of blocks measuring 1000 ft on a side. The grid was 25 columns by 38 rows, but only 516 nodes were actually used due to boundary conditions.

Another contaminant in evidence around the Arsenal was diisopropyl-methylphosphonate (DIMP). Robson (1981) developed and calibrated a solute-transport model for DIMP to evaluate (1) the mechanisms and parameters controlling DIMP migration, (2) future concentrations in nearby water wells, and (3) effectiveness of various groundwater barrier configurations in stopping polluted groundwater movement (43). The model included an area of about 90 mi² (230 km²) and assumed that DIMP is conservative. Using the

TABLE 5. - Status of ground-water modeling, U.S. Geological Survey (38)

	Phase of activity				Principal U.S. Geological Survey investigators	Selected references
	Devel- op- men- tal	Veri- fica- tion	Op- era- tion- al	Con- tinued im- prove- ment		
FLOW						
Saturated						
Two-dimensional						
Analytical-----	--	--	X	X	S.S. Papadopoulos, R.L. Cooley.	Cooper (1966), Papadopoulos (1967), Papadopoulos (1966), Cooper and others (1965).
R-C Analog Networks	--	--	X	X	S.M. Longwill	Skibitzke (1960), Patten (1965), Stallman (1963b).
Numerical-						
Finite Difference	--	--	X	X	P.O. Trescott	Trescott (1973), Pinder (1969), Maddock (1970).
Finite element	--	--	X	X	G.F. Pinder, R.L. Cooley	Pinder & Frind(1972)
-Galerkin						Frind & Pinder(1973)
Finite element-	--	--	X	--	R.T. Hurr	Hurr (1972).
Variational						
Three-dimensional						
R-C Analog Networks	--	--	X	X	S.M. Longwill	Skibitzke (1960), Stallman (1963a), Patten (1965),
Numerical (Finite difference)	--	--	X	X	P.C. Trescott	Trescott (1975), Bredehoeft and Pinder (1970).

TABLE 5. - Status of ground-water modeling, U.S. Geological Survey (38), (cont'd)

	Phase of activity			Con- tinued im- prove- ment	Principal U.S. Geological Survey investigators	Selected references
	Devel- op- men- tal	Veri- fica- tion	Op- era- tion- al			
Partly (or entirely) unsaturated						
One-dimensional Analytical ²	--	--	X	--	C.D. Ripple, J. Rubin, T.E.A. Van Hylckama.	Ripple, Rubin, and Van Hylckama (1972), Stallman & Reed (1966).
Numerical-						
Finite difference	--	--	X	X	J. Rubin and C.D. Ripple	Rubin (1967, 1968a).
Finite element-	--	X	--	--	do	
Galerkin						
Two-dimensional						
Numerical-						
Finite difference	--	--	X	X	do	Rubin (1968b).
Cylindrical Region						
Numerical-						
Finite difference-	--	X	--	--	do	Doherty (1972).
Galerkin						
LAND SUBSIDENCE-Induced by ground water extraction						
Analytical	--	--	X	--	F.S. Riley	Riley (1969).
R-C Analog & Analytical	--	--	X	--	D.G. Jorgensen	Jorgensen (1975).
Numerical & Analytical	--	--	X	--	D.C. Helm	Helm (1974, 1975).
COUPLED GROUND WATER-stream systems						
Numerical-Finite	--	X	--	--	G.F. Pinder and S.P. Sauer	Pinder & Sauer (1971)
Difference						
Numerical & Analytical	--	--	X	--	A.F. Moench, V.B. Sauer, M.E. Jennings	Moench Sauer, and Jennings (1974); Lucky and Livingston (1975).

TABLE 5. - Status of ground-water modeling, U.S. Geological Survey (38) (cont'd)

	Phase of activity			Con- tinued im- prove- ment	Principal U.S. Geological Survey investigators	Selected references
	Devel- op- men- tal	Veri- fica- tion	Op- era- tion- al			
COUPLED GROUND WATER-RAINFALL-RUNOFF MODELS - Numerical	--	X	--	--	J.E. Reed and M.S. Bedinger and John Terry.	
COUPLED GROUND WATER-ECONOMIC SYSTEMS- Numerical	--	--	X	X	T.Maddock, III and J.D. Bedinger and John Terry	Bredehoeft and Young (1970), Young and Bredehoeft (1972), Maddock (1972,1973, 1975).
COUPLED FLOW AND TRANSPORT OF CHEMICAL CONSTITUENTS						
Saturated system						
Conservative (or nonconservative trace constituents)						
Uniform density, inorganic						
Two-dimensional						
Analytical	--	--	X	--	A. Ogata	Ogata (1976,1970) Grove (1970).
Numerical- Characteristics	--	--	X	X	L.F. Konifow and J.D. Bredehoeft	Konikow & Bredehoeft (1973, Robertson (1974) Bredehoeft & Pinder (1973).
Finite difference	--	X	--	--	D.B. Grove	
Finite element- Galerkin	--	--	X	X	D.B. Grove, J.Rubin,	Pinder (1973) G.F. Pinder
Finite difference and finite element - Galerkin	--	X	--	--	D.B. Grove	
Variable Density						
Two-dimensional						

TABLE 5. - Status of ground-water modeling, U.S. Geological Survey (38) (cont'd)

	Phase of activity				Principal U.S. Geological Survey investigators	Selected references
	Devel- op- men- tal	Veri- fica- tion	Op- era- tion- al	Con- tinued im- prove- ment		
Analytical ²	--	X	--	--	A. Ogata	Henry (1964).
Analog & Analytical ²	--	--	X	--	G.D. Bennett	Bennett & others (1968)
Numerical	--	--	X	--	G.F. Pinder ¹	Pinder & Cooper
Characteristics						
Finite difference ²	--	X	--	--		(1970), Henry (1964)
Finite element- Galerkin	--	X	--	--	do	Segol, Pinder, & Gray (1975).
Three dimensional						
Numerical-Finite element- Galerkin	--	X	--	--	do	
Nonconservative, major constituents						
Uniform density						
Inorganic constituents (one-dimensional)- Numerical	--	X	--	--	D.B. Grove, W. W. Wood, J. Rubin, and R. V. James.	Rubin & James (1973)
Organic constituents (two-dimensional)- Numerical	X	--	--	--	J.B. Robertson and D. F. Goerlitz.	
Unsaturated						
Nonconservative, Major constituents						
Uniform density, inorganic constituents- Numerical	X	--	--	--	J. Rubin and R.V. James	
COUPLED FLOW AND TRANSPORT OF HEAT						
Single phase (hot water						
Two dimensional						
Numerical-Finite difference	--	X	--	--	C.R. Faust and J.W. Mercer	Faust & Mercer(1976)
Integrated						
Finite difference	--	X	--	--	M.L. Sorey	Sorey (1975).

TABLE 5. - Status of ground-water modeling, U.S. Geological Survey (38) (cont'd)

	Phase of activity				Principal U.S. Geological Survey investigators	Selected references
	Devel- op- men- tal	Veri- fica- tion	Op- era- tion- al	Con- tinued im- prove- ment		
Finite element- Galerkin	--	X	--	--	J.W. Mercer and G.F. Pinder ¹	Mercer, Pinder, & Donaldson (1975); Mercer & Pinder(1975)
Three dimensional Numerical-Finite difference- Galerkin	X	--	--	--	G.F. Pinder ¹	
Two Phase (steam water)						
Two dimensional Numerical-Finite difference	--	X	--	--	C.R. Faust & J.W. Mercer	Faust & Mercer(1976)
Finite element- Galerkin	--	X	--	--	J.W. Mercer & C.R. Faust	Mercer & Faust(1975) Faust & Mercer(1975)
Three dimensional Numerical-Finite element- Galerkin	X	--	--	--	G.F. Pinder ¹	
COUPLED FLOW AND TRANSPORT OF CONSERVATIVE (OR NONCONSERVATIVE TRACE) CONSTITUENTS AND HEAT (SINGLE PHASE)						
Two dimensional Numerical-Finite difference ^{2 3}	--	X	--	-		Henry & Hilleke(1972)
Three dimensional Numerical-Finite difference ³	--	X	--	--	D.B. Grove, S.P. Larson	Intercomp (1976).

¹Part-time investigator with USGS.²Model limited to steady-state conditions.³Model prepared for USGS under contract.

calibrated model, Robson was able to reconstruct the historical movement of DIMP in the aquifer between 1951 and 1975, to estimate DIMP concentrations in the south Platte River resulting from discharge of contaminated groundwater, and to predict future DIMP concentrations under a variety of assumed management alternatives (44).

In additional work concerning the Arsenal, Warner modeled a 2.5 mi² portion of the aquifer in much smaller detail (45). He predicted the impact on DIMP concentration by implementing a variety of interception schemes that incorporated variants of a basic plan that included elements of groundwater withdrawal, a barrier, and reinjection of treated water.

An overall systems-management model is currently in final development under the sponsorship of the U.S. Army. This computer model is expected to provide a valuable management and decision-making tool to aid in evaluating aquifer reclamation alternatives at the Rocky Mountain Arsenal. The model will be composed of numerous modules, including (1) groundwater flow, (2) solute transport, (3) groundwater interception and control, (4) surface-water control, (5) groundwater and surface-water treatment, (6) cost estimation, and (7) report and graphics output. The model will be evaluated and verified using the Rocky Mountain Arsenal as a test case because of the abundance of historical data there. After verification, selected alternatives for contamination control will be modeled with a goal of predicting long-term system responses and costs. If successful, this model will be applied to Installation Restoration programs under way at other locations (44).

Bond, et al (122) published a user's manual for the Variable Thickness Transient (VTT) groundwater flow model. The central thrust of the research was to implement numerical models for description and prediction of surface leachate movement in saturated and partially saturated flow systems in soil beneath Flue Gas Desulfurization (FGD) sludge disposal areas. A subtask of the project was to document the modeling technology to make it generally useful to EPRI and the power companies for evaluation of disposal of wastes and sludges. The model can be used to simulate either confined or unconfined aquifer conditions in either a steady state or transient mode, and can model one, two, or three geologic layers.

Another user's guide, (123) for adsorption and decay modifications to the U.S.G.S. Solute Transport Model, was published by the Nuclear Regulatory Commission in 1982. The models of radioactive decay, linear isotherm, Langmuir isotherm, and the Fruedlich isotherm were developed as well as the basic flow and conservative transport equations for a groundwater system. The report included the theoretical developments, numerical implementations, data input requirements, a listing of the computer code that was written to comply with Fortran 77 standards, sample input and sample output, and a bibliography of selected publications on various aspects of the transport problems.

Rockwell Hanford Operations studied the feasibility of using underground repositories for terminal waste storage (124). Numerical models were developed for specific use in modeling the disposal processes in fractured-porous rock systems. Transport of heat through the water-rock system was modeled in fully coupled manner with groundwater flow. Migration of dissolved nuclides was modeled by accounting for the transport processes of advection, dispersion/diffusion, sorption, and chain decay. A Galerkin finite-element approach was used in conjunction with a Newton-Raphson method to solve the set of governing equations. The numerical models were applied in a parametric sensitivity modeling study to evaluate the basic waste isolation characteristics of the Columbia River basalts beneath the Hanford Site. Simulation results show the time-dependent response of the basalt waste isolation system over long-term periods.

A comprehensive account of numerical modeling efforts in attacking two groundwater problems was given by Merritt of the USGS (120). Industrial, organic liquid waste was injected into permeable limestone of the Floridan aquifer since 1963 at one site and since 1975 at another, raising water levels in the injection zone throughout a large region of northwest Florida. Injection operation data were used for numerical modeling of injection effects in the region. The USGS 2-D flow model of Trescott (4) and the subsurface waste injection program (SWIP) of Intercomp (121) were used to simulate the water-level rises at various monitor wells since 1963. The 2-D flow model was successfully used to simulate the regional flow system and the observed injection zone water level changes at various observation wells. Attempts to incorporate a simulation of waste transport into the SWIP model were not as successful.

Additional reports (125-132) are available describing recent modeling efforts to solve water resource problems. Because they are chiefly water resource papers and not modeling papers, they are not discussed in detail but mentioned for completeness of reference.

Finite-difference models were used to simulate aquifer systems in Parker Valley, Arizona (125), northeastern Florida (126) and Big Sioux, South Dakota (127). Two-dimensional models simulated groundwater flow near Lake Wingra, Wisconsin (128), and Army Creek, Delaware (129), while a multilayer model was used at Satus Creek, Washington (130). Saulnier and Goddard used 3-D, finite difference models to simulate impacts of oil shale mining on groundwater hydrology (131). Maslia and Johnston evaluated hydrologic controls on groundwater flow at Niagara Falls, NY, using a Galerkin finite-element method to solve a saturated-unsaturated flow equation (132).

Profile Models

In a study of degraded groundwater near Barstow, California, Robson (41) investigated the use of a 2-D profile-oriented water-quality model for aquifer simulation. The profile model is oriented in the x-z plane, contrasting with the areal model oriented in the x-y plane. He states, "The program used for this work was developed by Bredehoeft and Pinder (42) and employs an implicit alternating-direction iterative technique to solve the ground-water flow equation coupled with a method of characteristics solution to the mass-transport equation. Although the program was originally written as an areal-oriented (x-y plane) model, the program modifications made in changing the x-y orientations of the program to an x-z orientation were of a supportive nature and did not alter the numerical methods used in the original program" (41).

There are advantages and disadvantages associated with profile models as compared with areal models in groundwater management situations. According to Robson (41):

"An areal water-quality model can be used to simulate areal changes in head and water quality in confined or unconfined aquifers with steady or nonsteady uniform or radial flow systems, but it is not suited to simulation of multiple aquifer systems and cannot simulate the vertical distribution of head and water quality in an aquifer. A profile water-quality model can readily

simulate the vertical distribution of head and water quality in a single aquifer or in a multiple-aquifer system. The model can simulate these aquifers as confined or unconfined aquifers under conditions of steady or nonsteady flow but is not suited to conditions involving radial ground-water flow. The profile model is further limited in that the longitudinal axis of the model must follow a ground-water flow path. Thus, if two or more points in a study area are to be considered in a profile model they must be located on the same ground-water flow path. It is further required that the flow path not be subject to significant changes in location in the aquifer during the time period to be modeled.

"The type of ground-water management practices to be investigated and the form of the model results necessary to make evaluations of the alternative practices play obvious roles in the choice of a model. Management practices that are concerned primarily with areal changes of head or water quality, such as changes in the locations of well fields or areas of natural recharge or discharge, are best considered in an areal model. By contrast, management practices that are concerned primarily with changes in the vertical distribution of head and water quality are best dealt with by use of profile model. Examples of management practices of this type include changes in the location of perforated intervals in pumping wells, changes from surface liquid-waste disposal to injection-well disposal, or evaluating the change in head and water quality in a shallow aquifer owing to pumping-induced leakage of water of differing quality from deeper or shallower aquifers.

"The availability of basic data necessary to define the model parameters also plays an essential role in the choice of a model. Although both the areal and profile models require similar types of parameter data, the parameters for the profile model are generally more difficult to define. Areal model parameters such as areal distributions of hydraulic conductivity, saturated thickness, storage coefficient, recharge and discharge, and water-level and water quality data may often be estimated using the existing

distribution of wells or other land surface data in the model area. In the profile model essentially the same parameters must be defined vertically through the saturated thickness to be modeled. The normal distribution of wells and perforated intervals would seldom be adequate to define the profile model parameters, thus necessitating the installation of additional wells or piezometers. The added time and expense that may be required to estimate the parameters for a profile model limit the applicability of the model to problems in which the changes in vertical distribution of head and water quality are of importance and cannot be adequately simulated by other techniques.

"The possibilities of using the profile model at some later date to evaluate the effects of other ground-water management practices are probably more limited than they would be with an areal model. This stems from the requirement that the profile model be aligned with, and only consider conditions along, a particular ground-water flow path. The chances of a subsequent problem in the study area being located on the flow path considered in the model are considerably less than the chances of the problem being located in the area considered by an areal model. One means of partially alleviating this problem would be to use the profile model in conjunction with an areal model. The combination of these models provides a better simulation of the real-life three-dimensional flow system than does either model separately.

"The calibration techniques needed to assure the accuracy of either an areal or a profile model are virtually the same. Head and water-quality contour maps are well suited to making comparisons between model-generated data and observed data when a continuous trend of change in head and water quality data is being simulated. Hydrographs of head and water quality data are usually more suitable if the model is simulating a period of fluctuating head and water-quality conditions in the aquifer.

"The computer costs for running an areal model are slightly less than for a profile model because it requires smaller core

storage and fewer computations resulting from the more nearly square grid spacing of the model. No significant differences exist between an areal and profile model study in the type of computer required or in the needed expertise of the hydrologist."

Advection and Dispersion in Modeling Concepts

Whereas advection refers to the transport of contaminants at the average groundwater velocity, dispersion, which is analogous to diffusion, denotes the outward spread of a stream or point source of contaminants flowing through the subsurface. In 1984, Gilham, et al (46), proposed an advection-diffusion concept for solute transport in heterogeneous unconsolidated porous media. The authors state that: "In layered permeable deposits with flow predominantly parallel to the bedding, advection causes rapid solute transport in the more permeable layers. As the solute advances more rapidly in these layers, solute mass is continually transferred to the less permeable layers as a result of molecular diffusion due to the concentrations gradient between the layers. The interlayer solute transfer causes the concentration to decline along the permeable layers at the expense of increasing the concentration in the less permeable layers, which produces strongly dispersed concentration profiles in the direction of flow. The key parameters affecting the dispersive capability of the layered system are the diffusion coefficients for the less permeable layers, the thicknesses of the layers, and the hydraulic conductivity contrasts between the layers. Because interlayer solute transfer by transverse molecular diffusion is a time-dependent process, the advection-diffusion concept predicts a rate of longitudinal spreading during the development of dispersion process that is inconsistent with the classical Fickian dispersion model. A second consequence of the solute-storage effect is offered by transverse diffusion into low-permeability layers that is less than the groundwater velocity. Although various lines of evidence are presented in support of the advection-diffusion concept, more work is required to determine the range of geological materials for which it is applicable and to develop mathematical expressions that will make it useful as a predictive tool for application to field cases of contaminant migration."

According to other researchers numerical difficulties occur in simulating advective dispersive contaminant transport where large Peclet numbers are

involved (47). A 2-D Galerkin finite element model for flow and Lagrangian mass transport in porous media was developed. The solution methodology involves a linear triangular mesh which tracks along streamlines calculated from a flow equation using the stream function as the dependent variable. The model was accurate and stable when compared to Eulerian, or fixed coordinate, type models, and required less computational effort.

Neuman and Simpson (48) performed a comparative analysis of numerical approaches to advection/dispersion. Eulerian-Lagrangian methods were thought to be the most promising, because they combine the computational power of the Lagrangian approach with the simplicity of a fixed Eulerian grid.

According to Remer and Carnahan (49), the temporal dependence of processes of mass transfer between fluid and solid phases during transport by moving groundwater can affect concentrations of solutes in ways that are not predictable by methods based solely upon consideration of chemical equilibria. In cases where the chemical reaction at the phase boundaries is either by ion exchange or adsorption, the most generally useful mathematical models for the reaction progress are based upon reversible, second-order reaction kinetics. The approximation of first-order kinetics can be coupled with advective/dispersive transport to obtain a system of linear equations that is capable of being solved analytically.

Coupling of advective/dispersive transport with a reversible, second-order kinetic model of interphase mass transfer, however, produces a system of equations not amenable to analytical solution. It was to this end that NONEQ was developed; a program that numerically solves the solute transport problem when the sorption is governed by a reversible, second-order rate law (50). NONEQ operates in a 3-D, infinite medium with unequal longitudinal and transverse dispersion, to describe a point release of a solute that can be sorbed on a solid phase. The governing transport equation is solved using an alternating-direction-implicit (ADI) method, while finite-difference techniques are applied to the mass conservation equation for solute in the solid phase.

Pickens (39) used a finite element method based on a Galerkin technique to formulate the problem of simulating the two-dimensional transient movement of conservative or nonconservative wastes in a steady state saturated groundwater flow system. The advection-dispersion equation was solved in two ways: in

the conventional Cartesian coordinate system and in a transformed coordinate system involving streamlines and normals to those lines. The two formulations produced identical results. A sensitivity analysis on the dispersion parameter dispersity was performed, establishing its importance in advection-dispersion problems.

Stochastic Modeling

Dagan used stochastic (probabilistic) modeling to study solute transport in a heterogeneous formation in which values for transmissivity and hydraulic conductivity were uncertain (53). The formation properties (hydraulic conductivity and transmissivity) and the flow variables (head, specific discharge, solute concentration) are treated as spatial random variables subjected to uncertainty, rather than deterministic variables. The influence of conditional probability of input variables on the statistical structure of dependent variables was analyzed. The traditional approach of predicting solute concentration by solving deterministic partial differential equations was deemed highly questionable in the case of heterogeneous formations.

Mizell, et al, used spectral analysis and the theory of random functions to analyze 2-D steady groundwater flow in a confined aquifer with spatially variable transmissivity (54). Conditions that insure a stationary head process were derived, and the head covariance function was studied. Multi-dimensional flow analysis resulted in significantly reduced head variance; head variance calculated from the stationary theory agreed with that of previous Monte Carlo simulations. Gutjahr showed that the covariance relationships are exact solutions for the nonlinearized equations no matter how large the input variance (55).

Modeling Flow in Fractured Porous Media

The traditional means of prediction of injection flow rate or well pressure behavior upon injection of fluids into fractured rocks is to use solutions of the general transient equations of fluid flow in porous media (56). Noorishad and Doe used a new coupled hydromechanical finite element technique to simulate more realistic behavior of a deep-lying fracture subjected to fluid injection under constant head and constant flow conditions (56).

A numerical model was developed to simulate mechanical transport under steady flow in a fracture network (57). Mechanical transport is caused by the movement of fluid through the conductive channels of the fracture system, and was the only transport process considered in this model. The model calculates the location of streamtubes in determining the distribution of arrival times for particles traveling from one side of a flow region to another, assuming that fluid flow occurs only with planar fractures in an impermeable rock matrix. The primary use of the model is to determine when a fractured reservoir may be treated as a porous medium, allowing analysis without requiring detailed fracture geometry or simulation of transport within each fracture.

Although numerical models of random 2-D fracture systems have been used to study directional permeability (59), Long, et al, describe the theoretical basis for extending these techniques to three dimensions (58): "A model is developed for three-dimensional fracture systems in which fractures are disks randomly located in space with orientation, radius, and aperture randomly assigned according to given distributions. Intersections between fractures are line segments called nodes. In each fracture, equations for flow between nodes are constructed analytically as a function of the average head at each node. The construction of these equations employs image theory and assumes that each node acts like a source of constant strength per unit line length. Once a set of mass balance equations is solved for the average head at each node, the flux between nodes and through the entire fracture network can be calculated."

Transient analysis can be important in studying groundwater flow in fractured rock because many behavioral patterns that need to be predicted are transient, as are most of the field tests to measure hydrologic properties (62). The objective of such tests is to gain an accurate measurement of the rock's equivalent continuum properties, facilitating numerical simulation. Criteria for defining the equivalent continuum permeability were developed for steady-state conditions (59), but the application of these criteria to the results of large-scale transient well tests has yet to be undertaken.

Since groundwater flow in fractured rock masses occurs primarily within the fractures, one approach to studying this flow is to study the properties of the fracture network. Kanehiro, et al (62) did this by approximating the

fracture system as a network of interconnected parallel plates with apertures identified to provide the appropriate flux under a given gradient. The numerical code, designated FRANET, is a finite element formulation that solves the transient flow equation for a 2-D fracture network. The code uses a Galerkin approach (60). Computational problems associated with transient flow are considerably more difficult than with steady-state flow, and computer storage requirements are greater. Treatment of large fracture networks is quite difficult, and no adequate analytical solutions exist. Thus the code was validated against 1-D problems where analytical solutions do exist, and against the steady-state code LINEL (61). A good match was achieved against the steady-state condition. Currently, chemical and radionuclide transport are being added to the code, considering convection, molecular diffusion, decay, and limited chemical interaction with the rock matrix. The authors (52) believe that the above capabilities will be valuable in the design and analyses of tracer tests and in the study of transport in fractured reservoirs.

At Oak Ridge National Laboratory, Yeh developed a generalized, analytical, transient one-, two-, or three-dimensional computer code (AT123D) for estimating waste transport in groundwater (142). Mechanisms of transport considered are advection, hydrodynamic dispersion, adsorption, decay/degeneration, and waste losses to the atmosphere. The combinations of three dimensions, three kinds of wastes (radioactivity, chemicals, heat), eight sets of source configurations, three kinds of source releases, and four variations of aquifer dimensions give the program 450 options. The author states that there are practically no limitations on the configuration and situation of source releases and types of boundary conditions. The report includes program documentation and examples.

Thermal Processes

Pruess, et al, discussed modeling of geothermal reservoirs, most of which are extensively fractured (63). The fractures provide the principal paths for fluid and heat flow, yet flow between fractures and the rock matrix may also have a profound effect on reservoir behavior. The porous-medium approximation used in most modeling studies of geothermal reservoirs is not generally representative. The multiple interacting continua method (MINC) was developed

based on the different response times of fractures and rock matrix. A generalization of the double porosity method (64), the MINC method partitions the reservoir into sequences of interacting continua, or flow pathways, such as the fracture network and the rock matrix.

The first treatment of the MINC method employed highly idealized regular fracture distributions. Pruess and Karasaki introduced the concept of "proximity function," which provides a convenient way to handle irregular fracture distributions also (65). The function and its first derivative are sufficient to completely define a computational mesh between fractures and rock matrix. A preprocessor program called GMINC employs user-specified proximity functions to transform a "primary" (porous-medium) mesh into a "secondary" mesh containing all partitions necessary for modeling interporosity flow. The output of GMINC is compatible with geothermal simulators SHAFT79 (66) and MULKOM (67).

According to Pruess (67), SHAFT79, until recently, was the workhorse of the reservoir modeling effort at Lawrence Berkeley Laboratory. It was applied to a wide variety of generic, laboratory, and field problems associated with porous medium and fractured medium situations, including thermohydrologic conditions near high-level nuclear waste repositories.

Although SHAFT79 was adopted for distribution by the National Energy Software Center in Argonne, Illinois, and is currently used in over 20 companies and research organizations, the chief limitation of the program is its representation of reservoir fluids as single-component water, neglecting the effects of non-condensable gases and dissolved solids.

Since geofluids are usually mixtures and compositional effects are important in most geothermal reservoirs, a new, much more flexible program was developed that is applicable to a large variety of flow systems. The author's description follows (67):

"MULKOM is an acronym for "multicomponent model," a computer program for simulating the flow of multicomponent, multiphase fluids, and heat in porous or naturally fractured reservoirs. The flow equations solved and the mathematical and numerical methods employed in MULKOM are similar to SHAFT79.

"The numerical approach in MULKOM is based on the integral finite difference method, which permits simulation of one-, two- or three-dimensional reservoir systems with regular or irregular grid blocks and complex topology. The difference equations are formulated fully implicitly. All mass- and energy-balance equations are solved simultaneously, using Newton/Raphson iteration and a direct solution technique. The linear algebra is performed with the Harwell solver MA28, which efficiently handles nonsymmetric matrices with random sparsity structure.

"MULKOM features a modular architecture, with separate modules for (1) initializing simulation problems, (2) representing PVT properties (equation of state) for the desired fluid mixture(s), (3) assembling the nonlinear transport equations, and (4) solving the set of linear equations arising in the iterative solution process for the nonlinear equations. The coding is done in such a way that the number of fluid components to be treated can be provided as a (variable) input parameter. The nature of the fluids and their thermophysical properties are specified by means of equation-of-state modules ("EOS"). The EOS expresses all thermodynamic and thermophysical properties ("secondary parameters") of multicomponent, multiphase fluid mixtures in terms of a set of "primary" dependent variables. For a system with NK components, the number of primary variables (degrees of freedom) is $NK+1$, i.e., there is one variable for each mass component and one variable for the heat "component." The EOS module communicates with the other modules of MULKOM by means of two large arrays. One array contains the latest values of all primary variables for all grid blocks. The other array contains a complete set of secondary parameters for the given primary variables. The physical meaning of the primary variables needs to be specified within the EOS module, but is not needed in the other modules. Therefore, primary variables can be chosen (and changed) in such a way that accuracy and efficiency of the thermophysical property calculations are optimized. This has permitted better absolute and relative accuracy in parameters controlling flow, so that convergence can be obtained for 5-10 times larger steps than

was possible with SHAFT79. Phase transitions can be easily handled by means of variable switching. For example, in simulations for pure water, pressure and temperature are used as primary variables throughout the single phase regions. When a phase transition to two-phase conditions occurs, the second primary variable is "switched" from temperature to vapor saturation. This leads to a very efficient and robust algorithm.

"In assembling the flow equations, only secondary parameters are needed. The array of secondary parameters as provided by the EOS module(s) has a specific structure that enables the transport part of MULKOM to obtain the needed thermophysical properties in definite storage locations, irrespective of the number of fluid components and phases present. It is this peculiar structure of the primary and secondary parameter arrays-and the architecture of the interface for the EOS module-that give MULKOM the flexibility to represent different mixtures of nonreactant fluids (67)."

In related work, Goyal and Narasimhan developed a mathematical model of a fault-controlled geothermal reservoir in which heated water rises through the fault to charge a reservoir overlain by a cap rock (69). The model was considered to be representative of liquid-dominated systems like the one at East Mesa in California's Imperial Valley. According to the authors, "The analysis can be applied to compute the velocity field in an aquifer in response to changes in its permeability or fluid viscosity under a prescribed inlet pressure. Moreover, if the geologic, geophysical, heat flux, and borehole logging data are known, it is possible to calculate the total fluid recharge rate to the geothermal system in addition to other physical parameters of interest.

"The concepts used to generate the model can be tested directly by comparison of the field data and the theoretical prediction. Current measurement techniques provide surface heat flux distributions, downhole temperature, and pressure distributions that can be compared with values obtained in a given model. The temperatures predicted by this model compare favorably in a qualitative sense with those measured in the East Mesa anomaly."

A comprehensive modeling study was done of the Krafla geothermal field in Iceland (70). The study consisted of four tasks: (1) analyzing well test data, (2) modeling the reservoir system in its unexploited state, (3) determining the generating capacity of the different reservoir regions, and (4) predicting well performance on the basis of different exploitation schemes.

A natural state model for the field was developed in which natural mass and heat flows in the reservoir were quantified, and heat and mass recharge to the system (boundary conditions) were established. Several models were developed using MULKOM, the best of which agreed with all Krafla well test data. Pressure profiles, temperature profiles, and steam losses were predicted. Also, a quasi-3D model was developed in which all producing wells were represented individually. A reasonable history match (flow rates and enthalpies) of all wells in the field was obtained. The chief parameters adjusted in doing this were reservoir porosities and permeabilities, and productivity indices for the wells. Using various reservoir management criteria, the future performance of the Krafla field was predicted.

Partially Saturated (Unsaturated) Fractured Media

Very little work has been recorded with respect to partially saturated fractured media (71,72). Lately, however, the disposal of hazardous wastes has directed attention to water movement in the deep unsaturated zones in arid areas, which are characterized by low rates of recharge to the groundwater system.

Many systems of interest for the disposal of high-level radioactive wastes are only partially saturated with water. Narasimhan and Wang (71) are considering the Yucca Mountain area of the Nevada Test Site in ongoing work in the above area. A conceptual model of the system has been devised; a statistical description of a rough-wall, variable aperture fracture is based on averaging the aperture distribution function over the fracture plane. Capillary theory and the cubic law for fracture flow were generalized to derive theoretical formulas for fracture saturation, conductivity, and effective fracture flow area. The formulas were evaluated for Yucca Mountain rock using the available matrix and fracture data: relative permeability,

density, fracture frequency, fracture surface coating, *in situ* conductivity, and matrix-saturated conductivity characteristic curve.

Unsaturated Zone - Porous Media

More common is research dealing with the unsaturated (vadose) zone when fractures are not considered. The need to dispose of radioactive wastes is primarily responsible for increased modeling efforts in this area. Proposed regulations would require disposal in the unsaturated zone above the fluctuations of the water table unless it can be conclusively demonstrated that diffusion would be the predominant mechanism of transport at the site (73).

In 1982, Oster conducted an extensive literature search along with correspondence with experts in the field, to determine computer models suitable for studying low-level radioactive waste disposal in the unsaturated zone (73). Fifty-five models were identified as being potentially useful, with ten chosen for further examination based on quality of documentation, variety of applications, and code availability. Table 6 summarizes the models according to type (flow, transport, or flow-transport).

Reisenauer and Narasimhan developed the model TRUST to study fluid flow problems arising in variably saturated porous media involving complicated geometry (74). Based on the original code TRUMP, by Edwards (75), it uses an integrated finite difference algorithm for numerically solving the governing equations. A mixed explicit-implicit numerical procedure internally controls the time step, providing a control of the potential numerical instabilities which could arise. Simulation may be done in one, two, or three dimensions. The following quote (73) enumerates uses for the model: "TRUST has the capabilities for treating the wetting-drying front problem which appears in arid regions where many potential low level waste repository sites occur. In addition, the following list enumerates some of the problems which have been solved in the past using TRUST: settlement and consolidation in soft-clay systems under constant or variable loads; deformation of organic soils undergoing drainage and desaturation; simulation of drainage and infiltration in variably saturated columns, ditches and sand boxes; slug tests, constant rate or constant drawdown well-tests in porous media with single or multiple-

fractures; internal drainage into mines expanding with time; response of aquifer-well system of earthquakes or earth tides."

At the U.S. Geological Survey, Lappala (76) developed VS2D (variably saturated, 2-D), a code to simulate multidimensional movement of liquid water in variably saturated porous media. To predict the fate of the pollutants on land or buried above the zone of permanent saturation, VS2D was designed to handle the "difficult" nonlinear problems caused by infiltration into dry soils, anisotropy, and discontinuities in permeability and porosity. "This capability is met by using finite differences to discretize spatial and temporal domains. Adequate solutions of nonlinear equations using finite elements discretization in space require such numerical tricks as lumping the capacity (storage) term over each element. The upstream weighting of relative hydraulic conductivities that may be required to prevent numerical oscillations is more difficult with finite elements than with finite differences. Finally, algebraic equations resulting from a finite-element

TABLE 6a. Flow Code Summary (73)

Code		Spatial Characteristics							Special Features	Past Applications	Principal Contact	Comments	
Name	No.	Dimensions			Discretization Method								
		1	2	3	FDM	IFDM	FEM	Other					
AMOCO	37			X	X				Three-phase oil, water, gas	Oil reservoir	AMOCO	Proprietary Code	
ALPURS	21			X	X						Mobil Corp.	Proprietary Code	
BETA-II	40			X	X					Oil reservoir	Intercomp.	Proprietary Code	
BRUTSAERT1	33		X		X					Experimental	Brutsaert		
BRUTSAERT2	39		X		X					Experimental/Laboratory	Brutsaert		
CMG	38			X	X				Two-phase oil & gas Roots, evapotranspiration	Oil reservoir	CMG	Proprietary Code	
COOK	29		X							Oil reservoir	Cook	Proprietary Code	
DELAAT	48		X				X			Ground-water extraction	De Laat	European Code	
FEMWATER	24		X				X			crop production		Yeh	
FLUMP	5		X				X					Narasimhan	
GRANDALF	30		X		X				Underground nuclear explosions		Morrison		
GPSIM	31			X	X							Exxon	Proprietary Code
MOMOLS	52	X			X					Experimental	Rojstoczer		
PORES	49			X	X					Oil reservoir	UKAEA	European Code	
REEVES-DUGUID	22		X				X			Radioactive decay		Reeves	
SHELL	42			X	X				Oil reservoir		Shell Oil Co.	Proprietary Code	
SSC	41			X						Oil reservoir	SSC	Proprietary Code	
STGWT/MOGWT	27	X			X						de Smedt	European Code	
SUM2	46		X				X			Roots, evapotranspiration	De Laat	European Code	
SUPERMOCK	47		X		X					Roots	Reed		
TRACR3D	55			X		X			1- or 2-phase flow with tracer in either phase (air or water) Freundlich, Langmuir sorption, radioactive decay, capillary effects 3-member decay chain	Tracer flow in unsat. conditions, Radionuclide transport, Tracer flow in fractured system	Travis	Can operate in 1, 2 or 3 dimensions	
TRIPM	51		X				X			Radioactive waste disposal	Gureghian		
TRUST	4			X			X				Narasimhan		
TS&E	32			X						Oil reservoir	Tech. Soft. & Eng.	Proprietary Code	
UNFLOW	7		X				X			Radioactive waste disposal	Pickens		
UNSAT1	28	X					X		Roots, evapotranspiration Roots		van Genuchten		
UNSAT1D	10	X			X					Crop studies	Bond		
UNSAT2	26		X				X			Engineering design	Neuman		
VERGE	8			X			X			Radioactive waste storage	Verge		
VS2D	45		X		X					Roots, evapotranspiration	Lappala		
WAFE	50		X			X			Coupled heat & 2-phase mass transport (air vapor & liquid) Accurate treatment of H ₂ O Separate velocity field phase	Confined underground radioactive waste disposal, In-situ fossil energy recovery studies, 2-phase flow and tracer studies	Travis	Can operate in 1 or 2 dimensions	

KEY: FDM = finite difference method.
 IFDM = integrated finite difference method.
 FEM = finite element method.

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TABLE.6b Transport Code Summary (73)

Code		Spatial Characteristics							Special Features	Past Applications	Principal Contact	Comments
		Dimensions			Discretization Method							
Name	No.	1	2	3	FDM	IFDM	FEM	Other				
BACHMAT	6	X			X				Surface/ground water Absorption & decay	Backmat	Middle-east Code	
DUGUID-REEVES	19		X				X			Duguid	Compatible with Code No. 22	
FECTRA	17		X				X		1st-order decay, sorption	Baca	Compatible with Code No. 22	
FEMWASTE	25		X				X			Yeh		
MLTRAN	54		X				X			Reisenauer	Compatible with Code No. 44	
MMT-DPRW	44		X					X	Ground-water studies	Simmons	Discrete Parcel Random Walk	
SCAT1D	35	X			X					Stochastic velocity field	Oster	Stochastic Code
SCAT2D	36		X		X				Stochastic velocity field	Oster	Stochastic Code	
TRNMDL	2	X			X					Av-Ron	Middle-east Code	

KEY: FDM = finite difference method.
 IFDM = integrated finite difference method.
 FEM = finite element method.

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TABLE 6c Flow-Transport Code Summary (73)

Code		Spatial Characteristics							Special Features	Past Applications	Principal Contact	Comments
		Dimensions			Discretization Method							
Name	No.	1	2	3	FDM	IFDM	FEM	Other				
HANKS	1	X			X				Roots	Crop production studies	Hanks	
MARINO	53			X			X		1st-order reactions		Marino	
MCCANN	20		X		X				Heat transfer		McCann	
MOBIDIC	14		X		X				Roots		Couchat	European Code
NMODEL		X			X						Selim	
SEGOL	9			X			X				Segol	
SHAMTU	43	X			X					Water loss by evaporation	Vaucelin	European Code
SUMATRA-1	11	X					X		0- & 1st-order decay		van Genuchten	
TARGET	18			X		X			Heat transfer, elegant numerical solution. 0- & 1st-order decay. Variable saturation. Radio-active decay products	Tailings and chemical waste disposal, radio-active waste disposal	Dames & Moore	Proprietary Code
TRANS	23		X				X				Walker	
TRANSONE	12	X					X				van Genuchten	
TRANS TWO	13		X		X						Shapiro	
UNFLW	3	X			X						Kapuler	
WATSOL	16	X			X					Salinity studies	Gaudet	European Code
WHC	34			X				X			Crooks	Integrated Compartment Method

KEY: FDM = finite difference method.
 IFDM = integrated finite difference method.
 FEM = finite element method.

spatial discretization scheme generally require more computer core storage and time to solve than those resulting from a finite difference scheme. General nonlinear source-sink terms are included to account for stresses, such as evapotranspiration" (73).

A common use for unsaturated zone models is the study of water movement in soils, plants, and into the atmosphere. Neuman, et. al. (77) wrote UNSAT2 (unsaturated 2-D) to investigate these types of problems. UNSAT1D was developed to simulate 1-D flow through a partially saturated flow system (81). It is a fully implicit finite difference model which simulates seepage, infiltration, and uptake by plant roots as a function of the hydraulic properties of the soil, soil layering, root growth characteristics, evapotranspiration rates, and frequency, rate, and amount of irrigation.

A finite-element model simulating water flow through saturated-unsaturated media, FEMWATER is capable of performing a 2-D simulation of an aquifer system (78). The response of the groundwater basin to rainfall, artificial withdrawal, and other recharge or discharge systems such as lakes and streams may be considered. FEMWATER produces not only a continuous pressure distribution, but also a continuous velocity field. This may be used as input to the companion program FEMWASTE, a finite element model simulating solute transport in saturated-unsaturated media. Transport mechanisms in FEMWASTE include: advection, hydrodynamic dispersion, chemical sorption, and first-order decay (79). The model is an extension of the 1976 work of Duguid and Reeves (80), in which the distribution of the pollutant constituent is obtained from mass balance equations.

SEGOL is a 3-D flow/transport code for variably saturated flow systems (82). Oster describes it in the following manner:

"The Galerkin-finite element method is used to obtain the approximate sets of governing equations. Advantage is taken of the banded nature of the arrays in using out-of-core equation solvers to reduce the computer storage requirements. A two-dimensional model is available, which is identical in all respects to the three-dimensional model except that the third dimension is discarded and that the solution is performed entirely in core. The two-dimensional model may be used to check, if necessary, the results obtained with the three-dimensional code in a case where

the third dimension may be irrelevant; it also provides the user with a means to quantify the importance of the three-dimensional nature of a particular problem and to decide whether or not the more expensive three-dimensional analysis is justified" (73).

Sharma developed an integrated finite difference model of groundwater flow and effluent transport under transient conditions (83). The model can account for heat transfer and decay of reacting chemical species being transported by the groundwater. It is capable of performing 3-D simulations of transient flow through variably saturated, multilayered soils. The code, known as TARGET, is proprietary, and is owned by Dames & Moore, Golden, Colorado.

A code known as SUMATRA-1 was devised by van Genuchten (84) to simulate the simultaneous flow of water and solute in a 1-D vertical soil profile under transient unsaturated/saturated conditions. It is based on a 'Hermitian,' or cubic, finite element solution of the governing transport equations, and includes such processes as linear equilibrium adsorption and zero- and first-order decay.

Reisenauer, et al (85) developed a non-dispersive kinetic transport model of 2-D transport of dissolved contaminants through mine tailings, pit linings, and layered geological sediments. Known as MLTRAN, it was designed to work in conjunction with the flow code TRUST (74). The program uses the fluxes defined by TRUST along with media properties and grid configurations to calculate pathlines, fronts, and contaminant movement. One- or 2-D geometries may be used. The model was specifically designed to study worst case situations of low level waste storage sites where the media is unsaturated.

Persistent difficulties that arise in forming numerical solutions of variably saturated flow problems include controlling the stability of nonlinear equation solvers, and devising a reliable and efficient method for determining the positions of seepage surfaces. Cooley (98) used a subdomain finite-element discretization of the governing flow equations to address these problems. According to the report, the subdomain finite element method used produces accurate results, and has an added advantage over finite difference methods of accomplishing a greater amount of nodal averaging of troublesome nonlinear quantities to improve stability. New procedures for solving the nonlinear matrix equation that results from the finite element method and for

locating the positions of seepage faces are capable of solving a wide variety of variable saturated flow problems.

OTHER RECENT DEVELOPMENTS

Groundwater Flow Models

The Pearl Harbor aquifer, an important groundwater resource for Oahu, Hawaii, contains an enormous fresh water lens, up to 1000 ft thick, floating above saline water (86). To facilitate management of the aquifer, a finite difference flow model was used to simulate the aquifer system. The model was calibrated by simulating the lens' response to actual historical pumping patterns over the prior 100 years. According to the authors, simulated heads compared favorably with observed heads over time and space (86).

In similar work in Hawaii, Eyre (87) reported that groundwater flow and effects of future water development were simulated using AQUIFEM (88), a 2-D finite element flow model. The model was modified to account for a sea-water/fresh-water interface, as above, and accurately simulated observed heads averaged over several years.

To obtain simulations of seasonal or annual fluctuations in the water table that also correctly locate the depth to the fresh-water/salt-water interface, a model is required that simulates vertical flow as well as the interaction between the freshwater and salt-water flow fields (87). SUTRA, a solute transport and density-dependent flow model developed by Voss (89) is being tested on a cross section of the Pearl Harbor aquifer on Oahu and will be able to produce more detailed simulations in the near future. Profile models that simulate the flow of both the fresh and salt water - for example, Mercer, Larson, and Faust (90) allow the lens to be in disequilibrium and may provide improved simulations of the detailed behavior of the lens.

Other work pertinent to saltwater intrusion was done at Clemson University by Anand and Pandit (100). A Galerkin 2-D finite element model was developed, in which the coupled governing equations were nondimensionalized and solved for a saturated aquifer in the vertical plane using an iterative solution procedure. The selection of an appropriate mesh, region, and time step size was found to be quite important to obtain correct solutions in saltwater intrusion problems. Saltwater intrusion was shown to be primarily a function

of the ratio of aquifer depth to the longitudinal dispersivity of the medium, and of gradient of the piezometric surface.

Neuman, et al (91) presented a quasi three-dimensional finite element model for the analysis of groundwater flow and land subsidence due to pumpage in multiaquifer systems. In the model, aquifers are simulated with the aid of two-dimensional horizontal finite element grids. Each aquifer is connected to its neighbors above and below by one-dimensional vertical finite element strings which allow leakage across aquitards and aquicludes. Land subsidence is modeled by varying the void ratio of each vertical element according to nonlinear version of Terzaghi's one-dimensional consolidation theory. A major feature of the new method is its ability to solve the finite element equations explicitly in one part of the mesh and implicitly in another part, depending on the ratio between the stability limit of each node and any given time step size. Since the hydraulic diffusivity of aquitards is usually very small compared to that of aquifers, it is often possible to solve the finite element equations explicitly for most, and sometimes all, aquitard nodes. This leads to a virtual decoupling of the aquifer equations during a given time step, which results in a significant saving of computer time and storage.

Often, the most successful models become cornerstones on which improvements and modifications are continually made. Within the USGS, Leahy (92) modified the Trescott (4) groundwater flow program to (1) treat aquifer and confining bed pinchouts more realistically, and (2) reduce computer memory requirements for input data. Torak (93) described modifications of previous USGS modeling efforts (40,41,42) in 3-D, finite difference simulation of groundwater flow. These modifications extend the application of this model to simulations involving head-dependent sources and sinks (i.e., rivers, evapotranspiration, and springs or drains). Other modifications were made that enhance the iterative-solution process of the Strongly Implicit Procedures (SIP). An acceleration (or dampening) factor was introduced to the matrix equation that is to be solved, and optional methods of computing iteration parameters were incorporated into the original model.

The model was used as a management tool to evaluate effects of pumping variations on the "2000 ft sand" of the Miocene aquifer, Baton Rouge, La., in which the potentiometric surface has receded 430 ft over the last sixty years (94). The parameter-estimation program aided verification of the model over this time period.

Saline water, believed to originate from early oil and gas development, is degrading the quality of the Equus Beds aquifer near Wichita, Kansas (95). A calibrated model was necessary to predict where and how fast the brine plume would travel. To obtain this, multiple regression analysis was used for parameter estimation of the steady-state groundwater flow equation applied to the aquifer. Chloride transport was also modeled, giving a satisfactory history match dating from the 1940's. A correlation coefficient of .992 was obtained between calculated and observed values of hydraulic heads.

Tharp developed an "enriched" finite-element model to simulate a well or drain in 2-D fluid flow through porous media (96). The enriched four-node element simulates the logarithmic head distribution about a well located at its center. It is compatible with unenriched elements at its boundaries and can represent head boundary conditions in the well. It is most accurate where the ratio of element diameter to well diameter is large.

The finite element method with a 4-node "linear quadrilateral isoparametric" surface element was used for analysis of square aquifers containing pumped wells (97). Comparisons with the finite-difference method were made; a wide range of time steps were used. FEM results for aquifer storativity and pumped-well draw agreed well with analytical results and FDM results for small time increments.

Nonhomogeneous and anisotropic unconfined aquifers with pumping wells and/or artificial recharge and of various type of boundary conditions were considered (99). A governing equation was formulated in terms of the finite-element process using the Galerkin approach and triangular elements in the x-y plane. The area, number and kind of triangles chosen depend on the shape and the area of the wells, rivers, or lakes; on the nonhomogeneity and anisotropy of the aquifer and on the slopes; and on the changes of free groundwater surface. The continuous time Galerkin approximation is used for the time dimension. The obtained nonlinear system of algebraic equations is solved by a predictor-corrector approximation and the authors concluded that, "From the

numerical examples of the paper it is shown that any shape of boundary with any conditions can be introduced very easily in the mathematical model and many problems of pumping and/or recharging can be solved. In addition, the anisotropy of the aquifers can be handled with no difficulties. Nonhomogeneous aquifers can be solved by dividing the solution region into homogeneous triangles. It is mentioned that in every element the hydraulic conductivity may be a known function of time.

Results obtained with different time steps have small differences. The errors depend on the shape and the area of the triangular elements. Clearly, we ought to use not obtuse-angled but acute-angled triangles, with angles of $\approx 60^\circ$. Finally it is found that, if the size of the triangles is sufficiently small, the results could be higher order of accuracy, as it can be proved theoretically."

Transport Models

Garavedian and Konikow (101) described a front-tracking finite difference model that simulates the convective transport of water or tracer particles through porous media. Applied to 1-D or 2-D steady-state or transient flow problems, the model tracks representative water or tracer particles as they move in response to the groundwater velocity field. Aquifer properties may be both anisotropic and nonhomogeneous. Program listing, input formats, and test problem results are included in the report.

The numerical model CHEMTRN was developed at Lawrence Berkeley Laboratory to provide (a) a better understanding of chemical processes important during the transport of radionuclides away from a repository, and (b) a comprehensive model of chemical transport in porous media (102). An extension of other work (103-105), it is based on a one-step procedure that consists of solving simultaneously a system of equations describing aqueous-phase chemical reactions and convective-dispersive transport with instantaneous mass transfer. The transport equations are finite-differenced in space to produce a set of ordinary differential equations in time. These equations are then combined with mass action equations, solubility products, and a site constraint equation to give a set of differential/algebraic equations solved by a Newton-Raphson iteration technique. The program includes many of the chemical mechanisms important in transport modeling with emphasis on nuclear

waste repositories. It was used to model precipitation, water dissociation, aqueous phase complexation, and sorption via ion exchange or surface complexation and was validated against known analytical solutions and field test results.

To simulate neutralization and contaminant migration in groundwater beneath uranium mill tailings piles, Narasimhan developed DYNAMIX, a program for multiple species chemical transport with precipitation and dissolution (106). According to the author,

"Precipitation and dissolution occur when fluids of dissimilar composition mix with each other. The chemical reactions controlling these processes are governed by pH, redox potential, and the mineral phases that coexist with the aqueous phases. The pH and the redox potential, in turn, are governed by the chemical interactions between the many chemical species that participate in the reactions.

Parkhurst, et al [(107)] developed a computer program called PHREEQE for geochemical calculations at relatively low temperatures which considers an electrolyte of many dissolved species. On the basis of aqueous ion-pairing, it calculates pH and redox potential. Using theoretical volumes and compositions, PHREEQE can simulate mixing of two solutions in the presence of prescribed mineral species and compute the composition of the resulting mixture and postulate which species were dissolved and/or precipitated.

Whereas the PHREEQE program simulates the mixing process, the overall groundwater transport problem also requires the transport of the dissolved species through advective, dispersive, diffusive, and decay processes, with or without adsorption. This transport capability is available with the computer program TRUMP [(75)], which analyzes the transport of a single chemical species. Because precipitation and dissolution require consideration of several chemical species, program DYNAMIX was developed by extending TRUMP to handle the transport of 10 chemical species and coupling it with PHREEQE. The preliminary version of DYNAMIX has been tested and found to reasonably simulate the dilution front

migrating downward within the tailings as a result of the long-term infiltration of rain water" (106).

Thermal Processes and Transport Models

Although much progress has been made in geothermal simulation, difficulties still exist in modeling the injection of cold water into hot two phase fluids. Numerical modeling of injection under these conditions is difficult because it involves movement of "sharp" fronts (thermal, chemical, hydrodynamic) making volume averaging techniques questionable (108). Conventional geothermal reservoir simulation techniques partition a flow domain into a number of discrete volume elements and compute fluid and heat flow between elements from differences in average thermodynamic conditions producing "spurious" (unphysical) flows in injection problems (109). When cold water is introduced into a hot two-phase fluid, the average temperature declines. Under two-phase conditions, there is one-to-one correspondence between temperatures and pressures, so that pressures also decline, causing a spurious flow of reservoir fluid toward the injection well.

Pruess described the occurrence of spurious flows and used a front-tracking modeling technique to overcome the associated errors (108):

"Spurious flows occur only when the hydrodynamic front, which separates single-phase liquid near the injection well from two-phase reservoir fluids, and the thermal front between hot and cold fluids reside in the same volume element. The thermal front is retarded in comparison to the hydrodynamic front by heat transfer from the reservoir rock. In a radial flow problem, the distance between hydrodynamic and thermal front will increase with time, and will eventually exceed the dimensions of the volume elements used in the computational mesh. Therefore, as was shown by Schroeder, et al (1982), the spurious flows disappear after some time, so that the associated error can be controlled.

"Unfortunately, such a "self-correction" of spurious flows will not in general take place when injection into thick two-phase or steam zones is considered where significant vertical flows occur. Numerical simulation has been used to verify that, near the top of the injection zone, the distance between hydrodynamic

and thermal fronts can remain small, so that persistent spurious flows can be minimized only at the expense of introducing many very small grid blocks.

"A formulation of the heat- and mass-transfer problem has been developed that avoids spurious flows altogether. This is accomplished by "front tracking": The coordinates of the hydrodynamic front are introduced explicitly as dependent variables of the problem and are treated on an equal footing with thermodynamic variables in volume elements. Grid blocks containing a piece of the hydrodynamic front are assigned two sets of thermodynamic averages, referring to conditions behind and ahead of the front, respectively. No volume averaging is performed across the front. To fix the location of the hydrodynamic front, additional equations for front coordinates must be introduced and appended to the set of mass- and energy-balance equations for grid blocks. Because pressures are continuous across the hydrodynamic front, these additional equations can be written in the form of pressure constraints. Thus a consistent set of equations for all thermodynamic and frontal "coordinates" has been obtained that is well suited for implementation in existing geothermal simulators."

At times heat transfer, fluid flow, rock deformation, and chemical reactions and transport are simultaneously involved in a groundwater problem. This is the case when a fractured rock nuclear waste repository is considered. Although the interdependence of the different processes is generally recognized, they are often modeled individually and equation coupling is neglected or approximated. Tsang, et al, discussed the importance of coupling the above processes in numerical modeling (110). They stated that a coupled model can determine the limits of validity of uncoupled models, determine parameter sensitivity, design field tests and repository structures, and provide a good tool for waste thermal impact. Very little progress has been made until recently in coupling more than two of the processes. The report (110) summarized an investigation of the three-way coupling of heat transfer, fluid flow, and mechanical deformation.

In addition, they stated that, "The coupling of the fluid pressure field and rock mechanical deformation is founded on the extension of Biot's

consolidation theory (111) for porous elastic media to nonlinear fracture behavior (56). The temperature field is coupled to fluid flow through convection, and to the stress-strain field through the thermal expansion of rock. The governing equations for pressure, temperature, and rock displacement are derived from the conservation laws of mass and energy, the Darcy fluid-flow law, and the law of static equilibrium. A direct-solution numerical procedure has been developed that involves a variational finite element formulation and a Galerkin integral to produce a set of three matrix equations. In this approach, the equations of static equilibrium and fluid flow appear in an implicitly coupled form, and the energy equation is explicitly coupled to these equations. A predictor-corrector scheme is used to obtain the time-marching solution of the implicitly coupled equations. The energy equation uses a Crank-Nicholson step-by-step procedure, with the solution of each time step being sought in the middle of the interval. With time discretization, the final matrix equations are solved by a two-step interlacing scheme" (110).

Another usage of the geothermal simulator MULKOM (67), is in resistivity modeling. Surface resistivity measurements are successfully employed in geothermal exploration and exploitation. Repetitive resistivity measurements made since 1979 at the geothermal project at Cerro Prieto, Mexico, have achieved a level of precision and reproducibility that make possible the clear identification of temporal changes attributable to the large-scale exploitation of the reservoir (112). Numerical modeling techniques were used to study the migration of waters of different temperature and salinity in response to production, and simulated salinity and temperature changes were used to predict changes in apparent surface resistivity. A 2-D finite difference code, RESIS2D (113-114) was used. The authors concluded that it is feasible to use resistivity surveys as a means for monitoring reservoir processes (112).

Modeling Using Personal Computer

Groundwater modeling programs are adaptable to personal computers and microcomputers. Molden, et al (115) use an Apple II 48 microcomputer to provide an analytical solution for recharge of a rectangular basin. According

to the authors, a large number of recharge strategies can be graphically worked out by hydrologists using the program.

A large finite element program was adapted to a PDP-11/23 minicomputer to obtain the advantages of an interactive computer system (116). The program used was UNSAT2, a code for unsteady, saturated and/or unsaturated flow of ground water. Some of the advantages of this interactive system are: ease of data input by the use of a digitizer; the opportunity to review all output files and to select for printing only those of interest; and the opportunity to change the physical boundaries of a problem at any time to make use of new information as a project progresses. The main disadvantage is increased computational time.

A modular 3-D finite difference groundwater flow model was recently developed by McDonald and Harbaugh, of the USGS, and was adapted for IBM-PC usage by the International Groundwater Modeling Center (IGWMC), Holcomb Research Institute (117). The simulator consists of a Main Program and a series of highly independent subroutines called modules. "The division of the program 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 and output systems of the computer program are also designed to permit maximum flexibility.

Ground-water flow within the aquifer is simulated using a block-centered finite-difference approach. Layers are simulated as confined, unconfined, or a combination of both. Flow from external stresses, such as flow to wells, areal recharge, evapotranspiration, flow to drains, and flow through riverbeds can be simulated. The program is written in FORTRAN '66 and will run without modification on most computers which have a FORTRAN '66 compiler. It will also run without modification with most extended FORTRAN '77 compilers and with minor modifications on standard FORTRAN '77 compilers. The program was run without modification on computers manufactured by IBM, Control Data, Prime, Amdahl, Digital Equipment, Harris and Cray. Documentation presented in the report includes a narrative description, a flow chart, a list of variables, and a program listing of each module" (77).

Another model recently implemented by IGWMC for IBM-PC usage is the USGS solute transport model of Konikow and Bredehoeft (5, 118). It can be applied

to a wide range of problem types and is applicable to one- or two-dimensional problems involving steady-state or transient flow. The simulator computes changes in concentration over time caused by the processes of convective transport, hydrodynamic dispersion, and mixing (or dilution) from fluid sources. "The model assumes that the solute is nonreactive and that gradients of fluid density, viscosity, and temperature do not affect the velocity distribution. However, the aquifer may be heterogeneous and (or) anisotropic. The report includes a listing of the computer program, which is written in FORTRAN IV and contains about 2,000 lines. The model is based on a rectangular, block-centered, finite-difference grid. It allows the specification of any number of injection or withdrawal wells and of spatially varying diffuse recharge or discharge, saturated thickness, transmissivity, boundary conditions, and initial heads and concentrations. The program also permits the designation of up to five nodes as observation points, for which a summary table of head and concentration versus time is printed at the end of the calculations" (118).

Olsthoorn (119), introduces "spreadsheet" programming to groundwater modeling. He believes that, "So-called spreadsheet programs are forerunners of new general software from which the ground-water engineer is likely to benefit - no more special programs each capable of fulfilling just that single task it was explicitly designed for, but programs suitable to do almost any job, where only the fantasy of the user limits the possibilities. Moreover, this new software shows us what user friendliness looks like and proves that it is completely superfluous to be a computer specialist to use it.

With a spreadsheet you can build a simple finite-difference model from scratch within one or two minutes. With some extra time a wide versatility of problems can be solved as the multiaquifer, three-dimensional, phreatic and transient ground-water flow examples prove. This way any hydrologist should be able to solve diverging groundwater models himself without depending on special numerical models. All he needs beyond a microcomputer and a spreadsheet program is a good knowledge of the water balance."

The author demonstrated a technique for quickly developing and running a simple finite-difference model with several hundred nodes, and described techniques for enlarging the work to handle problems such as: leaky aquifer conditions, multiple aquifers, 3-D flow, and transient flow. His Apple IIe

computer with 64k memory will handle approximately 100 nodes, but with the larger 16-bit, megabyte memory machines the number of possible nodes could be an order of magnitude higher.

Techniques of Model Development

According to Mercer and Faust (31), the statistical analysis of parameter estimates and model predictions is a very promising area of current research. As groundwater models become more routinely applied to large scale water resource problems, model calibration and future response prediction are usually involved. Parameter estimation techniques are used to overcome shortcomings in calibration procedures. The method usually consists of two basic components - one part that calculates the best fit ("automatic history matching"), and a second part that evaluates the statistical properties of the fit. A promising new technique is known as kriging, a stochastic interpolation procedure. Delhomme (133) describes the methodology and associated case studies; Skrivan and Karlinger documented a program for kriging (134).

Kitanidis and Vormvoris studied, from a geostatistical perspective, the estimation of permeability from input-output measurements (138). A random field of unknown parameters is estimated by a two-step process. First, the structure of the parameter field is identified, and second, linear estimation theory is applied to provide minimum variance and unbiased point estimates of hydrogeologic parameters, as in kriging. This deals with the "inverse problem," defined by Dagan (139) as: "determine the transmissivity at various points given the shape and boundary of the aquifer and recharge intensity and given a set of log-transmissivity (Y) and head (H) values at a few points. The log transmissivity distribution is regarded as a realization of a random function of normal and stationary unconditional probability density function (pdf). The solution of the inverse problem is the conditional normal pdf of Y, conditioned on measured H and Y, which is unconditional joint pdf of Y and H. The problem is reduced to determining the unconditional head-log-transmissivity covariance and head variogram for a selected Y covariance which depends on a few unknown parameters. This is achieved by solving a first-order approximation of the flow equations."

His report illustrated the use of the method. Efficient and accurate solution techniques become increasingly important as numerical models become more sophisticated. For certain types of problems, boundary integral methods (BIM) offer more efficient solutions than standard, finite-difference-based numerical techniques (31). They can be utilized for both confined aquifer and free surface problems in which the flow properties are homogeneous or the study area can be divided into a few homogeneous zones. To quote Mercer and Faust (31), "In the indirect method, matrix techniques are used to solve for a set of fictitious sources along the boundary that when superimposed add up to the given boundary conditions. When the boundary conditions are satisfied in this manner, the net effect of the sources on any internal point is equal to the internal physical state as dictated by the governing differential equation and given boundary conditions.

The direct method utilizes Green's theorem and matrix techniques to solve a set of integral equations of the unknown heads along the segments of the boundary where the flux is given and for the unknown fluxes along the remaining segments. Once all the heads and fluxes are known along the boundary, numerical integration can be used to solve for heads at internal points.

The primary advantage of the BIM is that matrix techniques are only used to solve for unknowns along the boundary. Effectively, this means that the problem is reduced by one dimension, reducing the size of the matrix involved. When the zone boundaries become geometrically complex and the number of zones numerous, this advantage disappears. A second advantage is that the BIM can be used to treat infinite domains. These properties not only make BIM quite efficient for certain problems but also mean that the use of the BIM in conjunction with other numerical techniques creates a powerful technique for solving more complicated problems. For more information on the BIM, see Liggett and Liu" (135) (31).

In other efforts to lessen the burdensome computational problems of 3-D transport codes, Babu and Pinder recently presented a two-step finite element-finite difference procedure (FEFD) as an accurate and efficient alternative to the standard methods (136). The model is based on a splitting algorithm that combines a finite element formulation in the areal plane with a finite difference system in the vertical. Numerical theory and a 3-D transport

example are presented by the authors, who state that "Heuristic stability analysis indicates the scheme is unconditionally stable."

Batu (140) also published work in which the FEM and FDM were both utilized. A finite element dual mesh method was developed to calculate the horizontal and vertical Darcy velocity components in a highly nonhomogeneous and anisotropic aquifer of constant porosity under steady flow conditions. The FEM is used to calculate the total head distribution; the FDM forms of the total head gradients are used to calculate the Darcy velocity components. Results compared quite well with an analytical solution and with the method of Yeh (78). The dual mesh method can be applied to any nonhomogeneous and anisotropic porous medium to calculate the nodal Darcy velocities (140).

Abriola and Pinder developed a multiphase approach to the modeling of porous media contamination by organic compounds (137). The "approach makes it possible to describe the simultaneous transport of a chemical contaminant in three physical forms: as a nonaqueous phase, as a soluble component of an aqueous phase, and as a mobile fraction of a gas phase. The contaminant may be composed of, at most, two distinct components, one of which may be volatile and slightly water soluble and the other of which is both nonvolatile and insoluble in water. Equations which describe this complex system are derived from basic conservation of mass principles by the application of volume averaging techniques and the incorporation of various constitutive relations and approximations. Effects of matrix and fluid compressibilities, gravity, phase composition, interphase mass exchange, capillary, diffusion, and dispersion are all considered. The resulting mathematical model consists of a system of three nonlinear partial differential equations subject to two equilibrium constraints. These equations relate five unknowns: two capillary pressures and three mass fractions."

Although this system is not amenable to solution by analytical means, an approximate solution can be sought by a finite difference discretization of the governing equations. A one-dimensional, implicit numerical model was developed in this manner. To handle the solution of the resultant system of nonlinear algebraic equations, a Newton-Raphson iteration scheme was employed. In order to apply the finite difference model to a specific problem a number of parameters must be evaluated, including three-phase relative

permeabilities, saturation-pressure relations, partition coefficients and mixture densities and viscosities. As a demonstration of the model's applicability, the migration of a two-component hydrocarbon mixture in a soil column was simulated. A mass balance was performed, and convergence of the iteration scheme as well as convergence of the difference scheme in space and time were examined heuristically. Abriola and Pinder concluded that, "Thus a workable model has been developed which can describe much of the complexity of subsurface contaminant migration heretofore unexamined" (137).

As an approach to modelling radionuclide migration away from a crystalline rock repository, Neretnieks and Rasmuson (141) proposed a numerical scheme based on the integrated finite difference method (IFDM) of Edwards (75). They expanded the MINC concept of Pruess, et al (63), by introducing a "pseudobody" to account for strongly varying block sizes and velocities along the flow path. Quoting the authors, "The methods proposed here have great advantages over exact calculations as regards computing effort. A problem which would need rigorous three-dimensional flow calculations coupled to transport calculations (also in three dimensions) accounting for interaction with a multitude of different sized blocks has been simplified to an equivalent one-dimensional transport calculation with a solid interaction description which is no more complex than that used in interaction calculations with equally sized regularly shaped bodies (slabs, cylinders, and spheres) by introduction of a pseudobody. Such simplifications are, of course, bound to be less accurate than rigorous methods, if such were available."

According to Fogg and Senger (143), the use of flow nets, composed of streamlines and streamtubes, is one of the best means of visualizing groundwater flow fields. However, accurate construction of flow nets can be very difficult in heterogeneous anisotropic media or in regional cross sections where vertical exaggeration of scale is great. The authors have recently introduced a method developed to automatically generate the streamlines of a flow net using conventional groundwater flow modelling algorithms. "The method can be implemented using most any of the existing computer programs for flow modeling, and no modification of the programs is necessary. One need only replace the hydraulic head and conductivity terms in the steady-state ground-water flow equation with the stream function and an inverse form of hydraulic conductivity, respectively. Possible boundary

conditions include prescribed stream function (Dirichlet type) and prescribed stream function gradient (Neumann type). The former can be determined from prior knowledge of recharge or discharge rates or from boundary fluxes computed in previous simulations of hydraulic head distribution. The latter can be determined from data on hydraulic head along the boundaries, raising the possibility of solving for the streamlines directly without first solving for the head distribution. The method is generally not appropriate when sources or sinks occur inside the flow region, and it will not handle transient conditions. Accuracy of the method is demonstrated in three hypothetical test problems and a vertical-plane model through the Palo Duro Basin of Texas and New Mexico."

The rapidly expanding volume of groundwater models and reservoir simulators has fostered the development of a methodology for evaluating the mathematical and computational capabilities of the models. Such a methodology was designed at Texas Tech University by Ford, et al (144). The process involves tests of numerical computational difficulties and compatibility and accuracy of fluid property representations and fluid flow correlations. It does not determine the validity or usefulness of a simulator for a given field test, but attempts to evaluate the capabilities of a given simulator which might be available.

The test is based on the solution of a system of ordinary differential equations, referred to as a Similarity Porous Media System (SPMS), rather than on a customary system of partial differential equations, or Porous Media System (PMS). Ford explains: "Simulation of an actual problem imposes field physical conditions on a solution of the PMS by the simulator. Evaluation of a simulator by use of the similarity concept involves imposition of selected samples from a solution of the SPMS as conditions on a solution of the PMS by the simulator. Then, this solution of the PMS can be checked against a solution predicted by the solution of the SPMS." The SPMS can be used for evaluation and validation of reservoir simulators in several ways, "two of which have been specifically identified and tested as part of the project. They can be briefly described as follows:

1. Various methods of computer representation and/or smoothing of density, viscosity, relative permeability, and capillary data can be used in the SPMS for the purpose of comparison of difficulties in solution of the ordinary differential equations defining the SPMS.
2. A SPMS can be solved and its solution can be used to impose initial-boundary conditions on a PMS, which can then be solved by an existing simulator using these imposed conditions. Since the inverse coordinate transformation, (ξ, η) to (x, t) or (r, t) , predicts the values the PMS simulator should obtain under the imposed initial-boundary conditions, the PMS simulator can be checked for errors as well as for inefficiencies" (144).

The report contains documentation of the code and examples of its usage.

Reservoir heterogeneities and their accurate description in modelling processes continue to be the major stumbling block to accurate predictions in groundwater modeling and EOR reservoir simulation. The Gulf Universities Research Consortium (GURC), under contract to DOE, has undertaken a program to attack this problem (145). The proposed approach is to use multivariate statistical analysis techniques to develop two descriptive/predictive models which can describe reservoir heterogeneity patterns in sufficient detail to predict their effects on EOR. The first model, a 'Geosystem Types Model,' would quantitatively address reservoir heterogeneity; the second, an 'EOR Performance Probability Path Model,' would quantitatively address EOR performance using reservoir descriptive and process design data.

They noted, "A principal emphasis in both these models is that the resulting predictions will be probabilistic rather than deterministic and will be based on statistical treatment of empirical observations. These two models are being developed under a unified concept which GURC calls -- a Statistically Oriented Reservoir Comparison and Evaluation System (SORCES). The product goal is a computer-interactive decision support system, patterned after the emerging 'expert system' concept" (145).

The research design of the project was organized into three consecutive implementation phases. The objectives of Phase I (covered in the current report) are these:

- o concept development of the two models,
- o development of multivariate statistical methodologies to be used for generating the two models, and
- o pilot-scale testing and evaluation of such methodologies.

Continuing, the GURC report states, "The concept of the Geosystem Types Model involves the application of known generic reservoir heterogeneity patterns, in the form of quantified descriptive variable relationships, to identify statistically distinct groups of similar reservoirs. Developed first using reservoir mean data values, or macro-scale values, this model can be refined by using intra-reservoir, or micro-scale attributes, to predict reservoir characteristics probabilistically at the scale necessary for input to EOR modeling.

"The concept of the EOR Performance Probability Path Model focuses on the predictive capability of the multivariate regression analytical technique. Based on statistical expressions of the relationships among reservoir descriptors, process design, and performance variables, the model will be able to predict process and performance values probabilistically. When refined by combining with the Geosystem Types Model, the predictions of the Performance Model should have even better confidence limits.

"Descriptive statistics, correlations, and regressions are the approaches which comprise the iterative methodology tested in Phase 1. For the Geosystem Types Model, 227 reservoirs representing four "types" were used, and 160 field tests representing five EOR methods were used for the EOR Performance Probability Path Model. The data for both models were examined for distinct variable relationship patterns, correlations, and statistically significant differences on the intra- and inter-group levels.

"The results of this Phase 1 test were promising, generally indicating that the proposed methodology is a satisfactory and feasible approach. Good correlations within groups and distinct variation among groups were evident in both models. Tests to determine "goodness of fit," however, showed generally poor results in both, indicating the need for further model refinement and development to achieve the desired predictive capability.

"This final model development is proposed to be carried out under Phase 2 for the Geosystem Types Model and Phase 3 for the EOR Performance Probability Path Model. Phase 3 will also encompass the design of protocols for applications of the models and the structuring of a decision support system, SOURCES" (145).

SUMMARY AND CONCLUSIONS

The study revealed that numerical models are used to solve problems in the following areas:

- 1). Reservoir simulation for petroleum production
 - a) Reservoir engineering
 - b) EOR technology
 - c) Contamination from oil field chemicals
- 2). Reservoir simulation for geothermal energy production
- 3). Reservoir simulation for fresh water production
- 4). Reservoir simulation for fresh water aquifer recharge
- 5). Reservoir simulation for ground water contamination from:
 - a) Radioactive waste repositories
 - b) Mining activities (e.g. coal, minerals, oil shale, uranium, etc.)
 - c) Deep well injection of wastes
 - i) Hazardous wastes
 - ii) Industrial or municipal wastes

Numerical simulation programs are available to solve reservoir problems in one, two, or three dimensions. Attempts have been made to simulate combinations of elements such as fluid flow, solute transport, heat transport, multiple chemical reactions, and rock deformation. For example, fluid flow may be single or multiphase, steady state or transient, and may occur in saturated or unsaturated porous media which can be homogenous, heterogenous, fractured, or not fractured. Starting with the relatively simple base case of one dimension flow in saturated homogenous porous media, the numerical simulation programming becomes increasingly complex as additional combination of elements are factored. Until recently, little progress was made in coupling three or more of the element combinations listed in the second sentence of this paragraph. Scant research has been accomplished on modeling the movement of water and solute in porous media under the influence of a temperature gradient (146).

Many erudite mathematical and numerical techniques are now being used to develop comprehensive, sophisticated models. At the same time, less complex models of adequate quality are being designed for use on mini- or micro-computers by personnel who are not computer specialists.

Numerical simulation capabilities are sufficient to produce models of adequate quality for almost all uses, given proper knowledge of the subsurface strata. Therein lies the problem -- the same old nemesis that plagues the EOR and injection well disposal industries -- reservoir heterogeneities and their description. Improved knowledge of reservoir heterogeneities is needed to improve the accuracy of simulation prediction models.

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